Energies of Dilute Fermi Gases
— and —
Universalities in BCS Theory

by

Asbjørn Bækgaard Lauritsen

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Committee in charge:

Eva Benková, Chair
Robert Seiringer
László Erdős
Jan Philip Solovej

Institute of Science and Technology Austria

The thesis of Asbjørn Bækgaard Lauritsen, titled *Energies of Dilute Fermi Gases and Universalities in BCS Theory*, is approved by:

Supervisor: Robert Seiringer, ISTA, Klosterneuburg, Austria

Signature: ____________________________________

Committee Member: László Erdős, ISTA, Klosterneuburg, Austria

Signature: ____________________________________

Committee Member: Jan Philip Solovej, University of Copenhagen, Copenhagen, Denmark

Signature: ____________________________________

Defense Chair: Eva Benková, ISTA, Klosterneuburg, Austria

Signature: ____________________________________

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Abstract

This thesis consists of two separate parts. In the first part we consider a dilute Fermi gas interacting through a repulsive interaction in dimensions $d = 1, 2, 3$. Our focus is mostly on the physically most relevant dimension $d = 3$ and the setting of a spin-polarized (equivalently spinless) gas, where the Pauli exclusion principle plays a key role. We show that, at zero temperature, the ground state energy density of the interacting spin-polarized gas differs (to leading order) from that of the free (i.e. non-interacting) gas by a term of order $a_p^d \rho^{2+2/d}$ with a_p the p-wave scattering length of the repulsive interaction and ρ the density. Further, we extend this to positive temperature and show that the pressure of an interacting spin-polarized gas differs from that of the free gas by a now temperature dependent term, again of order $a_p^d \rho^{2+2/d}$. Lastly, we consider the setting of a spin-$\frac{1}{2}$ Fermi gas in $d = 3$ dimensions and show that here, as an upper bound, the ground state energy density differs from that of the free system by a term of order $a_s \rho^2$ with an error smaller than $a_s \rho^2 (a_s \rho^{1/3})^{1-\varepsilon}$ for any $\varepsilon > 0$, where a_s is the s-wave scattering length of the repulsive interaction.

These asymptotic formulas complement the similar formulas in the literature for the dilute Bose and spin-$\frac{1}{2}$ Fermi gas, where the ground state energies or pressures differ from that of the corresponding free systems by a term of order $a_s \rho^2$ in dimension $d = 3$. In the spin-polarized setting, the corrections, of order $a_p^3 \rho^{8/3}$ in dimension $d = 3$, are thus much smaller and requires a more delicate analysis.

In the second part of the thesis we consider the Bardeen–Cooper–Schrieffer (BCS) theory of superconductivity and in particular its associated critical temperature and energy gap. We prove that the ratio of the zero-temperature energy gap and critical temperature $\Xi(T = 0)/T_c$ approaches a universal constant $\pi e^{-\gamma} \approx 1.76$ in both the limit of high density in dimension $d = 3$ and in the limit of weak coupling in dimensions $d = 1, 2$. This complements the proofs in the literature of this universal behaviour in the limit of weak coupling or low density in dimension $d = 3$. Secondly, we prove that the ratio of the energy gap at positive temperature and critical temperature $\Xi(T)/T_c$ approaches a universal function of the relative temperature T/T_c in the limit of weak coupling in dimensions $d = 1, 2, 3$.

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I wish to thank my advisor Robert Seiringer for many fruitful discussions and guidance during my time at ISTA. Additionally I wish to thank my collaborators Barbara Roos, Frederik Ravn Klausen and in particular Joscha Henheik, with whom I had the pleasure of working with on many projects on BCS theory.

Thanks to everyone both at ISTA and in Vienna I have met during my time in Austria. In particular the math-phys analysis groups, the chamber music and board game groups at ISTA and the TUOrchester. Thanks also to my friends and family back in Copenhagen.

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About the Author

Asbjørn Bækgaard Lauritsen completed his BSc and MSc in mathematics at the University of Copenhagen before joining ISTA in 2020. His main research interests include the study of many-body quantum mechanical systems. During his PhD studies he worked primarily on establishing asymptotic expansions for the ground state energy and pressure of a dilute spin-polarized Fermi gas together with his advisor Robert Seiringer and secondarily on the universal properties of the BCS energy gap and critical temperature with fellow PhD students Joscha Henheik and Barbara Roos.

List of Publications

Part I contains the following papers and preprints:

[GSEUpp] A. B. Lauritsen and R. Seiringer. "Ground state energy of the dilute spin-polarized Fermi gas: Upper bound via cluster expansion", *J. Funct. Anal.* **286**.7 (2024), p. 110320. DOI: 10.1016/j.jfa.2024.110320.

[GSELow] A. B. Lauritsen and R. Seiringer. "Ground state energy of the dilute spin-polarized Fermi gas: Lower bound". arXiv: 2402.17558 [math-ph]. 2024. DOI: 10.48550/arXiv.2402.17558.

[Spin-1/2] A. B. Lauritsen. "Almost Optimal Upper Bound for the Ground State Energy of a Dilute Fermi Gas via Cluster Expansion", *Ann. Henri Poincaré* (2024). DOI: 10.1007/s00023-024-01450-1.

[PressLow] A. B. Lauritsen and R. Seiringer. "Pressure of a dilute spin-polarized Fermi gas: Lower bound", *Forum of Mathematics, Sigma* **12** (2024), e78. DOI: 10.1017/fms.2024.56.

[PressUpp] A. B. Lauritsen and R. Seiringer. "Pressure of a dilute spin-polarized Fermi gas: Upper bound". arXiv: 2407.05990 [math-ph]. 2024. DOI: 10.48550/arXiv.2407.05990.

And the supplementary material:

[GGRscript] A. B. Lauritsen. "GGR-diagrams". 2023. URL: https://github.com/ABLauritsen/GGR-Diagrams.

Part II contains the following papers and preprints:

[LowDim] J. Henheik, A. B. Lauritsen, and B. Roos. "Universality in low-dimensional BCS theory", *Rev. Math. Phys.* (2023), p. 2360005. DOI: 10.1142/S0129055X2360005X.

[HighDen] J. Henheik and A. B. Lauritsen. "The BCS Energy Gap at High Density", *J Stat Phys* **189**.5 (2022). DOI: 10.1007/s10955-022-02965-9.

[AllTemp] J. Henheik and A. B. Lauritsen. "Universal behavior of the BCS energy gap". arXiv: 2312.11310 [cond-mat, physics:math-ph]. 2023. DOI: 10.48550/arXiv.2312.11310.

Further, during my PhD, I have (co-)authored the following papers, which are not included in the thesis:

[Borders] F. R. Klausen and A. B. Lauritsen. "Stochastic cellular automaton model of culture formation", *Phys. Rev. E* **108**.5 (2023), p. 054307. DOI: 10.1103/PhysRevE.108.054307. "Research data for: A stochastic cellular automaton model of culture formation". 2023. DOI: 10.15479/AT:ISTA:12869.
"Model-for-culture-formation". 2023. URL: https://github.com/FrederikRavnKlausen/model-for-culture-formation.

[Jellium] A. B. Lauritsen. "Floating Wigner crystal and periodic jellium configurations", *J. Math. Phys.* **62**.8 (2021), p. 083305. DOI: 10.1063/5.0053494.

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Preface

This thesis consists of two completely independent parts. They may be read in any order. Each part begins with an introduction to the subject matter studied in the respective part. These introductions are given in Chapters 1 and 8.

Apart from Chapters 1, 2 and 8 each chapter consists of one of the papers included in the thesis [GSEUpp; GSELow; Spin-1/2; PressLow; PressUpp; LowDim; HighDen; AllTemp]. As such, they are (mostly) self-contained and can in principle be read in any order. There are however a few recommended dependencies/prerequisites illustrated in Figure 0.0.1. Note that these chapters do not appear in chronological order of their arXiv submission date.

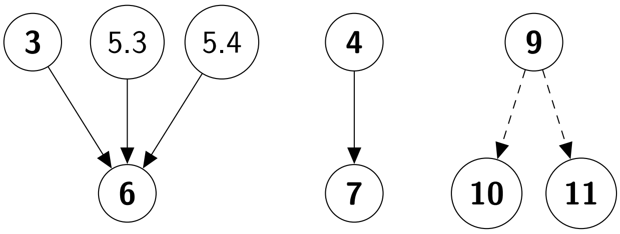


Figure 0.0.1: Recommended dependencies/prerequisites. The dashed arrows indicate that the preceding chapter contains many of the same ideas treated in a simpler setting and may thus suitably be read beforehand.

Chapters 1 and 2 serve as introduction and motivation for Chapters 3–7 and Chapter 8 serves as introduction for Chapters 9, 10 and 11.

Part I

Energies of Dilute Fermi Gases

Chapter 1

Introduction to the theory of dilute quantum gases

The study of dilute quantum gases with strong repulsive interactions has a long and rich history in theoretical physics going back to the 1950s and 1960s, when the energy asymptotics of both dilute Bose and Fermi gases were first computed to increasing levels of accuracy in the particle density [Dys57; Efi66; EA65; HY57; LHY57; Wu59]. Renewed interest was sparked by the experimental realization of Bose–Einstein condensates (BEC) [AEMWC95; Dav+95] and of dilute quantum gases with tunable interactions using Feshbach resonances, see [BDZ08; CGJT10; GPS08] and references therein. Further, in the recent years, it is now possible to tune the interaction in a dilute Fermi gas such that the fermions interact *as if they were spinless*, see references in [DZ19], where in particular the energy asymptotics of such a spinless Fermi gas is calculated.

The energy asymptotics of such dilute quantum gases are of a certain universal nature. They depend on the interaction only through a few parameters, being the s- and p-*wave scattering lengths* and (to higher order) the s- and p-*wave effective ranges*, but otherwise not on the microscopic details of the interaction. These are the relevant parameters of the interaction for particles that are far apart. The "dilute" in "dilute quantum gases" means exactly that the average interparticle distance is large compared to the length scale of the interaction. We define the scattering lengths in detail below and motivate why these are (to leading order) the only relevant parameters of the interaction.

On the mathematical physics side, the recent interest in the study of such dilute quantum gases was sparked by the seminal work of Lieb and Yngvason [LY98], wherein they give a rigorous lower bound for the leading order term in the asymptotic expansion of the ground state energy of a dilute Bose gas complementing the rigorous upper bound of Dyson [Dys57]. Since then, much effort has been devoted to prove rigorously the claimed asymptotic formulas from the 1950s and 1960s physics literature. These asymptotic formulas concern both the ground state energy and the free energy (or pressure) at positive temperature.

In large parts, the main object of study has been the 3-dimensional dilute Bose gas. Here only the s-wave scattering length of the interaction appears. For the Bose gas the validity of the leading order term has been extended to positive temperature [Sei08; Yin10] and recently also the next order term, the so-called Lee–Huang–Yang (LHY) term [LHY57] was proved both as upper [BCS21; YY09] and lower [FS20; FS23] bounds and extended to positive temperature [HHNST23; HHST24]. In addition, also the two-dimensional [FGJMO24; LY01] and one-dimensional [ARS22] Bose gases have been studied. While many of the asymptotic formulas have thus been put on rigorous ground, it remains an important open problem to verify the existence of Bose–Einstein condensation in a dilute interacting Bose gas [LSSY05].

The Fermi gas behaves quite differently compared to the Bose gas: For bosons, many of the particles may occupy the same one-particle state. This is not so for fermions. The Pauli exclusion principle dictates that at most q fermions may occupy the same one-particle state, q being the number of spin components. In particular, even the non-interacting Fermi gas has a non-zero ground state energy. Further, the effect of the interaction is highly dependent on the spin. For two fermions with different spin, there is no effect from the Pauli exclusion, and they interact similarly to two bosons. For fermions with the same spin, on the other hand, the Pauli exclusion suppresses the probability of the two particles being close, and the interaction is effectively much weaker. Following along this picture, Lieb, Seiringer and Solovej [LSS05] proved that the leading order correction to the ground state energy of the non-interacting Fermi gas is the same as that for the Bose gas if the number of spin components is $q \geq 2$. In particular here only the s-wave scattering length appears. This was later reproved using different methods and getting improved error bounds in [FGHP21; Gia23a] (see also [Gia23b]) and extended to positive temperature in [Sei06b]. The two-dimensional setting is studied in [LSS05; Sei06b] and the one-dimensional setting is discussed in the PhD thesis of Agerskov [Age23].

Notably absent from the rigorous analysis is the study of the spin-polarized (equivalently spinless) Fermi gas, with only one spin component $q = 1$. The only work on such a gas is in 1 dimension [ARS22]. As the fermions here all have the same spin, the Pauli exclusion plays an important role. An important consequence is that only the p-wave scattering length (and to higher order the p-wave effective range) matters, but not the s-wave parameters. Further, because of the Pauli exclusion suppressing the probability of two particles being close, the energy contribution coming from the interaction is much smaller than that for bosons or fermions of different spins. This means that the analysis of such a spinless Fermi gas is more delicate and requires a more precise analysis than that of the Bose gas or Fermi gas with spin in order to find the leading correction to the energy of a free (meaning non-interacting) gas.

Spin-polarized/spinless fermions may a priori seem somewhat academical — After all, real-world fermions have spin $\geq \frac{1}{2}$, meaning that the number of spin-components is $q \geq 2$. However, it is possible in experiments, using Feshbach resonances, to tune the interaction in a dilute Fermi gas such that the s-wave scattering length vanishes and so that only p-wave (and higher angular momentum) scattering appears, see references in [DZ19]. Such a Fermi gas then behaves *as if the particles were spinless* and may thus be studied by considering a spinless gas. A second physical setting, where a description of a spin-polarized/spinless Fermi gas is applicable is exactly (as the name suggests) that of a completely spin-polarized gas, where all the spins are aligned. This is for instance the case for a gas in a very strong magnetic field. If all the particles have the same spin we can equivalently forget about the spin, and treat the gas instead as a spinless gas. (This also explains the equivalence of the nomenclature of 'spin-polarized' and 'spinless'.)

1.1 Asymptotic formulas

We describe next the results and in broad strokes the methods of Part I of the thesis (Chapters 3–7) beginning with the precise statement of the asymptotic formulas for the energies (and pressures) of dilute Fermi gases.

To state the (conjectured) asymptotic formulas for the energies of dilute Fermi gases, we first define the system precisely. At zero temperature the relevant object is the ground state energy of an N-particle system in a large box $\Lambda = [-L/2, L/2]^d$ in d dimensions. (Our focus is mostly on the physically most relevant case $d = 3$.) The ground state energy is the lowest eigenvalue of the Hamiltonian describing the system. This Hamiltonian is

$$H_N = \sum_{j=1}^{N} \frac{-\hbar^2}{2m} \Delta_{x_j} + \sum_{1 \le j < k \le N} V(x_j - x_k),$$

and defined on some (appropriate domain in) some subspace of $L^2(\Lambda^N; \mathbb{C})$. (We shall work in natural units, where $\hbar = 1$ and $2m = 1$, to simplify the formulas by not having to carry around the factor $\hbar^2/2m$.) Concretely this means that if the particles are in the state $\psi_N \in L^2(\Lambda^N; \mathbb{C})$ (with $\|\psi_N\|^2_{L^2(\Lambda^N)} = \int \cdots \int_{\Lambda^N} |\psi_N(x_1, \ldots, x_N)|^2 \, \mathrm{d}x_1 \ldots \mathrm{d}x_N = 1$) then the energy is given by

$$\begin{aligned}\langle \psi_N | H_N | \psi_N \rangle = \int \cdots \int_{\Lambda^N} \Bigg[&\sum_{j=1}^{N} |\nabla_{x_j} \psi_N(x_1, \ldots, x_N)|^2 \\ &+ \sum_{1 \le j < k \le N} V(x_j - x_k) |\psi_N(x_1, \ldots, x_N)|^2 \Bigg] \mathrm{d}x_1 \ldots \mathrm{d}x_N.\end{aligned}$$

The ground state energy is then defined as the lowest possible energy:

$$E_N = \inf_{\psi_N : \|\psi_N\|_{L^2} = 1} \langle \psi_N | H_N | \psi_N \rangle ,$$

where the infimum is taken over appropriate states ψ_N. Exactly which states are appropriate depends on the type of particles, be it bosons or fermions with q spin components. In the following we restrict to the settings of fermions with either $q = 2$ or $q = 1$. Any gas of fermions with $q \ge 2$ behaves like a gas with $q = 2$ for our purposes, and it is notationally simpler to just consider $q = 2$. The spin-polarized (spinless) fermions with $q = 1$ behave significantly differently as discussed above. The particles being fermions, one has to consider antisymmetric wave-functions ψ_N. This is the Pauli exclusion principle. Concretely this means that for spin-polarized fermions, the relevant L^2-space is

$$\begin{aligned}L^2_a(\Lambda^N; \mathbb{C}) &= \bigwedge^N L^2(\Lambda^N; \mathbb{C}) \\ &= \left\{ \psi_N \in L^2(\Lambda^N; \mathbb{C}) : \psi_N(x_{\pi(1)}, \ldots, x_{\pi(N)}) = (-1)^\pi \psi_N(x_1, \ldots, x_N) \, \forall \pi \in \mathcal{S}_N \right\},\end{aligned}$$

with $\mathcal{S}_N$ the set of all permutations on N indices and $(-1)^\pi$ the sign of the permutation π. For spin-$\frac{1}{2}$ fermions (meaning $q = 2$) we can consider a fixed number $N_\uparrow$ of spin-$\uparrow$ and $N_\downarrow = N - N_\uparrow$ of spin-$\downarrow$ particles. Then the relevant space of ψ_N's is $L^2_a(\Lambda^{N_\uparrow}) \otimes L^2_a(\Lambda^{N_\downarrow})$. The ground state energy is then $E_{N_\uparrow, N_\downarrow}$.

We consider the thermodynamic limit, where N and L are both large, but such that the particle density $\rho = N/L^d$ stays finite. (In the spin-$\frac{1}{2}$ case with $q = 2$ we require the particle densities $\rho_\uparrow = N_\uparrow/L^d$ and $\rho_\downarrow = N_\downarrow/L^d = \rho - \rho_\uparrow$ of spin-$\uparrow$ respectively spin-$\downarrow$ particles to stay finite.) In this limit the ground state energy E_N is proportional to the number of particles (equivalently the volume L^d) and the following limits exist [Rob71]

$$e(\rho) = \lim_{\substack{N, L \to \infty \\ N/L^d = \rho}} \frac{E_N}{L^d}, \qquad e(\rho_\uparrow, \rho_\downarrow) = \lim_{\substack{N_\uparrow, N_\downarrow, L \to \infty \\ N_\uparrow/L^d = \rho_\uparrow \\ N_\downarrow/L^d = \rho_\downarrow}} \frac{E_{N_\uparrow, N_\downarrow}}{L^d}.$$

This defines the *ground state energy density* in the thermodynamic limit for both the spin-polarized and spin-$\frac{1}{2}$ Fermi gas. The asymptotic formulas of the energy discussed above are then expansions of the function(s) $e(\rho)$ (and $e(\rho_\uparrow, \rho_\downarrow)$) valid in the limit $\rho \to 0$. To state these we next define the scattering lengths properly.

Definition 1.1.1 (see also [LY01, Appendix A] and [SY20, Section 4])**.** The s- and p-*wave scattering lengths* a_s and a_p are defined (in 3 dimensions) by

$$
\begin{aligned}
4\pi a_s &= \inf\left\{\int_{\mathbb{R}^3} \left(|\nabla f|^2 + \frac{1}{2}V|f|^2\right) \mathrm{d}x : f(x) \to 1 \text{ for } |x| \to \infty\right\},\\
12\pi a_p^3 &= \inf\left\{\int_{\mathbb{R}^3} \left(|\nabla f|^2 + \frac{1}{2}V|f|^2\right) |x|^2 \,\mathrm{d}x : f(x) \to 1 \text{ for } |x| \to \infty\right\}.
\end{aligned}
$$

In case $V(x) = +\infty$ for some x we interpret $V(x)\,\mathrm{d}x$ as a measure. The minimizing f's are the s- and p-*wave scattering functions*. They are denoted f_s and f_p respectively and satisfy the scattering equations, being the Euler–Lagrange equations of the minimization problems:

$$
\begin{aligned}
-2\Delta f_s + V f_s &= 0, \qquad f_s(x) \to 1 \text{ for } |x| \to \infty,\\
-2\Delta f_p - 4\frac{x}{|x|^2}\cdot\nabla f_p + V f_p &= 0, \qquad f_p(x) \to 1 \text{ for } |x| \to \infty.
\end{aligned}
\tag{1.1.1}
$$

Remark 1.1.2. The scattering lengths can equivalently be defined using the scattering equations (1.1.1) as the numbers a_s and a_p appearing in $f_s(x) = 1 - a_s/|x|$ and $f_p(x) = 1 - a_p^3/|x|^3$ for x outside the support of V (for a compactly supported V). This is the approach used in Chapters 4 and 7 (where we consider the function $\varphi_p = 1 - f_p$ instead, however).

We give some intuition behind the scattering lengths in Chapter 2. They arise as the ground state energies of systems of two interacting fermions in a large box. (They are essentially defined by this fact.) Further, the ground state wave functions of such systems of two fermions in a large box are to leading order given by the scattering functions (s- or p-wave depending on the spins of the particles) times the ground states of the corresponding free (non-interacting) systems. For the details, see Chapter 2.

Admitting this fact, the relevance of the scattering lengths in the many-body problem can then be understood heuristically as follows: For the dilute system the particles are on average far apart (at distances of order $\rho^{-1/d} \gg \ell$ compared to some order one length scale ℓ set by the interaction). In particular, three particles being close enough to have all three particles interact simultaneously is a very rare event. Thus, the many-body problem is, at least to leading order, conceptually just given by a lot of two-particle problems, where the two particles are in some large box and don't interact with the remaining particles, which we can then ignore. As such, the energy of a two-particle system should play a key role in the energy of the many-body system.

Armed with this definition of the scattering lengths we can then state the conjectured formulas from the physics literature [AE68; DZ19; Efi66; EA65; HY57; WDS20]. For the spin-polarized Fermi gas (with $q = 1$ spin component), this formula reads (in 3 dimensions)

$$
\frac{e(\rho)}{\rho} = k_F^2\left[\frac{3}{5} + \frac{2}{5\pi}a_p^3k_F^3 - \frac{1}{35\pi}a_p^6 r_{p,\mathrm{eff}}^{-1}k_F^5 + \frac{2066 - 312\log 2}{10395\pi^2}a_p^6k_F^6 + o(a_p^6k_F^6)\right].
\tag{1.1.2}
$$

For the Fermi gas with $q = 2$ spin components of equal population $\rho/2$ the formula reads

$$\frac{e(\rho/2,\rho/2)}{\rho} = k_F^2\left[\frac{3}{5} + \frac{2}{3\pi}a_s k_F + \frac{4}{35\pi^2}(11 - 2\log 2)a_s^2 k_F^2 + O\left((a_s^3 + a_p^3 + a_s^2 r_{s,\text{eff}})k_F^3\right)\right]. \tag{1.1.3}$$

Here $k_F = (6\pi^2 q^{-1})^{1/3}\rho^{1/3}$ is the Fermi momentum, $r_{s,\text{eff}}$ and $r_{p,\text{eff}}$ are the s- and p-wave effective ranges and $O\left((a_s^3 + a_p^3 + a_s^2 r_{s,\text{eff}})k_F^3\right)$ is an explicit term of this order.

The main theorem of Part I of the thesis is the validity of the formula in (1.1.2) to order $a_p^3 k_F^5$.

Theorem 1.1.3. *Let $V \geq 0$ be radial and compactly supported. Then the ground state energy density of the 3-dimensional spin-polarized Fermi gas satisfies*

$$\frac{e(\rho)}{\rho} = k_F^2\left[\frac{3}{5} + \frac{2}{5\pi}a_p^3 k_F^3 + o(a_p^3 k_F^3)\right]$$

for sufficiently small $a_p k_F$.

The leading term $\frac{3}{5}k_F^2 = \frac{3}{5}(6\pi^2)^{2/3}\rho^{2/3}$ is the ground state energy per particle of a free (non-interacting) Fermi gas and the next term (of order $a_p^3 k_F^5$) is the leading correction arising from the interaction. The proof of Theorem 1.1.3 as an upper bound is given in Chapter 3 and as a lower bound in Chapter 4. Theorem 1.1.3 is illustrated in Figure 1.1.1.

Remark 1.1.4. We remark that the upper bound in Chapter 3 in fact captures the formula in (1.1.2) to order $a_p^6 r_{p,\text{eff}}^{-1} k_F^7$ and is valid also in dimensions $d = 1, 2$. The lower bound in Chapter 4 is valid also in dimension $d = 2$. Further, the 1-dimensional analogue of Theorem 1.1.3 is proved in [ARS22], see also [Age23]. For the details we refer to the respective chapters.

Finally, we note that the interaction V need not be well-behaved. In particular Theorem 1.1.3 allows for a hard core (also known as a hard sphere) interaction, where formally $V(x) = +\infty$ for $|x| \leq R_0$ and $V(x) = 0$ for $|x| > R_0$.

In Chapter 5 we prove the validity of the formula in (1.1.3) to order $a_s k_F^3$ as an upper bound with an error almost of order $a_s^2 k_F^4$. More precisely we show that

Theorem 1.1.5. *Let $V \geq 0$ be radial and compactly supported. Then for any $\varepsilon > 0$ there exists a constant $C_\varepsilon > 0$ such that the ground state energy density of the 3-dimensional spin-$\frac{1}{2}$ Fermi gas satisfies*

$$e(\rho_\uparrow, \rho_\downarrow) \leq \frac{3}{5}(6\pi^2)\left(\rho_\uparrow^{5/3} + \rho_\downarrow^{5/3}\right) + 8\pi a_s \rho_\uparrow \rho_\downarrow + C_\varepsilon a_s \rho^2 (a_s^3\rho)^{1/3-\varepsilon}$$

for sufficiently small $a_s^3\rho$.

This reproves the result of [LSS05] as an upper bound, but with an improved bound on the error. This formula was also reproved in [FGHP21; Gia23a] both as upper and lower bounds with improved errors compared to [LSS05] only there it is assumed that V is a smooth function. In particular the upper bound in [Gia23a] says that the error term is bounded by $a_s^2\rho^{7/3}$. The analysis in [FGHP21; Gia23a] only deals with smooth V, however, and thus in particular not the case of a hard core interaction. In Theorem 1.1.5 no smoothness or regularity on V is assumed, and we may take V to be a hard core interaction.

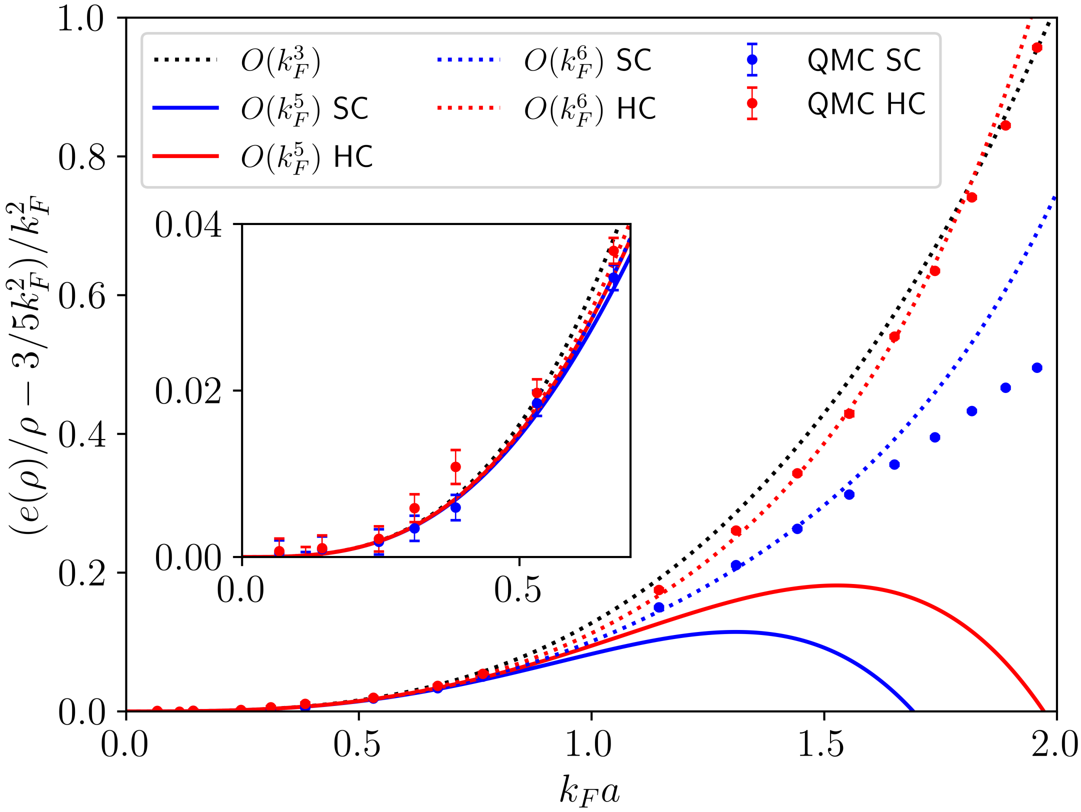


Figure 1.1.1: (Copied from Chapter 3.) Energies of dilute spin-polarized Fermi gases. The curves and points labelled *HC* are for a *Hard Core* interaction of radius a, with then $a_p = a$. The curves and points labelled *SC* are for a *Soft Core* interaction of radius $2a$ and strength V_0 chosen so that it's p-wave scattering length is a, (meaning $V(x) = V_0\chi_{(|x|\leq 2a)}$, χ being the characteristic function.) The points (labelled *QMC*) are *Quantum Monte Carlo* simulations from [BTP23]. The curves include the (conjectured) corrections up to the labelled order in $k_F = (6\pi^2\rho)^{1/3}$.

1.1.1 Positive temperature

Further, we consider in Chapters 6 and 7 the dilute spin-polarized gas at positive temperature. At positive temperature the natural quantity to consider is not the ground state energy (density) but instead the pressure. The pressure of the interacting and free systems are defined as

$$\psi(\beta,\mu) = \lim_{L\to\infty} \frac{1}{L^3\beta} \log \mathrm{Tr}_{\mathcal{F}}\, e^{-\beta(\mathcal{H}+\mathcal{V}-\mu\mathcal{N})}, \qquad \psi_0(\beta,\mu) = \lim_{L\to\infty} \frac{1}{L^3\beta} \log \mathrm{Tr}_{\mathcal{F}}\, e^{-\beta(\mathcal{H}-\mu\mathcal{N})},$$

with $\beta = 1/k_B T$ the inverse temperature, μ the chemical potential, $\mathcal{F}$ the fermionic Fock space, and $\mathcal{H}$, $\mathcal{V}$ and $\mathcal{N}$ the second quantized free Hamiltonian, interaction and number operator respectively. (Here k_B is Boltzmann's constant. We choose units so $k_B = 1$.)

The natural temperatures to consider are those at most on the order of the Fermi temperature of the free gas T_F. The Fermi temperature is the temperature scale at which the thermal (kinetic) energy per particle is comparable to the (kinetic) energy per particle arising from the Pauli exclusion. The thermal energy per particle is of order $k_B T = T$,[1] and the energy

[1]A monoatomic gas has a thermal (kinetic) energy per particle of $\frac{3}{2}k_B T$, for instance.

per particle from Pauli exclusion is of order $\rho_0^{2/3}$. That is, the Fermi temperature is of order $T_F \sim \rho_0^{2/3}$. The constraint that $T \lesssim T_F$ is the same as the constraint that the fugacity $z = e^{\beta\mu}$ satisfies $z \gtrsim 1$. For temperatures larger than the Fermi temperature the thermal energy exceeds that from quantum effects, and so the gas behaves more like a classical (high-temperature) gas.

We prove in Chapters 6 and 7 the positive temperature analogue of the formula in (1.1.2) to order $a_p^3 k_F^5$. This is the second main theorem of Part I of the thesis.

Theorem 1.1.6. *Let $V \geq 0$ be radial and of compact support. Then for small $a_p^3\rho_0$ we have*

$$\psi(\beta,\mu) = \psi_0(\beta,\mu) - 24\pi^2 \frac{-\operatorname{Li}_{5/2}(-z)}{(-\operatorname{Li}_{3/2}(-z))^{5/3}} a_p^3 \rho_0^{8/3} \left[1 + o_z(1)\right],$$

where $\rho_0 = \partial_\mu \psi_0(\beta,\mu)$ is the particle density of the free gas (in infinite volume), Li_s denotes the polylogarithm *of order s and $o_z(1)$ vanishes for $a_p^3\rho_0 \to 0$ uniformly for $z = e^{\beta\mu}$ in compact subsets of $(0,\infty)$.*

Remark 1.1.7. We note that the lower bound in Chapter 6 holds also in dimensions $d = 1, 2$ and is in fact uniform in $z \gtrsim 1$, meaning that $o_z(1)$ vanishes uniformly for bounded $1/z$. The upper bound in Chapter 7 holds also in dimension $d = 2$.

Note further that the pressure is decreasing in the Hamiltonian, describing the energy. Thus, a lower bound for the pressure corresponds to an upper bound for the ground state energy and vice versa.

We describe next the two different methods used in the following Chapters 3–7 to prove Theorems 1.1.3, 1.1.5 and 1.1.6. We discuss the reason for the two different methods in Remark 1.3.1 below.

1.2 Gaudin–Gillespie–Ripka expansion

At the centre of the argument in Chapters 3, 5 and 6 lies the Gaudin–Gillespie–Ripka (GGR) expansion [GGR71]. This is one example of a cluster expansion developed in the physics literature in order to deal with strongly correlated systems. To explain this expansion and its relevance in the many-body problem we first explain the overall structure of the proof of the bounds in Chapters 3, 5 and 6.

In Chapters 3 and 5 we prove upper bounds on the ground state energy of a spin-polarized and spin-$\frac{1}{2}$ Fermi gas respectively and in Chapter 6 we prove a lower bound on the pressure of a spin-polarized Fermi gas at positive temperature. All of these bounds arise from computing the energy (respectively pressure functional) of a trial state, being then an upper (respectively lower) bound for the ground state energy (respectively pressure) by the variational principle. The trial state we consider is of (Bijl–Dingle–)Jastrow type [Bij40; Din49; Jas55], meaning that (in the spin-polarized setting) the trial state is given by

$$\psi_{\mathsf{Jas}}(x_1,\ldots,x_N) = \frac{1}{\sqrt{C_N}} \prod_{1\leq j<k\leq N} f_p(x_j - x_k)\psi_0(x_1,\ldots,x_N), \tag{1.2.1}$$

where f_p is the p-wave scattering function defined in Definition 1.1.1, ψ_0 is the ground state of the free system, being a Slater determinant of the N smallest momenta, and C_N is a normalization constant. For the problem of spin-$\frac{1}{2}$ fermions or spin-polarized fermions at positive temperature analogous trial states are constructed. (For technical reasons the trial states we consider in Chapters 3, 5 and 6 are slightly modified.)

This type of trial state is motivated by the following picture: As discussed after Definition 1.1.1 above, we expect that the many-body system is essentially described by a bunch of two-particle interacting systems. More precisely, we expect that keeping all but two particles fixed, the wave function in the remaining two particles should be close to that of just the two-particle ground state. As discussed above, the ground state for the two-particle system in a large box is (to leading order) given by the scattering function times the ground state of the free two-particle system. That is, between any pair of particles the wave function should be modified by inclusion of the scattering function compared to the ground state of the free system. This naturally leads to the idea that the ground state of the free system modified by a factor $\prod_{1\leq j<k\leq N} f_p(x_j-x_k)$ should be a good approximation to the ground state of the many-body system. This motivates the choice of trial state in (1.2.1).

To calculate the energy of the trial state ψ_{Jas} we use the following observation: For any real-valued functions F, G we have

$$\int |\nabla(FG)|^2 = \int |\nabla F|^2|G|^2 + \int |F|^2 G(-\Delta)G. \tag{1.2.2}$$

(Verifying this is a simple exercise, which we leave to the reader.) We use (1.2.2) with $F=\prod f_p$ and $G=\psi_0$ and note that $\sum_j -\Delta_{x_j}\psi_0 = E_0\psi_0$ with E_0 the ground state energy of the free system. Then,

$$\begin{aligned}\langle\psi_{\mathsf{Jas}}|H_N|\psi_{\mathsf{Jas}}\rangle &= E_0 + \iint \rho^{(2)}_{\mathsf{Jas}}(x_1,x_2)\left(\left|\frac{\nabla f_p(x_1-x_2)}{f_p(x_1-x_2)}\right|^2 + \frac{1}{2}V(x_1-x_2)\right)\mathrm{d}x_1\,\mathrm{d}x_2\\ &\quad + \iiint \rho^{(3)}_{\mathsf{Jas}}(x_1,x_2,x_3)\frac{\nabla f_p(x_1-x_2)\nabla f_p(x_2-x_3)}{f_p(x_1-x_2)f_p(x_2-x_3)}\,\mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3,\end{aligned} \tag{1.2.3}$$

where $\rho^{(2)}_{\mathsf{Jas}}$ and $\rho^{(3)}_{\mathsf{Jas}}$ are the 2- and 3-particle reduced densities of ψ_{Jas}. Thus, to compute the energy, we need only compute the reduced densities $\rho^{(2)}_{\mathsf{Jas}}$ and $\rho^{(3)}_{\mathsf{Jas}}$. Calculating these reduced densities is essentially a complicated combinatorics problem. The solution of this combinatorics problem is the contents of the GGR expansion, giving the formulas for the q-particle reduced densities:

$$\rho^{(q)}_{\mathsf{Jas}}(x_1,\ldots,x_q) = \prod_{1\leq j<k\leq q} f_p(x_j-x_k)\left[\rho^{(q)}(x_1,\ldots,x_q) + \sum_{p=1}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\tilde{\mathcal{L}}_p^q}\Gamma^q_{\pi,G}(x_1,\ldots,x_q)\right]. \tag{1.2.4}$$

Here $\rho^{(q)}$ is the q-particle reduced density of the free state and the sets of diagrams $\tilde{\mathcal{L}}_p^q$ and their values $\Gamma^q_{\pi,G}$ are described in detail in Chapters 3, 5 and 6.

All the terms in the theorems of Chapters 3, 5 and 6 are contained in the contribution of the first two terms in (1.2.3) (suitably modified in the spin-$\frac{1}{2}$ setting or at positive temperature, see the respective chapters for the details). Moreover, for the expansion of $\rho^{(2)}_{\mathsf{Jas}}$ in (1.2.4) only the leading term contributes to the order we consider in Chapters 3, 5 and 6. The third term in (1.2.3) and the higher order terms in (1.2.4) are error terms. Ignoring these, we thus find the approximate formula (in the spin-polarized setting)

$$\langle\psi_{\mathsf{Jas}}|H_N|\psi_{\mathsf{Jas}}\rangle \approx E_0 + \iint \rho^{(2)}(x_1,x_2)\left[|\nabla f_p|^2 + \frac{1}{2}V\,|f_p|^2\right](x_1-x_2)\,\mathrm{d}x_1\,\mathrm{d}x_2.$$

It is a simple exercise to Taylor expand $\rho^{(2)}(x_1,x_2) \approx \frac{1}{5}k_F^2\rho^2|x_1-x_2|^2$ for x_1,x_2 close. Recalling the definition of the p-wave scattering length in Definition 1.1.1, we arrive at the formula in Theorem 1.1.3.

To control the errors in the above approximations we need to understand the expansions (1.2.4) in more detail. For the first few terms in the expansions we need somewhat precise calculations in order to control the errors from the remaining terms accurately enough. To aid in the calculation of these first few terms (the sets of diagrams $\tilde{\mathcal{L}}_p^q$ are quite big, even for small p's and q's) we wrote a short python-script [GGRscript]. Finally, bounding the tails of the expansions is again a complicated combinatorics problem. To bound these tails we need to replace f_p in the trial state in (1.2.1) by a slightly modified function and the Slater determinant ψ_0 by a slightly different Slater determinant, see the details in Chapters 3, 5 and 6.

1.3 Modified second order perturbation theory

In Chapter 4 we prove the lower bound in Theorem 1.1.3 and in Chapter 7 we prove the upper bound in Theorem 1.1.6. A central ingredient is a modified version of second order perturbation theory, where one considers part of the interaction to be part of the unperturbed operator. We explain here the main ideas, focussing on the approach in Chapter 4.

We introduce the particle hole transformation R factoring out the ground state of the free system, being the filled Fermi ball/sea. This satisfies $R\Omega = \psi_0$, with Ω the vacuum state and ψ_0 the ground state of the free system. Then

$$R^*H_NR \approx \langle\psi_0|H_N|\psi_0\rangle + \mathbb{H}_0 + \mathbb{Q}_2 + \mathbb{Q}_4,$$

with $\mathbb{H}_0 \geq 0$ an effective kinetic energy and $\mathbb{Q}_2$ and $\mathbb{Q}_4 \geq 0$ being effectively the 'off-diagonal' and 'diagonal' parts of the interaction, see Chapter 4 for the details. Then, second order perturbation theory is the claim that if B satisfies $[\mathbb{H}_0 + \mathbb{Q}_4, B] + \mathbb{Q}_2 \approx 0$ (this equation is essentially the scattering equation (1.1.1) for f_p in disguise), then $e^{-B}R^*H_NRe^B$ approximately has Ω as its ground state. Using a Baker–Campbell–Hausdorff expansion to second order in $\mathbb{Q}_2$ and B (this is the "second order" in "second order perturbation theory") we have

$$\begin{aligned} e^{-B}(\mathbb{H}_0 + \mathbb{Q}_2 + \mathbb{Q}_4)e^B &\approx \mathbb{H}_0 + \mathbb{Q}_4 + [\mathbb{H}_0 + \mathbb{Q}_4, B] + \mathbb{Q}_2 + \frac{1}{2}[[\mathbb{H}_0 + \mathbb{Q}_4, B], B] + [\mathbb{Q}_2, B] \\ &\approx \mathbb{H}_0 + \mathbb{Q}_4 + \frac{1}{2}[\mathbb{Q}_2, B]. \end{aligned}$$

Evaluating in the state Ω we find the following formula for the ground state energy:

$$E_N \approx \langle\psi_0|H_N|\psi_0\rangle + \langle\Omega|\mathbb{H}_0 + \mathbb{Q}_4|\Omega\rangle + \frac{1}{2}\langle\Omega|[\mathbb{Q}_2, B]|\Omega\rangle = \langle\psi_0|H_N|\psi_0\rangle + \frac{1}{2}\langle\Omega|[\mathbb{Q}_2, B]|\Omega\rangle .$$

These terms may then be evaluated to be the first two terms in the formula in (1.1.2).

The main argument in Chapter 4 consists of doing the computation above precisely, taking into account all the error terms. More precisely, we find the formula for the energy of any N-particle state ψ_N

$$\langle\psi_N|H_N|\psi_N\rangle = \langle\psi_0|H_N|\psi_0\rangle + \frac{1}{2}\langle\Omega|[\mathbb{Q}_2, B]|\Omega\rangle + \langle\xi_1|\mathbb{H}_0 + \mathbb{Q}_4|\xi_1\rangle + \mathcal{E}(\psi_N), \tag{1.3.1}$$

where $\xi_1 = R^* e^{-B} \psi_N$ and $\mathcal{E}(\psi_N)$ is an explicit error term, see Chapter 4 for the details. The first two terms evaluate to the claimed formula in Theorem 1.1.3 as above and the term $\langle \xi_1 | \mathbb{H}_0 + \mathbb{Q}_4 | \xi_1 \rangle$ can be dropped for a lower bound since $\mathbb{H}_0 + \mathbb{Q}_4 \geq 0$. The main work in Chapter 4 then concerns bounding the error term $\mathcal{E}(\psi_N)$.

In the positive temperature setting considered in Chapter 7 there is no natural particle hole transformation, since there is no filled Fermi ball. We can still conjugate the Hamiltonian by a unitary operator $e^{\mathcal{B}}$ with appropriately chosen $\mathcal{B}$, however. (The relevant $\mathcal{B}$ is related to the operator B above by $\mathcal{B} = RBR^*$.) We then conclude a formula similar to (1.3.1). In the positive temperature setting, the evaluation of (the positive temperature analogue of) the term $\langle \Omega | [\mathbb{Q}_2, B] | \Omega \rangle$ is further complicated. An essential part of the evaluation is showing the validity of *first order perturbation theory* at positive temperature in a certain appropriate regime.

We conclude this chapter with a discussion of the necessity of the two different methods; the GGR expansion and perturbation theory.

Remark 1.3.1 (Choice of method for upper versus lower bounds)**.** We use the GGR expansion to obtain upper bounds on the energy and modified second order perturbation theory to obtain lower bounds on the energy (and vice versa for the pressure). The reasons for not just using one method for both upper and lower bounds are as follows:

The GGR expansion is a trial state based approach computing the energy (or pressure functional) of a particular type of trial state. A priori it is not clear whether this class of states contain the ground state, however. Thus, the GGR expansion can inherently only prove upper bounds on the energy. It has the benefit of requiring no regularity of the interaction, however, and can in particular treat also hard core interactions. Further, it gives better bounds on the error term and works also in lower dimension, see Remarks 1.1.4 and 1.1.7.

The perturbation theory method, on the other hand, can be used to prove lower bounds on the energy. It works by conjugating the Hamiltonian by a particular unitary operator and in particular no class of states are excluded. The perturbation theory method can also be used to prove upper bounds, see Chapter 4. However, this doesn't work for too irregular interactions. Indeed, from the formula (1.3.1) we see that, in particular, we need that $\int V|x|^2 \, \mathrm{d}x < \infty$ for the expectation $\langle \psi_0 | H_N | \psi_0 \rangle$ to be finite. In fact, we need $V \in L^1$ to control also the error term, see Chapter 4. This is not an issue for proving lower bounds, since any interaction can be bounded from below by an integrable one, see Remark 4.1.4.

Chapter 2

Pair of particles in an infinite square well

Any introductory physics textbook on quantum mechanics considers the toy problem of a *particle in an infinite square well*, meaning that the particle is constrained to some box (being the bottom of the infinite well). This example serves to illustrate many important aspects of quantum mechanics. Following along these lines we consider here the problem of *two* particles in an infinite square well (equivalently localized to some box). We study this toy problem here for two main reasons:

1. It motivates clearly the definition of the scattering lengths in Definition 1.1.1, and
2. It illustrates and motivates the method of proof used in the following Chapters 3–7 to prove Theorems 1.1.3, 1.1.5 and 1.1.6.

More precisely, we consider the toy problem of two interacting indistinguishable fermions constrained to a large box Λ. For this system we shall determine the ground state energy to leading order in the volume of the box. We first describe the system more precisely.

We take the box to be $\Lambda = [-L/2, L/2]^3$ with L some large length. That is, we shall consider the limit $L \to \infty$. The particles interact through a radial interaction V, which we assume to be repulsive and short-ranged. Concretely this means that $V(x) \geq 0$ and that V has compact support. That is, there is some $R_0 > 0$ such that $V(x) = 0$ for $|x| > R_0$.

Working in units where the particle mass is $m = 1/2$ and $\hbar = 1$, the energy is then given by the Hamiltonian

$$H = -\Delta_x - \Delta_y + V(x-y).$$

Concretely this means that if the particles are in the state $\psi \in L^2(\Lambda^2; \mathbb{C})$ (with $\|\psi\|^2_{L^2(\Lambda^2;\mathbb{C})} = \iint_{\Lambda\times\Lambda} |\psi(x,y)|^2 \,\mathrm{d}x\,\mathrm{d}y = 1$) then the energy is given by

$$\langle\psi|H|\psi\rangle = \iint_{\Lambda\times\Lambda} \left(|\nabla_x\psi(x,y)|^2 + |\nabla_y\psi(x,y)|^2 + V(x-y)|\psi(x,y)|^2\right) \mathrm{d}x\,\mathrm{d}y.$$

The ground state energy is then defined as the lowest possible energy:

$$E = \inf_{\psi:\|\psi\|_{L^2}=1} \langle\psi|H|\psi\rangle,$$

where the infimum is taken over appropriate states ψ. Exactly which states are appropriate depends on the spins of the particles. We consider two settings:

1. Fermions of different spins: In this case the appropriate space for ψ is the product space $L^2(\Lambda;\mathbb{C}) \otimes L^2(\Lambda;\mathbb{C}) = L^2(\Lambda^2;\mathbb{C})$.

2. Fermions of the same spin: In this case the Pauli exclusion principle dictates that $\psi(x,y) = -\psi(y,x)$ and so the appropriate space for ψ is

$$L^2(\Lambda;\mathbb{C}) \wedge L^2(\Lambda;\mathbb{C}) = L^2_a(\Lambda^2;\mathbb{C}) = \left\{\psi(x,y) \in L^2(\Lambda^2;\mathbb{C}) : \psi(x,y) = -\psi(y,x)\right\}.$$

Further, we need to specify the boundary conditions. The particles being in an "infinite square well" the relevant boundary conditions would be Dirichlet boundary conditions, requiring that $\psi(x,y)$ vanishes whenever x or y are on the boundary. We shall instead consider the system with periodic boundary conditions. (Strictly speaking it would thus be more appropriate to call the system a "pair of particles in a periodic box".) These are the boundary conditions used in the finite systems in the following chapters and are slightly more convenient to work with. One can compute the ground state energy also for other choices of boundary conditions, but we do not do this here.

We calculate the ground state energy E in the limit of a large box in two ways:

1. Variationally, by considering trial states of a particular form, and

2. Perturbatively, using second order perturbation theory.

In both settings we shall solve the problem in a way familiar to many mathematicians by simply defining 'something' to be the solution and declaring victory. (This is a bit disingenuous. We still need to do *some* work.) This 'something' is the all-important *scattering length(s)* of the interaction defined in Definition 1.1.1. (One should really read Definition 1.1.1 then as defining the scattering length(s) to be the solution(s) of the present toy problem(s).)

Remark 2.0.1. The two different methods of calculating the ground state energy reflects the two different methods used in calculating the ground state energy of the many-body interacting system in the following chapters. In Chapters 3, 5 and 6 we use a trial state based on the variational methods here to find upper bounds on the ground state energies and a lower bound on the pressure of the many-body systems. In Chapters 4 and 7 we use a perturbation theory argument (modified compared to 'standard' perturbation theory as the argument given here) to give a lower bound on the ground state energy and an upper bound on the pressure of the many-body systems.

2.1 Non-interacting problem

To understand the interacting setting we first consider the simpler non-interacting setting, where $V = 0$. In the non-interacting setting the Hamiltonian is given by $H_0 = -\Delta_x - \Delta_y$, and we shall determine the ground state energy $E_0 = \inf_\psi \langle\psi|H_0|\psi\rangle$ and the ground state(s) ψ_0. Such ψ_0 satisfy $E_0 = \langle\psi|H_0|\psi\rangle$ and $H_0\psi_0 = E_0\psi_0$.

To find E_0 and ψ_0 we first note that the Hamiltonian H_0 is a sum of 1-body operators, $-\Delta_x$ and $-\Delta_y$. The eigenstates of $-\Delta_x$ are the planes waves $u_k(x) = L^{-3/2}e^{ikx}$ for momentum

$k \in \frac{2\pi}{L}\mathbb{Z}^3$. These have energy $\langle u_k|{-\Delta}|u_k\rangle = |k|^2$. Thus, the space of ground states is spanned by states of the form (see [Sol14, Theorem 8.6] for more details)

$$\psi_0 = \begin{cases} u_0 \otimes u_0 & \text{for different spins,} \\ u_0 \wedge u_k & \text{for same spins,} \end{cases} \qquad k = \pm\frac{2\pi}{L}e_j, \qquad e_j \in \{(0,0,1),(0,1,0),(1,0,0)\}.$$

For the case of different spins there is just one ground state $u_0 \otimes u_0$, whereas for the case of same spins the space of ground states is 6-dimensional. It will be convenient to choose a basis of real-valued ground states ψ_0. For instance the ground state space is spanned by the ground states

$$\psi_0(x,y) = \begin{cases} \dfrac{1}{L^3} & \text{for different spins,} \\ \dfrac{2}{L^3}\begin{Bmatrix}\cos \\ \sin\end{Bmatrix}\left(\dfrac{2\pi}{L}\dfrac{x^j+y^j}{2}\right)\sin\left(\dfrac{\pi}{L}(x^j-y^j)\right), \quad j=1,2,3 & \text{for same spins,} \end{cases} \tag{2.1.1}$$

where $\begin{Bmatrix}\cos \\ \sin\end{Bmatrix}$ means either $\cos$ or $\sin$ and x^j is the j'th coordinate of $x = (x^1,x^2,x^3)$. The ground state energy is

$$E_0 = \begin{cases} 0 & \text{for different spins,} \\ \dfrac{4\pi^2}{L^2} & \text{for same spins.} \end{cases}$$

2.2 Variational calculation

Next, we solve the interacting problem with a variational method. This serves as

1. Motivation for the definition of the scattering length(s) in Definition 1.1.1, and
2. Illustration and motivation for the method of proof used in Chapters 3, 5 and 6.

As a first step we claim that any ground state ψ of the interacting system can be written as $\psi(x,y) = f(x-y)\psi_0(x,y)$ with ψ_0 a ground state of the non-interacting system and f some function. Clearly, any state ψ can be written as $\psi(x,y) = f(x,y)\psi_0(x,y)$. The statement is that for the ground state it suffices to consider functions f only depending on the difference $x-y$. (Rather f should depend on the difference $x - y \,(\mathrm{mod}\,\Lambda)$, since f should be Λ-periodic by the periodic boundary conditions. Here $\mathrm{mod}\,\Lambda$ means that in each component one possibly adds or subtracts L such that the result is in the interval $[-L/2, L/2]$.)

To see this we change variables to the variables $(X,Y) \in \Lambda^2$. They represent the 'relative coordinate' $x-y$ and the 'centre-of-mass coordinate' $\frac{x+y}{2}$. The relative coordinate is more precisely given by $X = x - y \,(\mathrm{mod}\,\Lambda)$. For the centre-of-mass coordinate Y we possibly add or subtract a term L to one or more of the components of x or y, such that the resulting tuple (X,Y) satisfies $(X,Y) \in [-L/2, L/2]^6$, see Figure 2.2.1.[1] By the change of variables formula it follows that $\mathrm{d}x\,\mathrm{d}y = \mathrm{d}X\,\mathrm{d}Y$.

[1]Note that this change of variables is only really useful for functions that are $\Lambda/2$-periodic in the centre-of-mass variable, since the centre-of-mass is changed from $\frac{x+y}{2}$ by some integer vector multiple of $L/2$. Otherwise, (X,Y)-integrals would not factorize into products of the X- and Y-integrals. For ψ_0 a non-interacting ground state $|\psi_0|^2$ satisfies this, since $\sin(t+\pi) = -\sin t$ and $\cos(t+\pi) = -\cos t$. (Recall that a non-interacting ground state ψ_0 is spanned by states of the form in (2.1.1).)

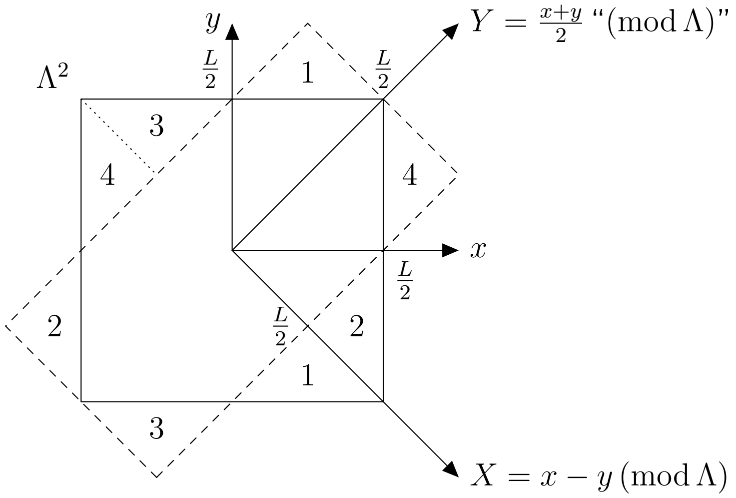


Figure 2.2.1: Change of coordinates to the 'centre-of-mass' coordinate Y and the 'relative' coordinate X. The picture is in one dimension and is applied to the three-dimensional setting component wise. Using the Λ-periodicity each of the regions labelled $1, 2, 3, 4$ are identified with the corresponding region for which $(X, Y) \in \Lambda^2$.

In these coordinates the Hamiltonian takes the form

$$H = -2\Delta_X - \frac{1}{2}\Delta_Y + V(X).$$

To evaluate the expectation of this in any state $\psi = f\psi_0$ we recall (1.2.2): For any real-valued functions F, G we have

$$\int |\nabla(FG)|^2 = \int |\nabla F|^2 |G|^2 + \int |F|^2 G(-\Delta)G.$$

We use this for $F = f$ and $G = \psi_0$. Then $(-2\Delta_X - \frac{1}{2}\Delta_Y)\psi_0 = E_0\psi_0$ since ψ_0 is a ground state of the non-interacting system. Thus,

$$\langle\psi|H|\psi\rangle = E_0 + \iint_{\Lambda\times\Lambda} \left(2|\nabla_X f|^2 + V|f|^2 + \frac{1}{2}|\nabla_Y f|^2\right) |\psi_0|^2 \,\mathrm{d}X\,\mathrm{d}Y. \tag{2.2.1}$$

To minimize this clearly $\nabla_Y f = 0$ and thus for the ground state ψ we may take f to depend only on X, i.e. on $x - y$. (Recall the Λ-periodicity.)

The ground state energy E is then given by (2.2.1) only with f depending only on X. Further, we expect that the effect of the interaction is somewhat localized to particles close enough, say $|x - y| \lesssim R_0$, since the interaction has range $R_0 \ll L$. If the particles are further apart the effect of the interaction should be small. We should thus expect that any ground state satisfies $\psi(x, y) \approx \psi_0(x, y)$ for $|x - y| \gg R_0$. That is, we expect that $f(X) \approx 1$ for large $|X|$.

2.2.1 Different spins

For the setting of different-spin fermions we have only one ground state for the non-interacting system $\psi_0(x, y) = 1/L^3$. Hence, the Y-integration in Equation (2.2.1) simply evaluates to $\int_\Lambda \mathrm{d}Y = L^3$. Further, f is constrained by the normalization that $\|\psi\|_{L^2} = 1$. Thus, the energy and optimal f (meaning the f for which the state $\psi(x,y) = f(x-y)\psi_0(x,y)$ has lowest energy) are given by the minimization problem

$$E = \frac{1}{L^3} \inf \left\{ \int (2|\nabla f|^2 + V|f|^2) \,\mathrm{d}X : \int |f|^2 \,\mathrm{d}X = L^3 \right\}.$$

Next, we replace the constraint that $\int |f|^2 \,\mathrm{d}X = L^3$ by the constraint that $f(X) \to 1$ for $|X| \to \infty$. In the limit of large L this is a good approximation. Indeed, by the discussion above we expect $f \approx 1$ for $|X| \gg R_0$ anyway, and this clearly satisfies the constraint $\int |f|^2 \,\mathrm{d}x = L^3$, at least to leading order in L.[2] This leads us to the definition of the *s-wave scattering length* as stated in Definition 1.1.1, and we thus find the formula

$$E \approx \frac{8\pi a_s}{L^3}$$

for the ground state energy of two different-spin fermions in a large periodic box.

2.2.2 Same spin

For the setting of same-spin fermions we again compute the Y-integral first. Noting that $\sin(t+\pi) = -\sin t$ and similarly for $\cos$ we see that for any non-interacting ground state ψ_0 the Y-integral evaluates to $\int_\Lambda \sin^2 = \int_\Lambda \cos^2 = \frac{1}{2}L^3$. (Recall that a non-interacting ground state ψ_0 is spanned by states of the form in (2.1.1).) Thus, combining Equations (2.1.1) and (2.2.1) we find that the ground state energy and optimal f are given by

$$E = \frac{4\pi^2}{L^2} + \frac{2}{L^3} \inf \left\{ \int (2|\nabla f|^2 + V|f|^2) \sin^2\left(\frac{\pi X^j}{L}\right) \,\mathrm{d}X : 2\int |f|^2 \sin^2\left(\frac{\pi X^j}{L}\right) \,\mathrm{d}X = L^3 \right\}.$$

As above, we replace the constraint by $f(X) \to 1$ for $|X| \to \infty$. As $\sin^2$ is $1/2$ "on average", this is a good approximation for large L exactly as above. Next, we expect the integrand in the first integral $(2|\nabla f|^2 + V|f|^2)\sin^2(\pi X^j/L)$ to be supported essentially only for $|X| \ll L$. (Clearly the term with V is by the compact support.) Thus, we Taylor expand the sine and find for large L that

$$E \approx \frac{4\pi^2}{L^2} + \frac{2\pi^2}{L^5} \inf \left\{ \int_{\mathbb{R}^3} (2|\nabla f|^2 + V|f|^2)|X^j|^2 \,\mathrm{d}X : f(X) \to 1 \text{ for } |X| \to \infty \right\}.$$

Further, this minimization problem is symmetric in relabelling the coordinates X^j, and thus we may replace $|X^j|^2$ by $|X|^2/3$. This leads us to the definition of the *p-wave scattering length* as stated in Definition 1.1.1. We conclude the formula

$$E \approx \frac{4\pi^2}{L^2} + \frac{16\pi^3 a_p^3}{L^5}$$

for the ground state energy of two same-spin fermions in a large periodic box.

[2] This can be done more rigorously as follows: By the Euler–Lagrange equations for the first minimization problem, f converges to some constant for large $|X|$. To leading order in L this constant has to be 1 in order to satisfy the constraint $\int |f|^2 \,\mathrm{d}X = L^3$.

2.3 Perturbation theory

Next, we illustrate how to solve the present toy problem using an appropriately modified version of second order perturbation theory. We do this for two main reasons:

1. It motivates an alternative definition of the scattering function using the scattering equation, (being the Euler–Lagrange of the variational definition given in Definition 1.1.1) and

2. It illustrates the method of proof used in Chapters 4 and 7.

Perturbation theory can be formulated in many equivalent ways. We use here a slightly modified form, where we treat only part of the interaction as the perturbation and formulate it using a unitary operator e^B.

To formulate this modified version of perturbation theory we split the interaction operator V into two parts; V_{D} the 'diagonal' part of V and V_{OD} the 'off-diagonal' part. To define them more precisely we introduce the projection operator P on $L^2(\Lambda)$ being a projection onto low-lying eigenvalues of $-\Delta$ such that $P \otimes P\psi_0 = \psi_0$. We can achieve this while simultaneously having the approximations $P \approx 0$ and $Q = \mathbb{1} - P \approx \mathbb{1}$.[3] For instance, one can consider $P = \chi_{(-\Delta \leq (2\pi/L)^2)}$ the projection onto the 0th and 1st excited modes of $-\Delta$.

To simplify notation we write $PP = P \otimes P$ and $QQ = Q \otimes Q$. We define then

$$V_{\mathsf{D}} = PPVPP + QQVQQ, \qquad V_{\mathsf{OD}} = PPVQQ + QQVPP,$$

and approximate $V \approx V_{\mathsf{D}} + V_{\mathsf{OD}}$. We then treat $H_0 + V_{\mathsf{D}} = -\Delta_x - \Delta_y + V_{\mathsf{D}}(x,y)$ as the unperturbed operator and V_{OD} as the perturbation. Using a Baker–Campbell–Hausdorff expansion to second order (in B and V_{OD}) we find

$$e^{-B}He^B \approx H_0 + V_{\mathsf{D}} + ([H_0 + V_{\mathsf{D}}, B] + V_{\mathsf{OD}}) + \left(\frac{1}{2}[[H_0 + V_{\mathsf{D}}, B], B] + [V_{\mathsf{OD}}, B]\right).$$

The statement of second order perturbation theory is then the following: If B is chosen so that $[H_0 + V_{\mathsf{D}}, B] + V_{\mathsf{OD}} \approx 0$, then ψ_0 is approximately the ground state of $e^{-B}He^B$.

We choose B to be (with s/p in the case of different/same spins)

$$B = PP(1 - f_{s/p})QQ - QQ(1 - f_{s/p})PP.$$

We claim then that this satisfies $[H_0 + V_{\mathsf{D}}, B] + V_{\mathsf{OD}} \approx 0$. (This boils down to $f_{s/p}$ satisfying the scattering equation as we show below.) Admitting this, the ground state energy is

$$\begin{aligned} E &\approx \left\langle \psi_0 \middle| -\Delta_x - \Delta_y + PPVPP + QQVQQ + \frac{1}{2}[V_{\mathsf{OD}}, B] \middle| \psi_0 \right\rangle \\ &= E_0 + \left\langle \psi_0 \middle| V + \frac{1}{2}[V_{\mathsf{OD}}, B] \middle| \psi_0 \right\rangle. \end{aligned}$$

[3] Here we are a bit vague regarding what exactly is meant. The analogous approximations in the many-body setting are made precise in Chapters 4 and 7. The same comment applies to subsequent operator approximations in this section.

For the commutator we have (approximating $Q \approx \mathbb{1}$ and $P \approx 0$ whenever they appear not as the first or last term of an operator)

$$\begin{aligned}[V_{\mathsf{OD}}, B] &= \Big[PPVQQ + QQVPP, PP(1 - f_{s/p})QQ\Big] + \text{h.c.} \\ &= QQVPP(1 - f_{s/p})QQ - PPVQQ(1 - f_{s/p})PP + \text{h.c.} \\ &\approx -2PPV(1 - f_{s/p})PP.\end{aligned}$$

Thus, we find that the energy is given by

$$E \approx E_0 + \Big\langle \psi_0 \Big| V f_{s/p} \Big| \psi_0 \Big\rangle . \tag{2.3.1}$$

To evaluate this and show that $[H_0 + V_{\mathsf{D}}, B] + V_{\mathsf{OD}} \approx 0$ we distinguish between the two settings of different or same spins.

2.3.1 Different spins

In the setting of the two particles having different spins, the ground state of the free system is $\psi_0(x, y) = 1/L^3$. Thus, by (2.3.1), we find the ground state energy of the interacting system as

$$E \approx 0 + \frac{1}{L^6} \iint_{\Lambda^2} V(x-y) f_s(x-y)\, \mathrm{d}x\, \mathrm{d}y = \frac{1}{L^3} \int V f_s\, \mathrm{d}x.$$

Using the scattering equation (1.1.1) and integrating by parts once we find $\int V f_s = 8\pi a_s$, and so we again find

$$E \approx \frac{8\pi a_s}{L^3}$$

for the ground state energy of two different-spin fermions in a large periodic box.

Next, to show that $[H_0 + V_{\mathsf{D}}, B] + V_{\mathsf{OD}} \approx 0$ we compute similarly to the commutator $[V_{\mathsf{OD}}, B]$ above

$$\begin{aligned}[H_0 + V_{\mathsf{D}}, B] + V_{\mathsf{OD}} &= PP\left[2\Delta f_s + 2\nabla f_s \cdot (\nabla_x - \nabla_y) + V\right] QQ \\ &\qquad + \left[PPVPP + QQVQQ, PP(1 - f_s)QQ\right] + \text{h.c.} \\ &\approx PP\left[2\Delta f_s + 2\nabla f_s \cdot (\nabla_x - \nabla_y) + V f_s\right] QQ + \text{h.c.}.\end{aligned}$$

Noting that $(\nabla f_s \cdot \nabla)^* = -\Delta f_s - \nabla f_s \cdot \nabla$ we can write this as

$$\begin{aligned}[H_0 + V_{\mathsf{D}}, B] + V_{\mathsf{OD}} &\approx QQ\left[-2\Delta f_s - 2\nabla f_s \cdot (\nabla_x - \nabla_y) + V f_s\right] PP + \text{h.c.} \\ &= -2QQ\nabla f_s \cdot (\nabla PP - P\nabla P) + \text{h.c.}\end{aligned}$$

by the scattering equation (1.1.1), where ∇P is the multiplication operator in momentum space multiplying by $k\hat{P}(k)$. Since P projects onto low-energy eigenstates of the Laplacian, k in the support of P is small. Thus, we see that $[H_0 + V_{\mathsf{D}}, B] + V_{\mathsf{OD}} \approx 0$.

We remark that for the scattering function f_s we used only the scattering equation (1.1.1), but not the variational formulation in Definition 1.1.1. Thus, the analysis above serves as motivation for taking the scattering equation (1.1.1) as the definition of the scattering function and length instead of the variational formulation in Definition 1.1.1. This is the definition used in Chapters 4 and 7, recall Remark 1.1.2.

2.3.2 Same spin

Similarly, as above we find by (2.3.1) the ground state energy to be

$$\begin{aligned} E &\approx \frac{4\pi^2}{L^2} + \frac{4}{L^6} \iint V(x-y) f_p(x-y) \begin{Bmatrix} \cos \\ \sin \end{Bmatrix}^2 \left(\frac{2\pi}{L} \frac{x^j + y^j}{2} \right) \sin^2\left(\frac{\pi}{L}(x^j - y^j) \right) \, \mathrm{d}x \, \mathrm{d}y \\ &= \frac{4\pi^2}{L^2} + \frac{2}{L^3} \int V(x) f_p(x) \sin^2\left(\frac{\pi}{L} x^j \right) \, \mathrm{d}x \end{aligned}$$

We Taylor expand the sine and replace $(x^j)^2$ by $|x|^2/3$ by the radial symmetry. Noting further that $\int V f_p |x|^2 = 24\pi a_p^3$, which follows from the scattering equation (1.1.1) and integrating by parts once, we find as above

$$E \approx \frac{4\pi^2}{L^2} + \frac{16\pi^3 a_p^3}{L^5}$$

for the ground state energy of two same-spin fermions in a large periodic box.

Next, to show that $[H_0 + V_{\mathsf{D}}, B] + V_{\mathsf{OD}}$ approximately vanishes we have as above

$$[H_0 + V_{\mathsf{D}}, B] + V_{\mathsf{OD}} \approx QQ \left[-2\Delta f_p - 2\nabla f_p \cdot (\nabla_x - \nabla_y) + V f_p \right] PP + \text{h.c.}.$$

Further, by exchanging the two particles, meaning interchanging x and y, we see that

$$[H_0 + V_{\mathsf{D}}, B] + V_{\mathsf{OD}} \approx QQ \left[-2\Delta f_p - 4\nabla f_p \cdot \nabla_x + V f_p \right] PP + \text{h.c.}.$$

For any state ψ we have that $(PP\psi)(x,y)$ vanishes for $x = y$ by the Pauli exclusion principle. Thus, we can Taylor expand it in x around $x = y$. That is

$$(PP\psi)(x,y) \approx (x-y) \cdot \left[\nabla_x (PP\psi)(x,y) \right]_{x=y} \approx (x-y) \cdot (\nabla PP\psi)(x,y).$$

Performing such a Taylor expansion for the two terms $-2\Delta f_p$ and $V f_p$ in the commutator above we find for any state ψ

$$\langle \psi | [H_0 + V_{\mathsf{D}}, B] + V_{\mathsf{OD}} | \psi \rangle \approx 2 \operatorname{Re} \langle \psi | QQ \left[-2(\cdot)\Delta f_p - 4\nabla f_p + (\cdot) V f_p \right] \cdot \nabla PP | \psi \rangle .$$

By the scattering equation (1.1.1), this vanishes, and we conclude that $[H_0 + V_{\mathsf{D}}, B] + V_{\mathsf{OD}} \approx 0$ as desired.

As in the different-spin setting considered above, we only used the scattering equation (1.1.1) for the scattering function f_p and not the variational formulation in Definition 1.1.1. Thus, the computation above serves as motivation for why one might take the scattering equation (1.1.1) as the definition of the scattering length instead.

2.4 Concluding remarks

From the variational calculation we saw that, for both the different- and same-spin settings, the ground state is approximately given by $f_{s/p}(x-y)\psi_0(x,y)$ with ψ_0 a non-interacting ground state. This serves as the motivation behind the Jastrow-type trial state considered in the many-body problem in Chapters 3, 5 and 6, see the discussion in Chapter 1.

From the perturbative calculation we saw that, for both the different- and same-spin settings, the ground state is approximately given by $e^B \psi_0$, with $B = PP(1 - f_{s/p})QQ - \text{h.c.}$. This motivates in part the analysis in Chapters 4 and 7.

The prefactor $f_{s/p}$ and the unitary operator e^B are two different methods of how to implement the correlations arising from the interaction. Their many-body generalizations are the basis for the implementation of the correlations in the following Chapters 3–7: The Jastrow type trial state used in Chapters 3, 5 and 6 is built using the scattering function $f_{s/p}$ and the unitary operator used in Chapters 4 and 7 is $e^{\mathcal{B}}$ with $\mathcal{B}$ the second quantization of B. (Up to technicalities.)

Finally, we saw quite clearly that the effect of the same-spin interaction is much weaker than that of the different-spin interaction. Indeed, $a_s/L^3 \gg a_p^3/L^5$ for large L. This point was already discussed in Chapter 1, but this toy problem serves as a simple concrete problem, where this effect is clearly illustrated.

Chapter 3

Ground state energy of the dilute spin-polarized Fermi gas: Upper bound via cluster expansion

This chapter contains the paper

[GSEUpp] A. B. Lauritsen and R. Seiringer. "Ground state energy of the dilute spin-polarized Fermi gas: Upper bound via cluster expansion", *J. Funct. Anal.* **286**.7 (2024), p. 110320. DOI: 10.1016/j.jfa.2024.110320.

Abstract. We prove an upper bound on the ground state energy of the dilute spin-polarized Fermi gas capturing the leading correction to the kinetic energy resulting from repulsive interactions. One of the main ingredients in the proof is a rigorous implementation of the fermionic cluster expansion of Gaudin, Gillespie and Ripka (Nucl. Phys. A, 176.2 (1971), pp. 237–260).

Contents

3.1 Introduction and main results

We consider a Fermi gas of N particles in a box $\Lambda = \Lambda_L = [-L/2, L/2]^d$ in d dimensions, $d = 1, 2, 3$. We will mostly focus on the case $d = 3$. The particles interact via a two-body interaction v, which we assume to be positive, radial and of compact support. In particular we allow for v to have a hard core, i.e. $v(x) = \infty$ for $|x| \le r$ for some $r > 0$. In natural units where $\hbar = 1$ and the mass of the particles is $m = 1/2$ the Hamiltonian of the system takes the form

$$H_N = \sum_{i=1}^{N} -\Delta_{x_i} + \sum_{j<k} v(x_j - x_k).$$

We are interested in spin-polarized fermions, meaning that all the spins are aligned. We may thus equivalently forget about the spin. This means that the Hamiltonian should be realized on the fermionic N-particle space of antisymmetric wavefunctions $L^2_a(\Lambda^N) = \bigwedge^N L^2(\Lambda)$. We consider the ground state energy density in the thermodynamic limit

$$e_d(\rho) = \lim_{\substack{L\to\infty \\ N/L^d\to\rho}} \inf_{\substack{\Psi_N \in L^2_a(\Lambda^N) \\ \|\Psi_N\|^2_{L^2}=1}} \frac{\langle \Psi_N | H_N | \Psi_N \rangle}{L^d}.$$

It is a result of Robinson [Rob71] that the thermodynamic limit exists, and that it is independent of boundary conditions (say, Dirichlet, Neumann or periodic).

We study the dilute limit, where the inter-particle spacing is large compared to the length scale set by the interaction. For spin-polarized fermions, the relevant lengthscale is the p-*wave scattering length* a which we define below. Our main theorem is the upper bound

$$e_{d=3}(\rho) \le \frac{3}{5}(6\pi^2)^{2/3}\rho^{5/3} + \frac{12\pi}{5}(6\pi)^{2/3}a^3\rho^{8/3}\left[1 - \frac{9}{35}(6\pi^2)^{2/3}a_0^2\rho^{2/3} + o\left((a^3\rho)^{2/3}\right)\right]$$

in the dilute limit $a^3\rho \ll 1$, where a_0 is another length related to the scattering length and effective range, also defined below. The leading term $\frac{3}{5}(6\pi^2)^{2/3}\rho^{5/3}$ is the kinetic energy density of the free Fermi gas. The next term $\frac{12\pi}{5}(6\pi)^{2/3}a^3\rho^{8/3}$ naturally results from the two-body interactions using that the two-body density vanishes quadratically at incident points, leading to the cubic behavior in the scattering length. Finally, the correction term of order $a^3a_0^2\rho^{10/3}$ is a consequence of the fourth-order behaviour of the two-particle density.

This formula is expected to be sharp [DZ19]. (How the length a_0 is related to the effective range appearing in [DZ19] is perhaps not immediate. We discuss this below.) To order $a^3\rho^{8/3}$ the formula follows by truncating expansion formulas of Jastrow [Jas55], Iwamoto and Yamada [IY57], Clark and Westhaus [CW68; WC68] or Gaudin, Gillespie and Ripka [GGR71]. Additionally the formula (to order $a^3\rho^{8/3}$) is claimed by Efimov and Amus'ya [Efi66; EA65], see also [WDS20] and references therein. Our result thus verifies this formula from the physics literature, at least as an upper bound. An important ingredient in our proof is a rigorous implementation of the cluster expansion introduced by Gaudin, Gillespie and Ripka [GGR71].

For the dilute Fermi gas one can also study the setting where different spins are present. This is studied in [FGHP21; Gia23a; LSS05], see also [Gia23b]. This system is realized by having the Hamiltonian H_N act on a definite spin-sector $L^2_a(\Lambda^{N_\uparrow}) \otimes L^2_a(\Lambda^{N_\downarrow})$, where one fixes the number of spin-up and -down particles to be $N_\uparrow$ and $N_\downarrow = N - N_\uparrow$ respectively. The energy density satisfies (in 3 dimensions)

$$e_{d=3}(\rho_\uparrow, \rho_\downarrow) = \frac{3}{5}(6\pi^2)^{2/3}\left(\rho_\uparrow^{5/3} + \rho_\downarrow^{5/3}\right) + 8\pi a_s \rho_\downarrow \rho_\uparrow + o(a_s\rho^2),$$

where ρ_σ denotes the density of particles of spin $\sigma \in \{\uparrow, \downarrow\}$ and $\rho = \rho_\downarrow + \rho_\uparrow$. Here a_s is the s-wave scattering length of the interaction. The leading term is again the kinetic energy density of a free Fermi gas. The next to leading order correction was first shown in [LSS05] and later in [FGHP21; Gia23a] using different methods. The next correction is conjectured to be the Huang–Yang term [HY57] of order $a_s^2\rho^{7/3}$, see [Gia23a; Gia23b]. Note that even the Huang–Yang term of order $a_s^2\rho^{7/3}$ is much larger than the leading correction in the spin-polarized case of order $a^3\rho^{8/3}$.

For the dilute Fermi gas with spin, effectively only fermions of different spins interact (to leading order). For fermions of different spins, the Pauli exclusion principle does not give any restriction, and the energy correction of the interaction is the same as for a dilute Bose gas (to leading order). For fermions of the same spin, the Pauli exclusion principle gives an inherent repulsion between the fermions. This gives the effect that the energy correction of the interaction is much smaller for fermions all of the same spin.

In addition to the dilute Fermi gas, much work has been done on dilute Bose gases. Here one realizes the Hamiltonian on the bosonic N-particle space of symmetric functions $L^2_s(\Lambda^N) = L^2(\Lambda)^{\otimes_{\mathsf{sym}} N}$ instead. One has the asymptotic formula (in 3 dimensions)

$$e_{d=3}(\rho) = 4\pi a_s \rho^2\left(1 + \frac{128}{15\sqrt{\pi}}(a_s^3\rho)^{1/2} + o\left((a_s^3\rho)^{1/2}\right)\right).$$

The leading term was shown by Dyson [Dys57] for an upper bound and Lieb and Yngvason [LY98] for the lower bound. The next correction, known as the Lee–Huang–Yang correction [LHY57], was shown as an upper bound in [BCS21; YY09] and as a lower bound in [FS20; FS23]. In some sense, the term $\frac{12\pi}{5}(6\pi)^{2/3}a^3\rho^{8/3}$ for the same-spin fermions is the fermionic analogue of the $4\pi a_s\rho^2$ for the bosons. It is the leading correction to the energy of the free Fermi/Bose gas.

Finally also some lower-dimensional problems have been studied. The 2-dimensional dilute Fermi gas with different spins present is studied in [LSS05], where the leading correction to the kinetic energy is shown. Recently also the bosonic problem has been studied in [FGJMO24]. We show that for the spin-polarized setting in 2 dimensions we have the upper bound

$$e_{d=2}(\rho) \leq 2\pi\rho^2 + 4\pi^2 a^2 \rho^3 [1 + o(1)] \qquad \text{as } a^2\rho \to 0.$$

Additionally, the 1-dimensional spin-polarized Fermi gas is studied in [ARS22]. Agerskov, Reuvers and Solovej [ARS22] show that

$$e_{d=1}(\rho) = \frac{\pi^2}{3}\rho^3 + \frac{2\pi^2}{3} a\rho^4 \left[1 + o(1)\right] \qquad \text{as } a\rho \to 0.$$

We give a new proof of this as an upper bound with an improved error term.

3.1.1 Precise statement of results

We now give the precise statement of our main theorems. We start with the 3-dimensional setting. First, we define the p-wave scattering length. (See also [LY01, Appendix A; SY20].)

Definition 3.1.1. The *p-wave scattering length* a of the interaction v is defined by the minimization problem

$$12\pi a^3 = \inf \left\{ \int_{\mathbb{R}^3} |x|^2 \left(|\nabla f_0(x)|^2 + \frac{1}{2} v(x) |f_0(x)|^2 \right) \mathrm{d}x : f_0(x) \to 1 \text{ as } |x| \to \infty \right\}.$$

The minimizer f_0 is the *(p-wave) scattering function*. (In case v has a hard core, i.e. $v(x) = \infty$ for $|x| \leq r$ one has to interpret $v(x)\,\mathrm{d}x$ as a measure. Necessarily then the minimizer has $f_0(x) = 0$ for $|x| \leq r$.)

We collect properties of the scattering function f_0 in Section 3.2.1. We define the length a_0 as follows.

Definition 3.1.2. The length a_0 is given by

$$3a_0^2 = \frac{1}{12\pi a^3} \int_{\mathbb{R}^3} |x|^4 \left(|\nabla f_0(x)|^2 + \frac{1}{2} v(x) |f_0(x)|^2 \right) \mathrm{d}x,$$

where f_0 is the scattering function of Definition 3.1.1. The normalization is chosen so that a hard core interaction of radius R_0 has $a_0 = a = R_0$, see Remark 3.2.3. (If v has a hard core we interpret $v(x)\,\mathrm{d}x$ as a measure as in Definition 3.1.1.)

We can now state our main theorem.

Theorem 3.1.3. *Suppose that $v \geq 0$ is radial and compactly supported. Then, for sufficiently small $a^3\rho$, the ground-state energy density satisfies*

$$\begin{aligned} e_{d=3}(\rho) \leq{}& \frac{3}{5}(6\pi^2)^{2/3}\rho^{5/3} \\ &+ \frac{12\pi}{5}(6\pi)^{2/3} a^3 \rho^{8/3} \left[1 - \frac{9}{35}(6\pi^2)^{2/3} a_0^2 \rho^{2/3} + O\left((a^3\rho)^{2/3+1/21} |\log(a^3\rho)|^6 \right) \right]. \end{aligned}$$

The essential steps in the proof are as follows.

(1) Show the absolute convergence of the formal cluster expansion formulas of [GGR71] for the reduced densities of a Jastrow-type trial state. The criterion for absolute convergence will not hold uniformly in the system size, and in order to allow for a larger particle number we need to introduce the "Fermi polyhedron", described in Section 3.2.2, as an approximation to the Fermi ball. The formulas of [GGR71] are computed in Sections 3.3.0.1, 3.3.0.2, 3.3.0.3 and 3.3.0.4 and stated in Theorem 3.3.4. The absolute convergence is proven in Section 3.3.1.

(2) Bound the energy of the Jastrow-type trial state. For this we shall in particular need bounds on "derivative Lebesgue constants" given in Lemma 3.4.9 and proven in Section 3.B. The computation of the energy of such a Jastrow-type trial state is given in Section 3.4.

(3) Use a box method to glue together trial states in smaller boxes to obtain a bound in the thermodynamic limit. This is done in Section 3.4.1.

Remark 3.1.4. The term of order $a^3a_0^2\rho^{10/3}$ is in fact the same as is claimed in [DZ19]. To see this we relate the *effective range* R_{eff} to the length a_0. In the physics literature the effective range is defined via the formula

$$k^3\cot\delta(k) = -\frac{3}{a^3} - \frac{1}{2R_{\text{eff}}}k^2 + \text{higher order in } k \qquad k\to 0 \tag{3.1.1}$$

for the phase shift $\delta(k)$ of low energy p-wave scattering. A formula for the effective range is found in [HL10, Equation (56)]. With this we find

Proposition 3.1.5. *The effective range is given by*

$$R_{\text{eff}}^{-1} = \frac{18}{5}a_0^2a^{-3}.$$

Using this formula we recover the formula [DZ19, Equation (15)] to order $\rho^{10/3}$. The formula of [DZ19] reads

$$\frac{e_{d=3}(\rho)}{\rho} = k_F^2\left[\frac{3}{5} + \frac{2}{5\pi}a^3k_F^3 - \frac{1}{35\pi}a^6R_{\text{eff}}^{-1}k_F^5 + \frac{2066-312\log 2}{10395\pi^2}a^6k_F^6 + \text{higher order}\right],$$

with $k_F = (6\pi^2\rho)^{1/3}$ the Fermi momentum. We give the proof of Proposition 3.1.5 in Section 3.2.1 below.

Remark 3.1.6 (Numerical investigation)**.** The validity of the formula in Theorem 3.1.3 is investigated numerically in [BTP23] using Quantum Monte Carlo simulations. We plot their findings in Figure 3.1.1 and compare them to the formula in Theorem 3.1.3 and the claimed formula to order $\rho^{11/3}$ of [DZ19, Equation (15)].

Remark 3.1.7. One may weaken the assumptions on the interaction v a bit at the cost of a longer proof. The compact support and that $v\geq 0$ are not strictly necessary. Essentially, we just need sufficiently good bounds on integrals of the scattering function f_0 as used in Sections 3.3.1 and 3.4 and that the "stability condition" of the tree-graph bound [PU09, Proposition 6.1; Uel18] used in Section 3.3.1 is satisfied.

Remark 3.1.8. With the same method one should be able to improve the error bound slightly. At best one could get the error to be $O_\varepsilon(\rho^{5/3}(a^3\rho)^{2-\varepsilon})$ for any $\varepsilon>0$ (i.e., the error-term in

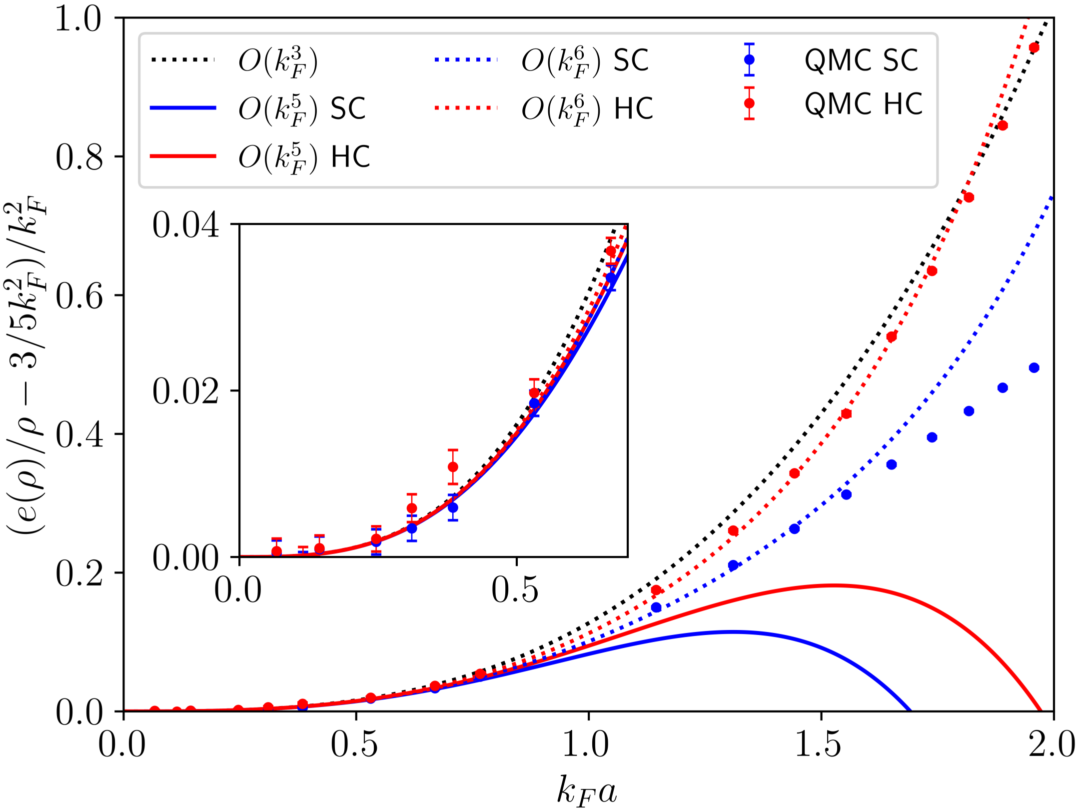


Figure 3.1.1: Energies of dilute Fermi gasses. The curves and points labelled *HC* are for a *Hard Core* interaction of radius a. The curves and points labelled *SC* are for a *Soft Core* interaction of radius $2a$ and strength V_0 chosen so that it's scattering length is a. (Meaning $v(x) = V_0\chi_{|x|\leq 2a}$, χ being the characteristic function.) The points (labelled *QMC*) are *Quantum Monte Carlo* simulations from [BTP23]. The curves include the (conjectured) corrections up to the labelled order in $k_F = (6\pi^2\rho)^{1/3}$.

Theorem 3.1.3, $O((a^3\rho)^{2/3+1/21}|\log(a^3\rho)|^6)$ could be replaced by $O_\varepsilon((a^3\rho)^{1-\varepsilon})$. The bound of the error-term in Theorem 3.1.3 arises from bounding the tail of the Gaudin-Gillespie-Ripka-expansion. Exact calculation for small diagrams (meaning small number of involved particles) reveal that this bound is very crude. Using such exact calculations for more diagrams would improve the error-bound as stated. This is somewhat similar to the recent work on the Bose gas [BCGOPS23]. We shall discuss this further in Remark 3.4.10.

We consider the lower-dimensional problems next. We start with 2 dimensions, where the scattering length is defined as follows.

Definition 3.1.9. The $(2$-dimensional$)$ p*-wave scattering length* a of the interaction v is defined by the minimization problem

$$4\pi a^2 = \inf\left\{\int_{\mathbb{R}^2} |x|^2\left(|\nabla f_0(x)|^2 + \frac{1}{2}v(x)|f_0(x)|^2\right)\,\mathrm{d}x : f_0(x) \to 1 \text{ as } |x|\to\infty\right\}$$

The minimizer f_0 is the $(2$-dimensional$)$ *(p-wave) scattering function*.

With this, we may state the 2-dimensional analogue of Theorem 3.1.3.

Theorem 3.1.10 (Two dimensions)**.** *Suppose that $v \geq 0$ is radial and compactly supported. Then, for sufficiently small $a^2\rho$, the ground-state energy density satisfies*

$$e_{d=2}(\rho) \leq 2\pi\rho^2 + 4\pi^2 a^2 \rho^3 \left[1 + O\left(a^2\rho|\log(a^2\rho)|^2\right)\right].$$

We sketch in Section 3.5.1 how to adapt the proof in the 3-dimensional setting to 2 dimensions.

Finally, we consider the 1-dimensional problem. The scattering length is defined as follows.

Definition 3.1.11. The (1-dimensional) *p-wave scattering length* a of the interaction v is defined by the minimization problem

$$2a = \inf \left\{ \int_{\mathbb{R}} |x|^2 \left(|\partial f_0(x)|^2 + \frac{1}{2} v(x) |f_0(x)|^2 \right) \mathrm{d}x : f_0(x) \to 1 \text{ as } |x| \to \infty \right\}$$

The minimizer f_0 is the (1-dimensional) *(p-wave) scattering function*.

We show in Proposition 3.5.12 that Definition 3.1.11 agrees with the (seemingly different) definition of the scattering length in [ARS22]. With this, we may state the 1-dimensional analogue of Theorem 3.1.3.

Theorem 3.1.12 (One dimension)**.** *Suppose that $v \geq 0$ is even and compactly supported. Suppose moreover that $\int \left(\frac{1}{2} v f_0^2 + |\partial f_0|^2\right) \mathrm{d}x < \infty$, where f_0 denotes the (p-wave) scattering function. Then, for sufficiently small $a\rho$, the ground-state energy density satisfies*

$$e_{d=1}(\rho) \leq \frac{\pi^2}{3}\rho^3 + \frac{2\pi^2}{3} a \rho^4 \left[1 + O\left((a\rho)^{9/13}\right)\right].$$

We remark that Agerskov, Reuvers and Solovej [ARS22] recently showed (almost) the same result with a matching lower bound $e_{d=1}(\rho) \geq \frac{\pi^2}{3}\rho^3 + \frac{2\pi^2}{3} a\rho^4(1 + o(1))$. Compared to their result we treat a slightly different class of potentials and obtain an improved error bound. The conjectured next contribution is of order $a^2\rho^5$, see [ARS22].

Remark 3.1.13 (On the assumptions on v)**.** Any smooth interaction or an interaction with a hard core (meaning that $v(x) = +\infty$ for $|x| \leq a_0$ for some $a_0 > 0$) satisfies $\int \left(\frac{1}{2} v f_0^2 + |\partial f_0|^2\right) \mathrm{d}x < \infty$, see Propositions 3.5.13 and 3.5.14.

We sketch in Section 3.5.2 how to adapt the proof in the 3-dimensional setting to 1 dimension. This turns out to be more involved than adapting the argument to 2 dimensions.

The paper is structured as follows. In Section 3.2 we give some preliminary computations and in particular we introduce the "Fermi polyhedron", a polyhedral approximation to the Fermi ball. In Section 3.3 we introduce the fermionic cluster expansion of Gaudin, Gillespie and Ripka [GGR71] and we find conditions on absolute convergence of the resulting formulas. In the subsequent Section 3.4 we compute the energy of a Jastrow-type trial state and glue many of them together using a box method to form trial states of arbitrary many particles. Finally, in Section 3.5 we sketch how to adapt the argument to the lower-dimensional settings. In Section 3.A we give computations of "small diagrams" needed for some bounds in Sections 3.4 and 3.5.2 and in Section 3.B we give the proof of Lemma 3.4.9, an important lemma used in Section 3.4.

3.2 Preliminary computations

We will construct a trial state using a box method, and bound the energy of such trial state. To use such a box method we need to use Dirichlet boundary conditions in each smaller box. In Lemma 3.4.3 we show that we may construct trial states with Dirichlet boundary condition out of trial states with periodic boundary conditions. We will thus use periodic boundary conditions in the box $\Lambda = [-L/2, L/2]^3$. For periodic boundary conditions, the Hamiltonian is given by

$$H_N = H_{N,L}^{\text{per}} = \sum_{j=1}^{N} -\Delta_j + \sum_{i<j} v_{\text{per}}(x_i - x_j),$$

where Δ_j denotes the Laplacian on the j'th coordinate and $v_{\text{per}}(x) = \sum_{n\in\mathbb{Z}^3} v(x+nL)$, the periodized interaction. By a slight abuse of notation we write $v = v_{\text{per}}$, since we will choose L bigger than the range of v.

The trial state in each smaller box is given by the Jastrow-type [Jas55] trial state (also known as a Bijl-Dingle-Jastrow-type trial state)

$$\psi_N = \frac{1}{\sqrt{C_N}} \prod_{i<j} f(x_i - x_j) D_N(x_1, \ldots, x_N), \tag{3.2.1}$$

where f is a scaled and cut-off version of the scatting function f_0, D_N is an appropriately chosen Slater determinant, and C_N is a normalization constant. More precisely,

$$f(x) = \begin{cases} \frac{1}{1-a^3/b^3} f_0(|x|) & |x| \le b, \\ 1 & |x| \ge b, \end{cases}$$

$$D_N(x_1, \ldots, x_N) = \det\left[u_k(x_i)\right]_{\substack{1\le i\le N \\ k\in P_F}}, \quad u_k(x) = \frac{1}{L^{3/2}} e^{ikx},$$

where f_0 is the p-wave scattering function, $|\cdot| := \min_{n\in\mathbb{Z}^3} |\cdot - nL|_{\mathbb{R}^3}$ (with $|\cdot|_{\mathbb{R}^3}$ denoting the norm on $\mathbb{R}^3$), $b > R_0$, the range of v, is some cut-off to be chosen later, P_F is a polyhedral approximation to the Fermi ball B_F of radius k_F described in Section 3.2.2, and the number of particles is $N = \# P_F$, the number of points in P_F. We choose b to be larger than the range of v; in particular, then f is continuous. (Note that the metric on the torus is $d(x,y) = |x-y|$. We will abuse notation slightly and denote by $|\cdot|$ also the absolute value of some number or the norm on $\mathbb{R}^3$.)

Before going further with the proof we first fix some notation.

Notation 3.2.1. We introduce the following.

- For any function h and edge (of some graph) $e = (i,j)$ we will write $h_e = h_{ij} = h(x_i - x_j)$.
- We denote by C a generic positive constant whose value may change line by line.
- For expressions A, B we write $A \lesssim B$ if there exists some constant $C > 0$ such that $A \le CB$. If both $A \lesssim B$ and $B \lesssim A$ we write $A \sim B$.
- For a vector $x = (x^1, \ldots, x^d) \in \mathbb{R}^d$ we write $x^1, \ldots, x^d$ for its components.

We will fix the Fermi momentum k_F and then choose L, N large but finite depending on k_F. The density of particles in the trial state ψ_N is $\rho := N/L^3$. The limit of small density $a^3\rho \to 0$ will be realized as $k_F a \to 0$.

To compute the energy of the trial state ψ_N note that for (real-valued) functions F, G we have

$$\int |\nabla(FG)|^2 = \int |\nabla F|^2 |G|^2 - \int |F|^2 G\Delta G.$$

Using this on $F = \prod_{i<j} f_{ij}$ and $G = D_N$ we have

$$\begin{aligned}
\langle \psi_N | H_N | \psi_N \rangle &= E_0 + 2\sum_{j<k} \left\langle \psi_N \middle| \left| \frac{\nabla f(x_j - x_k)}{f(x_j - x_k)} \right|^2 + \frac{1}{2} v(x_j - x_k) \middle| \psi_N \right\rangle \\
&\quad + 6 \sum_{i<j<k} \left\langle \psi_N \middle| \frac{\nabla f_{ij} \nabla f_{jk}}{f_{ij} f_{jk}} \middle| \psi_N \right\rangle \\
&= E_0 + \iint \rho^{(2)}_{\mathsf{Jas}}(x_1, x_2) \left(\left| \frac{\nabla f(x_1 - x_2)}{f(x_1 - x_2)} \right|^2 + \frac{1}{2} v(x_1 - x_2) \right) \mathrm{d}x_1 \, \mathrm{d}x_2 \\
&\quad + \iiint \rho^{(3)}_{\mathsf{Jas}}(x_1, x_2, x_3) \frac{\nabla f_{12} \nabla f_{23}}{f_{12} f_{23}} \, \mathrm{d}x_1 \, \mathrm{d}x_2 \, \mathrm{d}x_3,
\end{aligned} \tag{3.2.2}$$

where $E_0 = \sum_{k \in P_F} |k|^2$ is the kinetic energy of $\frac{1}{\sqrt{N!}} D_N$ and $\rho^{(n)}_{\mathsf{Jas}}$ denotes the n-particle reduced density of the trial state ψ_N, given by

$$\rho^{(n)}_{\mathsf{Jas}}(x_1, \ldots, x_n) = N(N-1)\cdots(N-n+1) \int \!\!\cdots\!\! \int |\psi_N(x_1, \ldots, x_N)|^2 \, \mathrm{d}x_{n+1} \ldots \mathrm{d}x_N, \qquad n = 1, \ldots, N. \tag{3.2.3}$$

The division by f is non-problematic even where $f = 0$, since it cancels with the corresponding factors of f in ψ_N. We need to compute $\rho^{(2)}_{\mathsf{Jas}}$ and bound $\rho^{(3)}_{\mathsf{Jas}}$. Before we start on this endeavour we first recall some properties of the scattering function.

3.2.1 The scattering function

The scattering function f_0 is defined by the minimization problem in Definition 3.1.1, see also [LY01, Appendix A; SY20]. In particular f_0 satisfies the corresponding Euler-Lagrange equation

$$-4x \cdot \nabla f_0 - 2|x|^2 \Delta f_0 + |x|^2 v f_0 = 0.$$

The minimizer f_0 is radial and with a slight abuse of notation we sometimes write $f_0(|x|) = f_0(x)$. In radial coordinates the Euler-Lagrange equations reads

$$-\partial_r^2 f_0 - \frac{4}{r} \partial_r f_0 + \frac{1}{2} v f_0 = 0, \tag{3.2.4}$$

where ∂_r denotes the derivative in the radial direction. This is the same equation as for s-wave scattering in 5 dimensions, see [LY01, Appendix A]. Thus, properties of this carry over. In particular $f_0(x) = 1 - \frac{a^3}{|x|^3}$ for x outside the support of v. Moreover

Lemma 3.2.2 ([LY01, Lemma A.1]). *The scattering function f_0 satisfies*

$$\left[1 - \frac{a^3}{|x|^3}\right]_+ \leq f_0(x) \leq 1$$

for all x and $|\nabla f_0(x)| \leq \frac{3a^3}{|x|^4}$ for $|x| > a$.

We give a short proof here for completeness.

Proof. From the radial Euler-Lagrange equation (3.2.4) we have $\partial_r(r^4 \partial_r f_0) = vr^4 f_0/2 \geq 0$. Denote by $f_{\mathsf{hc}} = \left[1 - \frac{a^3}{|x|^3}\right]_+$ the solution for a hard core potential of range a. Then

$$r^4 \partial_r f_{\mathsf{hc}} = \begin{cases} 3a^3 & r > a \\ 0 & r < a \end{cases}$$

In particular $\partial_r(r^4 \partial_r f_{\mathsf{hc}}) = 0$ for $r > a$. We thus see that $\partial_r f_0 \leq \partial_r f_{\mathsf{hc}} = 3a^3 r^{-4}$ and $f_0 \geq f_{\mathsf{hc}}$ for $r > a$ by integrating. Trivially $f_0 \geq 0 = f_{\mathsf{hc}}$ for $r \leq a$. $\square$

Remark 3.2.3. A hard core interaction of range $R_0 > 0$,

$$v_{\mathsf{hc}}(x) = \begin{cases} +\infty & |x| \leq R_0, \\ 0 & |x| > R_0, \end{cases}$$

has $f_0(x) = f_{\mathsf{hc}}(x) = \left[1 - \frac{a^3}{|x|^3}\right]_+$ and thus $a_0 = a = R_0$.

Finally, we give the

Proof of Proposition 3.1.5. Let R_0 denote the range of the interaction. Then the effective range is given by [HL10, Equation (56)]

$$-R_{\mathsf{eff}}^{-1} = -\frac{2}{R} - \frac{2R^2}{a^3} + \frac{2R^5}{5a^6} - 2\int_0^R u(r)^2 \, \mathrm{d}r, \qquad \text{for } R \geq R_0 \tag{3.2.5}$$

where u solves [HL10, Equation (22)]

$$-\partial_r^2 u + \frac{2}{r^2} u + \frac{1}{2} vu = 0$$

with ∂_r denoting the radial derivative. In particular then $f_0 = -\frac{a^3}{r^2} u$ satisfies the scattering equation, Equation (3.2.4). For $r \geq R_0$ we find using [HL10, Equation (27)] and Equation (3.1.1)

$$u(r) = \lim_{k \to 0} \frac{\sin(kr + \delta(k)) - kr\cos(kr + \delta(k))}{r \sin \delta(k)} = \frac{-r^2}{a^3}\left[1 - \frac{a^3}{r^3}\right].$$

We conclude that $f_0 = -\frac{a^3}{r^2} u$ is indeed the scattering function. Thus (3.2.5) reads

$$-R_{\mathsf{eff}}^{-1} = -\frac{2}{R} - \frac{2R^2}{a^3} + \frac{2R^5}{5a^6} - \frac{2}{a^6}\int_0^R r^4 f_0^2 \, \mathrm{d}r, \qquad \text{for } R \geq R_0$$

The remainder of the proof is a simple calculation using integration by parts and the scattering equation. We omit the details. This concludes the proof of Proposition 3.1.5. $\square$

3.2.2 The "Fermi polyhedron"

We introduce a polyhedral approximation P_F of the Fermi ball $B_F = \{k \in \frac{2\pi}{L}\mathbb{Z}^3 : |k| \le k_F\}$. The main properties we will need of the polyhedral approximation are given in Lemmas 3.2.12, 3.2.13 and 3.4.9. We discuss why we need such a polyhedral approximation in Remark 3.3.5. The problem is that

$$\int_{[0,L]^3} \frac{1}{L^3} \left| \sum_{k \in B(k_F) \cap \frac{2\pi}{L}\mathbb{Z}^3} e^{ikx} \right| \mathrm{d}x = \frac{1}{(2\pi)^3} \int_{[0,2\pi]^3} \left| \sum_{q \in B(cN^{1/3}) \cap \mathbb{Z}^3} e^{iqu} \right| \mathrm{d}u \sim N^{1/3}$$

for large N (see [GL19; Lif06] and references therein) is too big for our purposes. Note that this behaviour is a consequence of taking the absolute value. In fact we have that $\frac{1}{L^3} \int \sum_{k \in B(k_F) \cap \frac{2\pi}{L}\mathbb{Z}^3} e^{ikx} \, \mathrm{d}x = 1$.

This type of quantity is referred to as the *Lebesgue constant* [GL19; Lif06] of some domain Ω,

$$\mathcal{L}(\Omega) := \frac{1}{(2\pi)^3} \int_{[0,2\pi]^3} \left| \sum_{q \in \Omega \cap \mathbb{Z}^3} e^{iqu} \right| \mathrm{d}u$$

These kinds of integrals appear in estimates in Sections 3.3.1 and 3.4. For an overview of such Lebesgue constants, see [GL19; Lif06]. Of particular relevance for us is the fact that the Lebesgue constants are much smaller for polyhedral domains than for balls. Hence we introduce the polyhedron $P = P(N)$ as an approximation of the unit ball. Then the scaled version $P_F = k_F P \cap \frac{2\pi}{L}\mathbb{Z}^3$ approximates the Fermi ball. We will refer to P_F as the *Fermi polyhedron*. In [KL18, Theorem 4.1] it is shown that for any fixed convex polyhedron P' of s vertices

$$\mathcal{L}(RP') = \frac{1}{(2\pi)^3} \int_{[0,2\pi]^3} \left| \sum_{q \in RP' \cap \mathbb{Z}^3} e^{iqu} \right| \mathrm{d}u \le Cs(\log R)^3 + C(s)(\log R)^2 \tag{3.2.6}$$

for any $R > 2$, in particular for $R \sim N^{1/3}$, where $C(s)$ is some unknown function of s. We will improve on this bound for the specific polyhedron $P = P(N)$ to control the s-dependence of the subleading (in R) terms, i.e. of $C(s)$. For the specific polyhedron P we have $C(s) \le Cs$. This is the content of Lemma 3.2.12 below. We first give an almost correct definition of the polyhedron P.

"Definition" 3.2.4 (Simple definition)**.** The polyhedron P is chosen to be the convex hull of $s = s(N)$ points $\kappa_1, \ldots, \kappa_s$ on a sphere of radius $1 + \delta$, where δ is chosen such that $\mathrm{Vol}(P) = 4\pi/3$. We moreover choose the set of points to have the following properties.

- The points are *evenly distributed*, meaning that the distance d between any pair of points satisfies $d \gtrsim s^{-1/2}$, and that for any k on the sphere of radius $1+\delta$ the distance from k to the closest point is $\lesssim s^{-1/2}$. That is, for some constants $c, C > 0$ we have $d \ge cs^{-1/2}$ and $\inf_j |k - \kappa_j| \le Cs^{-1/2}$.
- P is invariant under any map $(k^1, k^2, k^3) \mapsto (\pm k^a, \pm k^b, \pm k^c)$ for $\{a, b, c\} = \{1, 2, 3\}$, i.e. reflection in or permutation of any of the axes.

The *Fermi polyhedron* is the rescaled version defined as $P_F := k_F P \cap \frac{2\pi}{L}\mathbb{Z}^3$, where L is chosen large (depending on k_F) such that $k_F L$ is large.

Remark 3.2.5. Note that the symmetry constraint adds a restriction on s. For instance, a generic point away from any plane of symmetry (i.e. k^1, k^2, k^3 all different and non-zero) has 48 images (including itself) when reflected by the maps $(k^1, k^2, k^3) \mapsto (\pm k^a, \pm k^b, \pm k^c)$ for $\{a, b, c\} = \{1, 2, 3\}$.

For s points on a sphere of radius $1 + \delta$, the natural lengthscale is $(1 + \delta)s^{-1/2} \sim s^{-1/2}$. The requirement that the points are evenly distributed then ensures that all pairs of close points (for any reasonable definition of "close points") have a pairwise distance of this order.

Remark 3.2.6. For all purposes apart from the technical argument in Section 3.B one may take this as the definition. In particular, the convergence criterion of the cluster expansion formulas of Gaudin, Gillespie and Ripka [GGR71], given in Theorem 3.3.4, holds also for this simpler definition of P. We provide this simpler definition to better give an intuition of the construction.

We now give the actual definition of P. We first give the construction. Then in Remark 3.2.9 we give a few comments and in Remark 3.2.10 we give a short motivation.

Definition 3.2.7 (Actual definition)**.** The polyhedron P with s corners and the "centre" z is constructed as follows.

- First, choose a big number Q, the "size of the primes" satisfying
$$Q^{-1/4} \le C s^{-1}, \qquad N^{4/3} \ll Q \le C N^C$$
in the limit $N \to \infty$.
- Pick three large distinct primes Q_1, Q_2, Q_3 with $Q_j \sim Q$.
- Place s *evenly distributed* points $\kappa_1^{\mathbb{R}}, \ldots, \kappa_s^{\mathbb{R}}$ on the sphere of radius $Q^{-3/4}$ and such that the set of points $\{\kappa_1^{\mathbb{R}}, \ldots, \kappa_s^{\mathbb{R}}\}$ is invariant under the symmetries $(k^1, k^2, k^3) \mapsto (\pm k^a, \pm k^b, \pm k^c)$ for $\{a, b, c\} = \{1, 2, 3\}$.

  Here, *evenly distributed* means that the distance between any pair of points is $d \gtrsim s^{-1/2} Q^{-3/4}$ and that for any k on the sphere of radius $Q^{-3/4}$ the distance from k to the nearest point is $\lesssim s^{-1/2} Q^{-3/4}$. That is, $d \ge c s^{-1/2} Q^{-3/4}$ and $\inf_j \left|k - \kappa_j^{\mathbb{R}}\right| \le C s^{-1/2} Q^{-3/4}$ for some constants $c, C > 0$.
- Find points $\kappa_1, \ldots, \kappa_s$ of the form
$$\kappa_j = \left(\frac{p_j^1}{Q_1}, \frac{p_j^2}{Q_2}, \frac{p_j^3}{Q_3}\right), \qquad p_j^\mu \in \mathbb{Z}, \quad \mu = 1, 2, 3, \quad j = 1, \ldots, s, \tag{3.2.7}$$
such that $\left|\kappa_j - \kappa_j^{\mathbb{R}}\right| \lesssim Q^{-1}$ for all $j = 1, \ldots, s$ and such that the set of points $\{\kappa_1, \ldots, \kappa_s\}$ is invariant under the symmetries $(k^1, k^2, k^3) \mapsto (\pm k^1, \pm k^2, \pm k^3)$.
- Define $\tilde{P}$ as the convex hull of all the points $\kappa_1, \ldots, \kappa_s$. That is, $\tilde{P} = \operatorname{conv}\{\kappa_1, \ldots, \kappa_s\}$.
- Define P as $\sigma \tilde{P}$, where σ is chosen such that $\operatorname{Vol}(P) = 4\pi/3$. We will refer to the scaled points $\sigma \kappa_j = \sigma(p_j^1/Q_1, p_j^2/Q_2, p_j^3/Q_3)$ for $j = 1, \ldots, s$ as *corners* of P.
- Define $P^{\mathbb{R}} = \sigma \operatorname{conv}\{\kappa_1^{\mathbb{R}}, \ldots, \kappa_s^{\mathbb{R}}\}$ as the scaled convex hull of all the initial points $\kappa_1^{\mathbb{R}}, \ldots, \kappa_s^{\mathbb{R}}$.

- Define the centre as $z = \sigma(1/Q_1, 1/Q_2, 1/Q_3)$.

The *Fermi polyhedron* is the rescaled version defined as $P_F := k_F P \cap \frac{2\pi}{L}\mathbb{Z}^3$, where L is chosen large (depending on k_F) such that $\frac{k_F L}{2\pi}$ is rational and large.

We additionally define $P_F^{\mathbb{R}} := k_F P^{\mathbb{R}} \cap \frac{2\pi}{L}\mathbb{Z}^3$.

Remark 3.2.8. We choose $N := \#P_F$, so that the Fermi polyhedron is filled. The dependence in N of, for instance, Q should therefore more precisely be given in terms of a dependence on $k_F L$. Note that $N = \rho L^3 \sim (k_F L)^3$ and $k_F = (6\pi^2\rho)^{1/3}(1 + O(N^{-1/3}))$.

We will choose also s depending on N (i.e. on $k_F L$) satisfying $s \to \infty$ as $N \to \infty$.

Remark 3.2.9 (Comments on and properties of the construction)**.** We collect here some properties of the Fermi polyhedron, some of which will only be needed in Section 3.B.

- The points $\kappa_1, \ldots, \kappa_s$ are *evenly distributed* on a thickened sphere of radius $Q^{-3/4}$ – their radial coordinates are $|\kappa_j| = Q^{-3/4} + O(Q^{-1})$. Indeed, the points $\kappa_1^{\mathbb{R}}, \ldots, \kappa_s^{\mathbb{R}}$ are *evenly distributed* and $Q^{-1} \ll s^{-1/2}Q^{-3/4}$. For s points on a thickened sphere of radius $Q^{-3/4}$, the natural lengthscale between points is $s^{-1/2}Q^{-3/4}$.

- There is some constraint on the number of points s. A generic point κ (with $\kappa^1, \kappa^2, \kappa^3$ all different and non-zero) has 48 images, including itself. The constraint on s is more or less the same as for the simpler ''Definition'' 3.2.4.

- By choosing the points $\kappa_1, \ldots, \kappa_s$ as in Equation (3.2.7) we break the symmetries of permuting the coordinates, i.e. $(k^1, k^2, k^3) \mapsto (k^a, k^b, k^c)$ if $(a, b, c) \neq (1, 2, 3)$. These symmetries are however still almost satisfied, see Lemma 3.2.11.

- We choose s, Q such that $Q^{-1/4} \ll s^{-1/2}$ in the limit of large N. Hence, for N sufficiently large, all the chosen points $\{\kappa_1, \ldots, \kappa_s\}$ are extreme points of $\tilde{P}$, i.e. all corners are extreme points of the polyhedron P. That is, the name "corner" is well-chosen, and we do not have any superfluous points in the construction.

- For any three points $(x_i, y_i, z_i) \in \mathbb{R}^3$, $i = 1, 2, 3$ the plane through them is given by the equation

$$\begin{pmatrix} (y_2 - y_1)(z_3 - z_1) - (y_3 - y_1)(z_2 - z_1) \\ (z_2 - z_1)(x_3 - x_1) - (z_3 - z_1)(x_2 - x_1) \\ (x_2 - x_1)(y_3 - y_1) - (x_3 - x_1)(y_2 - y_1) \end{pmatrix} \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \text{const.}$$

  Hence, for three points K_1, K_2, K_3 of the form $K_i = (p_i^1/Q_1, p_i^2/Q_2, p_i^3/Q_3), p_i^\mu \in \mathbb{Z}$, $i, \mu = 1, 2, 3$ the plane through them is given by

$$\frac{\alpha_1}{Q_2 Q_3} k^1 + \frac{\alpha_2}{Q_1 Q_3} k^2 + \frac{\alpha_3}{Q_1 Q_2} k^3 = \gamma \in \mathbb{Q}, \tag{3.2.8}$$

  where

$$\alpha_1 = (p_2^2 - p_1^2)(p_3^3 - p_1^3) - (p_3^2 - p_1^2)(p_2^3 - p_1^3) \in \mathbb{Z}$$

  and similarly for α_2, α_3. From these formulas it is immediate that for K_i's corners of P or the centre z we have $|\alpha_j| \leq C\sqrt{Q}$ for $j = 1, 2, 3$. For some planes we may have $\alpha_j = 0$ for some j.

- We claim that $\sigma = Q^{3/4}(1 + O(s^{-1}))$. In particular, that any point on the boundary ∂P has radial coordinate $1 + O(s^{-1})$. To see this, note that $Q^{3/4}\tilde{P}$ is a polyhedron whose corners are evenly spaced and have radial coordinates r with $r = 1 + O(Q^{-1/4})$. Thus, by scaling $Q^{3/4}\tilde{P}$ by $1 - CQ^{-1/4}$ we get that $(1 - CQ^{-1/4})Q^{3/4}\tilde{P} \subset B_1(0)$ so that this has volume $\leq \frac{4\pi}{3}$. It follows that $\sigma \geq Q^{3/4}(1 - CQ^{-1/4})$. On the other hand, scaling $Q^{3/4}\tilde{P}$ by $1 + Cs^{-1}$ we have that $(1 + Cs^{-1})Q^{3/4}\tilde{P} \supset B_1(0)$. Indeed, since the distance from any point k on the sphere of radius 1 to any corner of $Q^{3/4}\tilde{P}$ is $\lesssim s^{-1/2}$, and the sphere is locally quadratic, the smallest radial coordinate r of a point on the boundary $\partial(Q^{3/4}\tilde{P})$ is $r \geq 1 - Cs^{-1}$. It follows that $\sigma \leq (1 + Cs^{-1})Q^{3/4}$. Since $Q^{-1/4} \leq Cs^{-1}$ this shows the desired.

- Note moreover that σ is irrational. Indeed, the volume of a polyhedron with rational corners is rational. (This is easily seen for tetrahedra, of which any polyhedron is an essentially disjoint union.) Thus $\sigma^3 = \pi r$ for a rational r. Hence the equations of the planes defined by corners of P (i.e. scaled points) are of the form Equation (3.2.8) with an irrational constant $\sigma\gamma$ on the right-hand side. Indeed, the corners of P (and the central point z) are all scaled by σ compared to points of the form $(p^1/Q_1, p^2/Q_2, p^3/Q_3)$. The equation of the plane through three scaled points only differ by scaling the constant term. Since σ is irrational, and the constant term was rational for the unscaled points, this shows the desired.

- We now construct a triangulation of ∂P. For all (2-dimensional) triangular faces of P simply consider these as part of the triangulation. That is, we construct edges between any pair of the three corners of such a triangle. Some of the (2-dimensional) faces of P may be polygons of more than 3 sides (1-dimensional faces). Construct edges between all pairs of corners sharing a side (i.e. a 1-dimensional face) and choose one corner and construct edges from this corner to all other corners of the polygon.

  Doing this constructs a triangulation of ∂P and we will refer to all pairs of corners with an edge between them as *close* or *neighbours*. Since the points $\{\kappa_1, \ldots, \kappa_s\}$ are evenly distributed, that the distance between any pair of close corners is $d \sim s^{-1/2}$.

- Additionally, one may note that the corners of P have $\leq C$ many neighbours since the points are evenly distributed.

- The reason we need $\frac{Lk_F}{2\pi}$ rational will only become apparent in Section 3.B and will be explained there.

Remark 3.2.10 (Motivation of construction)**.** The purpose of the construction is twofold. Firstly we avoid a casework argument as in the proof of [KL18, Lemma 3.5] of whether the coefficients of the planes are rational or not. The argument in Lemmas 3.B.6 and 3.B.7 is heavily inspired by [KL18, Lemmas 3.6, 3.9], where such casework is required. Secondly we have good control over how many (and which) lattice points (i.e. points in $\frac{2\pi}{L}\mathbb{Z}^3$) can lie on each plane (or, rather, a closely related plane, see Section 3.B for the details).

These are technical details only needed in Section 3.B. We reiterate, that apart from the arguments in Section 3.B, the reader may have the simpler "Definition" 3.2.4 in mind instead.

As mentioned in Remark 3.2.9 the Fermi polyhedron is almost symmetric under permutation of the axes. This is formalized as follows.

Lemma 3.2.11. *For $\mu \neq \nu$ let $F_{\mu\nu}$ be the map that permutes k^μ and k^ν (i.e. $F_{12}(k^1, k^2, k^3) = (k^2, k^1, k^3)$, etc.). Then for any function $t \geq 0$ we have*

$$\sum_{k \in \frac{2\pi}{L}\mathbb{Z}^3} \left| \chi_{(k \in P_F)} - \chi_{(k \in F_{\mu\nu}(P_F))} \right| t(k) \lesssim Q^{-1/4} N \sup_{|k| \sim k_F} t(k) \lesssim N^{2/3} \sup_{|k| \sim k_F} t(k),$$

where Q is as in Definition 3.2.7 and χ denotes the indicator function.

Proof. Note that

$$\begin{aligned} &\sum_{k \in \frac{2\pi}{L}\mathbb{Z}^3} \left| \chi_{(k \in P_F)} - \chi_{(k \in F_{\mu\nu}(P_F))} \right| t(k) \\ &\qquad \leq \sum_{k \in \frac{2\pi}{L}\mathbb{Z}^3} \left| \chi_{(k \in P_F)} - \chi_{(k \in P_F^{\mathbb{R}})} \right| t(k) + \sum_{k \in \frac{2\pi}{L}\mathbb{Z}^3} \left| \chi_{(k \in F_{\mu\nu}(P_F))} - \chi_{(k \in F_{\mu\nu}(P_F^{\mathbb{R}}))} \right| t(k) \end{aligned} \tag{3.2.9}$$

since $P_F^{\mathbb{R}}$ is invariant under permutation of the axes, i.e. $F_{\mu\nu}(P_F^{\mathbb{R}}) = P_F^{\mathbb{R}}$. The points $\{\kappa_j\}_{j=1,\ldots,s}$ only differ from $\{\kappa_j^{\mathbb{R}}\}_{j=1,\ldots,s}$ by at most $\sim Q^{-1}$ thus the points $\{\sigma\kappa_j\}_{j=1,\ldots,s}$ (the corners of P) only differ from the points $\{\sigma\kappa_j^{\mathbb{R}}\}_{j=1,\ldots,s}$ by $\sim Q^{-1/4}$. Hence, the support of $\chi_{(k \in P_F)} - \chi_{(k \in P_F^{\mathbb{R}})}$ is contained in a shell of width $\sim k_F Q^{-1/4}$ around the surface $\partial(k_F P)$. That is,

$$\operatorname{supp}\left(\chi_{(k \in P_F)} - \chi_{(k \in P_F^{\mathbb{R}})}\right) \subset \left\{ k \in \frac{2\pi}{L}\mathbb{Z}^3 : \operatorname{dist}(k, \partial(k_F P)) \lesssim k_F Q^{-1/4} \right\}.$$

The surface $\partial(k_F P)$ has area $\sim k_F^2$ so

$$\operatorname{Vol}\left(\left\{ k \in \mathbb{R}^3 : \operatorname{dist}(k, \partial(k_F P)) \lesssim k_F Q^{-1/4} \right\} \right) \lesssim k_F^3 Q^{-1/4}.$$

The spacing between the k's in $\frac{2\pi}{L}\mathbb{Z}^3$ is $\sim L^{-1}$ and any k with $\operatorname{dist}(k, \partial(k_F P)) \lesssim k_F Q^{-1/4}$ has $|k| \sim k_F$. Thus

$$\sum_{k \in P_F} \left| \chi_{(k \in P_F)} - \chi_{(k \in P_F^{\mathbb{R}})} \right| t(k) \lesssim L^3 k_F^3 Q^{-1/4} \sup_{|k| \sim k_F} t(k) \sim Q^{-1/4} N \sup_{|k| \sim k_F} t(k).$$

The same argument applies to the second summand in Equation (3.2.9). We conclude the desired. □

We now improve on Equation (3.2.6) for our polyhedron.

Lemma 3.2.12. *The Lebesgue constant of the Fermi polyhedron satisfies*

$$\int_\Lambda \frac{1}{L^3} \left| \sum_{k \in P_F} e^{ikx} \right| \mathrm{d}x = \frac{1}{(2\pi)^3} \int_{[0,2\pi]^3} \left| \sum_{q \in \left(\frac{L k_F}{2\pi} P\right) \cap \mathbb{Z}^3} e^{iqu} \right| \mathrm{d}u \leq Cs(\log N)^3.$$

The proof is (almost) the same as given in [KL18, Theorem 4.1]. We need to be a bit more careful in the decomposition into tetrahedra.

Proof. Define $R = \frac{Lk_F}{2\pi}$. We decompose RP into tetrahedra using the "central" point z from the construction of P. We triangulate the surface of RP as in Remark 3.2.9. For each triangle in the triangulation add the point Rz to form a tetrahedron. Note that $Rz \notin \mathbb{Z}^3$ since $|Rz| \leq CRQ^{-1/4} \ll 1$ and $z \neq 0$. This gives $m = O(s)$ many (closed) tetrahedra $\{T_j\}$ such that $RP = \bigcup T_j$ and that $T_j \cap T_{j'}$ is a tetrahedron of lower dimension (i.e. the central point Rz, a line segment or a triangle). Then, as in [KL18, Theorem 4.1] by the inclusion–exclusion principle we have

$$\begin{aligned}\mathcal{L}(RP) &= \frac{1}{(2\pi)^3}\int \left| \sum_j \sum_{q\in T_j\cap\mathbb{Z}^3} e^{iqu} - \sum_{j<j'} \sum_{q\in T_j\cap T_{j'}\cap\mathbb{Z}^3} e^{iqu} + \cdots \right| \mathrm{d}u \\ &\leq \sum_{\ell=1}^{m} \sum_{j_1<\ldots<j_\ell} \mathcal{L}(T_{j_1}\cap\ldots\cap T_{j_\ell}).\end{aligned}$$

In [KL18, Theorem 4.1] it is shown that for a d-dimensional tetrahedron T with $T \subset [0,n_1]\times\ldots\times[0,n_d]$ we have $\mathcal{L}(T) \leq C(d)\prod_{i=1}^d \log(n_i+1)$. All the tetrahedra in our construction are d-dimensional for $d \leq 3$ and contained in boxes $[0,CR]^d$ (after translations by lattice vectors $\kappa \in \mathbb{Z}^3$). Hence for all tuples $T_{j_1},\ldots,T_{j_\ell}$ we have

$$\mathcal{L}(T_{j_1}\cap\ldots\cap T_{j_\ell}) \leq C(\log R)^d \leq C(\log N)^3.$$

We need to count how many summands we have. The 3-dimensional tetrahedra each appear just once, and there are $m = O(s)$ many of them. The 2-dimensional tetrahedra (triangles) appear just once, namely in the term $\mathcal{L}(T_j \cap T_{j'})$ where the triangle is the intersection $T_j \cap T_{j'}$. Hence there are $O(s)$ many such terms. The 1-dimensional tetrahedra (line segments) may appear more times, with $3,4,\ldots,C$ many T_j's. Indeed an edge may be shared by more tetrahedra, but only a bounded number of them. (This follows from the points being well-distributed, so each corner of P has a bounded number of neighbours.) Since there is also only $O(s)$ many 1-dimensional line segments this gives also just a contribution $O(s)$. The central point appears many times, but all appearances contribute 0, since $Rz \notin \mathbb{Z}^3$. We conclude that $\mathcal{L}(RP) \leq Cs(\log N)^3$ as desired. $\square$

By replacing B_F with P_F we make an error in the kinetic energy. (The Fermi ball B_F is the set of momenta of the Slater determinant with lowest kinetic energy.) We now bound the error made with this approximation. That is, we consider

$$\sum_{k\in P_F} |k|^2 - \sum_{k\in B_F} |k|^2.$$

Note that there might not be the same number of summands in both sums. To compute this difference we interpret the sums as Riemann-sums and replace them with the corresponding integrals. It is a simple exercise to show that the error made in this replacement is $Ck_F^2N^{2/3}$. That is,

$$\sum_{k\in P_F} |k|^2 - \sum_{k\in B_F} |k|^2 = \frac{L^3}{(2\pi)^3}\left(\int_{k_FP} |k|^2\,\mathrm{d}k - \int_{B(k_F)} |k|^2\,\mathrm{d}k\right) + O\left(k_F^2N^{2/3}\right).$$

The integrals can be computed in spherical coordinates,

$$\int_{k_FP} |k|^2\,\mathrm{d}k - \int_{B(k_F)} |k|^2\,\mathrm{d}k = \int_{\mathbb{S}^2}\left(\int_0^{k_FR(\omega)} r^4\,\mathrm{d}r - \int_0^{k_F} r^4\,\mathrm{d}r\right)\mathrm{d}\omega$$

For $k_F P$ the radial limit is $k_F R(\omega) = k_F(1+\varepsilon(\omega))$, where $\varepsilon(\omega) = O(s^{-1})$ uniformly in ω by the argument in Remark 3.2.9. Expanding the powers of R we thus get

$$\int_{k_F P} |k|^2 \,\mathrm{d}k - \int_{B(k_F)} |k|^2 \,\mathrm{d}k = k_F^5 \int_{\mathbb{S}^2} \left(\varepsilon(\omega) + O(s^{-2})\right) \mathrm{d}\omega.$$

By construction, P has volume $4\pi/3$. That is, $k_F P$ and $B(k_F)$ have the same volume. This means that

$$0 = \int_{\mathbb{S}^2} \left(\int_0^{k_F R(\omega)} r^2 \,\mathrm{d}r - \int_0^{k_F} r^2 \,\mathrm{d}r \right) \mathrm{d}\omega = k_F^3 \int_{\mathbb{S}^2} \left(\varepsilon(\omega) + O(s^{-2})\right) \mathrm{d}\omega.$$

We thus get that

$$\sum_{k \in P_F} |k|^2 - \sum_{k \in B_F} |k|^2 = O(k_F^2 N s^{-2}) + O\left(k_F^2 N^{2/3}\right).$$

We conclude the following.

Lemma 3.2.13. *The kinetic energy of the (Slater determinant with momenta in the) Fermi polyhedron satisfies*

$$\begin{aligned} \sum_{k \in P_F} |k|^2 &= \sum_{k \in B_F} |k|^2 \left(1 + O(N^{-1/3}) + O(s^{-2})\right) \\ &= \frac{3}{5}(6\pi)^{2/3} \rho^{2/3} N \left(1 + O(N^{-1/3}) + O(s^{-2})\right). \end{aligned}$$

Proof. The computation above gives the first equality. The second follows by noting that $\sum_{k \in B_F} |k|^2$ is a Riemann sum for

$$\frac{L^3}{(2\pi)^3} \int_{|k| \le k_F} |k|^2 \,\mathrm{d}k = \frac{4\pi}{5(2\pi)^3} k_F^5 L^3 = \frac{3}{5}(6\pi^2)^{2/3} \rho^{2/3} N(1 + O(N^{-1/3})). \qquad \square$$

Completely analogously one can show that

$$\sum_{k \in P_F} |k|^4 = \frac{18\pi^2}{7} (6\pi)^{1/3} \rho^{4/3} N \left(1 + O(N^{-1/3}) + O(s^{-2})\right). \tag{3.2.10}$$

We need this formula for Lemma 3.2.14 below. Additionally we need a formula for $\sum_{k \in P_F} |k^1|^4$, where k^1 refers to the first coordinate of $k = (k^1, k^2, k^3)$. Here we have

$$\sum_{k \in P_F} |k^1|^4 = \frac{18\pi^2}{35} (6\pi)^{1/3} \rho^{4/3} N \left(1 + O(N^{-1/3}) + O(s^{-1})\right). \tag{3.2.11}$$

To see this we compare it to $\sum_{k \in B_F} |k^1|^4$. The only difference from above is when doing the spherical integral. We have

$$\begin{aligned} &\sum_{k \in P_F} |k^1|^4 - \sum_{k \in B_F} |k^1|^4 \\ &= \frac{L^3}{(2\pi)^3} \int_0^{2\pi} \mathrm{d}\theta \int_0^{\pi} \mathrm{d}\phi \cos(\phi)^4 \left(\int_0^{k_F(1+\varepsilon(\phi,\theta))} r^6 \,\mathrm{d}r - \int_0^{k_F} r^6 \,\mathrm{d}r \right) + O(k_F^4 N^{2/3}) \\ &= O(k_F^4 N s^{-1}) + O(k_F^4 N^{2/3}), \end{aligned}$$

since we can't use the volume constraint that $\int_{\mathbb{S}^2} \varepsilon(\omega) \,\mathrm{d}\omega = O(s^{-2})$ but only that $\varepsilon(\omega) = O(s^{-1})$. Thus we only get an error of (relative) size s^{-1}. The sum over B_F may be readily computed by computing the corresponding integral.

3.2.3 Reduced densities of the Slater determinant

We now consider the 2-particle reduced density of the (normalized) Slater determinant. We have the following.

Lemma 3.2.14. *The 2-particle reduced density of the (normalized) Slater determinant $\frac{1}{\sqrt{N!}}D_N$ satisfies*

$$\rho^{(2)}(x_1,x_2) = \frac{(6\pi^2)^{2/3}}{5}\rho^{8/3}|x_1-x_2|^2\bigg(1 - \frac{3(6\pi^2)^{2/3}}{35}\rho^{2/3}|x_1-x_2|^2 + O(N^{-1/3}) + O(s^{-2}) + O(N^{-1/3}\rho^{2/3}|x_1-x_2|^2) + O(\rho^{4/3}|x_1-x_2|^4)\bigg).$$

This follows from a Taylor expansion akin to the argument in [ARS22, Lemma 11].

Proof. The Slater determinant is in particular a quasi-free state, hence we get by Wick's rule that

$$\rho^{(2)}(x_1,x_2) = \rho^{(1)}(x_1)\rho^{(1)}(x_2) - \gamma_N^{(1)}(x_1;x_2)\gamma_N^{(1)}(x_2,x_1), \tag{3.2.12}$$

where $\gamma_N^{(1)}$ denotes the (kernel of the) reduced 1-particle density matrix of the Slater determinant. We have

$$\gamma_N^{(1)}(x_1;x_2) = \sum_{k\in P_F} u_k(x_1)\overline{u_k(x_2)} = \frac{1}{L^3}\sum_{k\in P_F} e^{ik(x_1-x_2)}, \qquad \rho^{(1)}(x_1) = \rho.$$

By translation invariance, $\gamma_N^{(1)}(x_1;x_2)$ is a function of x_1-x_2 only, and we shall Taylor expand $\gamma_N^{(1)}$ in x_1-x_2. By construction P_F is reflection symmetric in the axes, see Definition 3.2.7. This means that all odd orders vanish and that all off-diagonal second order terms vanish. Thus, by defining $x_{12} = (x_{12}^1, x_{12}^2, x_{12}^3) = x_1 - x_2$ and expanding all the exponentials we get

$$\begin{aligned}
&\gamma_N^{(1)}(x_1;x_2) \\
&\quad = \frac{1}{L^3}\sum_{k\in P_F}\left(1 - \frac{1}{2}(k\cdot(x_1-x_2))^2 + \frac{1}{24}(k\cdot(x_1-x_2))^4 + O(|k|^6|x_1-x_2|^6)\right) \\
&\quad = \rho - \frac{1}{2L^3}\sum_{k\in P_F}\left[|k^1|^2|x_{12}^1|^2 + |k^2|^2|x_{12}^2|^2 + |k^3|^2|x_{12}^3|^2\right] \\
&\qquad + \frac{1}{24L^3}\Bigg(\sum_{k\in P_F}\left[|k^1|^4|x_{12}^1|^4 + |k^2|^4|x_{12}^2|^4 + |k^3|^4|x_{12}^3|^4\right] \\
&\qquad\quad + 6\sum_{k\in P_F}\left[|k^1|^2|k^2|^2|x_{12}^1|^2|x_{12}^2|^2 + |k^1|^2|k^3|^2|x_{12}^1|^2|x_{12}^3|^2 + |k^2|^2|k^3|^2|x_{12}^2|^2|x_{12}^3|^2\right]\Bigg) \\
&\qquad + O(\rho^3|x_1-x_2|^6).
\end{aligned}$$

By Lemma 3.2.11 we may write

$$\sum_{k\in P_F}|k^\mu|^2 = \frac{1}{3}\sum_{k\in P_F}|k|^2 + O\left(N^{2/3}k_F^2\right)$$

and similar for the $\sum|k^\mu|^4$ and $\sum|k^\mu|^2|k^\nu|^2$-sums. Using this the second order term is given by

$$-\frac{1}{6L^3}\sum_{k\in P_F}|k|^2|x_{12}|^2 + O(\rho^{5/3}|x_{12}|^2N^{-1/3}).$$

Similarly by also rewriting everything in terms of $|x_{12}|^4$ and $[|x_{12}^1|^4 + |x_{12}^2|^4 + |x_{12}^3|^4]$ the fourth order term is given by

$$\frac{1}{48L^3}\Bigg[\Bigg(\sum_{k\in P_F}|k|^4 - 3\sum_{k\in P_F}|k^1|^4\Bigg)|x_{12}|^4 \\ + \Bigg(5\sum_{k\in P_F}|k^1|^4 - \sum_{k\in P_F}|k|^4\Bigg)\Big[|x_{12}^1|^4 + |x_{12}^2|^4 + |x_{12}^3|^4\Big]\Bigg] + O(\rho^{7/3}|x_{12}|^4 N^{-1/3}).$$

Using Lemma 3.2.13 and Equations (3.2.10) and (3.2.11) we get that

$$\begin{aligned}\gamma_N^{(1)}(x_1;x_2) = \rho &- \frac{(6\pi^2)^{2/3}}{10}\rho^{5/3}|x_1-x_2|^2 + \frac{3\pi^2(6\pi^2)^{1/3}}{140}\rho^{7/3}|x_1-x_2|^4 \\ &+ O(\rho^{5/3}N^{-1/3}|x_1-x_2|^2) + O(\rho^{5/3}s^{-2}|x_1-x_2|^2) \\ &+ O(\rho^{7/3}N^{-1/3}|x_1-x_2|^4) + O(\rho^{7/3}s^{-1}|x_1-x_2|^4) + O(\rho^3|x_1-x_2|^6).\end{aligned}$$

Plugging this into Equation (3.2.12) we conclude the desired. □

Finally, we have the following bound on the 3-particle reduced density

Lemma 3.2.15. *The 3-particle reduced density of the (normalized) Slater determinant* $\frac{1}{\sqrt{N!}}D_N$ *satisfies*

$$\rho^{(3)}(x_1,x_2,x_3) \le C\rho^{3+4/3}|x_1-x_2|^2|x_1-x_3|^2.$$

Proof. Note that $\rho^{(3)}$ vanishes whenever any 2 of the 3 particles are incident and moreover that $\rho^{(3)}$ is symmetric under exchange of the particles. We may bound derivatives of $\rho^{(3)}$ as we did for $\rho^{(2)}$. By Taylor's theorem we conclude the desired. □

3.3 Gaudin–Gillespie–Ripka expansion

We now present the cluster expansion of Gaudin, Gillespie and Ripka [GGR71]. The argument given here is essentially the same as in [GGR71], only we give sufficient conditions for the formulas [GGR71, Equations (3.19), (4.9) and (8.4)], given in Theorem 3.3.4, to hold, i.e., for absolute convergence of the expansion.

Recall the definition of the trial state ψ_N in Equation (3.2.1). We calculate the the normalization constant C_N and the reduced densities $\rho^{(1)}_{\mathsf{Jas}}, \rho^{(2)}_{\mathsf{Jas}}$ and $\rho^{(3)}_{\mathsf{Jas}}$ defined in Equation (3.2.3)

We remark that the computation given in the following is not just valid for the function f and (square of a) Slater determinant $|D_N|^2$ we choose, but these can be replaced by a more general function and determinant of a more general matrix. We comment on this further in Remark 3.3.3.

3.3.0.1 Calculation of the normalization constant

First we give the calculation of C_N. Rewriting the f's in terms of $g = f^2 - 1$ we have

$$C_N = \int\!\!\cdots\!\!\int \prod_{i<j} f_{ij}^2 |D_N|^2 \,\mathrm{d}x_1 \ldots \mathrm{d}x_N = \int\!\!\cdots\!\!\int \prod_{i<j}(1+g_{ij})|D_N|^2 \,\mathrm{d}x_1 \ldots \mathrm{d}x_N$$

We factor out the g_{ij} and group terms with the same number of values x_i. (For instance $g_{12}g_{23}$ and $g_{45}g_{46}g_{56}$ both have 3 values x_i appearing, the values x_1, x_2, x_3 and x_4, x_5, x_6, respectively). To state the result we define $\mathcal{G}_p$ as the set of all graphs on $\{1, \ldots, p\}$ such that each vertex has degree at least 1 (i.e. is incident to at least one edge) and define

$$W_p(x_1, \ldots, x_p) := \sum_{G \in \mathcal{G}_p} \prod_{e \in G} g_e.$$

(Note that for $p = 0, 1$ we have $\mathcal{G}_p = \varnothing$ and so $W_p = 0$.) By the symmetry of permuting the coordinates we have

$$\begin{aligned} C_N &= \int\!\!\cdots\!\!\int \left[1 + \frac{N(N-1)}{2} W_2(x_1, x_2) + \frac{N(N-1)(N-2)}{3!} W_3(x_1, x_2, x_3) + \ldots\right] \\ &\qquad \times |D_N|^2 \, \mathrm{d}x_1 \ldots \mathrm{d}x_N \\ &= N! \left[1 + \sum_{p=2}^{N} \frac{1}{p!} \int\!\!\cdots\!\!\int W_p(x_1, \ldots, x_p) \rho^{(p)}(x_1, \ldots, x_p) \, \mathrm{d}x_1 \ldots \mathrm{d}x_p\right], \end{aligned}$$

where again the reduced densities are normalised as

$$\rho^{(p)}(x_1, \ldots, x_p) = N(N-1)\cdots(N-p+1) \int\!\!\cdots\!\!\int \frac{1}{N!} |D_N(x_1, \ldots, x_N)|^2 \, \mathrm{d}x_{p+1} \ldots \mathrm{d}x_N.$$

A simple calculation using the Wick rule shows that

$$\rho^{(p)} = \det\left[\gamma_N^{(1)}(x_i; x_j)\right]_{1 \le i,j \le p} = \det\left[\sum_{k \in P_F} \overline{u_k(x_i)} u_k(x_j)\right]_{1 \le i,j \le p} = \det[S_p^* S_p],$$

where S_p is the $P_F \times p$ "Slater"-matrix with entries $u_k(x_i)$. This has rank $\min\{N, p\} = p$ and so by taking this determinant as the definition of $\rho^{(p)}$ for $p > N$ we have $\rho^{(p)} = 0$ for $p > N$. Thus we may extend the summation to ∞. We now expand out the determinant and the W_p. That is

$$\frac{C_N}{N!} = 1 + \sum_{p=2}^{\infty} \frac{1}{p!} \sum_{\substack{G \in \mathcal{G}_p \\ \pi \in \mathcal{S}_p}} (-1)^\pi \int\!\!\cdots\!\!\int \prod_{e \in G} g_e \prod_{j=1}^{p} \gamma_N^{(1)}(x_j, x_{\pi(j)}) \, \mathrm{d}x_1 \ldots \mathrm{d}x_p,$$

where $\mathcal{S}_p$ denotes the symmetric group on p elements. We will consider π and G together as a diagram (π, G). We give a slightly more general definition for what a diagram is, as we will need such for the calculation of the reduced densities.

Definition 3.3.1. Define the set $\mathcal{G}_p^q$ as the set of all graphs on q "external" vertices $\{1, \ldots, q\}$ and p "internal" vertices $\{q+1, \ldots, q+p\}$ such that all internal vertices have degree at least 1, i.e. each internal vertex has at least one incident edge, and such that there are no edges between external vertices. The external edges are allowed to have degree zero, i.e. have no incident edges. For $q = 0$ we recover $\mathcal{G}_p^0 = \mathcal{G}_p$.

A *diagram* (π, G) on q "external" and p "internal" vertices is a pair of a permutation $\pi \in \mathcal{S}_{q+p}$ (viewed as a directed graph on $\{1, \ldots, q+p\}$) and a graph $G \in \mathcal{G}_p^q$. We denote the set of all diagrams on q "external" vertices and p "internal" vertices by $\mathcal{D}_p^q$.

We will sometimes refer to edges in G as g-edges, directed edges in π as $\gamma_N^{(1)}$-edges and the graph G as a g-graph. The value of a diagram $(\pi, G) \in \mathcal{D}_p^q$ is the function

$$\Gamma_{\pi,G}^q(x_1, \ldots, x_q) := (-1)^\pi \int\!\!\cdots\!\!\int \prod_{e \in G} g_e \prod_{j=1}^{q+p} \gamma_N^{(1)}(x_j, x_{\pi(j)}) \, \mathrm{d}x_{q+1} \ldots \mathrm{d}x_{q+p}.$$

For $q = 0$ we write $\Gamma_{\pi,G} = \Gamma^0_{\pi,G}$ and $\mathcal{D}_p = \mathcal{D}^0_p$.

A diagram (π, G) is said to be *linked* if the graph $\tilde{G}$ with edges the union of edges in G and directed edges in π is connected. The set of all linked diagrams on q "external" and p "internal" vertices is denoted $\mathcal{L}^q_p$. For $q = 0$ we write $\mathcal{L}_p = \mathcal{L}^0_p$.

By the translation invariance we have that $\Gamma^1_{\pi,G}$ is a constant for any diagram (π, G).

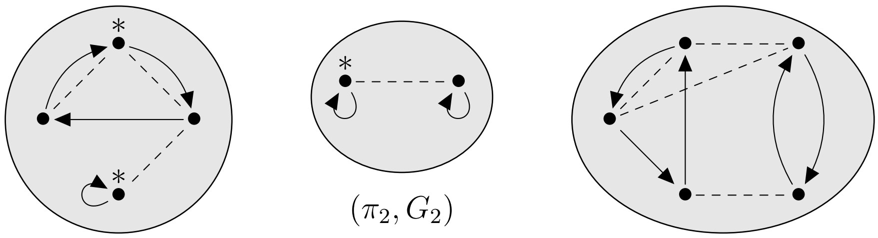
(π_1, G_1)  (π_2, G_2) (π_3, G_3)

Figure 3.3.1: A diagram $(\pi, G) \in \mathcal{D}^3_8$ decomposed into linked components. The dashed lines denote g-edges and the arrows (i, j) denote that $\pi(i) = j$. Vertices labelled with $*$ denote external vertices.

In terms of diagrams we thus have

$$\frac{C_N}{N!} = 1 + \sum_{p=2}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{D}_p} \Gamma_{\pi,G}.$$

If (π, G) is not linked we may decompose it into its linked components. Here the integration factorizes. We split the sum according to the number of linked components. Each linked component has at least 2 vertices, since each vertex must be connected to another vertex with an edge in the corresponding graph. We get

$$\frac{C_N}{N!} = 1 + \sum_{p=2}^{\infty} \underbrace{\sum_{k=1}^{\infty}}_{\#\ \text{lnk. cps.}} \frac{1}{k!} \underbrace{\sum_{p_1\geq 2} \cdots \sum_{p_k\geq 2}}_{\text{sizes linked cps.}} \chi_{(\sum p_\ell = p)} \underbrace{\sum_{(\pi_1,G_1)\in\mathcal{L}_{p_1}} \cdots \sum_{(\pi_k,G_k)\in\mathcal{L}_{p_k}}}_{\text{linked components}} \frac{\Gamma_{\pi_1,G_1}}{p_1!} \cdots \frac{\Gamma_{\pi_k,G_k}}{p_k!} \tag{3.3.1}$$

Here χ is the indicator function. The factor $1/(k!)$ comes from counting the possible labellings of the k linked components. The factors $1/(p_1!), \ldots, 1/(p_k!)$ come from counting how to distribute the p vertices $\{1, \ldots, p\}$ between the linked components of prescribed sizes $p_1, \ldots, p_k$. This gives the factor $\binom{p}{p_1,\ldots,p_k} = \frac{p!}{p_1!\ldots p_k!}$, which together with the factor $1/p!$ already present gives the claimed formula.

We want to pull the p-summation inside the $p_1, \ldots, p_k$-summation. This is allowed once we check that $\sum_p \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p} \Gamma_{\pi,G}$ is absolutely convergent. More precisely we need that the p-sum is absolutely convergent, i.e. $\sum_p \frac{1}{p!} \left|\sum_{(\pi,G)\in\mathcal{L}_p} \Gamma_{\pi,G}\right| < \infty$. This is the content of Lemma 3.3.2 below. We conclude that if the assumptions of Lemma 3.3.2 are satisfied then

$$\begin{aligned} \frac{C_N}{N!} &= 1 + \sum_{k=1}^{\infty} \frac{1}{k!} \sum_{p_1\geq 2} \cdots \sum_{p_k\geq 2} \sum_{(\pi_1,G_1)\in\mathcal{L}_{p_1}} \cdots \sum_{(\pi_k,G_k)\in\mathcal{L}_{p_k}} \frac{\Gamma_{\pi_1,G_1}}{p_1!} \cdots \frac{\Gamma_{\pi_k,G_k}}{p_k!} \\ &= 1 + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\sum_{p=2}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p} \Gamma_{\pi,G} \right)^k = \exp\left(\sum_{p=2}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p} \Gamma_{\pi,G} \right). \end{aligned} \tag{3.3.2}$$

3.3.0.2 Calculation of the 1-particle reduced density

We consider now the 1-particle reduced density of the Jastrow trial state. We have by the translation invariance that $\rho^{(1)}_{\mathsf{Jas}} = \rho^{(1)} = \rho$. We nonetheless compute it here, as we need the formula in terms of (linked) diagrams. We have similarly as before

$$
\begin{aligned}
\rho^{(1)}_{\mathsf{Jas}}(x_1) &= \frac{N}{C_N} \int\!\!\cdots\!\!\int \prod_{2\le i\le N} f_{1i}^2 \prod_{2\le i<j\le N} f_{ij}^2 |D_N|^2 \,\mathrm{d}x_2 \ldots \mathrm{d}x_N \\
&= \frac{N!}{C_N}\left[\rho^{(1)}(x_1) + \sum_{p=1}^{\infty} \frac{1}{p!} \int\!\!\cdots\!\!\int X_p^1 \rho^{(p+1)} \,\mathrm{d}x_2 \ldots \mathrm{d}x_{p+1}\right],
\end{aligned}
$$

where

$$
X_p^1 = \sum_{G\in\mathcal{G}_p^1} \prod_{e\in G} g_e,
$$

with $\mathcal{G}_p^1$ as in Definition 3.3.1. Again this is what one gets by just expanding all the products in the first line and grouping them in terms of how many x_i's appear. The sum is again extended to ∞, since $\rho^{(p)} = 0$ for $p > N$.

We again expand out the determinant and the X_p^1's. For each summand $\pi \in \mathcal{S}_{p+1}$ and $G \in \mathcal{G}_p^1$ we again think of them together as a diagram $(\pi, G) \in \mathcal{D}_p^1$. The formula for $\rho^{(1)}_{\mathsf{Jas}}$ in terms of diagrams is

$$
\rho^{(1)}_{\mathsf{Jas}} = \frac{N!}{C_N} \sum_{p=0}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{D}_p^1} \Gamma^1_{\pi,G} = \frac{N!}{C_N}\left[\rho^{(1)} + \sum_{p=1}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{D}_p^1} \Gamma^1_{\pi,G}\right].
$$

As for the normalization we write out the diagrams in terms of their linked components. There is a distinguished linked component, namely the one containing the vertex $\{1\}$. We will write its size as p_*. It is convenient to take "size" to mean number of internal vertices, i.e. $p_* = 0$ if $\{1\}$ is not connected to any other vertex by either an edge in G or an edge in π. Similarly "number of linked components" means disregarding the distinguished one.

Analogously to the computation in Equation (3.3.1) we thus get for any $p \ge 0$

$$
\begin{aligned}
\frac{1}{p!} \sum_{(\pi,G)\in\mathcal{D}_p^1} \Gamma^1_{\pi,G} &= \sum_{(\pi_*,G_*)\in\mathcal{L}_p^1} \frac{\Gamma^1_{\pi_*,G_*}}{p!} \\
&\quad + \left[\sum_{k=1}^{\infty} \frac{1}{k!} \sum_{p_*\ge 0} \sum_{p_1\ge 2} \cdots \sum_{p_k\ge 2} \chi_{(\sum_{\ell\in\{*,1,\ldots,k\}} p_\ell = p)} \sum_{(\pi_*,G_*)\in\mathcal{L}^1_{p_*}} \frac{\Gamma^1_{\pi_*,G_*}}{p_*!}\right. \\
&\quad \left. \times \sum_{(\pi_1,G_1)\in\mathcal{L}_{p_1}} \cdots \sum_{(\pi_k,G_k)\in\mathcal{L}_{p_k}} \frac{\Gamma_{\pi_1,G_1}}{p_1!} \cdots \frac{\Gamma_{\pi_k,G_k}}{p_k!}\right],
\end{aligned}
$$

where the superscript 1 refers to the slightly modified structure as described in Definition 3.3.1, where there may be no g-edges connecting to $\{1\}$, and there is no integration over x_1. Note that $(\pi_1, G_1) \in \mathcal{L}_{p_1}, \ldots, (\pi_k, G_k) \in \mathcal{L}_{p_k}$ only deal with internal vertices.

Again here we take the sum over p's. We are allowed to permute the p-sum inside of the p_*- and $p_1, \ldots, p_k$-sums if the sums over linked diagrams are absolutely summable. That is, if

$$
\sum_{p\ge 0} \frac{1}{p!} \left| \sum_{(\pi,G)\in\mathcal{L}_p^1} \Gamma^1_{\pi,G} \right| < \infty, \qquad \sum_{p\ge 2} \frac{1}{p!} \left| \sum_{(\pi,G)\in\mathcal{L}_p} \Gamma_{\pi,G} \right| < \infty,
$$

then we have, as for the normalization in Equation (3.3.2), that

$$
\begin{aligned}
\rho^{(1)}_{\mathsf{Jas}} &= \frac{N!}{C_N}\sum_{p=0}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{D}^1_p}\Gamma^1_{\pi,G} \\
&= \frac{N!}{C_N}\left[\sum_{p_*\geq 0}\sum_{(\pi_*,G_*)\in\mathcal{L}_{p_*}}\frac{\Gamma^1_{\pi_*,G_*}}{p_*!}\right]\times\left[\sum_{k=0}^{\infty}\frac{1}{k!}\left(\sum_{p\geq 2}\sum_{(\pi,G)\in\mathcal{L}_p}\frac{\Gamma_{\pi,G}}{p!}\right)^k\right] \\
&= \sum_{p\geq 0}\sum_{(\pi,G)\in\mathcal{L}^1_p}\frac{\Gamma^1_{\pi,G}}{p!} = \rho^{(1)} + \sum_{p\geq 1}\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}^1_p}\Gamma^1_{\pi,G},
\end{aligned}
$$

where we used Equation (3.3.2) and that the $p=0$ term just gives the 1-particle density of the Slater determinant. Thus, by translation invariance, we have

$$
\rho = \rho^{(1)} = \rho^{(1)}_{\mathsf{Jas}} = \sum_{p\geq 0}\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}^1_p}\Gamma^1_{\pi,G}.
$$

3.3.0.3 Calculation of the 2-particle reduced density

Let us now compute the 2-particle reduced density. As before by expanding all the $f^2 = 1+g$ factors apart from the factor f_{12} we get

$$
\rho^{(2)}_{\mathsf{Jas}} = \frac{N!}{C_N}f_{12}^2\sum_{p=0}^{\infty}\int X^2_p\rho^{(p+2)}\,\mathrm{d}x_3\ldots\,\mathrm{d}x_{p+2}, \qquad X^2_p = \sum_{G\in\mathcal{G}^2_p}\prod_{e\in G}g_e,
$$

where $\mathcal{G}^2_p$ is as in Definition 3.3.1.

We again decompose the diagrams into linked components. However, we need to distinguish between the cases where $\{1\}$ and $\{2\}$ are both in the same component or in two different components. The computation is analogous to the computation above. We get

$$
\begin{aligned}
\rho^{(2)}_{\mathsf{Jas}}(x_1,x_2) &= f_{12}^2\Bigg(\underbrace{\sum_{p_1,p_2\geq 0}\sum_{\substack{(\pi_1,G_1)\in\mathcal{L}^1_{p_1}\\(\pi_2,G_2)\in\mathcal{L}^1_{p_2}}}\frac{\Gamma^1_{\pi_1,G_1}(x_1)\Gamma^1_{\pi_2,G_2}(x_2)}{p_1!p_2!}}_{\{1\}\text{ and }\{2\}\text{ in different linked components}} \\
&\qquad + \underbrace{\sum_{p_{12}\geq 0}\sum_{(\pi_{12},G_{12})\in\mathcal{L}^2_{p_{12}}}\frac{\Gamma^2_{\pi_{12},G_{12}}(x_1,x_2)}{p_{12}!}}_{\{1\}\text{ and }\{2\}\text{ in same linked component}}\Bigg) \\
&= f_{12}^2\left(\rho^{(1)}_{\mathsf{Jas}}(x_1)\rho^{(1)}_{\mathsf{Jas}}(x_2) + \sum_{p_{12}\geq 0}\frac{1}{p_{12}!}\sum_{(\pi_{12},G_{12})\in\mathcal{L}^2_{p_{12}}}\Gamma^2_{\pi_{12},G_{12}}(x_1,x_2)\right)
\end{aligned}
$$

after pulling in the sum over $p\geq 0$. The $p_{12}=0$ term together with the term $\rho^{(1)}_{\mathsf{Jas}}(x_1)\rho^{(1)}_{\mathsf{Jas}}(x_2) = \rho^{(1)}(x_1)\rho^{(1)}(x_2) = \rho^2$ gives $\rho^{(2)}$ by Wick's rule. The condition of absolute convergence is

$$
\sum_{p\geq 2}\frac{1}{p!}\left|\sum_{(\pi,G)\in\mathcal{L}_p}\Gamma_{\pi,G}\right| < \infty, \quad \sum_{p\geq 0}\frac{1}{p!}\left|\sum_{(\pi,G)\in\mathcal{L}^1_p}\Gamma^1_{\pi,G}\right| < \infty, \quad \sum_{p\geq 0}\frac{1}{p!}\left|\sum_{(\pi,G)\in\mathcal{L}^2_p}\Gamma^2_{\pi,G}\right| < \infty.
$$

3.3.0.4 Calculation of the 3-particle reduced density

The calculation of the 3-particle reduced density follows along the same arguments as for the 2-particle reduced density. We introduce the relevant diagrams and decompose these according to their linked components. As for the 2-particle reduced density we distinguish between the cases according to whether the external vertices $\{1, 2, 3\}$ are in the same or different linked components. They are either in $1, 2$ or 3 different components. Thus, schematically

$$\rho^{(3)}_{\text{Jas}} = f_{12}^2 f_{13}^2 f_{23}^2 \Bigg[\sum_{\text{all in different}} \Gamma^1\Gamma^1\Gamma^1 + \Bigg(\sum_{\text{2 in one}} \Gamma^1(x_1)\Gamma^2(x_2, x_3) + \text{permutations} \Bigg) + \sum_{\text{all in same}} \Gamma^3 \Bigg].$$

Any case where one external vertex is in its own linked component, the contribution for such a linked component is $\rho^{(1)}_{\text{Jas}} = \rho^{(1)} = \rho$ (assuming absolute convergence). Thus,

$$\begin{aligned} &\rho^{(3)}_{\text{Jas}}(x_1, x_2, x_3) \\ &\quad = f_{12}^2 f_{13}^2 f_{23}^2 \Bigg[\rho^3 + \rho \sum_{p \geq 0} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p^2} \Big(\Gamma^2_{\pi,G}(x_1, x_2) + \Gamma^2_{\pi,G}(x_1, x_3) + \Gamma^2_{\pi,G}(x_2, x_3) \Big) \\ &\qquad + \sum_{p \geq 0} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p^3} \Gamma^3_{\pi,G}(x_1, x_2, x_3) \Bigg]. \end{aligned}$$

All the $p = 0$-terms together give $\rho^{(3)}$ by Wick's rule. The condition for absolute convergence is that for any $q \leq 3$ we have $\sum_{p\geq 0} \frac{1}{p!} \left| \sum_{(\pi,G)\in\mathcal{L}_p^q} \Gamma^q_{\pi,G} \right| < \infty$.

3.3.0.5 Summarising the results

For the absolute convergence we have

Lemma 3.3.2. *There exists a constant $c > 0$ such that if $sa^3\rho\log(b/a)(\log N)^3 < c$, then*

$$\sum_{p\geq 0} \frac{1}{p!} \left| \sum_{(\pi,G)\in\mathcal{L}_p^q} \Gamma^q_{\pi,G} \right| < \infty$$

for any $0 \leq q \leq 3$.

Remark 3.3.3. As mentioned in the beginning of the section, the calculation just given is still valid if we replace f by some general function $h \geq 0$ and replace $|D_N|^2$ by some more general determinant $\det[\gamma(x_i - x_j)]_{1\leq i,j\leq N}$, where $\gamma(x - y)$ is the kernel of some rank N projection (for instance the one-particle density matrix of a Slater determinant of N particles). The criterion for absolute convergence reads

$$\sup_{x_1,\ldots,x_n} \prod_{1\leq i<j\leq n} h(x_i - x_j) \leq C^n \text{ for all } n \in \mathbb{N},$$

$$\frac{1}{L^3} \sum_{k\in\frac{2\pi}{L}\mathbb{Z}^3} |\hat{\gamma}(k)| \int_\Lambda \left| h^2 - 1 \right| \,\mathrm{d}x \int_\Lambda |\gamma| \,\mathrm{d}y < c$$

for some constants $c, C > 0$, where the first condition is the "stability condition" of the tree-graph bound [PU09, Proposition 6.1; Uel18] and $\hat{\gamma}(k) := \int_\Lambda \gamma(x)e^{-ikx}\,\mathrm{d}x$.

We give the proof of Lemma 3.3.2 in Section 3.3.1. Thus, we have the following.

Theorem 3.3.4. *There exists a constant $c > 0$ such that if $sa^3\rho\log(b/a)(\log N)^3 < c$, then*

$$
\begin{aligned}
\frac{C_N}{N!} &= \exp\left(\sum_{p=2}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p}\Gamma_{\pi,G}\right),\\
\rho^{(1)}_{\mathsf{Jas}} &= \rho^{(1)} + \sum_{p=1}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p^1}\Gamma^1_{\pi,G},\\
\rho^{(2)}_{\mathsf{Jas}} &= f_{12}^2\left[\rho^{(2)} + \sum_{p=1}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p^2}\Gamma^2_{\pi,G}\right].\\
\rho^{(3)}_{\mathsf{Jas}} &= f_{12}^2f_{13}^2f_{23}^2\Bigg[\rho^{(3)} + \rho\sum_{p\geq 1}\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p^2}\Big(\Gamma^2_{\pi,G}(x_1,x_2)+\Gamma^2_{\pi,G}(x_1,x_3)+\Gamma^2_{\pi,G}(x_2,x_3)\Big)\\
&\qquad + \sum_{p\geq 1}\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p^3}\Gamma^3_{\pi,G}\Bigg].
\end{aligned}
\tag{3.3.3}
$$

The first three formulas are the same as those of [GGR71, Equations (3.19), (4.9) and (8.4)]. Our main contribution is to give a criterion for convergence, and hence for validity of the formulas.

Remark 3.3.5. The factor $s(\log N)^3$ results from the bound in Lemma 3.2.12. If we had not introduced the Fermi polyhedron, and instead used the Fermi ball, we would instead have a factor $N^{1/3}$ as mentioned in Section 3.2.2. That is, the condition for absolute convergence would be $N^{1/3}a^3\rho\log(b/a) < c$ for some constant $c > 0$.

In either case, the N-dependence prevents us from taking a thermodynamic limit directly, and we instead use a box method of gluing together multiple smaller boxes, where we may put some finite number of particles in each box, see Section 3.4.1. For the case of using a Slater determinant with momenta in the Fermi ball, there is no way to choose the number of particles in each smaller box so that both the absolute convergence holds ($N^{1/3}a^3\rho\log(b/a) < c$), and the finite-size error made in the kinetic energy ($\sim N^{2/3}\rho^{2/3}$, see Lemma 3.2.13) is smaller than the claimed energy contribution from the interaction ($\sim Na^3\rho^{5/3}$, see Theorem 3.1.3). For this reason we need the polyhedron of Section 3.2.2.

Remark 3.3.6. The formulas for $\rho^{(2)}_{\mathsf{Jas}}$ and $\rho^{(3)}_{\mathsf{Jas}}$ only hold for periodic boundary conditions, since in this case $\rho^{(1)}_{\mathsf{Jas}} = \rho^{(1)} = \rho$. For different boundary conditions, one has to take into account that this equality is not valid. In general one has for $\rho^{(2)}_{\mathsf{Jas}}$ that

$$
\begin{aligned}
\rho^{(2)}_{\mathsf{Jas}} &= f_{12}^2\left[\rho^{(2)} + \sum_{p=1}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p^2}\Gamma^2_{\pi,G} + \Big(\rho^{(1)}_{\mathsf{Jas}}(x_1)\rho^{(1)}_{\mathsf{Jas}}(x_2) - \rho^{(1)}(x_1)\rho^{(1)}(x_2)\Big)\right]\\
&= f_{12}^2\left[\rho^{(2)} + \sum_{p=1}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p^2}\Gamma^2_{\pi,G} + \sum_{\substack{p_1,p_2\geq 0\\ p_1+p_2\geq 1}}\frac{1}{p_1!p_2!}\sum_{\substack{(\pi_1,G_1)\in\mathcal{L}^1_{p_1}\\ (\pi_2,G_2)\in\mathcal{L}^1_{p_2}}}\Gamma^1_{\pi_1,G_1}(x_1)\Gamma^1_{\pi_2,G_2}(x_2)\right].
\end{aligned}
$$

One of the reasons we work with periodic boundary conditions is that by doing so, we don't have the complication of dealing with the additional term.

Remark 3.3.7. By following the same procedure as in the previous sections, one can equally well get formulas for the higher order reduced particle densities. Similarly one can extend the absolute convergence, Lemma 3.3.2, to any q, only one may have to change the constant $c > 0$ to depend on q.

3.3.1 Absolute convergence

We now prove Lemma 3.3.2, i.e. that the appropriate sums are absolutely convergent.

Proof of Lemma 3.3.2. We consider the four sums $\sum_{p\geq 0} \frac{1}{p!}\left|\sum_{(\pi,G)\in\mathcal{L}_p^q} \Gamma^q_{\pi,G}\right|$, $q = 0,1,2,3$ one by one.

3.3.1.1 Absolute convergence of the Γ-sum

Consider first $\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p}\Gamma_{\pi,G}$. Split the sum according to the number of connected components of G, labelled as $(G_1,\ldots,G_k)$ of sizes $n_1,\ldots,n_k$. We call these *clusters*. (Note that "connected" only refers to the graph G, and is independent of the permutation π.) Name the vertices in G_1 as $\{1,\ldots,n_1\}$, in G_2 as $\{n_1+1,\ldots,n_1+n_2\}$ and so on. Then we have (for $p\geq 2$)

$$\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p}\Gamma_{\pi,G} = \sum_{k=1}^{\infty}\frac{1}{k!}\sum_{n_1,\ldots,n_k\geq 2}\frac{1}{n_1!\cdots n_k!}\chi_{(\sum n_\ell = p)}\sum_{\substack{G_1,\ldots,G_k\\ G_\ell\in\mathcal{C}_{n_\ell}}}\sum_{\pi\in\mathcal{S}_p}(-1)^\pi\chi_{((\pi,\cup G_\ell)\in\mathcal{L}_p)}$$
$$\times\int\!\cdots\!\int\prod_{\ell=1}^{k}\prod_{e\in G_\ell} g_e\prod_{j=1}^{p}\gamma_N^{(1)}(x_j;x_{\pi(j)})\,\mathrm{d}x_1\ldots\mathrm{d}x_p,$$

where $\mathcal{C}_n$ denotes the set of connected graphs on n (labelled) vertices. The factorial factors are similar to those of Equation (3.3.1). Indeed, the factor $1/(k!)$ comes from counting the possible labelling of the clusters, and the factors $1/(n_1!),\ldots,1/(n_k!)$ come from counting the number of ways to distribute the $p=\sum n_\ell$ vertices into the clusters and using the factor $1/(p!)$ already present.

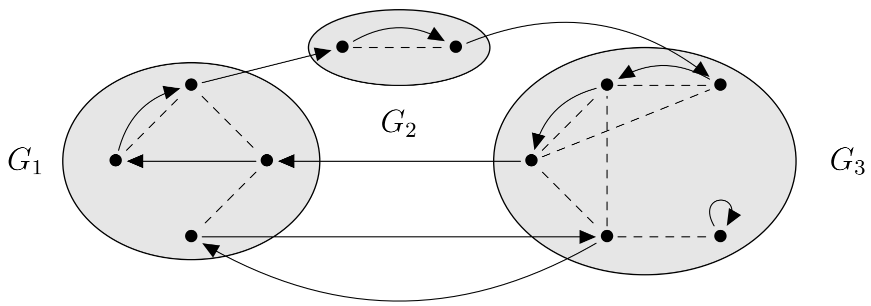


Figure 3.3.2: A linked diagram $(\pi,G)\in\mathcal{L}_{11}$ decomposed into clusters G_1,G_2,G_3. Dashed lines denote g-edges, and arrows (i,j) denote that $\pi(i)=j$.

For the analysis we will need the following.

Definition 3.3.8. Let $A_1,\ldots,A_k$ denote disjoint non-empty sets. The *truncated* correlation function is

$$\rho_{\mathsf{t}}^{(A_1,\ldots,A_k)} := \sum_{\pi\in\mathcal{S}_{\cup_\ell A_\ell}}(-1)^\pi\chi_{((\pi,\cup G_\ell)\text{ linked})}\prod_{j\in\cup_\ell A_\ell}\gamma_N^{(1)}(x_j;x_{\pi(j)}). \tag{3.3.4}$$

for some choice of connected graphs $G_\ell \in \mathcal{C}_{A_\ell}$. The definition does not depend on the choice of graphs G_ℓ.

If the underlying sets $A_1, \ldots, A_k$ are clear we will simply denote the truncated correlation by their sizes,

$$\rho_{\mathsf{t}}^{(|A_1|,\ldots,|A_k|)} = \rho_{\mathsf{t}}^{(A_1,\ldots,A_k)}.$$

The truncated correlation functions are also sometimes referred to as *connected* correlation functions [GMR21, Appendix D].

Remark 3.3.9. We write the characteristic function in Equation (3.3.4) as $\chi_{((\pi,\cup G_\ell)\text{ linked})}$ for ease of generalizability to the cases in Sections 3.3.1.2 and 3.3.1.3 where we will need the notion of truncated correlations also for some of the vertices being external. For the truncated correlations it doesn't matter which (if any) vertices are external, only which vertices are in which clusters.

Since $0 \le f \le 1$ we have $-1 \le g \le 0$. Thus, by the tree-graph bound [PU09, Proposition 6.1; Uel18] we have

$$\left| \sum_{G\in\mathcal{C}_n} \prod_{e\in G} g_e \right| \le \sum_{T\in\mathcal{T}_n} \prod_{e\in T} |g_e|,$$

where $\mathcal{T}_n$ is the set of all trees on n (labelled) vertices. Thus we get

$$\begin{aligned} &\sum_{p=2}^{\infty} \frac{1}{p!} \left| \sum_{(\pi,G)\in\mathcal{L}_p} \Gamma_{\pi,G} \right| \\ &\quad \le \sum_{k=1}^{\infty} \frac{1}{k!} \sum_{n_1,\ldots,n_k\ge 2} \frac{1}{n_1!\cdots n_k!} \int\!\!\cdots\!\!\int \sum_{\substack{T_1,\ldots,T_k \\ T_\ell\in\mathcal{T}_{n_\ell}}} \prod_{\ell=1}^{k} \prod_{e\in T_\ell} |g_e| \left|\rho_{\mathsf{t}}^{(n_1,\ldots,n_k)}\right| \,\mathrm{d}x_1 \ldots \mathrm{d}x_{\sum n_\ell}. \end{aligned} \tag{3.3.5}$$

Here the vertices in T_ℓ are the same as in G_ℓ, i.e. T_1 has vertices $\{1,\ldots,n_1\}$, T_2 has vertices $\{n_1+1,\ldots,n_1+n_2\}$ and so on.

In [GMR21, Equation (D.53)] the following formula, known as the Brydges-Battle-Federbush (BBF) formula, is shown for the truncated correlation functions

$$\rho_{\mathsf{t}}^{(A_1,\ldots,A_k)} = \sum_{\tau\in\mathcal{A}^{(A_1,\ldots,A_k)}} \prod_{(i,j)\in\tau} \gamma_N^{(1)}(x_i;x_j) \int \mathrm{d}\mu_\tau(r) \det\mathcal{N}(r), \tag{3.3.6}$$

where $\mathcal{A}^{(A_1,\ldots,A_k)}$ is the set of all anchored trees on k clusters with vertices $A_1,\ldots,A_k$. (If the sets $A_1,\ldots,A_k$ are clear we will write $\mathcal{A}^{(|A_1|,\ldots,|A_k|)} = \mathcal{A}^{(A_1,\ldots,A_k)}$ as for the truncated correlations.) An *anchored tree* is a directed graph on all the $\cup_\ell A_\ell$ vertices, such that each vertex has at most one incoming and at most one outgoing edge (note that these are all $\gamma_N^{(1)}$-edges, and that the g-edges don't matter for this construction) and such that upon identifying all vertices in each cluster, the resulting graph is a (directed) tree. The measure μ_τ is a probability measure on $\{(r_{\ell\ell'})_{1\le\ell\le\ell'\le k} : 0 \le r_{\ell\ell'} \le 1\} = [0,1]^{k(k-1)/2}$ and depends only on τ but not on the factors $\gamma_N^{(1)}(x_i;x_j)$. Finally, $\mathcal{N}$ is an $I\times J$ (square) matrix with entries $\mathcal{N}_{ij} = r_{c(i)c(j)}\gamma_N^{(1)}(x_i;x_j)$, where $c(i)$ is the (label of the) cluster containing the vertex $\{i\}$ and $r_{\ell\ell'} := r_{\ell'\ell}$ if $\ell > \ell'$. Here

$$I = \left\{ i \in \textstyle\bigcup_{\ell=1}^k A_\ell : \nexists j : (i,j)\in\tau \right\}, \qquad J = \left\{ j \in \textstyle\bigcup_{\ell=1}^k A_\ell : \nexists i : (i,j)\in\tau \right\},$$

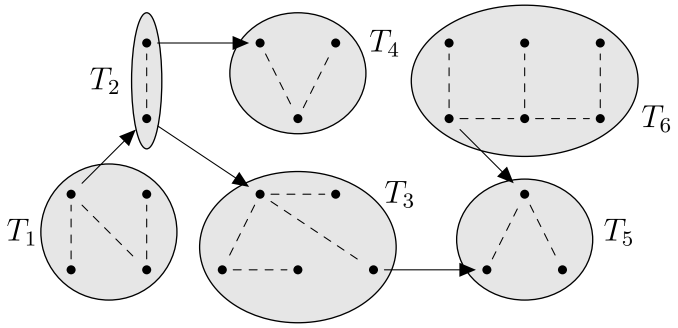


Figure 3.3.3: An anchored tree τ (arrows) and trees $T_1, \ldots, T_6$ (dashed lines).

are the set of i's (respectively j's) not appearing as i's (respectively j's) in the anchored tree τ.

From [GMR21, Equation (D.57)] it follows that $|\det \mathcal{N}| \leq \rho^{\sum n_\ell - (k-1)}$. To see this, one has to adapt the argument in [GMR21, Lemma D.2] slightly. We sketch the argument here.

Lemma 3.3.10 ([GMR21, Lemmas D.2 and D.6])**.** *The matrix $\mathcal{N}(r)$ satisfies $|\det \mathcal{N}(r)| \leq \rho^{\sum n_\ell - (k-1)}$ for all $r \in [0,1]^{k(k-1)/2}$.*

Proof. First we bound $\rho^{(p)} = \det[\gamma_N^{(1)}(x_i; x_j)]_{1 \leq i,j \leq p}$ following the strategy of [GMR21, Lemma D.2]. This is done by writing (as in [GMR21, Equations (D.8), (D.9)])

$$\gamma_N^{(1)}(x_i; x_j) = \langle \alpha_i | \beta_j \rangle_{\ell^2((2\pi/L)\mathbb{Z}^3)},$$

where for $k \in \frac{2\pi}{L}\mathbb{Z}^3$

$$\alpha_i(k) = L^{-3/2} e^{-ikx_i} \chi_{(k \in P_F)} \qquad \beta_j(k) = L^{-3/2} e^{-ikx_j} \chi_{(k \in P_F)} = \alpha_j(k).$$

By the the Gram-Hadamard inequality [GMR21, Lemma D.1] we have

$$\left|\rho^{(p)}\right| = \left|\det[\gamma_N^{(1)}(x_i; x_j)]_{1 \leq i,j \leq p}\right| \leq \prod_{i=1}^{p} \|\alpha_i\|_{\ell^2((2\pi/L)\mathbb{Z}^3)} \|\beta_i\|_{\ell^2((2\pi/L)\mathbb{Z}^3)} = \rho^p.$$

By modifying this argument exactly as described in the proof of [GMR21, Lemma D.6] and noting that $r_{\ell\ell'} \leq 1$ one concludes the desired. ☐

Remark 3.3.11. We denote the functions as α_j and β_j (even though they denote the same function) for ease of modifying the argument later in order to prove Equation (3.4.16).

In particular one concludes the bound

$$\left|\rho_{\mathsf{t}}^{(n_1,\ldots,n_k)}\right| \leq \rho^{\sum n_\ell - (k-1)} \sum_{\tau \in \mathcal{A}^{(n_1,\ldots,n_k)}} \prod_{(i,j) \in \tau} \left|\gamma_N^{(1)}(x_i; x_j)\right|. \tag{3.3.7}$$

Plugging this into Equation (3.3.5) above we get

$$\sum_{p=2}^{\infty} \frac{1}{p!} \left| \sum_{(\pi,G) \in \mathcal{L}_p} \Gamma_{\pi,G} \right| \leq \sum_{k=1}^{\infty} \frac{1}{k!} \sum_{n_1,\ldots,n_k \geq 2} \frac{1}{n_1! \cdots n_k!} \rho^{\sum n_\ell - (k-1)} \sum_{\substack{T_1,\ldots,T_k \\ T_\ell \in \mathcal{T}_{n_\ell}}} \sum_{\tau \in \mathcal{A}^{(n_1,\ldots,n_k)}}$$
$$\times \int \!\! \cdots \!\! \int \mathrm{d}x_1 \ldots \mathrm{d}x_{\sum n_\ell} \prod_{\ell=1}^{k} \prod_{e \in T_\ell} |g_e| \prod_{(i,j) \in \tau} \left|\gamma_N^{(1)}(x_i; x_j)\right|.$$

To compute these integrals we note that by Lemma 3.2.2

$$
\begin{aligned}
\int |g(x)| \, \mathrm{d}x &= \int \left(1 - f(x)^2\right) \mathrm{d}x \\
&\leq \frac{4\pi}{(1 - a^3/b^3)^2} \int_a^b \left(\left(1 - \frac{a^3}{b^3}\right)^2 - \left(1 - \frac{a^3}{r^3}\right)^2 \right) r^2 \, \mathrm{d}r \leq C a^3 \log \frac{b}{a}.
\end{aligned}
$$

That is, each factor of g_e gives a contribution $Ca^3 \log(b/a)$ after integration. The $\gamma_N^{(1)}$-factors we can bound by Lemma 3.2.12 as

$$
\int \left| \gamma_N^{(1)}(x; y) \right| \mathrm{d}y \leq Cs (\log N)^3.
$$

This takes care of all but one integration, which gives the volume factor L^3. We shall compute the integrations in the following order:

(1.) Pick any leaf $\{j_0\}$ of the anchored tree τ lying in some cluster ℓ, meaning that there is exactly one edge of τ incident in ℓ.

(2.) Consider $\{j_0\}$ as the root of T_ℓ and pick any leaf $\{j\}$ of T_ℓ and integrate over x_j. Since $\{j\}$ is a leaf of T_ℓ and $\{j_0\}$ is a leaf of τ we have that the only place x_j appears in the integrand is in some factor g_{ij} for $\{i\}$ the unique vertex connected to $\{j\}$ by a g-edge. Hence the x_j-integral contributes $\int |g|$ by the translation invariance.

Remove $\{j\}$ and its incident edge from T_ℓ.

Repeat for all vertices in the cluster until only $\{j_0\}$ remain. (At this point the entirety of T_ℓ has been removed.)

(3.) Integrate over x_{j_0}. Since $\{j_0\}$ is a leaf of τ the only place x_{j_0} appears (in the remaining integrand) is in the $\gamma_N^{(1)}$-factor from τ. Thus, the x_{j_0}-integral gives a contribution $\int |\gamma_N^{(1)}|$ by the translation invariance.

Remove $\{j_0\}$ and its incident edge from τ.

(4.) Repeat steps (1.)-(3.) until all integrals have been computed. The final integral gives the volume factor L^3.

Steps (1.)-(3.) compute all integrations in one cluster. Repeating this process we integrate over the clusters one by one and thus compute all the integrals. Note that each integration is always over a coordinate associated to a leaf of the relevant graphs. This is a key point, since then by translation invariance each integration contributes exactly $\int |g|$ or $\int |\gamma_N^{(1)}|$ whichever is appropriate. In total we thus have the bound

$$
\begin{aligned}
&\int \!\cdots\! \int \mathrm{d}x_1 \ldots \mathrm{d}x_{\sum n_\ell} \prod_{\ell=1}^{k} \prod_{e \in T_\ell} |g_e| \prod_{(i,j) \in \tau} \left| \gamma_N^{(1)}(x_i; x_j) \right| \\
&\quad \leq \left(Ca^3 \log(b/a) \right)^{\sum n_\ell - k} \left(Cs (\log N)^3 \right)^{k-1} L^3.
\end{aligned}
$$

This bound is for each summand $\tau, T_1, \ldots, T_k$. By Cayley's formula $\#\mathcal{T}_n = n^{n-2} \leq C^n n!$, and by [GMR21, Appendix D.5] $\#\mathcal{A}^{(n_1,\ldots,n_k)} \leq k! 4^{\sum n_\ell}$. Thus, we get

$$\begin{aligned}
\sum_{p=2}^{\infty} \frac{1}{p!} \left| \sum_{(\pi,G)\in\mathcal{L}_p} \Gamma_{\pi,G} \right| &\leq CN \sum_{k=1}^{\infty} \left[Cs(\log N)^3 \right]^{k-1} \left[\sum_{n=2}^{\infty} (Ca^3\rho\log(b/a))^{n-1} \right]^k \\
&\leq CNa^3\rho\log(b/a) \sum_{k=1}^{\infty} \left[Csa^3\rho\log(b/a)(\log N)^3 \right]^{k-1} \\
&\leq CNa^3\rho\log(b/a) < \infty,
\end{aligned}$$

for $sa^3\rho\log(b/a)(\log N)^3$ sufficiently small. This shows that $\sum_p \frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p}\Gamma_{\pi,G}$ is absolutely convergent under this condition.

3.3.1.2 Absolute convergence of the Γ^1-sum

Consider now $\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p^1}\Gamma^1_{\pi,G}$. The argument is almost identical to the argument above. We again split the sum according to the connected components of G. Call these $G_*, G_1, \ldots, G_k$, where G_* is the distinguished connected component (cluster) containing the distinguished vertex $\{1\}$. Exactly as for $\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p}\Gamma_{\pi,G}$ we have that (for $p=0$ one has to interpret the empty product of integrals as 1, so $\sum_{(\pi,G)\in\mathcal{L}_0^1}\Gamma^1_{\pi,G} = \rho$)

$$\begin{aligned}
&\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p^1} \Gamma^1_{\pi,G}(x_1) \\
&\quad = \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{n_*\geq 0} \sum_{n_1,\ldots,n_k\geq 2} \frac{1}{n_*! n_1! \cdots n_k!} \chi_{\left(\sum_{\ell\{*,1,\ldots,k\}} n_\ell = p\right)} \sum_{\substack{G_1\in\mathcal{C}_{n_1},\ldots,G_k\in\mathcal{C}_{n_k} \\ G_*\in\mathcal{C}_{n_*+1}}} \sum_{\pi\in\mathcal{S}_{p+1}} (-1)^\pi \\
&\qquad \times \chi_{\left((\pi,\cup_{\ell\in\{*,1,\ldots,k\}} G_\ell)\in\mathcal{L}_p^1\right)} \int\!\!\cdots\!\!\int \prod_{\ell\in\{*,1,\ldots,k\}} \prod_{e\in G_\ell} g_e \prod_{j=1}^{p+1} \gamma_N^{(1)}(x_j; x_{\pi(j)}) \,\mathrm{d}x_2 \ldots \mathrm{d}x_{p+1}.
\end{aligned}$$

Here for the $k=0$ term one should think of the $n_1,\ldots,n_k$-sums as being an empty product before it is an empty sum, i.e. it should give a factor 1. That is, the $k=0$ term reads

$$\sum_{G_*\in\mathcal{C}_{p+1}} \sum_{\pi\in\mathcal{S}_{p+1}} (-1)^\pi \int\!\!\cdots\!\!\int \prod_{e\in G_*} g_e \prod_{j=1}^{p+1} \gamma_N^{(1)}(x_j; x_{\pi(j)}) \,\mathrm{d}x_2 \ldots \mathrm{d}x_{p+1},$$

since (π, G_*) is trivially linked, since G_* is connected. From here on, we won't write out the $k=0$ term separately to make the formulas more concise. As before we use the tree-graph inequality and the truncated correlation function (see Remark 3.3.9) to get

$$\begin{aligned}
&\sum_{p\geq 0} \frac{1}{p!} \left| \sum_{(\pi,G)\in\mathcal{L}_p^1} \Gamma^1_{\pi,G} \right| \\
&\quad \leq \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{n_*\geq 0} \sum_{n_1,\ldots,n_k\geq 2} \frac{1}{n_*! n_1! \cdots n_k!} \sum_{\substack{T_1\in\mathcal{T}_{n_1},\ldots,T_k\in\mathcal{T}_{n_k} \\ T_*\in\mathcal{T}_{n_*+1}}} \\
&\qquad \times \int\!\!\cdots\!\!\int \prod_{\ell\in\{*,1,\ldots,k\}} \prod_{e\in T_\ell} |g_e| \left| \rho_{\mathrm{t}}^{(n_*+1,n_1,\ldots,n_k)} \right| \mathrm{d}x_2 \ldots \mathrm{d}x_{\sum_{\ell\in\{*,1,\ldots,k\}} n_\ell + 1}.
\end{aligned}$$

To bound this we use the same bound, Equation (3.3.7), on the truncated correlations as before. It reads

$$\left|\rho_{\mathrm{t}}^{(n_*+1,n_1,\ldots,n_k)}\right| \le \rho^{\sum_{\ell\in\{*,1,\ldots,k\}} n_\ell+1-(k+1-1)} \sum_{\tau\in\mathcal{A}^{(n_*+1,n_1,\ldots,n_k)}} \prod_{(i,j)\in\tau} \left|\gamma_N^{(1)}(x_i;x_j)\right|.$$

Computing the integrals is as before, with a few differences. During each repeat (apart from the last one) of step (1.) we pick not just any leaf j_0 but a leaf j_0 not in the cluster containing $\{1\}$. (Since any tree has at least 2 leaves, this is always possible.) For each of these repeats, the argument is the same as before. For the last repeat of step (1.) where only the cluster containing $\{1\}$ remains we follow step (2.) with the slight change, that the root is chosen to be $\{1\}$. (There are no $\gamma_N^{(1)}$-factors left, so we are free to choose any vertex as the root.) There is then no step (3.) since we do not integrate over x_1.

This has the following effect. First, the last variable x_1 is not integrated over, so there is no volume factor L^3. And second, there are k integrals $\int|\gamma_N^{(1)}|$ instead of $k-1$ (since there are $k+1$ many clusters including the distinguished one). For the bounds of the sum of all terms we use that $\#\mathcal{A}^{(n_*+1,n_1,\ldots,n_k)} \le (k+1)!4^{\sum_{\ell\in\{*,1,\ldots,k\}} n_\ell+1}$. Thus, uniformly in x_1

$$\begin{aligned}
&\sum_{p\ge0}\frac{1}{p!}\left|\sum_{(\pi,G)\in\mathcal{L}_p^1}\Gamma_{\pi,G}^1\right| \\
&\quad\le C\rho\left(\sum_{n_*=0}^\infty\left[Ca^3\rho\log(b/a)\right]^{n_*}\right)\left(\sum_{k=0}^\infty(k+1)\left[Cs(\log N)^3\right]^k\left[\sum_{n=2}^\infty(Ca^3\rho\log(b/a))^{n-1}\right]^k\right)\\
&\quad\le C\rho<\infty,
\end{aligned}$$

for $sa^3\rho\log(b/a)(\log N)^3$ sufficiently small. This shows that $\sum_p\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p^1}\Gamma_{\pi,G}^1$ is absolutely convergent under this condition.

3.3.1.3 Absolute convergence of the Γ^2-sum

For the third sum the argument is mostly analogous. There are a few changes needed for the argument. First, one has to distinguish between the two cases of whether or not the two distinguished vertices $\{1,2\}$ are in the same connected component (cluster) of the graph or not. One computes

$$\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p^2}\Gamma_{\pi,G}^2 = \Sigma_{\text{different}}+\Sigma_{\text{same}}, \tag{3.3.8}$$

where

$$\begin{aligned}
\Sigma_{\text{different}} &= \sum_{k=0}^\infty\frac{1}{k!}\sum_{n_*,n_{**}\ge0}\sum_{n_1,\ldots,n_k\ge2}\frac{1}{\prod_\ell n_\ell!}\chi_{(\sum n_\ell=p)}\sum_{\substack{G_1\in\mathcal{C}_{n_1},\ldots,G_k\in\mathcal{C}_{n_k}\\ G_*\in\mathcal{C}_{n_*+\{1\}}\\ G_{**}\in\mathcal{C}_{n_{**}+\{2\}}}}\\
&\quad\times\int\!\!\cdots\!\!\int\prod_\ell\prod_{e\in G_\ell}g_e\rho_{\mathrm{t}}^{(n_*+\{1\},n_{**}+\{2\},n_1,\ldots,n_k)}\,\mathrm{d}x_3\ldots\mathrm{d}x_{p+2},\\
\Sigma_{\text{same}} &= \sum_{k=0}^\infty\frac{1}{k!}\sum_{n_*\ge1}\sum_{n_1,\ldots,n_k\ge2}\frac{1}{\prod_\ell n_\ell!}\chi_{(\sum n_\ell=p)}\sum_{\substack{G_1\in\mathcal{C}_{n_1},\ldots,G_k\in\mathcal{C}_{n_k}\\ G_*\in\mathcal{C}_{n_*+\{1,2\}}\\ (1,2)\notin G_*}}\\
&\quad\times\int\!\!\cdots\!\!\int\prod_\ell\prod_{e\in G_\ell}g_e\rho_{\mathrm{t}}^{(n_*+\{1,2\},n_1,\ldots,n_k)}\,\mathrm{d}x_3\ldots\mathrm{d}x_{p+2}.
\end{aligned}\tag{3.3.9}$$

Here $\sum_\ell$ and $\prod_\ell$ are over $\ell \in \{*, **, 1, \ldots, k\}$ or $\ell \in \{*, 1, \ldots, k\}$, whichever is appropriate. With a slight abuse of notation we write $n_* + \{1\}$ for the set of vertices in the cluster containing the external vertex $\{1\}$ (similarly for $n_{**} + \{2\}, n_* + \{1,2\}$). This set has exactly n_* internal vertices. For $p = 0$ one has to interpret the empty product of integrals as a factor 1.

The first part is the contribution where $\{1\}$ and $\{2\}$ are in distinct clusters (labelled $*$ and $**$), the second part is the contribution from where they are in the same (labelled $*$). Note that in the second contribution we have $n_* \geq 1$. Indeed, $\{1\}$ and $\{2\}$ are connected, but not by an edge. Hence they must be connected by a path of length ≥ 2, which necessarily goes through at least one vertex $\{j\}, j \neq 1, 2$.

We treat the two cases separately. In the case where the two distinguished vertices are in different clusters we may readily apply both the tree-graph bound and the bound on the truncated correlation Equation (3.3.7). The latter reads

$$\left|\rho_{\mathrm{t}}^{(n_*+\{1\}, n_{**}+\{2\}, n_1, \ldots, n_k)}\right| \\ \leq \rho^{(\sum_{\ell\in\{*,**,1,\ldots,k\}} n_\ell + 2) - (k+2-1)} \sum_{\tau \in \mathcal{A}^{(n_*+\{1\}, n_{**}+\{2\}, n_1, \ldots, n_k)}} \prod_{(i,j)\in\tau} \left|\gamma_N^{(1)}(x_i; x_j)\right|.$$

The integration procedure is slightly modified compared to that of Section 3.3.1.2. In the anchored tree there is a path between (the cluster containing) $\{1\}$ and (the cluster containing) $\{2\}$. For the edge incident to (the cluster containing) $\{1\}$ on this path, we bound $|\gamma_N^{(1)}| \leq \rho$. This cuts the anchored tree into two anchored trees τ_1, τ_2 such that (with a slight abuse of notation) $1 \in \tau_1$ and $2 \in \tau_2$. We may follow the integration procedure exactly as for the Γ^1-sum for each of the anchored trees τ_1 and τ_2. Recall the bound

$$\#\mathcal{A}^{(n_*+\{1\}, n_{**}+\{2\}, n_1, \ldots, n_k)} \leq (k+2)! 4^{\sum_{\ell\in\{*,**,1,\ldots,k\}} n_\ell + 2} \leq C(k^2+1) k! 4^{\sum_{\ell\in\{*,**,1,\ldots,k\}} n_\ell}.$$

We thus get for the contribution of all terms where the two distinguished vertices are in different clusters (assuming that $sa^3\rho\log(b/a)(\log N)^3$ is sufficiently small)

$$\begin{aligned} |\Sigma_{\text{different}}| &\leq C\rho^2 \left(\sum_{n_*=0}^{\infty} \left[Ca^3\rho\log(b/a) \right]^{n_*} \right)^2 \\ &\quad \times \left(\sum_{k=0}^{\infty} (k^2+1) \left[Cs(\log N)^3 \right]^k \left[\sum_{n=2}^{\infty} (Ca^3\rho\log(b/a))^{n-1} \right]^k \right) \\ &\leq C\rho^2 < \infty. \end{aligned} \tag{3.3.10}$$

Now we consider the case where $\{1\}$ and $\{2\}$ are in the same distinguished cluster. Here we may readily apply the bound in Equation (3.3.7) on the truncated correlation but we need to be a bit careful in applying the tree-graph bound. Indeed, then the sum over graphs in the cluster containing the two vertices is not $\sum_{G_*\in\mathcal{C}_{n_*+2}}$, but instead $\sum_{G_*\in\mathcal{C}_{n_*+2}, (1,2)\notin G_*}$, since in the construction, no g-edges are allowed between $\{1\}$ and $\{2\}$. To still apply the tree-graph bound, we define

$$\tilde{g}_e := \begin{cases} g_e & e \neq (1,2) \\ 0 & e = (1,2). \end{cases}$$

Then $-1 \leq \tilde{g}_e \leq 0$ so we can apply the tree-graph bound with these edge-weights to get

$$\left| \sum_{G_*\in\mathcal{C}_{n_*+2}, (1,2)\notin G_*} \prod_{e\in G_*} g_e \right| = \left| \sum_{G_*\in\mathcal{C}_{n_*+2}} \prod_{e\in G_*} \tilde{g}_e \right| \leq \sum_{T_*\in\mathcal{T}_{n_*+2}} \prod_{e\in T_*} |\tilde{g}_e| = \sum_{T_*\in\mathcal{T}_{n_*+2}, (1,2)\notin T_*} \prod_{e\in T_*} |g_e|.$$

We again have to modify the integrations slightly. The integrations over all clusters apart from the distinguished one may be computed as for the Γ- and Γ^1-sums. For the distinguished cluster with $\{1\}$ and $\{2\}$ there is some path of g-edges connecting them. Pick the unique edge on this path incident with $\{1\}$ and bound $|g| \leq 1$ for this factor. This splits the tree T_* into two trees T_*^1 and T_*^2 with $1 \in T_*^1$ and $2 \in T_*^2$. We may compute the integrations over all the variables with index in the distinguished cluster exactly as for the Γ^1-sum for each tree T_*^1 and T_*^2 separately. One gets for the contribution (assuming that $sa^3\rho\log(b/a)(\log N)^3$ is sufficiently small)

$$\begin{aligned} |\Sigma_{\mathsf{same}}| &\leq C\rho^2 \left(\sum_{n_*=1}^{\infty}\left[Ca^3\rho\log(b/a)\right]^{n_*}\right) \\ &\quad\times\left(\sum_{k=0}^{\infty}(k+1)\left[Cs(\log N)^3\right]^k\left[\sum_{n=2}^{\infty}(Ca^3\rho\log(b/a))^{n-1}\right]^k\right) \\ &\leq Ca^3\rho^3\log(b/a) < \infty. \end{aligned} \tag{3.3.11}$$

We conclude that

$$\sum_{p\geq 0}\frac{1}{p!}\left|\sum_{(\pi,G)\in\mathcal{L}_p^2}\Gamma^2_{\pi,G}\right| \leq C\rho^2 < \infty,$$

uniformly in x_1, x_2 for sufficiently small $sa^3\rho\log(b/a)(\log N)^3$.

3.3.1.4 Absolute convergence of the Γ^3-sum

The argument for the last sum is completely analogous to the argument for the Γ^2-sum. We have to distinguish between different cases of the clusters containing the external vertices $\{1,2,3\}$. Either there is one cluster containing all of them, one cluster containing two of them and one cluster containing the last vertex, or they are all in distinct clusters. One then deals with the different cases exactly as we did for the Γ^2-sum. We skip the details. This concludes the proof of Lemma 3.3.2. □

3.4 Energy of the trial state

In this section we bound the energy of the trial state ψ_N defined in Equation (3.2.1). Recall Equation (3.2.2). By Theorem 3.3.4 we have (for $sa^3\rho\log(b/a)(\log N)^3$ sufficiently small)

$$\rho^{(2)}_{\mathsf{Jas}}(x_1,x_2) = f(x_1-x_2)^2\left(\rho^{(2)}(x_1,x_2) + \sum_{p=1}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p^2}\Gamma^2_{\pi,G}\right).$$

We can expand $\rho^{(2)}$ in $x_1 - x_2$ using Lemma 3.2.14. The second term is an error term we have to control. Additionally, also the three-body term is an error we have to control. We claim that

Lemma 3.4.1. *There exist constants $c, C > 0$ such that if $sa^3\rho\log(b/a)(\log N)^3 < c$ and $N = \#P_F > C$, then*

$$\begin{aligned}
&\left|\sum_{p=1}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p^2}\Gamma_{\pi,G}^2\right| \\
&\quad\leq Ca^6\rho^4(\log(b/a))^2\Big[s^3a^6\rho^2(\log b/a)^2(\log N)^9+1\Big] \\
&\qquad+Ca^3\rho^{3+2/3}|x_1-x_2|^2\Big[s^5a^{12}\rho^4(\log(b/a))^5(\log N)^{16}+b^2\rho^{2/3}+\log(b/a)\Big].
\end{aligned}$$

Lemma 3.4.2. *There exists a constant $c > 0$ such that if $sa^3\rho\log(b/a)(\log N)^3 < c$, then*

$$\rho^{(3)}_{\mathsf{Jas}} = f_{12}^2f_{13}^2f_{23}^2\left[\rho^{(3)} + O\left(a^3\rho^4\log(b/a)\left[s^3a^6\rho^2(\log(b/a))^2(\log N)^9+1\right]\right)\right]$$

where the error is uniform in x_1, x_2, x_3.

We give the proof of these lemmas in Sections 3.4.2 and 3.4.3 below. For the three-body term, we additionally have the bound $\rho^{(3)} \leq C\rho^{3+4/3}|x_1-x_2|^2|x_2-x_3|^2$ by Lemma 3.2.15. Combining now Lemmas 3.2.13, 3.2.14, 3.4.1 and 3.4.2, Theorem 3.3.4 and Equation (3.2.2) we thus get (for $sa^3\rho\log(b/a)(\log N)^3$ sufficiently small and N sufficiently large)

$$\begin{aligned}
&\langle\psi_N|H_N|\psi_N\rangle \\
&\quad= \frac{3}{5}(6\pi)^{2/3}\rho^{2/3}N\left(1+O(N^{-1/3})+O(s^{-2})\right) + L^3\int \mathrm{d}x\left(|\nabla f(x)|^2+\frac{1}{2}v(x)f(x)^2\right) \\
&\qquad\times\Bigg[\frac{(6\pi^2)^{2/3}}{5}\rho^{8/3}|x|^2\Bigg(1-\frac{3(6\pi^2)^{2/3}}{35}\rho^{2/3}|x|^2 \\
&\qquad\qquad+O(N^{-1/3})+O(s^{-2})+O(N^{-1/3}\rho^{2/3}|x|^2)+O(\rho^{4/3}|x|^4)\Bigg) \\
&\qquad\quad+O\left(a^6\rho^4(\log(b/a))^2\Big[s^3a^6\rho^2(\log b/a)^2(\log N)^9+1\Big]\right) \\
&\qquad\quad+O\left(a^3\rho^{3+2/3}|x|^2\Big[s^5a^{12}\rho^4(\log(b/a))^5(\log N)^{16}+b^2\rho^{2/3}+\log(b/a)\Big]\right)\Bigg] \\
&\quad+\iiint \mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3 f_{12}\nabla f_{12}f_{23}\nabla f_{23}f_{13}^2\Big[O(\rho^{3+4/3}|x_1-x_2|^2|x_2-x_3|^2) \\
&\qquad+O\left(a^3\rho^4\log(b/a)\left[s^3a^6\rho^2(\log(b/a))^2(\log N)^9+1\right]\right)\Big].
\end{aligned} \tag{3.4.1}$$

We will choose N (really L, see Remark 3.2.8) some large negative power of $a^3\rho$, so errors with $N^{-1/3}$ are subleading. We may compute

$$\begin{aligned}
&\int \mathrm{d}x\left(|\nabla f(x)|^2+\frac{1}{2}v(x)f(x)^2\right)|x|^2 \\
&\quad= \frac{1}{(1-a^3/b^3)^2}\int_{|x|\leq b}\mathrm{d}x\left(|\nabla f_0(x)|^2+\frac{1}{2}v(x)f_0(x)^2\right)|x|^2 \\
&\quad\leq 12\pi a^3\left(1+O(a^3/b^3)\right),
\end{aligned} \tag{3.4.2}$$

by Definition 3.1.1 since $f = \frac{1}{1-a^3/b^3}f_0$ for $|x| \leq b$ and $b > R_0$, the range of v. For the higher moments we recall that $|\nabla f_0| \leq |\nabla f_{\mathsf{hc}}| = \frac{3a^3}{|x|^4}$ for $|x| \geq a$ by Lemma 3.2.2. Then we have

(for $n = 4, 6$)

$$\begin{aligned}
&\int \mathrm{d}x \left(|\nabla f(x)|^2 + \frac{1}{2} v(x) f(x)^2 \right) |x|^n \\
&= \frac{1}{(1-a^3/b^3)^2} \int_{|x|\le b} \mathrm{d}x \left(|\nabla f_0(x)|^2 + \frac{1}{2} v(x) f_0(x)^2 \right) |x|^n \\
&\le \frac{1}{2} R_0^{n-2} \int v |f_0|^2 |x|^2 \,\mathrm{d}x + \int_{|x|\ge a} \left(\frac{3a^3}{|x|^4} \right)^2 |x|^n \,\mathrm{d}x + a^{n-2} \int_{|x|\le a} |\nabla f_0|^2 |x|^2 \,\mathrm{d}x \\
&\lesssim C R_0^{n-2} a^3.
\end{aligned} \tag{3.4.3}$$

For $n = 4$ we have more precisely

$$\begin{aligned}
&\int \mathrm{d}x \left(|\nabla f(x)|^2 + \frac{1}{2} v(x) f(x)^2 \right) |x|^4 \\
&\le \int \mathrm{d}x \left(|\nabla f_0(x)|^2 + \frac{1}{2} v(x) f_0(x)^2 \right) |x|^4 \left(1 + O(a^3 b^{-3}) \right) \\
&= 36\pi a^3 a_0^2 + O(a^6 a_0^2 b^{-3}).
\end{aligned}$$

For the lower moment, we have by Equation (3.2.4)

$$\begin{aligned}
\int \mathrm{d}x \left(|\nabla f(x)|^2 + \frac{1}{2} v(x) f(x)^2 \right) &= 4\pi \int_0^b \left(|\partial_r f|^2 r^2 + r^2 f \partial_r^2 f + 4 r f \partial_r f \right) \mathrm{d}r \\
&= \frac{12\pi a^3/b^2}{1 - a^3/b^3} + 8\pi \int_0^b r f \partial_r f \,\mathrm{d}r
\end{aligned} \tag{3.4.4}$$

where ∂_r denotes the radial derivative, and we integrated by parts using that $f(r) = \frac{1-a^3/r^3}{1-a^3/b^3}$ outside the support of v. By Lemma 3.2.2 we have

$$2 \int_0^b r f \partial_r f \,\mathrm{d}r = b - \int_0^b f^2 \,\mathrm{d}r \le b - \frac{1}{(1-a^3/b^3)^2} \int_a^b \left(1 - \frac{a^3}{r^3} \right)^2 \mathrm{d}r \le Ca. \tag{3.4.5}$$

Hence

$$\int \mathrm{d}x \left(|\nabla f(x)|^2 + \frac{1}{2} v(x) f(x)^2 \right) \le Ca.$$

This concludes the bounds on all the terms in Equation (3.4.1) arising from the 2-body term. To bound those arising from the 3-body term we bound $f_{13} \le 1$. By the translation invariance one integration gives a volume factor L^3. The remaining two integrals then both give the same contribution. That is,

$$\begin{aligned}
&\iiint \mathrm{d}x_1 \,\mathrm{d}x_2 \,\mathrm{d}x_3 f_{12} \nabla f_{12} f_{23} \nabla f_{23} f_{13}^2 \Big[O(\rho^{3+4/3} |x_1 - x_2|^2 |x_2 - x_3|^2) \\
&\qquad + O\left(a^3 \rho^4 \log(b/a) \left[s^3 a^6 \rho^2 (\log(b/a))^2 (\log N)^9 + 1 \right] \right) \Big] \\
&\le C N \rho^{2+4/3} \left(\int |x|^2 f \partial_r f \,\mathrm{d}x \right)^2 \\
&\qquad + C N a^3 \rho^3 \log(b/a) \left[s^3 a^6 \rho^2 (\log(b/a))^2 (\log N)^9 + 1 \right] \left(\int f \partial_r f \,\mathrm{d}x \right)^2 .
\end{aligned}$$

Using integration by parts and Lemma 3.2.2, we have that

$$\begin{aligned}\frac{1}{4\pi}\int |x|^n f\partial_r f \, \mathrm{d}x &= \int_0^b r^{n+2} f\partial_r f \, \mathrm{d}r = \frac{b^{n+2}}{2} - \frac{n+2}{2}\int_0^b r^{n+1} f^2 \, \mathrm{d}r \\ &\leq \frac{b^{n+2}}{2} - \frac{n+2}{2}\int_a^b r^{n+1}\left(\frac{1-a^3/r^3}{1-a^3/b^3}\right)^2 \mathrm{d}r \leq \begin{cases} Ca^2 & n=0, \\ Ca^3 b & n=2. \end{cases}\end{aligned} \tag{3.4.6}$$

Plugging all this into Equation (3.4.1) we thus get for the energy density

$$\begin{aligned}\frac{\langle \psi_N | H_N | \psi_N \rangle}{L^3} &= \frac{3}{5}(6\pi)^{2/3}\rho^{5/3} + \frac{12\pi}{5}(6\pi^2)^{2/3} a^3 \rho^{8/3} - \frac{108\pi(6\pi^2)^{4/3}}{175} a^3 a_0^2 \rho^{10/3} \\ &\quad + O\left(s^{-2}\rho^{5/3}\right) + O\left(N^{-1/3}\rho^{5/3}\right) \\ &\quad + O\left(a^6 b^{-3}\rho^{8/3}\right) + O\left(a^6 a_0^2 b^{-3}\rho^{10/3}\right) + O\left(R_0^4 a^3 \rho^4\right) \\ &\quad + O\left(a^7\rho^4(\log(b/a))^2\Big[s^3 a^6\rho^2(\log b/a)^2(\log N)^9 + 1\Big]\right) \\ &\quad + O\left(a^6\rho^{3+2/3}\Big[s^5 a^{12}\rho^4(\log(b/a))^5(\log N)^{16} + b^2\rho^{2/3} + \log(b/a)\Big]\right) \\ &\quad + O\left(a^6 b^2 \rho^{3+4/3}\right) + O\left(a^7\rho^4 \log(b/a)\left[s^3 a^6 \rho^2(\log(b/a))^3(\log N)^9 + 1\right]\right).\end{aligned} \tag{3.4.7}$$

We choose $L \sim a(a^3\rho)^{-10}$ still ensuring that $\frac{Lk_F}{2\pi}$ is rational. (More precisely one chooses $L \sim a(k_F a)^{-30}$, since ρ is defined in terms of L.) Then $N \sim (a^3\rho)^{-29}$. Choose moreover

$$b = a(a^3\rho)^{-\beta}, \qquad s \sim (a^3\rho)^{-\alpha}|\log(a^3\rho)|^{-\delta}.$$

Note that we need

$$\frac{2}{9} < \beta < \frac{1}{2}, \qquad \frac{5}{6} < \alpha < \frac{13}{15}$$

for the error terms to be smaller than the desired accuracy of order $a^3 a_0^2 \rho^{10/3}$. We get

$$\begin{aligned}\frac{\langle \psi_N | H_N | \psi_N \rangle}{L^3} &= \frac{3}{5}(6\pi)^{2/3}\rho^{5/3} + \frac{12\pi}{5}(6\pi^2)^{2/3} a^3 \rho^{8/3} - \frac{108\pi(6\pi^2)^{4/3}}{175} a^3 a_0^2 \rho^{10/3} \\ &\quad + O(\rho^{5/3}(a^3\rho)^{\gamma_1}|\log(a^3\rho)|^{\gamma_2}).\end{aligned}$$

where

$$\gamma_1 = \min\left\{2\alpha, 1+3\beta, \frac{13}{3} - 3\alpha, 6 - 5\alpha, \frac{8}{3} - 2\beta\right\},$$

and γ_2 is given by the power of the logarithmic factors of the largest error term. Optimising in α, β, δ we see that for the choice

$$\beta = \frac{1}{3}, \qquad \alpha = \frac{6}{7}, \qquad \delta = 3$$

we have $\gamma_1 = \frac{12}{7}$ and $\gamma_2 = 6$, i.e.

$$\begin{aligned}&\frac{\langle \psi_N | H_N | \psi_N \rangle}{L^3} \\ &= \frac{3}{5}(6\pi)^{2/3}\rho^{5/3} \\ &\quad + \frac{12\pi}{5}(6\pi^2)^{2/3} a^3 \rho^{8/3}\left[1 - \frac{9}{35}(6\pi^2)^{2/3} a_0^2 \rho^{2/3} + O((a^3\rho)^{2/3+1/21}|\log(a^3\rho)|^6)\right]\end{aligned} \tag{3.4.8}$$

for $a^3\rho$ small enough. Note that for this choice of s, N we have $s \sim N^{6/203}(\log N)^3$. Thus any Q with $N^{4/3} \ll Q \leq CN^C$ satisfies the condition $Q^{-1/4} \leq Cs^{-1}$ of Definition 3.2.7.

3.4.1 Thermodynamic limit via a box method

In this section we construct a trial state in the thermodynamic limit using a box method of gluing trial states for finite n together. Such a method has been used for many studies of dilute Bose and Fermi gases, see for instance [BCS21; FGJMO24; LSS05; YY09]. First we show that we may choose periodic boundary conditions in the small boxes instead of using Dirichlet boundary conditions. The setting and argument is due to Robinson [Rob71, Lemmas 2.1.12 and 2.1.13]. We present a slightly modified version in [MS20, Section C].

Lemma 3.4.3 ([MS20; Rob71])**.** *Let $0 < d < L/2$ be a cut-off, let*

$$H^D_{N,L+2d} = \sum_{j=1}^{N} -\Delta^D_{j,L+2d} + \sum_{i<j} v(x_i - x_j)$$

denote the N-particle Hamiltonian with Dirichlet boundary conditions on a box of sides $L+2d$, and let

$$H^{\text{per}}_{N,L} = \sum_{j=1}^{N} -\Delta^{\text{per}}_{j,L} + \sum_{i<j} v_{\text{per}}(x_i - x_j)$$

denote the N-particle Hamiltonian with periodic boundary conditions on a box of sides L, with the interaction $v_{\text{per}}(x) = \sum_{n\in\mathbb{Z}^3} v(x+nL)$, the periodized interaction.

Then, there exists an isometry $V : L^2_a(\Lambda_L^N) \to L^2_a(\Lambda^N_{L+2d})$ such that for all ψ in the form-domain of $H^{\text{per}}_{N,L}$ we have $V\psi$ in the form-domain of $H^D_{N,L+2d}$ and

$$\left\langle V\psi \middle| H^D_{N,L+2d} \middle| V\psi \right\rangle \le \left\langle \psi \middle| H^{\text{per}}_{N,L} \middle| \psi \right\rangle + \frac{6N}{d^2} \|\psi\|^2$$

Proof. This is a trivial modification of [MS20, Lemma 4], noting that the explicitly constructed V respects the anti-symmetry. □

We now glue together trial states. For any (sufficiently small) density ρ we have above found that we may construct a (normalized) trial state ψ_n on the torus $\Lambda_\ell = [-\ell/2, \ell/2]^3$ satisfying Equation (3.4.8) with $\ell \sim a(a^3\rho)^{-10}$, i.e. $n \sim (a^3\rho)^{-29}$. We now use the isometry V from Lemma 3.4.3 to find a trial state $V\psi_n$ with Dirichlet boundary conditions on $\Lambda_{\ell+2d}$. Our trial state Ψ_N for $N = M^3 n$ is then obtained by gluing together M^3 copies of $V\psi_n$ arranged in boxes, with a distance b between them, so that there is no interaction between the boxes. We choose the same b as before. More precisely, for configurations where the first n particles are in box 1 and so on,

$$\Psi_N(x_1, \ldots, x_N) = \prod_{j=1}^{M^3} V\psi_n(x_{n(j-1)+1} - \tau_j, \ldots, x_{nj} - \tau_j),$$

where $\tau_j \in \mathbb{R}^3$ denotes the centre of box number j. The state Ψ_N is then the antisymmetrization of this. Its energy is

$$\left\langle \Psi_N \middle| H^D_{N,M(\ell+2d+b)} \middle| \Psi_N \right\rangle = M^3 \left\langle V\psi_n \middle| H^D_{n,\ell+2d} \middle| V\psi_N \right\rangle \le M^3 \left(\left\langle \psi_n \middle| H^{\text{per}}_{n,\ell} \middle| \psi_n \right\rangle + \frac{6n}{d^2} \right).$$

The particle density of the state Ψ_N is $\tilde\rho = \frac{n}{(\ell+2d+b)^3} = \rho(1 + O(d/\ell) + O(b/\ell))$. The energy density is

$$\begin{aligned} e(\tilde\rho) &\le \liminf_{M\to\infty} \frac{\left\langle \Psi_N \middle| H^D_{N,M(\ell+2d+b)} \middle| \Psi_N \right\rangle}{M^3(\ell+2d+b)^3} = \frac{\left\langle V\psi_n \middle| H^D_{n,\ell+2d} \middle| V\psi_N \right\rangle}{(\ell+2d+b)^3} \\ &\le \frac{\left\langle \psi_n \middle| H^{\text{per}}_{n,\ell} \middle| \psi_n \right\rangle}{\ell^3} \left[1 + O(d/\ell) + O(b/\ell)\right] + O(\rho d^{-2}). \end{aligned} \tag{3.4.9}$$

Choosing $d = a(a^3\rho)^{-5}$ and using Equation (3.4.8) we conclude that for $a^3\rho$ sufficiently small

$$\begin{aligned} e(\tilde\rho) &\le \frac{3}{5}(6\pi)^{2/3}\rho^{5/3} \\ &\quad + \frac{12\pi}{5}(6\pi^2)^{2/3}a^3\rho^{8/3}\left[1 - \frac{9}{35}(6\pi^2)^{2/3}a_0^2\rho^{2/3} + O\left((a^3\rho)^{2/3+1/21}|\log(a^3\rho)|^6\right)\right] \\ &= \frac{3}{5}(6\pi)^{2/3}\tilde\rho^{5/3} \\ &\quad + \frac{12\pi}{5}(6\pi^2)^{2/3}a^3\tilde\rho^{8/3}\left[1 - \frac{9}{35}(6\pi^2)^{2/3}a_0^2\tilde\rho^{2/3} + O\left((a^3\tilde\rho)^{2/3+1/21}|\log(a^3\tilde\rho)|^6\right)\right] \end{aligned}$$

since $\tilde\rho = \rho(1 + O((a^3\rho)^5))$, so $\rho = \tilde\rho(1 + O((a^3\tilde\rho)^5))$. This concludes the proof of Theorem 3.1.3.

It remains to give the proofs of Lemmas 3.4.1 and 3.4.2.

3.4.2 Subleading 2-particle diagrams (proof of Lemma 3.4.1)

In this section we give the proof of Lemma 3.4.1. Before doing this, we first discuss why we don't just use the bounds of these terms from the proof of Lemma 3.3.2.

Remark 3.4.4 (Why not use bounds of Lemma 3.3.2?)**.** Inspecting the proof of Lemma 3.3.2 (more precisely Equations (3.3.10) and (3.3.11) of Section 3.3.1.3) we can extract the following bound

$$\left|\sum_{p=1}^\infty \frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p^2}\Gamma_{\pi,G}^2\right| \le Csa^3\rho^3\log(b/a)(\log N)^3.$$

This is immediate by considering the bounds Equations (3.3.10) and (3.3.11) and noting that since we have $p \ge 1$ in the sum $\sum_{p=1}^\infty \frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p^2}\Gamma_{\pi,G}^2$, the summands either have $k \ge 1$ or $n_* \ge 1$ or $n_{**} \ge 1$. Using this bound we would thus get for the error in the ground state energy density the bound $\sim sa^4\rho^3$ (ignoring the $\log$-factors). However, as we saw in Section 3.4, using Lemma 3.2.13, the s-dependent error of the kinetic energy density is $\sim s^{-2}\rho^{5/3}$. There is no way to choose s, such that both of these errors are smaller that $a^3\rho^{8/3}$, which is the precision we need in order to prove the leading correction to the kinetic energy in Theorem 3.1.3.

Similarly, by following the proof of Lemma 3.3.2 one could get the bound

$$\rho^{(3)}_{\mathrm{Jas}} \le C\rho^3 f_{12}^2 f_{13}^2 f_{23}^2.$$

This bound is not problematic in terms of getting all the error terms in the energy density smaller than $a^3\rho^{8/3}$. However, we improve on this bound in Lemma 3.4.2 in order to get a better error bound in Theorem 3.1.3.

Proof of Lemma 3.4.1. Note first that by translation invariance

$$\sum_{p=1}^\infty \frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p^2}\Gamma_{\pi,G}^2$$

is a function of $x_1 - x_2$ only. Recall Equations (3.3.8) and (3.3.9). We split the diagrams in $\mathcal{L}_p^2$ into three groups. To define these three groups we first define for any diagram $(\pi, G) \in \mathcal{L}_p^2$

the number $k = k(\pi, G)$ as the number of clusters entirely containing internal vertices. (This k is exactly the same k as in the proof of Lemma 3.3.2.) Then we define

$$\nu = \nu(\pi, G) = \textstyle\sum_{\ell=1}^{k} n_\ell - 2k, \qquad \nu^* = \nu^*(\pi, G) = n_* + n_{**},$$

with the understanding that $n_{**} = 0$ if $\{1\}$ and $\{2\}$ are in the same cluster. We think of $\nu + \nu^*$ as the "number of added vertices". Indeed, given a k the smallest number of vertices in a diagram $(\pi, G) \in \mathcal{L}_p^2$ with k clusters is $2k + 2$ and in this case we have $p = 2k$. For such a diagram, there are $p = 2k$ internal vertices and 2 external vertices. The graph G of such a diagram looks like

$$G = \quad \overset{*}{\underset{1}{\bullet}} \qquad \left.\begin{array}{c} \bullet\text{-----}\bullet \\ \vdots \\ \bullet\text{-----}\bullet \end{array}\right\} k \quad \overset{*}{\underset{2}{\bullet}} \; .$$

Then $\nu + \nu^*$ is the number of (internal) vertices a diagram has more than this lowest number.

By following the bound in Equations (3.3.10) and (3.3.11) we see that for $p = \nu_0 + 2k_0$

$$\left| \frac{1}{p!} \sum_{\substack{(\pi,G)\in\mathcal{L}_p^2 \\ \nu(\pi,G)+\nu^*(\pi,G)=\nu_0 \\ k(\pi,G)=k_0}} \Gamma_{\pi,G}^2 \right| \leq C\rho^2 (Cs(\log N)^3)^{k_0} (Ca^3\rho\log(b/a))^{k_0+\nu_0}. \tag{3.4.10}$$

We split diagrams into different groups depending on whether or not they are "large" and whether or not we will do a Taylor expansion of their values. We first give some motivation for what "large" means.

Remark 3.4.5. Here "large" and "small" should be interpreted in the sense of how many vertices appear in the diagram. Equation (3.4.10) describe how diagrams with more vertices (larger values of k, ν, ν^*) have a smaller value. More precisely, "large" should be thought of in terms of the bound in Equation (3.4.10) in the following sense.

Recall that the (s-dependent) error in the kinetic energy density is $s^{-2}\rho^{5/3}$. For this error to be smaller than the desired accuracy of order $a^3a_0^2\rho^{10/3}$ we need $s \gg (a^3\rho)^{-5/6}$. If we think of, say $s \sim (a^3\rho)^{-6/7}$, then (ignoring $\log$-factors) Equation (3.4.10) reads $\lesssim \rho^2(a^3\rho)^{k_0/7+\nu_0}$. The large diagrams (with $\nu^* \geq 1$) are those for which this bound gives a contribution to the energy density $\ll a^5\rho^{10/3}$, i.e. with $\nu + \nu^* + k/7 \geq 4/3$ by counting powers of ρ. For diagrams with $\nu^* = 0$ we obtain a differentiated version of the bound in Equation (3.4.10), where one effectively gains a power $a^2\rho^{2/3}$, see the details of the proof. The large diagrams (with $\nu^* = 0$) are those for which the differentiated version gives a contribution to the energy density $\ll a^5\rho^{10/3}$, i.e. with $\nu + k/7 \geq 2/3$.

We split the diagrams into three (exhaustive) groups:

1. Small diagrams with
   - (A) $\{1\}$ and $\{2\}$ in different clusters and $1 \leq k \leq 4, \nu = 0, \nu^* = 0$,
   - (B) $\{1\}$ and $\{2\}$ in different clusters and $0 \leq k \leq 2, \nu = 0, \nu^* = 1$,
   - (C) $\{1\}$ and $\{2\}$ in the same cluster and $0 \leq k \leq 2, \nu = 0, \nu^* = 1$.
2. Large diagrams with $\nu^* = 0$ (in particular $\{1\}$ and $\{2\}$ are in different clusters) and

(A) $k \geq 5, \nu = 0$ or

(B) $k \geq 1, \nu \geq 1$.

3. Large diagrams with $\nu^* \geq 1$ and

(A) $k \geq 3, \nu = 0$ or

(B) $\nu + \nu^* \geq 2$.

Note that we have $p \geq 1$, so the diagrams with $k = 0, \nu = 0, \nu^* = 0$ are not present. Moreover, if $k = 0$ then clearly also $\nu = 0$. For drawings of the small diagrams see Figure 3.A.1 in Section 3.A.1. We then write

$$\sum_{p=1}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p^2} \Gamma_{\pi,G}^2 = \xi_{\textsf{small},0} + \xi_{\textsf{small},\geq 1} + \xi_0 + \xi_{\geq 1}, \tag{3.4.11}$$

where $\xi_{\textsf{small},0}$ is the contribution of all small diagrams of types (A) and (B), $\xi_{\textsf{small},\geq 1}$ is the contribution of all small diagrams of type (C), ξ_0 is the contribution of all large diagrams with $\nu^* = 0$, and $\xi_{\geq 1}$ is the contribution of all large diagrams with $\nu^* \geq 1$.

The notation is motivated by that of the large diagrams, which were split into two groups depending on whether $\nu^* = 0$ or $\nu^* \geq 1$. We will treat the small diagrams of types (A) and (B) somewhat similar to the large diagrams in ξ_0 (hence the notation $\xi_{\textsf{small},0}$) and the small diagrams of type (C) somewhat similar to the large diagrams in $\xi_{\geq 1}$ (hence the notation $\xi_{\textsf{small},\geq 1}$). Indeed, we will do a Taylor expansion of $\xi_{\textsf{small},0}$ and ξ_0 but not of $\xi_{\textsf{small},\geq 1}$ or $\xi_{\geq 1}$.

Using the bound in Equation (3.4.10) and the absolute convergence (Lemma 3.3.2) we get

$$\begin{aligned} |\xi_{\geq 1}(x_1,x_2)| &\leq \underbrace{C\rho^2(s(\log N)^3)^3(a^3\rho\log(b/a))^4}_{\text{type } (A) \text{ diagrams}} + \underbrace{C\rho^2(a^3\rho\log(b/a))^2}_{\text{type } (B) \text{ diagrams}} \\ &\leq Ca^6\rho^4(\log(b/a))^2\left[s^3(\log N)^9 a^6\rho^2(\log(b/a))^2 + 1\right] \end{aligned} \tag{3.4.12}$$

uniformly in x_1, x_2. For $\xi_{\textsf{small},\geq 1}$ we have

Lemma 3.4.6. *For the small diagrams of type (C) we have the bound*

$$|\xi_{\textsf{small},\geq 1}| \leq Ca^3b^2\rho^{3+4/3}|x_1 - x_2|^2 + Ca^6\rho^4(\log(b/a))^2.$$

The proof of this lemma is a (not very insightful) computation. We give it in Section 3.A.1. Slightly more insightful however, is why we split off the small diagrams from the large diagrams.

Remark 3.4.7 (Why one gets better bounds by computing small diagrams)**.** We could treat all the small diagrams exactly as we treat ξ_0 and $\xi_{\geq 1}$. We do however gain better error bounds by treating them more directly, i.e. computing more precisely what the values of these small diagrams are. In exact calculations we can make use the fact that $\int \gamma_N^{(1)} = 1$, instead of bounding the absolute value as $\int |\gamma_N^{(1)}| \leq Cs(\log N)^3$.

We Taylor expand $\xi_{\textsf{small},0}$ and ξ_0 to second order around the diagonal. We first claim that

$$\xi_{\textsf{small},0}(x_2,x_2) + \xi_0(x_2,x_2) + \xi_{\textsf{small},\geq 1}(x_2,x_2) + \xi_{\geq 1}(x_2,x_2) = 0 \tag{3.4.13}$$

Indeed by Theorem 3.3.4 we have

$$\begin{aligned}\xi_{\mathsf{small},0} + \xi_0 + \xi_{\mathsf{small},\geq 1} + \xi_{\geq 1} &= \frac{\rho^{(2)}_{\mathsf{Jas}}}{f_{12}^2} - \rho^{(2)} \\ &= \frac{N(N-1)}{C_N} \int\!\!\cdots\!\!\int \prod_{\substack{i<j \\ (i,j)\neq(1,2)}} f_{ij}^2 D_N \, \mathrm{d}x_3 \ldots \mathrm{d}x_N - \rho^{(2)}.\end{aligned}$$

(Formally to do the division by f in the first equality in case $f = 0$ somewhere one uses Theorem 3.3.4 with all instances of f replaced by $\tilde{f}^{(n)}$ for some sequence $\tilde{f}^{(n)} > 0$ with $\tilde{f}^{(n)} \searrow f$. Then one readily applies the Lebesgue dominated convergence theorem to exchange the limit $\tilde{f}^{(n)} \to f$ with the relevant sums and integrals.) Taking $x_1 = x_2$ in this we have $D_N = 0$ and $\rho^{(2)} = 0$. This shows Equation (3.4.13). We may thus bound the zeroth order term of $\xi_{\mathsf{small},0}$ and ξ_0 by

$$\begin{aligned}&|\xi_{\mathsf{small},0}(x_2,x_2) + \xi_0(x_2,x_2)| \\ &\quad\leq |\xi_{\mathsf{small},\geq 1}(x_2,x_2)| + |\xi_{\geq 1}(x_2,x_2)| \\ &\quad\leq Ca^6\rho^4(\log(b/a))^2\left[s^3(\log N)^9 a^6\rho^2(\log(b/a))^2 + 1\right].\end{aligned} \tag{3.4.14}$$

Since both $\xi_{\mathsf{small},0}$ and ξ_0 are symmetric in x_1 and x_2 all first order terms vanish. We are left with bounding the second derivatives. For $\xi_{\mathsf{small},0}$ we have

Lemma 3.4.8. *For any $\mu, \nu = 1,2,3$ we have*

$$\left|\partial^\mu_{x_1}\partial^\nu_{x_1}\xi_{\mathsf{small},0}\right| \leq Ca^3\rho^{3+2/3}\log(b/a)$$

uniformly in x_1, x_2. Here $\partial^\mu_{x_1}$ denotes the derivative in the x_1^μ-direction.

The proof of this lemma is a (not very insightful) computation. We give it in Section 3.A.1.

Next we consider $\partial^\mu_{x_1}\partial^\nu_{x_1}\xi_0$. We write ξ_0 in terms of truncated densities as in Equation (3.3.9), i.e.

$$\begin{aligned}\xi_0 = \sum_{k=0}^\infty \frac{1}{k!} \sum_{n_1,\ldots,n_k\geq 2} \chi_{(k\geq 5, n_\ell = 2 \text{ or } k\geq 1, \sum n_\ell = 2k+1)} \frac{1}{\prod_\ell n_\ell!} \sum_{\substack{G_1,\ldots,G_k \\ G_\ell\in\mathcal{C}_{n_\ell}}} \\ \times \int\!\!\cdots\!\!\int \prod_\ell \prod_{e\in G_\ell} g_e \rho_{\mathsf{t}}^{(\{1\},\{2\},n_1,\ldots,n_k)} \, \mathrm{d}x_3 \ldots \mathrm{d}x_{p+2}.\end{aligned}$$

Since we consider terms with $n_* = n_{**} = 0$, there are no g-factors that depend on x_1 and thus all derivatives are of $\rho_{\mathsf{t}}^{(\{1\},\{2\},n_1,\ldots,n_k)}$. We thus need to calculate $\partial^\mu_{x_1}\partial^\nu_{x_1}\rho_{\mathsf{t}}^{(\{1\},\{2\},n_1,\ldots,n_k)}$. For this we use the definition in Equation (3.3.4) rather than the formula in Equation (3.3.6). In Equation (3.3.4) the variable x_1 appears exactly twice: Once in an outgoing $\gamma_N^{(1)}$-edge from $\{1\}$ and once in an incoming $\gamma_N^{(1)}$-edge to $\{1\}$. Taking the derivatives then amounts to replacing either one of these edges by its second derivative or both of them by their first derivatives. Thus, using that $\gamma_N^{(1)}(x_i;x_j) = \gamma_N^{(1)}(x_j;x_i)$ since $\gamma_N^{(1)}$ is real, and that for $(\pi, \cup G_\ell)$

to be linked necessarily $\pi(1) \neq 1$, we have (for $p = 2 + \sum_\ell n_\ell$)

$$
\begin{aligned}
&\partial_{x_1}^\mu \partial_{x_1}^\nu \rho_{\mathrm{t}}^{(\{1\},\{2\},n_1,\ldots,n_k)} \\
&\quad = \partial_{x_1}^\mu \partial_{x_1}^\nu \sum_{\pi \in \mathcal{S}_p} (-1)^\pi \chi_{((\pi,\cup G_\ell)\in\mathcal{L}_p)} \prod_{j=1}^p \gamma_N^{(1)}(x_j; x_{\pi(j)}) \\
&\quad = \sum_{\pi \in \mathcal{S}_p} (-1)^\pi \chi_{((\pi,\cup G_\ell)\in\mathcal{L}_p)} \prod_{j\neq 1, j\neq \pi^{-1}(1)} \gamma_N^{(1)}(x_j; x_{\pi(j)}) \Big[2\partial_{x_1}^\mu \partial_{x_1}^\nu \gamma_N^{(1)}(x_1; x_{\pi(1)}) \gamma_N^{(1)}(x_{\pi^{-1}(1)}; x_1) \\
&\qquad + 2\partial_{x_1}^\mu \gamma_N^{(1)}(x_1; x_{\pi(1)}) \partial_{x_1}^\nu \gamma_N^{(1)}(x_{\pi^{-1}(1)}; x_1) \Big] .
\end{aligned}
\tag{3.4.15}
$$

With this formula we may then redo the computation of [GMR21, Equation (D.53)] only now some of the $\gamma_N^{(1)}$-factors (precisely 1 or 2 of them) carry derivatives. The $\gamma_N^{(1)}$-factors with derivatives may end up in the anchored tree, or they may end up in the matrix $\mathcal{N}(r)$. If they end up in $\mathcal{N}(r)$ it is explained around [GMR21, Equation (D.9)] how to modify Lemma 3.3.10. One simply includes factors ik^μ in the definition of (some of) the functions α_i (and not of β_j) in the proof of Lemma 3.3.10. Since we may bound $|k| \leq C\rho^{1/3}$ for $k \in P_F$ we get

$$
\left|\det \tilde{\mathcal{N}}(r)\right| \leq \begin{cases} \rho^{\sum n_\ell + 2 - (k+2-1)} & \text{if no derivatives end up in } \mathcal{N}, \\ C\rho^{\sum n_\ell + 2 - (k+2-1) + 1/3} & \text{if one derivative ends up in } \mathcal{N}, \\ C\rho^{\sum n_\ell + 2 - (k+2-1) + 2/3} & \text{if two derivatives end up in } \mathcal{N}, \end{cases}
\tag{3.4.16}
$$

where $\tilde{\mathcal{N}}(r)$ is the appropriate modification of $\mathcal{N}(r)$. To get the formula for ρ_{t} we need also to consider two cases for how the anchored tree looks. There could be both an incoming and an outgoing edge to/from the vertex $\{1\}$. And if there is just one edge to/from $\{1\}$ it could be either an incoming or an outgoing edge. Since $\gamma_N^{(1)}$ is real, incoming and outgoing edges gives the same factor $\gamma_N^{(1)}(x_1; x_j)$. A simple calculation (essentially just undoing the product rule) then shows that

$$
\begin{aligned}
&\partial_{x_1}^\mu \partial_{x_1}^\nu \rho_{\mathrm{t}}^{(\{1\},\{2\},n_1,\ldots,n_k)} \\
&\quad = \sum_{\partial \in \{1, \partial_{x_1}^\mu, \partial_{x_1}^\nu, \partial_{x_1}^\mu \partial_{x_1}^\nu\}} \Bigg[\sum_{\substack{\tau \in \mathcal{A}^{(\{1\},\{2\},n_1,\ldots,n_k)} \\ \text{two edges to/from } \{1\}}} \partial \left[\gamma_N^{(1)}(x_{j_2}, x_1) \gamma_N^{(1)}(x_1; x_{j_1}) \right] \\
&\qquad + \sum_{\substack{\tau \in \mathcal{A}^{(\{1\},\{2\},n_1,\ldots,n_k)} \\ \text{one edge to/from } \{1\}}} \partial \gamma_N^{(1)}(x_1; x_{j_1}) \Bigg] \prod_{\substack{(i,j)\in\tau \\ i,j\neq 1}} \gamma_N^{(1)}(x_i; x_j) \int \mathrm{d}\mu_\tau(r) \det \tilde{\mathcal{N}}_\partial(r),
\end{aligned}
\tag{3.4.17}
$$

where j_1 and j_2 denote the vertices connected to $\{1\}$ by the relevant edges in τ and $\tilde{\mathcal{N}}_\partial$ is the appropriately modified version of $\mathcal{N}$, where the derivatives not in ∂ end up in $\mathcal{N}$, i.e. Equation (3.4.16) reads

$$
\left|\det \tilde{\mathcal{N}}_\partial(r)\right| \leq C\rho^{\sum n_\ell + 2 - (k+2-1) + (2-\#\partial)/3},
$$

where $\#\partial$ denotes the number of derivatives in ∂, i.e. $\#1 = 0, \#\partial_{x_1}^\mu = 1$ and $\#\partial_{x_1}^\mu \partial_{x_1}^\nu = 2$.

We denote the contribution of the two terms in Equation (3.4.17) to $\partial_{x_1}^\mu \partial_{x_1}^\nu \xi_0$ by $(\partial_{x_1}^\mu \partial_{x_1}^\nu \xi_0)^{\to\bullet\to}$ and $(\partial_{x_1}^\mu \partial_{x_1}^\nu \xi_0)^{\bullet\to}$ respectively.

We first deal with the second term of Equation (3.4.17) where there is just one edge to/from $\{1\}$ in the anchored tree. We may bound the contribution of this term almost exactly as in the proof of Lemma 3.3.2. We give a sketch here. Using Equation (3.4.16) we get the bound

$$\begin{aligned} &\leq C \sum_{\partial \in \{1, \partial_{x_1}^\mu, \partial_{x_1}^\nu, \partial_{x_1}^\mu \partial_{x_1}^\nu\}} \rho^{(2-\#\partial)/3} \sum_{\tau \in \mathcal{A}^{(\{1\},\{2\},n_1,\ldots,n_k)}} \left| \partial \gamma_N^{(1)}(x_1; x_{j_1}) \right| \\ &\quad \times \prod_{\substack{(i,j)\in\tau \\ i,j\neq 1}} \left| \gamma_N^{(1)}(x_i; x_j) \right| \rho^{(\sum_\ell n_\ell + 2) - (k+2-1)}, \end{aligned} \tag{3.4.18}$$

where again $\#\partial$ denotes the number of derivatives in ∂.

To bound the integrations we again follow the strategy of the proof of the Γ^2-sum of Lemma 3.3.2, Section 3.3.1.3. The only difference is that the $\gamma_N^{(1)}$-edge on the path in the anchored tree between $\{1\}$ and $\{2\}$ incident to $\{1\}$ is the edge with derivatives, $\partial\gamma_N^{(1)}(x_1; x_{j_1})$. This we bound by $|\partial\gamma_N^{(1)}| \leq C\rho^{1+\#\partial/3}$. The integrations can then be performed exactly as in Section 3.3.1.3. We conclude the bound

$$\begin{aligned} &\int \!\!\cdots\!\! \int \prod_{\ell=1}^k \prod_{e\in T_\ell} |g_e| \left|\partial\gamma_N^{(1)}(x_1;x_{j_1})\right| \prod_{\substack{(i,j)\in\tau \\ i,j\neq 1}} \left|\gamma_N^{(1)}(x_i;x_j)\right| \,\mathrm{d}x_3 \ldots \mathrm{d}x_{\sum n_\ell + 2} \\ &\quad \leq \rho^{1+\#\partial/3} \left(Ca^3\log(b/a)\right)^{\sum n_\ell - k} \left(Cs(\log N)^3\right)^k. \end{aligned}$$

Again, as in the proof of Lemma 3.3.2 we have by Cayley's formula that $\#\mathcal{T}_n = n^{n-2} \leq C^n n!$ and by [GMR21, Appendix D.5] that $\#\mathcal{A}^{(\{1\},\{2\},n_1,\ldots,n_k)} \leq (k+2)! 4^{\sum n_\ell + 2} \leq C(k^2+1)k! 4^{\sum n_\ell}$. Following the same arguments as for Equation (3.4.10) and recalling that the diagrams in ξ_0 have either $k \geq 5$ or $\nu \geq 1$ we get the contribution to $\partial_{x_1}^\mu \partial_{x_1}^\nu \xi_0$ of

$$\begin{aligned} \left| (\partial_{x_1}^\mu \partial_{x_1}^\nu \xi_0)^{\bullet\to} \right| &\leq C\rho^{2+2/3} \Big[\underbrace{(s(\log N)^3)^5 (a^3\rho\log(b/a))^5}_{\text{type } (A) \text{ diagrams}} + \underbrace{s(\log N)^3 (a^3\rho\log(b/a))^2}_{\text{type } (B) \text{ diagrams}} \Big] \\ &\leq Ca^6\rho^{4+2/3}(\log(b/a))^2 s(\log N)^3 \left[s^4(\log N)^{12} a^9 \rho^3 (\log(b/a))^3 + 1 \right] \end{aligned} \tag{3.4.19}$$

uniformly in x_1, x_2.

Next consider the first term of Equation (3.4.17). The argument is almost the same, only we have to distinguish between which $\gamma_N^{(1)}$-factor(s) the derivatives in ∂ hits. We consider the case $\partial = \partial_{x_1}^\mu \partial_{x_1}^\nu$. The other cases are similar. Suppose that the $\gamma_N^{(1)}$-edge on the path (in the anchored tree) from $\{1\}$ to $\{2\}$ is $\gamma_N^{(1)}(x_1; x_{j_1})$ and the $\gamma_N^{(1)}$-factor not on the path is $\gamma_N^{(1)}(x_{j_2}; x_1)$. We distinguish between three cases:

1. If both derivatives are on $\gamma_N^{(1)}(x_1; x_{j_1})$ we may bound this exactly as above.
2. If one derivative is on $\gamma_N^{(1)}(x_1; x_{j_1})$ (say $\partial_{x_1}^\nu$) and one derivative (say $\partial_{x_1}^\mu$) is on $\gamma_N^{(1)}(x_{j_2}; x_1)$ we bound $|\partial_{x_1}^\nu \gamma_N^{(1)}(x_1; x_{j_1})| \leq C\rho^{4/3}$. Then the argument is similar, only now one of the $\gamma_N^{(1)}$-integrations is with $\partial^\mu \gamma_N^{(1)}$ instead. Thus, in the computation leading to Equation (3.4.19) we should replace one factor $Cs\rho^{1/3}(\log N)^3$ with $\int |\partial^\mu \gamma_N^{(1)}| \,\mathrm{d}x$.
3. If both derivatives are on $\gamma_N^{(1)}(x_{j_2}; x_1)$ then analogously we bound $|\gamma_N^{(1)}(x_1; x_{j_1})| \leq C\rho$ and in the computation leading to Equation (3.4.19) we should replace one factor $Cs\rho^{2/3}(\log N)^3$ with $\int |\partial^\mu \partial^\nu \gamma_N^{(1)}| \,\mathrm{d}x$.

In total we have the contribution to $\partial_{x_1}^\mu \partial_{x_1}^\nu \xi_0$ of

$$\leq C\rho^2 \left(\rho^{2/3} s(\log N)^3 + \rho^{1/3}\int_\Lambda \left|\partial^\mu \gamma_N^{(1)}\right| \,\mathrm{d}x + \rho^{1/3}\int_\Lambda \left|\partial^\nu \gamma_N^{(1)}\right| \,\mathrm{d}x + \int_\Lambda \left|\partial^\mu\partial^\nu \gamma_N^{(1)}\right| \,\mathrm{d}x\right) \times \left[(s(\log N)^3)^4 (a^3\rho\log(b/a))^5 + (a^3\rho\log(b/a))^2\right]$$

uniformly in x_1, x_2. One may do a similar computation for the other cases of ∂ and conclude that

$$\begin{aligned}&\left|(\partial_{x_1}^\mu \partial_{x_1}^\nu \xi_0)^{\rightarrow\bullet\rightarrow}\right| \\ &\quad\leq C\rho^2 \left(\rho^{2/3} s(\log N)^3 + \rho^{1/3}\int_\Lambda \left|\partial^\mu \gamma_N^{(1)}\right| \,\mathrm{d}x + \rho^{1/3}\int_\Lambda \left|\partial^\nu \gamma_N^{(1)}\right| \,\mathrm{d}x + \int_\Lambda \left|\partial^\mu\partial^\nu \gamma_N^{(1)}\right| \,\mathrm{d}x\right) \\ &\qquad\times \left[(s(\log N)^3)^4 (a^3\rho\log(b/a))^5 + (a^3\rho\log(b/a))^2\right]\end{aligned} \tag{3.4.20}$$

uniformly in x_1, x_2. Thus, we need to bound the integrals

$$\int_\Lambda \left|\partial^\mu \gamma_N^{(1)}\right| \,\mathrm{d}x = \int_\Lambda \frac{1}{L^3}\left|\sum_{k\in P_F} k^\mu e^{ikx}\right| \,\mathrm{d}x = \frac{1}{(2\pi)^2 L}\int_{[0,2\pi]^3} \left|\sum_{q\in\left(\frac{Lk_F}{2\pi}P\right)\cap\mathbb{Z}^3} q^\mu e^{iqu}\right| \,\mathrm{d}u,$$

and

$$\int_\Lambda \left|\partial^\mu\partial^\nu \gamma_N^{(1)}\right| \,\mathrm{d}x = \int_\Lambda \frac{1}{L^3}\left|\sum_{k\in P_F} k^\mu k^\nu e^{ikx}\right| \,\mathrm{d}x = \frac{1}{2\pi L^2}\int_{[0,2\pi]^3} \left|\sum_{q\in\left(\frac{Lk_F}{2\pi}P\right)\cap\mathbb{Z}^3} q^\mu q^\nu e^{iqu}\right| \,\mathrm{d}u.$$

Here we have

Lemma 3.4.9. *The polyhedron P from Definition 3.2.7 satisfies for any $\mu,\nu = 1,2,3$ that*

$$\int_{[0,2\pi]^3} \left|\sum_{q\in\left(\frac{Lk_F}{2\pi}P\right)\cap\mathbb{Z}^3} q^\mu e^{iqu}\right| \,\mathrm{d}u \leq CsN^{1/3}(\log N)^3,$$

$$\int_{[0,2\pi]^3} \left|\sum_{q\in\left(\frac{Lk_F}{2\pi}P\right)\cap\mathbb{Z}^3} q^\mu q^\nu e^{iqu}\right| \,\mathrm{d}u \leq CsN^{2/3}(\log N)^4$$

for sufficiently large N.

The proof of Lemma 3.4.9 is a long and technical computation, which we give in Section 3.B. Applying the lemma we conclude that

$$\int_\Lambda \left|\partial^\mu \gamma_N^{(1)}\right| \,\mathrm{d}x \leq Cs\rho^{1/3}(\log N)^3, \qquad \int_\Lambda \left|\partial^\mu\partial^\nu \gamma_N^{(1)}\right| \,\mathrm{d}x \leq Cs\rho^{2/3}(\log N)^4.$$

By combining this with Equations (3.4.19) and (3.4.20) we get

$$\left|\partial_{x_1}^\mu \partial_{x_1}^\nu \xi_0\right| \leq Ca^6\rho^{4+2/3}(\log(b/a))^2 s(\log N)^4\left[s^4(\log N)^{12}a^9\rho^3(\log(b/a))^3 + 1\right] \tag{3.4.21}$$

uniformly in x_1, x_2. Combining Lemmas 3.4.6 and 3.4.8 and Equations (3.4.12), (3.4.14) and (3.4.21) and using that for any real number $t > 0$ and integer $n \geq 1$ we may bound $t \lesssim t^n + 1$ this shows the desired. □

Remark 3.4.10 (Treating more diagrams as small)**.** One can improve the error bound in Theorem 3.1.3 slightly by treating more diagrams as small, i.e. calculating their values more precisely. This is similar to what is done in [BCGOPS23] for the dilute Bose gas. (In [BCGOPS23] the Bose gas is treated with a method very similar to a cluster expansion. Their expansion is performed to some arbitrarily high order [denoted by M in [BCGOPS23]], which if chosen sufficiently large yields the bounds of [BCGOPS23].) We sketch the overall idea.

If we choose $s \sim (a^3\rho)^{-1+\varepsilon/2}$ then the error from the s-dependent term in the kinetic energy to the energy density is $\rho^{5/3}(a^3\rho)^{2-\varepsilon}$. Then choose as "large" the diagrams for which the bound in Equation (3.4.10) gives contributions to the energy density much smaller than $\rho^{5/3}(a^3\rho)^{2-\varepsilon}$. This happens for $k_0 > K$ for some large $K \sim \varepsilon^{-1}$. We can then evaluate all small diagrams as in Section 3.A and conclude that their contributions are as given in Section 3.A only with some K-dependent constants, since there is some K-dependent number of small diagrams. In total we would then get an error of size $O_\varepsilon(\rho^{5/3}(a^3\rho)^{2-\varepsilon})$ in Theorem 3.1.3.

3.4.3 Subleading 3-particle diagrams (proof of Lemma 3.4.2)

Proof of Lemma 3.4.2. Recall the formula for $\rho^{(3)}_{\text{Jas}}$ of Theorem 3.3.4. In this formula there are terms like $\rho\sum_{p\geq 1}\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p^2}\Gamma^2_{\pi,G}(x_2,x_3)$. We have

$$\rho = \rho^{(1)}_{\text{Jas}}(x_1) = \sum_{p'\geq 1}\frac{1}{p'!}\sum_{(\pi',G')\in\mathcal{L}^1_{p'}}\Gamma^1_{\pi',G'}(x_1)$$

by translation invariance. Joining the two diagrams $(\pi,G)\in\mathcal{L}_p^2$ and $(\pi',G')\in\mathcal{L}^1_{p'}$ we get a new (no longer linked) diagram $(\pi'',G'')\in\mathcal{D}^3_{p+p'}$ with two linked components, one of which contains the vertices $\{2\}$ and $\{3\}$ and one of which contains the vertex $\{1\}$. Doing this for all three terms of this type, we are led to define the set

$$\tilde{\mathcal{L}}_p^3 := \mathcal{L}_p^3 \cup \bigcup_{q+q'=p}(\mathcal{L}_q^2\oplus\mathcal{L}^1_{q'}),$$

where $\oplus$ refers to the operation of joining two diagrams as above. The set $\tilde{\mathcal{L}}_p^3$ is then the set of diagrams on 3 external and p internal vertices such that there is at most two linked components, and that each linked component contains at least one external vertex. With this, the formula for $\rho^{(3)}_{\text{Jas}}$ of Theorem 3.3.4 reads (assuming that $sa^3\rho\log(b/a)(\log N)^3$ is sufficiently small)

$$\rho^{(3)}_{\text{Jas}} = f_{12}^2f_{13}^2f_{23}^2\left[\rho^{(3)} + \sum_{p\geq 1}\frac{1}{p!}\sum_{(\pi,G)\in\tilde{\mathcal{L}}_p^3}\Gamma^3_{\pi,G}\right].$$

We split the diagrams in $\tilde{\mathcal{L}}_p^3$ into two groups, large and small similarly to the proof of Lemma 3.4.1. To do this, we similarly define for a diagram $(\pi,G)\in\tilde{\mathcal{L}}_p^3$ the number $k=k(\pi,G)$ as the number of clusters entirely containing internal vertices. (This k is exactly the same k as in the proof of Lemma 3.3.2.) Then we define

$$\nu = \nu(\pi,G) = \textstyle\sum_{\ell=1}^k n_\ell - 2k, \qquad \nu^* = \nu^*(\pi,G) = n_* + n_{**} + n_{***},$$

where we understand $n_{**}=0$ and/or $n_{***}=0$ if $\{1,2,3\}$ are not all in different clusters. (One defines n_{***} as the number of internal vertices in the cluster containing $\{3\}$ if all $\{1,2,3\}$ are in different clusters, exactly as for the n_{**} and n_* of Sections 3.3.1.2 and 3.3.1.3.) We may still think of $\nu + \nu^*$ as the "number of added vertices". As for Equation (3.4.10) we have (for $p = 2k_0 + \nu_0$)

$$\left| \frac{1}{p!} \sum_{\substack{(\pi,G)\in\tilde{\mathcal{L}}_p^3 \\ \nu(\pi,G)+\nu^*(\pi,G)=\nu_0 \\ k(\pi,G)=k_0}} \Gamma_{\pi,G}^3 \right| \leq C\rho^3 (Cs(\log N)^3)^{k_0} (Ca^3\rho\log(b/a))^{k_0+\nu_0}. \tag{3.4.22}$$

The main difference compared to Equation (3.4.10) is that we here allow diagrams that are not linked. This doesn't matter, since when we compute the integrals (as in Section 3.3.1.3) we anyway have to cut the diagram up into 3 parts (either by bounding g-edges or $\gamma_N^{(1)}$-edges) as described in Section 3.3.1.3. We split the diagrams into two (exhaustive) groups:

1. Small diagrams with $1 \leq k \leq 2, \nu = 0, \nu^* = 0$, and
2. Large diagrams as the rest, i.e. with
   (A) $k \geq 3$, or
   (B) $\nu + \nu^* \geq 1$.

As in Section 3.4.2, the splitting is motivated by counting powers in Equation (3.4.22). Note that for $p \geq 1$ the diagrams with $k = 0, \nu = 0, \nu^* = 0$ are not present. We write

$$\sum_{p\geq 1} \frac{1}{p!} \sum_{(\pi,G)\in\tilde{\mathcal{L}}_p^3} \Gamma_{\pi,G}^3 = \xi_{\text{small}}^3 + \xi_{\text{large}}^3,$$

where ξ_{small}^3 and ξ_{large}^3 are the contributions of small and large diagrams respectively. Exactly as in Equation (3.4.12) we may bound, using Equation (3.4.22)

$$\begin{aligned} |\xi_{\text{large}}^3| &\leq \underbrace{C\rho^3(s(\log N)^3)^3(a^3\rho\log(b/a))^3}_{\text{type } (A) \text{ diagrams}} + \underbrace{C\rho^3 a^3\rho\log(b/a)}_{\text{type } (B) \text{ diagrams}} \\ &\leq Ca^3\rho^4\log(b/a)\left[s^3a^6\rho^2(\log(b/a))^2(\log N)^9 + 1\right]. \end{aligned}$$

For the small diagrams we have

Lemma 3.4.11. *We have*

$$|\xi_{\text{small}}^3| \leq Ca^3\rho^4\log(b/a)$$

uniformly in x_1, x_2, x_3.

As with Lemma 3.4.8, the proof is simply a computation, which we give in Section 3.A.2. We conclude the desired. □

3.5 One and two dimensions

In this section we sketch the necessary changes one needs to make for the argument to apply in dimensions $d = 1$ and $d = 2$. We will abuse notation slightly and denote by the same symbols as in Sections 3.2, 3.3 and 3.4 the relevant 1- and 2-dimensional analogues.

3.5.1 Two dimensions

Similarly to the 3-dimensional setting, the p-wave scattering function f_0 in 2 dimensions is radial and solves the equation

$$-\partial_r^2 f_0 - \frac{3}{r}\partial_r f_0 + \frac{1}{2} v f_0 = 0, \tag{3.5.1}$$

see Section 3.2.1 and recall Definition 3.1.9. Thus, it is the same as the s-wave scattering function in 4 dimensions. In particular it satisfies the bound

Lemma 3.5.1 ([LY01, Lemma A.1], Lemma 3.2.2)**.** *The scattering function satisfies*

$$\left[1 - \frac{a^2}{|x|^2}\right]_+ \leq f_0(x) \leq 1$$

for all x and $|\nabla f_0(x)| \leq \frac{2a^2}{|x|^3}$ for $|x| > a$.

As for the 3-dimensional setting we consider the trial state

$$\psi_N(x_1, \ldots, x_N) = \frac{1}{\sqrt{C_N}} \prod_{i<j} f(x_i - x_j) D_N(x_1, \ldots, x_N),$$

where f is a rescaled scattering function

$$f(x) = \begin{cases} \frac{1}{1-a^2/b^2} f_0(|x|) & |x| \leq b, \\ 1 & |x| \geq b \end{cases}$$

and

$$D_N(x_1, \ldots, x_N) = \det[u_k(x_i)]_{\substack{1 \leq i \leq N, \\ k \in P_F}}, \qquad u_k(x) = \frac{1}{L} e^{ikx}, \qquad N = \# P_F.$$

Here P_F denotes the "Fermi polygon", the 2-dimensional analogue of the "Fermi polyhedron" P_F. It is defined as follows. (Compare to Definition 3.2.7.)

Definition 3.5.2. The polygon P is defined as follows.

- First pick Q, satisfying

  $$Q^{-1/2} \leq C s^{-2}, \qquad N^{3/2} \ll Q \leq C N^C$$

  in the limit $N \to \infty$. (The exponents arise as $\frac{-1}{2} = \frac{-1}{2(d-1)}$, $-2 = \frac{-2}{d-1}$ and $\frac{3}{2} = \frac{d+1}{d}$ for $d = 2$.)

- Pick two distinct primes $Q_1, Q_2 \sim Q$.

- Place s *evenly distributed* points $\kappa_1^{\mathbb{R}}, \ldots, \kappa_s^{\mathbb{R}}$ on the circle of radius $Q^{-1/2}$ such that the points are invariant under the symmetries $(k^1, k^2) \mapsto (\pm k^a, \pm k^b)$ for $\{a, b\} = \{1, 2\}$. (Here the exponent arises as $\frac{-1}{2} = \frac{1}{2(d-1)} - 1$ for $d = 2$.)

  Evenly distributed means that the distance between any pair of points is $d \gtrsim s^{-1} Q^{-1/2}$ and that for any k on the sphere of radius $Q^{-1/2}$ the distance from k to the nearest point is $\lesssim s^{-1} Q^{-1/2}$. (On the circle we can naturally order the points. Then the condition for being *evenly distributed* reads that consecutive points are separated by a distance $\sim s^{-1} Q^{-1/2}$.)

- Find now points $\kappa_1, \ldots, \kappa_s$ of the form

$$\kappa_j = \left(\frac{p_j^1}{Q_1}, \frac{p_j^2}{Q_2}\right), \qquad p_j^\mu \in \mathbb{Z}, \quad \mu = 1,2, \quad j = 1, \ldots, s$$

  such that the points are invariant under the symmetries $(k^1, k^2) \mapsto (\pm k^1, \pm k^2)$ and such that for any $j = 1, \ldots, s$ we have $\left|\kappa_j - \kappa_j^{\mathbb{R}}\right| \lesssim Q^{-1}$.

- Define $\tilde{P}$ as the convex hull of the points $\kappa_1, \ldots, \kappa_s$ and $P = \sigma\tilde{P}$ where σ is such that $\mathrm{Vol}(P) = \pi$.

- Define the centre $z = \sigma(1/Q_1, 1/Q_2)$.

The "Fermi polygon" is the rescaled version defined as $P_F = k_F P \cap \frac{2\pi}{L}\mathbb{Z}^2$, where L is chosen large (depending on k_F) such that $\frac{k_F L}{2\pi}$ is rational and large.

Similarly as in Remark 3.2.9 we have that σ is irrational and $\sigma = Q^{1/2}(1 + O(s^{-2}))$. In particular, any point on the boundary ∂P has radial coordinate $1 + O(s^{-2})$. (The power of s here comes from the circle being locally quadratic and the distance between close points being $\sim s^{-1}$. Compare to Remark 3.2.9.) Moreover, P_F is almost symmetric under the map $(k^1, k^2) \mapsto (k^2, k^1)$ similarly to Lemma 3.2.11.

Lemma 3.5.3. *Let F_{12} be the map $(k^1, k^2) \mapsto (k^2, k^1)$. For any function $t \geq 0$ we have*

$$\sum_{k \in \frac{2\pi}{L}\mathbb{Z}^2} \left|\chi_{(k \in P_F)} - \chi_{(k \in F_{12}(P_F))}\right| t(k) \lesssim Q^{-1/2} N \sup_{|k| \sim k_F} t(k) \lesssim N^{1/4} \sup_{|k| \sim k_F} t(k),$$

where Q is as in Definition 3.5.2.

The analogue of Lemma 3.2.12 is then

Lemma 3.5.4. *The Lebesgue constant of the Fermi polygon satisfies*

$$\int_\Lambda \frac{1}{L^2} \left| \sum_{k \in P_F} e^{ikx} \right| \mathrm{d}x = \frac{1}{(2\pi)^2} \int_{[0,2\pi]^2} \left| \sum_{q \in \left(\frac{Lk_F}{2\pi} P\right) \cap \mathbb{Z}^2} e^{iqu} \right| \mathrm{d}u \leq Cs(\log N)^2.$$

We can again compute the kinetic energy of the Slater determinant analogously to Lemma 3.2.13 and its 2-particle reduced density analogously to Lemma 3.2.14.

Lemma 3.5.5. *The kinetic energy of the (Slater determinant with momenta in the) Fermi polygon satisfies*

$$\sum_{k \in P_F} |k|^2 = \sum_{k \in B_F} |k|^2 \left(1 + O(N^{-1/2}) + O(s^{-4})\right) = 2\pi\rho N \left(1 + O(N^{-1/2}) + O(s^{-4})\right).$$

Lemma 3.5.6. *The 2-particle reduced density of the (normalized) Slater determinant satisfies*

$$\rho^{(2)}(x_1, x_2) = \pi\rho^3 |x_1 - x_2|^2 \left(1 + O(N^{-1/2}) + O(s^{-4}) + O(\rho|x_1 - x_2|^2)\right).$$

The computations in Section 3.3 make no reference to the dimension and are thus also valid in dimension $d = 2$. For the absolute convergence in Section 3.3.1 and Lemma 3.3.2 one should simply replace occurrences of g and $\gamma_N^{(1)}$ with their 2-dimensional analogues. Here we have the bounds (using Lemmas 3.5.1 and 3.5.4)

$$\begin{aligned}\int_\Lambda |g| &\lesssim a^2 + \frac{1}{(1-a^2/b^2)^2}\int_a^b \left[\left(1-\frac{a^2}{b^2}\right)^2 - \left(1-\frac{a^2}{x^2}\right)^2\right] x \,\mathrm{d}x \lesssim a^2\log(b/a), \\ \int_\Lambda |\gamma_N^{(1)}| &\lesssim s(\log N)^2.\end{aligned} \tag{3.5.2}$$

Thus the absolute convergence holds as long as $sa^2\rho\log(b/a)(\log N)^2$ is sufficiently small. That is, the analogue of Theorem 3.3.4 reads

Theorem 3.5.7. *There exists a constant $c > 0$ such that if $sa^2\rho\log(b/a)(\log N)^2 < c$, then the formulas in Equation* (3.3.3) *hold (with $\rho^{(n)}_{\mathsf{Jas}}$ and $\Gamma^n_{\pi,G}$ interpreted as appropriate in the two-dimensional setting).*

The analogues of Lemmas 3.4.1 and 3.4.2 read

Lemma 3.5.8. *There exist constants $c, C > 0$ such that if $sa^2\rho\log(b/a)(\log N)^2 < c$ and $N = \#P_F > C$, then*

$$\begin{aligned}\left|\sum_{p=1}^\infty \frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p^2}\Gamma^2_{\pi,G}\right| &\leq Ca^4\rho^4(\log(b/a))^2\Big[s^3a^4\rho^2(\log b/a)^2(\log N)^6 + 1\Big] \\ &\quad + Ca^2\rho^4|x_1-x_2|^2\Big[s^5a^8\rho^4(\log(b/a))^5(\log N)^{11} + b^2\rho + \log(b/a)\Big],\end{aligned}$$

and

$$\begin{aligned}\rho^{(3)}_{\mathsf{Jas}} \leq Cf_{12}^2f_{13}^2f_{23}^2\Big[&\rho^5|x_1-x_2|^2|x_2-x_3|^2 \\ &+ a^2\rho^4\log(b/a)\left[s^3a^4\rho^2(\log(b/a))^2(\log N)^6 + 1\right]\Big].\end{aligned}$$

The proof is again similar to the 3-dimensional case replacing the bounds on $\int|g|$ and $\int|\gamma_N^{(1)}|$ as in Equation (3.5.2) above. Apart from this, there are two main changes. The first is in the proof of the analogue of Lemma 3.4.6, namely Equation (3.A.1), where one bounds $\int|x|^2|1-f^2|$. In two dimensions this bound is, using Lemma 3.5.1,

$$\begin{aligned}\int_{\mathbb{R}^2}\left(1-f(x)^2\right)|x|^2\,\mathrm{d}x &\leq Ca^4 + \frac{C}{(1-a^2/b^2)^2}\int_a^b\left[\left(1-\frac{a^2}{b^2}\right)^2 - \left(1-\frac{a^2}{r^2}\right)^2\right] r^3\,\mathrm{d}r \\ &\leq Ca^2b^2.\end{aligned}$$

The other main difference is for the analogue of Lemma 3.4.9. Here the 2-dimensional analogue reads

Lemma 3.5.9. *The polygon P from Definition 3.5.2 satisfies for any $\mu,\nu = 1,2$ that*

$$\int_{[0,2\pi]^2}\left|\sum_{q\in\left(\frac{Lk_F}{2\pi}P\right)\cap\mathbb{Z}^2} q^\mu e^{iqu}\right|\mathrm{d}u \leq CsN^{1/2}(\log N)^2,$$

$$\int_{[0,2\pi]^2}\left|\sum_{q\in\left(\frac{Lk_F}{2\pi}P\right)\cap\mathbb{Z}^2} q^\mu q^\nu e^{iqu}\right|\mathrm{d}u \leq CsN(\log N)^3$$

for sufficiently large N.

The proof is similar to that of Lemma 3.4.9 given in Section 3.B only one skips Section 3.B.2 and notes that $R = \frac{Lk_F}{2\pi} \sim N^{1/2}$.

Putting together the formulas in Theorem 3.5.7 with the bounds in Lemmas 3.5.5, 3.5.6 and 3.5.8 we easily find the analogue of Equation (3.4.1). We then need to bound a few terms. Following the type of arguments of Section 3.4, namely Equations (3.4.2), (3.4.3), (3.4.4), (3.4.5) and (3.4.6) and using Lemma 3.5.1 we get the bounds

$$\int \left(|\nabla f(x)|^2 + \frac{1}{2}v(x)f(x)^2\right)|x|^n \,\mathrm{d}x \leq \begin{cases} C, & n=0, \\ 4\pi a^2 + O(a^4 b^{-2}), & n=2, \\ Ca^4\log(b/a) + CR_0^2 a^2, & n=4, \end{cases}$$

$$\int |x|^n f \partial_r f \,\mathrm{d}x \leq \begin{cases} Ca, & n=0, \\ Ca^2 b, & n=2. \end{cases}$$

Plugging this into the analogue of Equation (3.4.1) we get the analogue of Equation (3.4.7),

$$\begin{aligned}\frac{\langle\psi_N|H_N|\psi_N\rangle}{L^2} &= 2\pi\rho^2 + 4\pi^2 a^2\rho^3 \\ &\quad + O\left(s^{-4}\rho^2\right) + O\left(N^{-1/2}\rho^2\right) \\ &\quad + O\left(a^4 b^{-2}\rho^3\right) + O\left(a^4\rho^4\log(b/a)\right) + O\left(R_0^2 a^2\rho^4\right) \\ &\quad + O\left(a^4\rho^4(\log(b/a))^2\left[s^3 a^4\rho^2(\log b/a)^2(\log N)^6 + 1\right]\right) \\ &\quad + O\left(a^4\rho^4\left[s^5 a^8\rho^4(\log(b/a))^5(\log N)^{11} + b^2\rho + \log(b/a)\right]\right) \\ &\quad + O\left(a^4 b^2\rho^5\right) + O\left(a^4\rho^4\log(b/a)\left[s^3 a^4\rho^2(\log(b/a))^3(\log N)^6 + 1\right]\right).\end{aligned} \tag{3.5.3}$$

As above, we can choose $L \sim a(a^2\rho)^{-10}$ still ensuring that $\frac{Lk_F}{2\pi}$ is rational. (More precisely one chooses $L \sim a(k_F a)^{-20}$, since ρ is defined in terms of L.) Then $N \sim (a^2\rho)^{-19}$. Choose moreover

$$b = a(a^2\rho)^{-\beta}, \qquad s \sim (a^2\rho)^{-\alpha}|\log(a^2\rho)|^{-\gamma}.$$

Optimising in α,β,γ we see that for the choice

$$\beta = \frac{1}{2}, \qquad \alpha = \frac{4}{7}, \qquad \gamma = \frac{10}{7}$$

we have

$$\frac{\langle\psi_N|H_N|\psi_N\rangle}{L^3} = 2\pi\rho^2 + 4\pi^2 a^2\rho^3\left[1 + O\left(a^2\rho|\log(a^2\rho)|^2\right)\right] \tag{3.5.4}$$

for $a^2\rho$ small enough. Note that for this choice of s, N we have $s \sim N^{4/133}(\log N)^{10/7}$. Thus any Q with $N^{3/2} \ll Q \leq CN^C$ satisfies the condition $Q^{-1/2} \leq Cs^{-2}$ of Definition 3.5.2.

The extension to the thermodynamic limit of Section 3.4.1 is readily generalized. We thus conclude the proof of Theorem 3.1.10.

3.5.2 One dimension

Similarly to the 2- and 3-dimensional settings, the p-wave scattering function f_0 in 1 dimension is even and solves the equation (here ∂^2 denotes the second derivative)

$$-\partial^2 f_0 - \frac{2}{r}\partial f_0 + \frac{1}{2}v f_0 = 0, \tag{3.5.5}$$

see Section 3.2.1 and recall Definition 3.1.11. Thus, it is the same as the s-wave scattering function in 3 dimensions. In particular it satisfies the bound

Lemma 3.5.10 ([LY01, Lemma A.1], Lemma 3.2.2)**.** *The scattering function satisfies*

$$\left[1-\frac{a}{|x|}\right]_+ \leq f_0(x) \leq 1$$

for all x and $|\partial f_0(x)| \leq \frac{a}{|x|^2}$ for $|x| > a$.

Before giving the proof of Theorem 3.1.12 we first compare our definition of the scattering length to that of [ARS22]. In [ARS22] the following definition is given.

Definition 3.5.11 ([ARS22, Section 1.3])**.** The *odd-wave scattering length* a_{odd} is given by

$$\frac{4}{R-a_{\mathsf{odd}}} = \inf\left\{\int_{-R}^{R}\left(2|\partial h|^2+v|h|^2\right)\,\mathrm{d}x : h(R)=-h(-R)=1\right\}$$

for any $R > R_0$, the range of v.

The value of a_{odd} is independent of $R > R_0$ so a_{odd} is well-defined. We claim that

Proposition 3.5.12. *The* p-wave scattering length a *defined in Definition 3.1.11 and the* odd-wave scattering length a_{odd} *defined in Definition 3.5.11 agree, i.e. $a = a_{\mathsf{odd}}$.*

Proof. Note first that $h \mapsto \mathcal{E}(h) = \int_{-R}^{R}(2|\partial h|^2 + v|h|^2)\,\mathrm{d}x$ is convex, so by replacing h by $(h(x)-h(-x))/2$ we can only lower its value. Thus, we have

$$\frac{4}{R-a_{\mathsf{odd}}} = \inf\left\{\int_{-R}^{R}\left(2|\partial h|^2+v|h|^2\right)\,\mathrm{d}x : h(x)=-h(-x),\, h(R)=1\right\}.$$

Any h we write as $h(x) = \frac{xf(x)}{R}$. Using this and integration by parts we get

$$\begin{aligned}
&\frac{4}{R-a_{\mathsf{odd}}} \\
&= \frac{1}{R^2}\inf\left\{\int_{-R}^{R}\left(2|f|^2+4xf\partial f+2|x|^2|\partial f|^2+v|f|^2|x|^2\right)\,\mathrm{d}x : f(x)=f(-x),\, f(R)=1\right\} \\
&= \frac{4}{R}+\frac{2}{R^2}\inf\left\{\int_{-R}^{R}\left(|\partial f|^2+\frac{1}{2}v|f|^2\right)|x|^2\,\mathrm{d}x : f(x)=f(-x),\, f(R)=1\right\}.
\end{aligned}$$

That is,

$$2R\left(\frac{1}{1-a_{\mathsf{odd}}/R}-1\right) = \inf\left\{\int_{-R}^{R}\left(|\partial f|^2+\frac{1}{2}v|f|^2\right)|x|^2\,\mathrm{d}x : f(x)=f(-x),\, f(R)=1\right\}.$$

Taking $R \to \infty$ in this we recover the definition of a. We conclude that $a = a_{\mathsf{odd}}$. ☐

Concerning the assumption on v that $\int\left(\frac{1}{2}vf_0^2+|\partial f_0|^2\right)\,\mathrm{d}x < \infty$ we have the following two propositions.

Proposition 3.5.13. *Suppose that $v \geq 0$ is even and compactly supported and that for some interval $[x_1,x_2]$, $0 \leq x_1 < x_2$ we have $v(x) = \infty$ for $x_1 \leq x \leq x_2$. Then $\int\left(\frac{1}{2}vf_0^2+|\partial f_0|^2\right)\,\mathrm{d}x < \infty$, where f_0 denotes the p-wave scattering function.*

Proof. Let $[x_1, x_2]$ be an interval where $v(x) = \infty$ for $x_1 \leq x \leq x_2$ and note that $f_0(x) = 0$ for all $|x| \leq x_2$. Then we have

$$\int \left(\frac{1}{2} v f_0^2 + |\partial f_0|^2\right) \mathrm{d}x \leq \frac{1}{x_2^2} \int_{|x| \geq x_2} \left(\frac{1}{2} v f_0^2 + |\partial f_0|^2\right) |x|^2 \, \mathrm{d}x = 2 a x_2^{-2} < \infty. \qquad \square$$

Proposition 3.5.14. *Suppose that $v \geq 0$ is even, compactly supported and smooth. Then $\int \left(\frac{1}{2} v f_0^2 + |\partial f_0|^2\right) \mathrm{d}x < \infty$, where f_0 denotes the p-wave scattering function.*

Proof. For smooth v also the scattering function f_0 is smooth. Recall the scattering equation (3.5.5). Then a simple calculation using integration by parts shows that

$$\begin{aligned}\int \left(\frac{1}{2} v f_0^2 + |\partial f_0|^2\right) \mathrm{d}x &= 2 \int_0^\infty \left(f_0 \partial^2 f_0 + \frac{2 f_0 \partial f_0}{x} + (\partial f_0)^2\right) \mathrm{d}x \\ &= 2 \int_0^\infty \frac{f_0(x)^2 - f_0(0)^2}{x^2} \, \mathrm{d}x.\end{aligned}$$

The function f_0 is smooth and even. Thus for small x we have $f(x) = f(0) + O(|x|^2)$, hence the integral converges around 0. By the decay of $\frac{1}{x^2}$ the integral converges at ∞. We conclude the desired. $\square$

We now give the proof of Theorem 3.1.12. We consider the trial state given in Equation (3.2.1) where f is a rescaled scattering function

$$f(x) = \begin{cases} \frac{1}{1 - a/b} f_0(|x|) & |x| \leq b, \\ 1 & |x| \geq b \end{cases}$$

and

$$D_N(x_1, \ldots, x_N) = \det[u_k(x_i)]_{\substack{1 \leq i \leq N, \\ k \in B_F}}, \qquad u_k(x) = \frac{1}{L^{1/2}} e^{ikx}, \qquad N = \# B_F.$$

In 1 dimension, there is no difference between a ball and a polyhedron, so we may use the Fermi ball $B_F = \{k \in \frac{2\pi}{L}\mathbb{Z} : |k| \leq k_F\}$ for the momenta in the Slater determinant. In this case we have (see [KL18, Lemma 3.2] or Lemma 3.B.11)

Lemma 3.5.15. *The Lebesgue constant of the Fermi ball satisfies*

$$\int_{-L/2}^{L/2} \frac{1}{L} \left| \sum_{k \in B_F} e^{ikx} \right| \mathrm{d}x = \frac{1}{2\pi} \int_0^{2\pi} \left| \sum_{q \in \left(B\left(\frac{L k_F}{2\pi}\right)\right) \cap \mathbb{Z}^2} e^{iqu} \right| \mathrm{d}u \leq C \log N.$$

As for the 2-dimensional setting one easily generalizes the computation of the kinetic energy in Lemma 3.2.13 and the calculation of the 2-particle reduced density for a Slater determinant in Lemma 3.2.14. That is,

Lemma 3.5.16. *The kinetic energy of the (Slater determinant with momenta in the) Fermi ball satisfies*

$$\sum_{k \in B_F} |k|^2 = \frac{\pi^2}{3} \rho^2 N \left(1 + O(N^{-1})\right).$$

Lemma 3.5.17. *The* 2*-particle reduced density of the (normalized) Slater determinant satisfies*

$$\rho^{(2)}(x_1,x_2) = \frac{\pi^2}{3}\rho^4|x_1-x_2|^2\left(1+O(N^{-1})+O(\rho^2|x_1-x_2|^2)\right).$$

For the Gaudin-Gillespie-Ripka-expansion we replace occurrences of g and $\gamma_N^{(1)}$ with their 1-dimensional analogues as for the 2-dimensional setting. Here we have the bounds (using Lemmas 3.5.10 and 3.5.15)

$$\int_\Lambda |g| \lesssim a\log(b/a), \qquad \int_\Lambda |\gamma_N^{(1)}| \lesssim \log N. \tag{3.5.6}$$

Then, the 1-dimensional analogue of Theorem 3.3.4 reads

Theorem 3.5.18. *There exists a constant $c>0$ such that if $a\rho\log(b/a)\log N < c$, then the formulas in Equation* (3.3.3) *hold (with $\rho_{\mathsf{Jas}}^{(n)}$ and $\Gamma_{\pi,G}^n$ interpreted as appropriate for the* 1*-dimensional setting.)*

For the analogues of Lemmas 3.4.1 and 3.4.2 we have to a bit more careful. In order to get errors smaller than the desired accuracy of the leading interaction term (of order $a\rho^4$ for the energy density) we need to also do a Taylor expansion of (some of) the 3-particle diagrams. (Pointwise we only have the bound $\left|\Gamma_{\pi,G}^3\right| \le Ca\rho^4\log(b/a)\log N$ (see Sections 3.A.2 and 3.4.3) for any subleading diagram (π,G), i.e. for $(\pi,G)\in\tilde{\mathcal{L}}_p^3$ with $p\ge 1$.)

Remark 3.5.19 (Why this was not a problem for dimensions $d=2,3$)**.** In dimensions $d=1,2,3$ the analoguous bound reads $\left|\Gamma_{\pi,G}^3\right| \le Csa^d\rho^4\log(b/a)(\log N)^d$ (if $d=1$ then there is no s) for any subleading diagram, see Equation (3.4.22). This bound should be compared to the energy density of the leading interaction term of order $a^d\rho^{2+2/d}$. Considering just the power of ρ, we see that such terms are subleading compared to the interaction term for $d\neq 1$.

Similarly the argument for Γ^2 is also slightly different compared to that of Lemma 3.4.1. We have the bounds

Lemma 3.5.20. *There exists a constant $c>0$ such that if $a\rho\log(b/a)\log N<c$, then*

$$\begin{aligned}\left|\sum_{p=1}^\infty \frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p^2}\Gamma_{\pi,G}^2\right| &\le Ca^2\rho^4\left[a\rho(\log(b/a))^3(\log N)^3 + b^4\rho^4\right] \\ &\quad + Ca\rho^5|x_1-x_2|^2\left[b^2\rho^2 + Nab^4\rho^5 + \log(b/a)\right]\end{aligned}$$

and

$$\begin{aligned}\rho_{\mathsf{Jas}}^{(3)} \le Cf_{12}^2f_{13}^2f_{23}^2\Big[&\rho^7|x_1-x_2|^2|x_2-x_3|^2 + a^2\rho^5(\log(b/a))^2(\log N)^2 \\ &+ a\rho^6\left((b^2\rho^2+\log(b/a))\right)\left[|x_1-x_2|^2+|x_1-x_3|^2+|x_2-x_3|^2\right]\Big].\end{aligned}$$

The proof is similar to that of Lemmas 3.4.1 and 3.4.2. We postpone it to the end of this section. Note here that the N-dependence is not just via logarithmic factors. Thus, we need to be more careful in choosing the size of the smaller boxes when applying the box method arguments of Section 3.4.1. With this we get the analogue of Equation (3.4.1) in 1 dimension,

$$
\begin{aligned}
&\langle \psi_N | H_N | \psi_N \rangle \\
&\quad = \frac{\pi^2}{3}\rho^2 N \left(1 + O(N^{-1})\right) + L \int \mathrm{d}x \left(|\partial f(x)|^2 + \frac{1}{2} v(x) f(x)^2 \right) \\
&\qquad \times \left[\frac{\pi^2}{3}\rho^4 |x|^2 \left(1 + O(N^{-1}) + O(\rho^2|x|^2)\right) + O\left(a\rho^5|x|^2\left[b^2\rho^2 + Nab^4\rho^5 + \log(b/a)\right]\right) \right. \\
&\qquad\quad \left. + O\left(a^2\rho^4\left[a\rho(\log b/a)^3(\log N)^3 + b^4\rho^4\right]\right) \right] \\
&\qquad + \iiint \mathrm{d}x_1 \,\mathrm{d}x_2 \,\mathrm{d}x_3 \, f_{12}\partial f_{12} f_{23} \partial f_{23} f_{13}^2 \\
&\qquad\quad \times \left[O(\rho^7 |x_1 - x_2|^2 |x_2 - x_3|^2) + O\left(a^2\rho^5 (\log(b/a))^2 (\log N)^2\right) \right. \\
&\qquad\qquad \left. + O\left(a\rho^6\left[b^2\rho^2 + \log(b/a)\right]\left[|x_1 - x_2|^2 + |x_1 - x_3|^2 + |x_2 - x_3|^2\right]\right) \right].
\end{aligned}
\tag{3.5.7}
$$

For the 2-body error terms we may follow the type of arguments of Section 3.4, namely Equations (3.4.2), (3.4.3), (3.4.4), (3.4.5) and (3.4.6) exactly as for the 2-dimensional case. By using Lemma 3.5.10 we get the bounds

$$
\int \left(|\partial f(x)|^2 + \frac{1}{2} v(x) f(x)^2 \right) |x|^n \,\mathrm{d}x \le \begin{cases} 2a, & n = 2, \\ Ca^2 b, & n = 4, \end{cases}
$$

$$
\int |x|^n f \partial f \,\mathrm{d}x \le \begin{cases} C, & n = 0, \\ Ca\log(b/a), & n = 1, \\ Cab, & n = 2. \end{cases}
$$

Define a_0 by

$$
\frac{1}{2a_0} = \int \left(|\partial f(x)|^2 + \frac{1}{2} v(x) f(x)^2 \right) \mathrm{d}x
$$

and recall by assumption on v that $a_0 > 0$, i.e. that $1/a_0 < \infty$. For the 3-body terms we may do as for the 3-dimensional case, Section 3.4. For the first term we bound $f_{13} \le 1$. By the translation invariance one integration gives a volume (i.e. length) factor L. That is,

$$
\begin{aligned}
&\iiint \mathrm{d}x_1 \,\mathrm{d}x_2 \,\mathrm{d}x_3 \left| f_{12}\partial f_{12} f_{23} \partial f_{23} f_{13}^2 \right| \\
&\quad \times \left[O(\rho^7 |x_1 - x_2|^2 |x_2 - x_3|^2) + O\left(a^2\rho^5 (\log(b/a))^2 (\log N)^2\right) \right. \\
&\qquad \left. + O\left(a\rho^6\left[b^2\rho^2 + \log(b/a)\right]\left[|x_1 - x_2|^2 + |x_1 - x_3|^2 + |x_2 - x_3|^2\right]\right) \right] \\
&\le CN\rho^6 \left(\int_0^b |x|^2 f\partial f \,\mathrm{d}x \right)^2 + CNa^2\rho^4 (\log(b/a))^2 (\log N)^2 \left(\int_0^b f\partial f \right)^2 \\
&\quad + CNa\rho^5 \left[b^2\rho^2 + \log(b/a)\right] \left[\left(\int_0^b |x|^2 f\partial f \,\mathrm{d}x \right) \left(\int_0^b f\partial f \,\mathrm{d}x \right) + \left(\int_0^b |x| f\partial f \,\mathrm{d}x \right)^2 \right]. \\
&\le CNa^2\rho^4 \left[b^2\rho^2 + (\log(b/a))^2 (\log N)^2 + b\rho\left[b^2\rho^2 + \log(b/a)\right] \right].
\end{aligned}
$$

We conclude the analogue of Equation (3.4.7) in dimension 1

$$\begin{aligned}\frac{\langle\psi_N|H_N|\psi_N\rangle}{L} = &\frac{\pi^2}{3}\rho^3 + \frac{2\pi^2}{3}a\rho^4 + O\left(N^{-1}\rho^3\right) + O\left(a^2b^{-1}\rho^4\right) + O\left(a^2b\rho^6\right) \\ &+ O\left(a^2\rho^4a_0^{-1}\left[a\rho(\log(b/a))^3(\log N)^3 + b^4\rho^4\right]\right) \\ &+ O\left(a^2\rho^5\left[b^2\rho^2 + Nab^4\rho^5 + \log(b/a)\right]\right) \\ &+ O\left(a^2\rho^5\left[b^2\rho^2 + (\log(b/a))^2(\log N)^2 + b\rho\left[b^2\rho^2 + \log(b/a)\right]\right]\right).\end{aligned} \tag{3.5.8}$$

We need to be careful how we choose N (i.e. how we choose L), since the error depends on N not just via logarithmic terms. We choose

$$N = (a\rho)^{-\alpha}, \quad \alpha > 1 \qquad b = a(a\rho)^{-\beta}, \quad 0 < \beta < 1$$

where the bounds on α, β are immediate for all the error-terms to be smaller than the desired accuracy (there is similarly also an upper limit for α, which we do not write). Keeping then only the leading error terms we get

$$\begin{aligned}\frac{\langle\psi_N|H_N|\psi_N\rangle}{L} = &\frac{\pi^2}{3}\rho^3 + \frac{2\pi^2}{3}a\rho^4 \\ &+ O\left(N^{-1}\rho^3\right) + O\left(a^2b^{-1}\rho^4\right) + O\left(a^2a_0^{-1}b^2\rho^6\right) + O\left(Na^3b^4\rho^{10}\right).\end{aligned} \tag{3.5.9}$$

Using the box method similarly as in Section 3.4.1 we also have to be careful with how we choose the parameter d. As in Equation (3.4.9) we get

$$\begin{aligned}e(\tilde\rho) &\leq \frac{\langle\psi_n|H_n|\psi_n\rangle}{\ell}\left[1 + O(d/\ell) + O(b/\ell)\right] + O\left(\rho d^{-2}\right) \\ &\leq \frac{\pi^2}{3}\rho^3 + \frac{2\pi^2}{3}a\rho^4 + O\left(n^{-1}\rho^3\right) + O\left(a^2b^{-1}\rho^4\right) + O\left(a^2a_0^{-1}b^2\rho^6\right) + O\left(na^3b^4\rho^{10}\right) \\ &\quad + O\left(d\ell^{-1}\rho^3\right) + O\left(b\ell^{-1}\rho^3\right) + O\left(\rho d^{-2}\right).\end{aligned}$$

Here we change notation from N to n and choose $d = a(a\rho)^{-\delta}$. To get the error smaller than desired, we see that we need to choose $\delta > 3/2$. In particular then the error is $O(\rho^3(a\rho)^\gamma)$, where

$$\gamma = \min\{1+\beta, 5-4\beta, 7-\alpha-4\beta, \alpha+1-\delta, 2\delta-2\}.$$

Then, also $\tilde\rho = \rho\left(1 + O((a\rho)^\gamma)\right)$ so $\rho = \tilde\rho(1 + O((a\tilde\rho)^\gamma))$. Optimising in α, β, δ we see that for

$$\alpha = \frac{33}{13}, \qquad \beta = \frac{9}{13}, \qquad \delta = \frac{24}{13} \tag{3.5.10}$$

we get $\gamma = 22/13$, i.e.

$$e(\tilde\rho) \leq \frac{\pi^2}{3}\tilde\rho^3 + \frac{2\pi^2}{3}a\tilde\rho^4\left(1 + O\left((a\tilde\rho)^{9/13}\right)\right).$$

This concludes the proof of Theorem 3.1.12.

It remains to give the

Proof of Lemma 3.5.20. Note first that, completely analogously to (3.4.10) and (3.4.22), we have

$$
\begin{aligned}
\frac{1}{p!}\left|\sum_{\substack{(\pi,G)\in\mathcal{L}_p^2\\ \nu(\pi,G)+\nu^*(\pi,G)=\nu_0\\ k(\pi,G)=k_0}}\Gamma^2_{\pi,G}\right| &\le C\rho^2(C\log N)^{k_0}(Ca\rho\log(b/a))^{k_0+\nu_0},\quad p=2k_0+\nu_0\\
\frac{1}{p!}\left|\sum_{\substack{(\pi,G)\in\tilde{\mathcal{L}}_p^3\\ \nu(\pi,G)+\nu^*(\pi,G)=\nu_0\\ k(\pi,G)=k_0}}\Gamma^3_{\pi,G}\right| &\le C\rho^3(C\log N)^{k_0}(Ca\rho\log(b/a))^{k_0+\nu_0},\quad p=2k_0+\nu_0.
\end{aligned}
\tag{3.5.11}
$$

We will use this to split the diagrams of $\mathcal{L}_p^2$ and $\tilde{\mathcal{L}}_p^3$ into groups. We split diagrams in $\mathcal{L}_p^2$ into three (exhaustive) groups:

1. Small diagrams with $1\le k+\nu+\nu^*\le 2$, $\{1\}$ and $\{2\}$ in different clusters
   - (A) and $k\ge 1$,
   - (B) and $k=0,\nu^*=1$.
2. Small diagrams with $1\le k+\nu+\nu^*\le 2$ and
   - (A) $\{1\}$ and $\{2\}$ in different clusters and $k=0,\nu^*=2$,
   - (B) $\{1\}$ and $\{2\}$ in the same cluster,
3. Large diagrams with $k+\nu+\nu^*\ge 3$.

We then split

$$\sum_{p=1}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p^2}\Gamma^2_{\pi,G}=\xi_{\mathsf{small},0}+\xi_{\mathsf{small},\ge 1}+\xi_{\ge 1},$$

where $\xi_{\mathsf{small},0}$ is the contribution of all small diagram in the first group, $\xi_{\mathsf{small},\ge 1}$ is the contribution of all small diagrams in the second group and $\xi_{\ge 1}$ is the contribution of all large diagrams. We will then do a Taylor expansion of $\xi_{\mathsf{small},0}$ but not of the other terms.

We split diagrams in $\tilde{\mathcal{L}}_p^3$ into three (exhaustive) groups:

1. Small diagrams with $k+\nu+\nu^*=1$ and $\{1\}$, $\{2\}$ and $\{3\}$ in 3 different clusters. (Then $\nu=0$.)
2. Small diagrams with $k+\nu+\nu^*=1$ and $\{1\}$, $\{2\}$ and $\{3\}$ in <3 different clusters. (Then $k=\nu=0$.)
3. Large diagrams with $k+\nu+\nu^*\ge 2$.

We then split

$$\sum_{p=1}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\tilde{\mathcal{L}}_p^3} \Gamma_{\pi,G}^3 = \xi_{\text{small},0}^3 + \xi_{\text{small},\geq 1}^3 + \xi_{\geq 1}^3,$$

where $\xi_{\text{small},0}^3$ is the contribution of all small diagram in the first group, $\xi_{\text{small},\geq 1}^3$ is the contribution of all small diagrams in the second group and $\xi_{\geq 1}^3$ is the contribution of all large diagrams. Again, we do a Taylor expansion of $\xi_{\text{small},0}^3$ but not of the other terms. For simplicity we will only compute the derivatives $\partial_{x_1}^2$. With this bound the error term for the energy density is $O(a^2 b\rho^6 \log(b/a))$ and so it is even smaller than the accuracy $a^2\rho^5$ with b chosen as in Equation (3.5.10). (By the symmetry, we could bound $\xi_{\text{small},0}$ by bounding its 6th derivative $\partial_{x_1}^2\partial_{x_2}^2\partial_{x_3}^2$ instead.) To keep the result symmetric in x_1, x_2, x_3 we will symmetrize the result afterwards.

We have immediately by Equation (3.5.11) that

$$|\xi_{\geq 1}| \leq C a^3\rho^5 (\log(b/a))^3 (\log N)^3, \qquad \left|\xi_{\geq 1}^3\right| \leq C a^2 \rho^5 (\log(b/a))^2 (\log N)^2. \tag{3.5.12}$$

Similarly as in the proof of Lemma 3.4.1 we have for $x_1 = x_2$

$$\begin{aligned} \xi_{\text{small},0}(x_2,x_2) + \xi_{\text{small},\geq 1}(x_2,x_2) + \xi_{\geq 1}(x_2,x_2) &= 0, \\ \xi_{\text{small},0}^3(x_2,x_2,x_3) + \xi_{\text{small},\geq 1}^3(x_2,x_2,x_3) + \xi_{\geq 1}^3(x_2,x_2,x_3) &= 0. \end{aligned}$$

Hence we may bound the zeroth order by

$$\begin{aligned} |\xi_{\text{small},0}(x_2,x_2)| &\leq |\xi_{\text{small},\geq 1}(x_2,x_2)| + |\xi_{\geq 1}(x_2,x_2)|, \\ \left|\xi_{\text{small},0}^3(x_2,x_2,x_3)\right| &\leq \left|\xi_{\text{small},\geq 1}^3(x_2,x_2,x_3)\right| + \left|\xi_{\geq 1}^3(x_2,x_2,x_3)\right|. \end{aligned}$$

For the diagrams in $\xi_{\text{small},0}$ and $\xi_{\text{small},0}^3$ we have similarly to Lemma 3.4.8 that

$$\left|\partial_{x_1}^2 \xi_{\text{small},0}\right| \leq C a\rho^5 \log(b/a), \qquad \left|\partial_{x_1}^2 \xi_{\text{small},0}^3\right| \leq C a \rho^6 \log(b/a) \tag{3.5.13}$$

uniformly in x_1, x_2, x_3. For the diagrams in $\xi_{\text{small},\geq 1}$ and $\xi_{\text{small},\geq 1}^3$ the analysis is somewhat similar to the proof of Lemma 3.4.6. We have

Lemma 3.5.21. *For the small diagrams in $\xi_{\text{small},\geq 1}$ and $\xi_{\text{small},\geq 1}^3$ we have the bounds*

$$|\xi_{\text{small},\geq 1}| \leq C a^2 b^4 \rho^8 + C a b^2 \rho^7 |x_1 - x_2|^2 \left[1 + N a b^2 \rho^3\right], \tag{3.5.14}$$

$$\left|\xi_{\text{small},\geq 1}^3\right| \leq C a b^2 \rho^8 \left(|x_1 - x_2|^2 + |x_1 - x_3|^2 + |x_2 - x_3|^2\right) \tag{3.5.15}$$

uniformly in x_1, x_2, x_3.

We give the proof of Lemma 3.5.21 in Section 3.A.3. Combining Lemma 3.5.21 and Equations (3.5.12) and (3.5.13) concludes the proof of Lemma 3.5.20. □

3.A Small diagrams

In this appendix we compute the contributions of all the small diagrams of Lemmas 3.4.6, 3.4.8, 3.4.11 and 3.5.21. We first consider those of Lemmas 3.4.6 and 3.4.8.

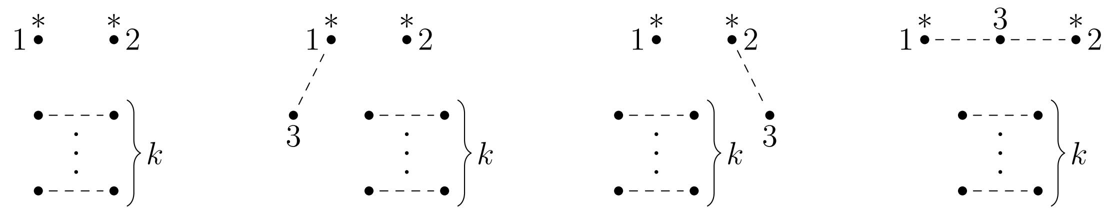
3.A.1 Small 2-particle diagrams (proof of Lemmas 3.4.6 and 3.4.8)

Recall from the proof of Lemma 3.4.1, Section 3.4.2 that

$$\xi_{\text{small},0} + \xi_{\text{small},\geq 1} = \sum_{p=1}^{\infty} \frac{1}{p!} \sum_{\substack{(\pi,G)\in\mathcal{L}_p^2 \\ (\pi,G) \text{ small}}} \Gamma^2_{\pi,G}.$$

The criterion for being small is defined in the proof of Lemma 3.4.1 around Equation (3.4.11), and will be recalled below. The diagrams are split into types $(A),(B)$ and (C) according their underlying graphs G as in the proof of Lemma 3.4.1. We further split the type (B) into two types (B_1) and (B_2). The diagrams of type (B_1) are those diagrams for which the extra vertex $\{3\}$ in the distinguished clusters is in the cluster containing $\{1\}$, i.e. connected to $\{1\}$. The diagrams of type (B_2) are those diagrams for which the extra vertex $\{3\}$ is in the cluster containing $\{2\}$, i.e. connected to $\{2\}$. That is, the different types are as follows. See also Figure 3.A.1.

- (A) $\{1\}$ and $\{2\}$ in different clusters and $1 \leq k \leq 4, \nu = 0, \nu^* = 0$,
- (B) $\{1\}$ and $\{2\}$ in different clusters and $0 \leq k \leq 2, \nu = 0, \nu^* = 1$,
  - (B_1) and $n_* = 1, n_{**} = 0$,
  - (B_2) and $n_* = 0, n_{**} = 1$,
- (C) $\{1\}$ and $\{2\}$ in the same cluster and $0 \leq k \leq 2, \nu = 0, \nu^* = 1$.



(a) Type $(A), 1 \leq k \leq 4$ (b) Type $(B_1), 0 \leq k \leq 2$ (c) Type $(B_2), 0 \leq k \leq 2$ (d) Type $(C), 0 \leq k \leq 2$

Figure 3.A.1: g-graphs of small diagrams of different types. For each diagram only the graph G is drawn. The relevant diagrams come with permutations π such that the diagrams are linked.

We first give the

Proof of Lemma 3.4.6. Consider first all diagrams of type (C) of smallest size, i.e. with g-graph

$$G_0 = 1\overset{*}{\bullet}\text{-----}\bullet\text{-----}\overset{*}{\bullet}2$$

Since this graph is connected, all $\pi \in \mathcal{S}_3$ give rise to a linked diagram (π, G_0). By Wick's rule, the π-sum then gives the factor $\rho^{(3)}$. That is,

$$\sum_{\pi\in\mathcal{S}_3:(\pi,G_0)\in\mathcal{L}_1^2} \Gamma^2_{\pi,G_0} = \int g_{13}g_{23} \sum_{\pi\in\mathcal{S}_3} (-1)^\pi \prod_{j=1}^{3} \gamma_N^{(1)}(x_j, x_{\pi(j)}) \,\mathrm{d}x_3 = \int g_{13}g_{23}\rho^{(3)} \,\mathrm{d}x_3.$$

Recall the bound $\rho^{(3)} \leq C\rho^{3+4/3}|x_1 - x_2|^2|x_1 - x_3|^2$ from Lemma 3.2.15. Now we bound $|g_{23}| \leq 1$. Thus

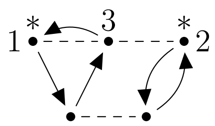
$$\left| \sum_{\pi \in \mathcal{S}_3 : (\pi, G_0) \in \mathcal{L}_1^2} \Gamma^2_{\pi, G_0} \right| \leq C\rho^{3+4/3}|x_1 - x_2|^2 \int \left(1 - f(x)^2\right) |x|^2 \,\mathrm{d}x.$$

Recalling Lemma 3.2.2 we may bound

$$\int \left(1 - f(x)^2\right) |x|^2 \,\mathrm{d}x \leq Ca^5 + \frac{C}{(1 - a^3/b^3)^2} \int_a^b \left[\left(1 - \frac{a^3}{b^3}\right)^2 - \left(1 - \frac{a^3}{r^3}\right)^2 \right] r^4 \,\mathrm{d}r \leq Ca^3b^2. \tag{3.A.1}$$

We conclude that all diagrams of smallest size contribute $\leq Ca^3b^2\rho^{3+4/3}|x_1 - x_2|^2$.

For the larger diagrams, we consider an example diagram

$(\pi, G) =$ 

For this diagram we have

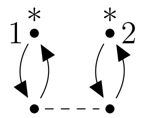
$$\begin{aligned}
\Gamma^2_{\pi,G} &= (-1)^\pi \iiint \gamma_N^{(1)}(x_1; x_4)\gamma_N^{(1)}(x_4; x_3)\gamma_N^{(1)}(x_3; x_1)\gamma_N^{(1)}(x_2; x_5)\gamma_N^{(1)}(x_5; x_2) \\
&\quad \times g_{13}g_{23}g_{45} \,\mathrm{d}x_3 \,\mathrm{d}x_4 \,\mathrm{d}x_5 \\
&= \frac{-1}{L^{15}} \sum_{k_1,\ldots,k_5 \in P_F} \iiint e^{ik_1(x_1 - x_4)} e^{ik_2(x_4 - x_3)} e^{ik_3(x_3 - x_1)} e^{ik_4(x_2 - x_5)} e^{ik_5(x_5 - x_2)} \\
&\quad \times g_{13}g_{23}g_{45} \,\mathrm{d}x_3 \,\mathrm{d}x_4 \,\mathrm{d}x_5 \\
&= \frac{-1}{L^{15}} \sum_{k_1,\ldots,k_5 \in P_F} e^{i(k_1 - k_3)x_1} e^{i(k_4 - k_5)x_2} \int \mathrm{d}x_3 \, e^{i(k_3 - k_2)x_3} g(x_1 - x_3) g(x_2 - x_3) \\
&\quad \times \int \mathrm{d}x_4 \left[e^{i(k_2 - k_1 + k_5 - k_4)x_4} \int \mathrm{d}x_5 \, e^{-i(k_5 - k_4)(x_4 - x_5)} g(x_4 - x_5) \right] \\
&= \frac{-1}{L^{12}} \sum_{k_1,\ldots,k_5 \in P_F} e^{i(k_1 - k_3)x_1} e^{i(k_4 - k_5)x_2} \int \mathrm{d}x_3 \, e^{i(k_3 - k_2)x_3} g(x_1 - x_3) g(x_2 - x_3) \\
&\quad \times \chi_{(k_2 - k_1 = k_4 - k_5)} \hat{g}(k_5 - k_4),
\end{aligned}$$

where $\hat{g}(k) := \int_\Lambda g(x)e^{-ikx} \,\mathrm{d}x$. Bounding $|g_{23}| \leq 1$ and $|\hat{g}(k)| \leq \int |g| \leq a^3 \log(b/a)$ we get that

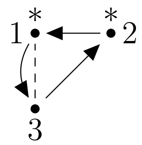
$$\left|\Gamma^2_{\pi,G}\right| \leq Ca^6\rho^4(\log(b/a))^2.$$

One may do a similar computation for all the remaining diagrams. By computing the integrations of the vertices in the internal clusters first, these give some factor $\hat{g}(k_i - k_j)$ and a factor $L^3\chi_{(k_i - k_j = k_{i'} - k_{j'})}$. By bounding as above we conclude that the contribution of small diagrams of type (C) is bounded as desired. □

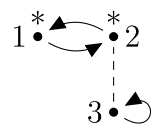
Proof of Lemma 3.4.8. As with the larger diagrams of type (C) we only give calculations for a few example diagrams and explain how the calculation for the remaining diagrams are similar. We consider the examples in Figure 3.A.2.



(a) Example of a type (A) diagram of smallest size



(b) Example of a type (B_1) diagram of smallest size



(c) Example of a type (B_2) diagram of smallest size

Figure 3.A.2: Exemplary diagrams of types $(A), (B_1)$ and (B_2). The dashed lines denote g-edges, and the arrows denote (directed) edges of the permutation.

The contribution of the diagram in Figure 3.A.2a to $\partial_{x_1}^\mu \partial_{x_1}^\nu \xi_{\mathsf{small}}$ is

$$
\begin{aligned}
&\frac{1}{2}\partial_{x_1}^\mu \partial_{x_1}^\nu \Gamma_{\pi,G}^2 \\
&= \frac{-1}{2L^{12}} \sum_{k_1,\ldots,k_4\in P_F} (k_1^\mu - k_2^\mu)(k_1^\nu - k_2^\nu) \\
&\quad \times \iint e^{ik_1(x_1-x_3)} e^{ik_2(x_3-x_1)} e^{ik_3(x_2-x_4)} e^{ik_4(x_4-x_2)} g_{34} \, \mathrm{d}x_3 \, \mathrm{d}x_4 \\
&= \frac{-1}{2L^{12}} \sum_{k_1,\ldots,k_4\in P_F} (k_1^\mu - k_2^\mu)(k_1^\nu - k_2^\nu) e^{i(k_1-k_2)x_1} e^{i(k_3-k_4)x_2} \\
&\quad \times \iint e^{-i(k_4-k_3)(x_3-x_4)} e^{i(k_2-k_1+k_4-k_3)x_3} g(x_3 - x_4) \, \mathrm{d}x_3 \, \mathrm{d}x_4 \\
&= \frac{-1}{2L^9} \sum_{k_1,\ldots,k_4\in P_F} (k_1^\mu - k_2^\mu)(k_1^\nu - k_2^\nu) e^{i(k_1-k_2)x_1} e^{i(k_3-k_4)x_2} \chi_{(k_2-k_1=k_3-k_4)} \hat{g}(k_4 - k_3) \\
&= O(\rho^{3+2/3} a^3 \log(b/a))
\end{aligned}
$$

using that $\hat{g}(k) = \int_\Lambda g(x) e^{-ikx} \, \mathrm{d}x$ satisfies $|\hat{g}(k)| \leq \int |g| \leq Ca^3 \log(b/a)$. The same type of computation is valid for all other diagrams of type (A).

Consider now the diagram in Figure 3.A.2c of type (B_2). This contributes

$$
\begin{aligned}
&\partial_{x_1}^\mu \partial_{x_1}^\nu \frac{-1}{L^9} \sum_{k_1,k_2,k_3\in P_F} \int e^{ik_1(x_1-x_2)} e^{ik_2(x_2-x_1)} g(x_2 - x_3) \, \mathrm{d}x_3 \\
&\quad = \frac{1}{L^9} \sum_{k_1,k_2,k_3\in P_F} (k_1^\mu - k_2^\mu)(k_1^\nu - k_2^\nu) e^{i(k_1-k_2)x_1} e^{i(k_2-k_1)x_2} \int g(x_2 - x_3) \, \mathrm{d}x_3 \\
&\quad = O(\rho^{3+2/3} a^3 \log(b/a))
\end{aligned}
$$

exactly as for type (A). Similarly, all other diagrams of type (B_2) may be bounded using the same method as for types (A).

Finally, we consider the diagram in Figure 3.A.2b of type (B_1). Here we have

$$
\begin{aligned}
\partial_{x_1}^\mu \partial_{x_1}^\nu \Gamma_{\pi,G}^2 &= \partial_{x_1}^\mu \partial_{x_1}^\nu \frac{1}{L^9} \sum_{k_1,k_2,k_3\in P_F} \int e^{ik_1(x_1-x_3)} e^{ik_2(x_3-x_2)} e^{ik_3(x_2-x_1)} g(x_1 - x_3) \, \mathrm{d}x_3 \\
&= \partial_{x_1}^\mu \partial_{x_1}^\nu \frac{1}{L^9} \sum_{k_1,k_2,k_3\in P_F} e^{i(k_2-k_3)x_1} e^{i(k_3-k_2)x_2} \int e^{-i(k_2-k_1)(x_1-x_3)} g(x_1 - x_3) \, \mathrm{d}x_3 \\
&= \frac{-1}{L^9} \sum_{k_1,k_2,k_3\in P_F} (k_2^\mu - k_3^\mu)(k_2^\nu - k_3^\nu) e^{i(k_2-k_3)x_1} e^{i(k_3-k_2)x_2} \hat{g}(k_2 - k_1) \\
&= O(\rho^{3+2/3} a^3 \log(b/a)).
\end{aligned}
$$

All larger diagrams of type (B_1) may be bounded similarly. We conclude the desired. $\square$

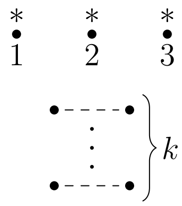
3.A.2 Small 3-particle diagrams (proof of Lemma 3.4.11)

We now give the

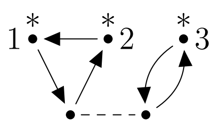
Proof of Lemma 3.4.11. Recall that

$$\xi^3_{\text{small}} = \sum_{p=1}^{\infty} \frac{1}{p!} \sum_{\substack{(\pi,G)\in\tilde{\mathcal{L}}^3_p \\ (\pi,G)\ \text{small}}} \Gamma^3_{\pi,G},$$

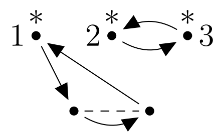
where "small" refers to diagrams with G-graph

$G =$  $k = 1, 2$

and permutation π such that (π, G) has at most two linked components, both of which contain at least one external vertex. As in the proof of Lemmas 3.4.6 and 3.4.8 in Section 3.A.1 we compute the value of a few examples and explain how to compute the value of the remaining diagrams. We consider the examples of Figure 3.A.3



(a) Example of a diagram of smallest size with one linked component



(b) Example of a diagram of smallest size with two linked components

Figure 3.A.3: Exemplary small diagrams in $\tilde{\mathcal{L}}^3_2$.

The contribution of the diagram in Figure 3.A.3a is

$$\begin{aligned}
\Gamma^3_{\pi,G} &= \frac{-1}{L^{15}} \sum_{k_1,\ldots,k_5\in P_F} \iint e^{ik_1(x_1-x_4)} e^{ik_2(x_4-x_2)} e^{ik_3(x_2-x_1)} e^{ik_4(x_3-x_5)} e^{ik_5(x_5-x_3)} g_{45} \,\mathrm{d}x_4 \,\mathrm{d}x_5 \\
&= \frac{-1}{L^{12}} \sum_{k_1,\ldots,k_5\in P_F} e^{i(k_1-k_3)x_1} e^{i(k_3-k_2)x_2} e^{i(k_4-k_5)x_3} \chi_{(k_2-k_1=k_4-k_5)} \hat{g}(k_5-k_4) \\
&= O(a^3\rho^4\log(b/a)).
\end{aligned}$$

Similarly, the contribution of the diagram in Figure 3.A.3b is

$$\begin{aligned}
\Gamma^3_{\pi,G} &= \frac{-1}{L^{15}} \sum_{k_1,\ldots,k_5\in P_F} \iint e^{ik_1(x_1-x_4)} e^{ik_2(x_4-x_5)} e^{ik_3(x_5-x_1)} e^{ik_4(x_2-x_3)} e^{ik_5(x_3-x_2)} g_{45} \,\mathrm{d}x_4 \,\mathrm{d}x_5 \\
&= \frac{-1}{L^{12}} \sum_{k_1,\ldots,k_5\in P_F} e^{i(k_1-k_3)x_1} e^{i(k_4-k_5)x_2} e^{i(k_5-k_4)x_3} \chi_{(k_2-k_1=k_2-k_3)} \hat{g}(k_3-k_2) \\
&= O(a^3\rho^4\log(b/a)).
\end{aligned}$$

One may follow this kind of computation for any diagram. The central property we used is that the internal vertices are all in the same linked component as some external vertex. This means that the integrals over internal vertices either gives a factor of $\hat{g}(k_i - k_j)$ or a factor of $L^3\chi_{(k_i-k_j=k_{i'}-k_{j'})}$. We conclude the desired. $\square$

3.A.3 Small diagrams in 1 dimension (proof of Lemma 3.5.21)

We now give the

Proof of Lemma 3.5.21. We first give the proof of Equation (3.5.14). We split the two cases (A) and (B) of small diagrams further. They are given as follows.

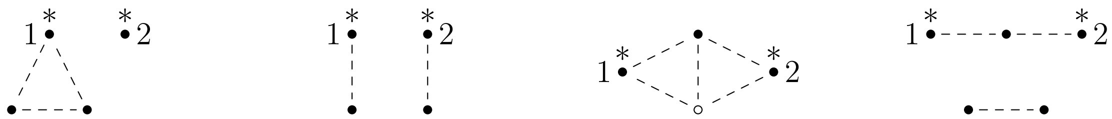
(A) $\{1\}$ and $\{2\}$ in different clusters and $k = 0, \nu^* = 2$,

- (A_1) $n_* = 2, n_{**} = 0$ (or $n_* = 0, n_{**} = 2$),
- (A_2) $n_* = 1, n_{**} = 1$.

(B) $\{1\}$ and $\{2\}$ in the same cluster and $1 \le k + \nu + \nu^* \le 2$,

- (B_1) $k = 0$,
- (B_2) $k = 1$.

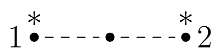
See also Figure 3.A.4.



(a) Type (A_1) (b) Type (A_2) (c) Type (B_1) (d) Type (B_2)

Figure 3.A.4: g-graphs of small diagrams of different types. For each diagram only the graph G is drawn. The relevant diagrams come with permutations π such the the diagrams are linked. The diagrams of type (A_1) and (B_1) may have some of the drawn g-edges not present, but the same connected components. Moreover, the diagrams of type (B_1) may have one of the internal vertices drawn not present (indicated by a $\circ$). With the modification of the drawings described here these are all small diagrams.

We will consider some examples of diagrams. Namely those drawn in Figure 3.A.4 (but not modified as described in the caption), except for the diagram of type (B_1), where we will consider diagrams of smallest size, with g-graph

$G_0 =$  (3.A.2)

All other diagrams can be treated in a similar fashion. For the argument we will need a different formula for ρ_{t}. Recall the definition in Equation (3.3.4). We may write the characteristic function as

$$\chi((\pi, \cup G_\ell) \text{ linked}) = 1 - \chi((\pi, \cup G_\ell) \text{ not linked}).$$

That is,

$$\rho_{\mathsf{t}}^{(A_1,\dots,A_k)} = \sum_{\pi\in\mathcal{S}_{\cup A_\ell}} (-1)^\pi \prod_{j\in\cup A_\ell} \gamma_N^{(1)}(x_j;x_{\pi(j)}) - \sum_{\pi\in\mathcal{S}_{\cup A_\ell}} (-1)^\pi \chi_{((\pi,\cup G_\ell)\text{ not linked})} \prod_{j\in\cup A_\ell} \gamma_N^{(1)}(x_j;x_{\pi(j)}).$$

For our case we only need to consider cases where there are at most two clusters. If there is just one cluster then $\rho_{\mathsf{t}}^{(A)} = \rho^{(|A|)}((x_j)_{j\in A})$. So suppose we have two clusters A_1, A_2. Here, all the π's for which $(\pi,\cup G_\ell)$ is not linked are exactly those arising as products $\pi=\pi_1\pi_2$, where $\pi_1\in\mathcal{S}_{A_1}$ and $\pi_2\in\mathcal{S}_{A_1}$ are permutations of the vertices in the 2 clusters. Thus,

$$\begin{aligned}\rho_{\mathsf{t}}^{(A_1,A_2)}((x_j)_{j\in A_1\cup A_2}) &= \sum_{\pi\in\mathcal{S}_{A_1\cup A_2}} (-1)^\pi \prod_{j\in A_1\cup A_2} \gamma_N^{(1)}(x_j;x_{\pi(j)}) \\ &\quad - \sum_{\pi_1\in\mathcal{S}_{A_1}} (-1)^{\pi_1} \prod_{j\in A_1} \gamma_N^{(1)}(x_j;x_{\pi_1(j)}) \sum_{\pi_2\in\mathcal{S}_{A_2}} (-1)^{\pi_2} \prod_{j\in A_2} \gamma_N^{(1)}(x_j;x_{\pi_2(j)}) \\ &= \rho^{(|A_1|+|A_2|)}((x_j)_{j\in A_1\cup A_2}) - \rho^{(|A_1|)}((x_j)_{j\in A_1})\rho^{(|A_2|)}((x_j)_{j\in A_2}).\end{aligned} \tag{3.A.3}$$

We now consider the diagrams in Figures 3.A.4a, 3.A.4b and 3.A.4d and (3.A.2). We get

$$\begin{aligned}
\text{Type } (A_1): &\quad \sum_{\pi\in\mathcal{S}_4:(\pi,G_0)\in\mathcal{L}_2^2} \Gamma^2_{\pi,G_0} = \iint g_{13}g_{14}g_{34}\rho_{\mathsf{t}}^{(\{1,3,4\},\{2\})}\,\mathrm{d}x_3\,\mathrm{d}x_4,\\
\text{Type } (A_2): &\quad \sum_{\pi\in\mathcal{S}_4:(\pi,G_0)\in\mathcal{L}_2^2} \Gamma^2_{\pi,G_0} = \iint g_{13}g_{24}\rho_{\mathsf{t}}^{(\{1,3\},\{2,4\})}\,\mathrm{d}x_3\,\mathrm{d}x_4,\\
\text{Type } (B_1): &\quad \sum_{\pi\in\mathcal{S}_3:(\pi,G_0)\in\mathcal{L}_1^2} \Gamma^2_{\pi,G_0} = \int g_{13}g_{23}\rho^{(3)}\,\mathrm{d}x_3,\\
\text{Type } (B_2): &\quad \sum_{\pi\in\mathcal{S}_5:(\pi,G_0)\in\mathcal{L}_3^2} \Gamma^2_{\pi,G_0} = \iiint g_{13}g_{23}g_{45}\rho_{\mathsf{t}}^{(\{1,2,3\},\{4,5\})}\,\mathrm{d}x_3\,\mathrm{d}x_4\,\mathrm{d}x_5.
\end{aligned} \tag{3.A.4}$$

Using Equation (3.A.3) and (the 1-dimensional versions of) Lemmas 3.2.14 and 3.2.15 and similar bounds for the 4- and 5-particle reduced densities we get the bounds on the truncated correlations

$$\begin{aligned}
(A_1) &\qquad \left|\rho_{\mathsf{t}}^{(\{1,3,4\},\{2\})}\right| \le \rho^{(4)}(x_1,\dots,x_4) + \rho^{(3)}(x_1,x_3,x_4)\rho^{(1)}(x_2)\\
&\qquad\qquad \le C\rho^8|x_1-x_3|^2|x_1-x_4|^2,\\
(A_2) &\qquad \left|\rho_{\mathsf{t}}^{(\{1,3\},\{2,4\})}\right| \le \rho^{(4)}(x_1,\dots,x_4) + \rho^{(2)}(x_1,x_3)\rho^{(2)}(x_2,x_4)\\
&\qquad\qquad \le C\rho^8|x_1-x_3|^2|x_2-x_4|^2,\\
(B_1) &\qquad \rho^{(3)} \le C\rho^7|x_1-x_2|^2|x_1-x_3|^2,\\
(B_2) &\qquad \left|\rho_{\mathsf{t}}^{(\{1,2,3\},\{4,5\})}\right| \le \rho^{(5)}(x_1,\dots,x_5) + \rho^{(3)}(x_1,x_2,x_3)\rho^{(2)}(x_4,x_5)\\
&\qquad\qquad \le C\rho^{11}|x_1-x_2|^2|x_1-x_3|^2|x_4-x_5|^2.
\end{aligned}$$

Bounding moreover, $g_{34}\le 1$ for the diagram of type (A_1) we thus get by the translation invariance

$$\left|\sum_{\substack{\pi\in\mathcal{S}_4:(\pi,G_0)\in\mathcal{L}_2^2\\ \text{type } (A_1)}} \Gamma^2_{\pi,G_0}\right| \le C\rho^8\left(\int |g(x)||x|^2\,\mathrm{d}x\right)^2.$$

For the diagram of type (A_2) we get

$$\left| \sum_{\substack{\pi \in \mathcal{S}_4 : (\pi, G_0) \in \mathcal{L}_2^2 \\ \text{type } (A_2)}} \Gamma^2_{\pi, G_0} \right| \leq C\rho^8 \left(\int |g(x)||x|^2 \, \mathrm{d}x \right)^2 .$$

For the diagram of type (B_1) we get by bounding $g_{23} \leq 1$ (as in the proof of Lemma 3.4.6)

$$\left| \sum_{\substack{\pi \in \mathcal{S}_3 : (\pi, G_0) \in \mathcal{L}_1^2 \\ \text{type } (B_1)}} \Gamma^2_{\pi, G_0} \right| \leq C\rho^7 |x_1 - x_2|^2 \int |g(x)||x|^2 \, \mathrm{d}x.$$

Finally, for the diagram of type (B_2) we get in the same way

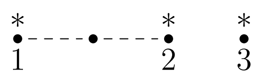
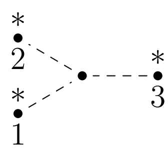
$$\left| \sum_{\substack{\pi \in \mathcal{S}_5 : (\pi, G_0) \in \mathcal{L}_3^2 \\ \text{type } (B_2)}} \Gamma^2_{\pi, G_0} \right| \leq CN\rho^{10} |x_1 - x_2|^2 \left(\int |g(x)||x|^2 \, \mathrm{d}x \right)^2 .$$

We may bound $\int |x|^2 |g| \, \mathrm{d}x$ similarly as in 3 and 2 dimensions,

$$\int_{\mathbb{R}} \left(1 - f(x)^2\right) |x|^2 \, \mathrm{d}x \leq Ca^3 + \frac{C}{(1 - a/b)^2} \int_a^b \left[\left(1 - \frac{a}{b}\right)^2 - \left(1 - \frac{a}{r}\right)^2 \right] r^2 \, \mathrm{d}r \leq Cab^2.$$

The other diagrams of types (A_1) and (B_1) (there are no other diagrams of type (A_2) or (B_2)) we may treat similarly by bounding some of the g-edges by $|g| \leq 1$. Combining these bounds we conclude the proof of Equation (3.5.14).

To prove Equation (3.5.15) we recall that we consider all diagrams with g-graph

$G_0 =$  or $G_1 =$ 

(and graphs that look like G_0 where $\{1, 2, 3\}$ are permuted). One may treat this similarly as the diagrams above, with the result that

$$\left| \sum_{\pi \in \mathcal{S}_4 : (\pi, G_0) \in \mathcal{L}_1^3} \Gamma^3_{\pi, G_0} \right| \leq \int |g_{14}||g_{24}| \left| \rho_{\mathrm{t}}^{(\{1,2,4\},\{3\})} \right| \mathrm{d}x_4 \leq Cab^2 \rho^8 |x_1 - x_2|^2$$

$$\left| \sum_{\pi \in \mathcal{S}_4 : (\pi, G_1) \in \mathcal{L}_1^3} \Gamma^3_{\pi, G_1} \right| \leq \int |g_{14}||g_{24}||g_{34}| \rho^{(4)} \, \mathrm{d}x_4 \leq Cab^2 \rho^8 |x_1 - x_2|^2.$$

Summing this over all the permutations of $\{1, 2, 3\}$ we conclude the proof of Equation (3.5.15).

∎

3.B Derivative Lebesgue constants (proof of Lemma 3.4.9)

In this appendix we give the proof of Lemma 3.4.9. We recall the statement in slightly different notation for convenience.

Lemma 3.4.9. *The polyhedron P from Definition 3.2.7 satisfies for any $\mu, \nu = 1, 2, 3$ that*

$$\int_{[0,2\pi]^3} \left| \sum_{k \in RP \cap \mathbb{Z}^3} k^\mu e^{ikx} \right| \mathrm{d}x \leq CsR(\log R)^3, \quad \int_{[0,2\pi]^3} \left| \sum_{k \in RP \cap \mathbb{Z}^3} k^\mu k^\nu e^{ikx} \right| \mathrm{d}x \leq CsR^2(\log R)^4$$

for sufficiently large $R = \frac{Lk_F}{2\pi}$.

Recall that by construction $R \sim N^{1/3}$ is rational.

The proof follows quite closely the argument in [KL18]. In particular the structure is that of induction. The 3-dimensional integral is bounded one dimension at a time. We start by introducing some notation from [KL18].

Notation 3.B.1. For any real number x we will write $[x]$ for either $\lfloor x \rfloor$ or $\lceil x \rceil$. Similarly we will write $\langle x \rangle = x - [x]$, i.e. $\langle x \rangle$ is either the fractional part $\{x\} = x - \lfloor x \rfloor$ or $x - \lceil x \rceil$. For any computation we do below, the definition of $[x]$ is fixed, but the computations hold with either choice.

Additionally for a d-dimensional vector $x = (x^1, \ldots, x^d)$ we write $x^{(\tilde{d})} = (x^1, \ldots, x^{\tilde{d}})$ for the first $\tilde{d} \leq d$ components.

We emphasize that expressions like $k^2, x^3, \ldots$ do not denote squares or cubes of numbers k, x, but instead refer to coordinates of vectors k, x. The instances where we do want to denote a square, cube or higher power should be clear.

By potentially relabelling the coordinates it suffices to consider the cases $\mu = 1$, $\mu = \nu = 1$ and $\mu = 1, \nu = 2$. (Alternatively, by appealing to Lemma 3.2.11 and choosing $Q \gtrsim N^4$ in Definition 3.2.7 we have a symmetry of coordinates up to error-terms which are subleading compared to Lemma 3.4.9.) Hence define

$$t_1(k) = k^1, \qquad t_2(k) = k^1 k^1 = (k^1)^2, \qquad t_3(k) = k^1 k^2.$$

We want to show that

$$\int_{[0,2\pi]^3} \left| \sum_{k \in RP \cap \mathbb{Z}^3} t_j(k) e^{ikx} \right| \mathrm{d}x \leq \begin{cases} CsR(\log R)^3 & j = 1, \\ CsR^2(\log R)^4 & j = 2, 3. \end{cases}$$

As in the proof of Lemma 3.2.12 we write RP as a union of $O(s)$ closed tetrahedra. We also recall that $Rz \notin \mathbb{Z}^3$. As in the proof of Lemma 3.2.12 we get by the inclusion exclusion principle $O(s)$ terms with tetrahedra of lower dimension (triangles or line segments). All the 3-dimensional (closed) tetrahedra are convex and hence of the form

$$T = \left\{ k \in \mathbb{Z}^3 : \lambda_1 \leq k^1 \leq \Lambda_1, \lambda_2(k^1) \leq k^2 \leq \Lambda_2(k^1), \lambda_3(k^1, k^2) \leq k^3 \leq \Lambda_3(k^1, k^2) \right\},$$

for some piecewise affine functions $\lambda_i, \Lambda_i, i = 1, 2, 3$. They are the equations of the planes bounding the tetrahedron T. Since any $k \in T$ has integer coordinates we can replace Λ_j by

$\lfloor \Lambda_j \rfloor$ and λ_j by $\lceil \lambda_j \rceil$. It will be convenient to not distinguish between $\lfloor \cdot \rfloor$ and $\lceil \cdot \rceil$ and use instead the notation $[\cdot]$ introduced in Notation 3.B.1. Then the tetrahedra are of the form

$$T = \Big\{ k \in \mathbb{Z}^3 : [\lambda_1] \le k^1 \le [\Lambda_1], [\lambda_2(k^1)] \le k^2 \le [\Lambda_2(k^1)], \\ [\lambda_3(k^1,k^2)] \le k^3 \le [\Lambda_3(k^1,k^2)] \Big\}, \tag{3.B.1}$$

where we allow $[\cdot]$ to be different in any of the 6 instances it appears.

Sums over lower-dimensional tetrahedra can be written as differences of sums over 3-dimensional tetrahedra (with potentially different meanings of $[\cdot]$). We will thus only consider 3-dimensional tetrahedra. That is, for a tetrahedron T of the form Equation (3.B.1), we need to bound

$$\int_{[0,2\pi]^3} \left| \sum_{k \in T\cap \mathbb{Z}^3} t_j(k) e^{ikx} \right| \mathrm{d}x \le \begin{cases} CR(\log R)^3 & j=1, \\ CR^2(\log R)^4 & j=2,3. \end{cases} \tag{3.B.2}$$

Gluing together tetrahedra as in Lemma 3.2.12 we conclude the desired bound, Lemma 3.4.9. The remainder of this section gives the proof of Equation (3.B.2).

3.B.1 Reduction to simpler tetrahedron

We first reduce to the case of a simpler tetrahedron T. Consider what happens by shifting all k's by some fixed lattice vector $\kappa \in \mathbb{Z}^3$ with $|\kappa| \le CR$. For t_2 we have

$$\begin{aligned} \sum_{k \in T\cap\mathbb{Z}^3} (k^1)^2 e^{ikx} &= \sum_{k\in (T-\kappa)\cap \mathbb{Z}^3} (k^1+\kappa^1)^2 e^{ikx} \\ &= \sum_{k\in (T-\kappa)\cap \mathbb{Z}^3} (k^1)^2 e^{ikx} + 2\kappa^1 \sum_{k\in (T-\kappa)\cap \mathbb{Z}^3} k^1 e^{ikx} + (\kappa^1)^2 \sum_{k\in (T-\kappa)\cap \mathbb{Z}^3} e^{ikx}. \end{aligned}$$

A similar computation holds for t_1, t_3. We may bound $|\kappa| \le CR$ and thus we may assume that $T \subset [0, CR]^3$. (Recall that $\int_{[0,2\pi]^3} \left| \sum_{k\in T\cap\mathbb{Z}^3} e^{ikx} \right| \mathrm{d}x \le C(\log R)^3$ by [KL18, Theorem 4.1], see the proof of Lemma 3.2.12.)

For any tetrahedron of the form (3.B.1) we may write the k-sum as three 1-dimensional sums

$$\sum_{k\in T\cap\mathbb{Z}^3} = \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} \sum_{k^3=[\lambda_3(k^1,k^2)]}^{[\Lambda_3(k^1,k^2)]} = \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} \left(\sum_{k^3=0}^{[\Lambda_3(k^1,k^2)]} - \sum_{k^3=0}^{[\lambda_3(k^1,k^2)-1]} \right),$$

where the λ_j's and Λ_j's are the equations of the planes bounding the tetrahedron T, i.e. piecewise affine functions. As in Equation (3.B.1) each instance of $[\cdot]$ may be either of the definitions of Notation 3.B.1. By splitting the k^1, k^2 sums into at most 4 parts, we may ensure that both Λ_3 and $\lambda_3 - 1$ are only from one bounding plane, i.e. they are affine functions. When we do this splitting, we have to choose (in each new tetrahedron) which definition of $[\cdot]$ to use for the new bounding plane. This may give rise to some "boundary term", if we choose definitions of $[\cdot]$ in the new tetrahedra such that the k's on the splitting face are either in both or in neither of the two tetrahedra sharing this face. These boundary terms are sums over lower-dimensional tetrahedra, and may thus be bounded by sums over 3-dimensional ones as above.

Remark 3.B.2. One may similarly let the k^1- and k^2-sums go from 0 by writing e.g.

$$\sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} = \sum_{k^2=0}^{[\Lambda_2(k^1)]} - \sum_{k^2=0}^{[\lambda_2(k^1)-1]}.$$

However, the upper limits $\Lambda_3(k^1,k^2)$ and $\lambda_3(k^1,k^2)-1$ for the k^3-sum may become much larger than R for $k^2 \le \lambda_2(k^1)$. This is why we don't do this.

The terms with Λ_3 and $\lambda_3 - 1$ may be treated the same way, so we just look at the one with Λ_3. We thus want to bound

$$\int_{[0,2\pi]^3} \left| \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) \sum_{k^3=0}^{[\Lambda_3(k^1,k^2)]} e^{ikx} \right| \mathrm{d}x \lesssim \begin{cases} R(\log R)^3 & j=1, \\ R^2(\log R)^4 & j=2,3. \end{cases}$$

3.B.2 Reduction from $d=3$ to $d=2$

We show that we may bound the three-dimensional integrals by analogous two-dimensional integrals up to a factor of $(\log R + \log Q) \sim \log N$.

First, before shifting by a constant $\kappa \in \mathbb{Z}^3$, Λ_3 is given by either the plane through 3 close corners of RP (points $R\sigma(p^1/Q_1, p^2/Q_2, p^3/Q_3)$) or of two close corners and the centre Rz. This follows from the construction of P in Definition 3.2.7, since forming the edges between pairs of close points constructs a triangulation of P.

The equation for a plane through the three points $R\sigma(p^1_j/Q_1, p^2_j/Q_2, p^3_j/Q_3)$, $j=1,2,3$ is given by

$$\frac{\alpha_1}{Q_2Q_3}k^1 + \frac{\alpha_2}{Q_1Q_3}k^2 + \frac{\alpha_3}{Q_1Q_2}k^3 = R\sigma\gamma$$

where by construction of P, see Definition 3.2.7, we have

$$\sigma \notin \mathbb{Q}, \qquad \gamma \in \mathbb{Q}, \qquad \alpha_j \in \mathbb{Z}, \qquad |\alpha_j| \le C\sqrt{Q}, \quad j=1,2,3.$$

We might have that $\alpha_j = 0$. If $\alpha_3 = 0$ then this plane is parallel to the k^3-axis and so does not give rise to a bound on the k^3-sum. Hence $\alpha_3 \ne 0$. By choice of L, we have that R is rational, and so $R\sigma\gamma \notin \mathbb{Q}$. (The choice of L such that R is rational, is exactly so that $R\sigma\gamma \notin \mathbb{Q}$.) The equation for Λ_3 is an integer shift of this plane, hence it is of the form

$$\begin{aligned} \Lambda_3(k^1,k^2) = n_3 - m^1k^1 - m^2k^2 = n_3 - \frac{Q_1\alpha_1}{Q_3\alpha_3}k^1 - \frac{Q_2\alpha_2}{Q_3\alpha_3}k^2, \\ n_3 \notin \mathbb{Q}, \quad |\alpha_j| \le C\sqrt{Q},\ j=1,2,3. \end{aligned} \tag{3.B.3}$$

Define for $j=1,2,3$ the quantities

$$\begin{aligned} D^j_3(x) &:= \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) \sum_{k^3=0}^{[\Lambda_3(k^1,k^2)]} e^{ik^{(3)}x^{(3)}}, \\ \tilde{D}^j_2(x) &:= \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}}, \\ G^j_3(x) &:= \frac{1}{e^{ix^3}-1}\left(e^{i(n_3+1)x^3}\tilde{D}^j_2(x^{(2)} - m^{(2)}x^3) - \tilde{D}^j_2(x^{(2)})\right), \\ F^j_3(x) &:= \frac{e^{i(n_3+1)x^3}}{e^{ix^3}-1} \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}(x^{(2)}-m^{(2)}x^3)} \left(e^{-i\langle\Lambda_3(k^{(2)})\rangle x^3} - 1\right), \end{aligned} \tag{3.B.4}$$

where $m^{(2)} = (m^1,m^2)$ is defined in Equation (3.B.3). We shall prove the following bound.

Lemma 3.B.3. *We have for some $k_0^{(2)} \in \mathbb{Z}^2$, some (non-zero) $\kappa = \kappa^{(2)} \in \mathbb{Z}^2$ and a $h \in \mathbb{Z}$, $h \geq 0$ with $|k_0^{(2)}| \leq CR$ and $h|\kappa^{(2)}| \leq CR$ that for any $j = 1,2,3$*

$$\begin{aligned}
&\int_{[0,2\pi]^3} \left|D_3^j(x^{(3)})\right| \,\mathrm{d}x^{(3)} \\
&\quad\lesssim (\log R + \log Q) \int_{[0,2\pi]^2} \left|\tilde{D}_2^j(x^{(2)})\right| \,\mathrm{d}x^{(2)} + 1 + \int_0^{2\pi} \left|\sum_{\tau=0}^{h} t_j\left(k_0^{(2)} + \tau\kappa^{(2)}\right) e^{i\tau|\kappa^{(2)}|x^1}\right| \,\mathrm{d}x^1.
\end{aligned}$$

As a first step, consider the case where both $\alpha_1 = \alpha_2 = 0$ in Equation (3.B.3). Then the k^3-sum and x^3-integral in Lemma 3.B.3 factors out. Using [KL18, Lemma 3.2] to evaluate the k^3-sum and x^3-integral we conclude the desired. Hence we can assume that at most one of α_1, α_2 is 0. (This will be relevant for Lemma 3.B.8, but only then.)

A simple calculation shows that [KL18, Lemma 3.1]

$$D_3^j(x) = G_3^j(x) + F_3^j(x), \quad j = 1,2,3. \tag{3.B.5}$$

By a straightforward modification of the argument in [KL18, Lemma 3.3] (including the factor t_j) we have

Lemma 3.B.4 ([KL18, Lemma 3.3])**.** *For any $j = 1,2,3$ we have*

$$\int_{[0,2\pi]^3} \left|G_3^j(x)\right| \,\mathrm{d}x \lesssim \log R \int_{[0,2\pi]^2} \left|\tilde{D}_2^j(x^{(2)})\right| \,\mathrm{d}x^{(2)}.$$

We thus want to bound the integral of F_3^j. Again, by a straightforward modification of the argument in [KL18, Lemma 3.7] (including the factor t_j) we have

Lemma 3.B.5 ([KL18, Lemma 3.7])**.** *For any $j = 1,2,3$ we have*

$$\int_{[0,2\pi]^3} \left|F_3^j(x)\right| \,\mathrm{d}x \lesssim \sum_{r=1}^{\infty} \frac{(2\pi)^r}{r!} \int_{[0,2\pi]^2} \left|\sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} \left\langle \Lambda_3(k^{(2)})\right\rangle^r\right| \,\mathrm{d}x^{(2)}.$$

To bound the right hand side of Lemma 3.B.5 we bound either definition of $\langle\cdot\rangle$ by the fractional part $\{\cdot\}$. This follows the strategy in [KL18]. In analogy with [KL18, Lemma 3.6] we have

Lemma 3.B.6 ([KL18, Lemma 3.6])**.** *For either definition of $\langle\cdot\rangle$ we have the bound*

$$\begin{aligned}
&\int_{[0,2\pi]^2} \left|\sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} \left\langle \Lambda_3(k^{(2)})\right\rangle^r\right| \,\mathrm{d}x^{(2)} \\
&\quad\leq \int_{[0,2\pi]^2} \left|\tilde{D}_2^j(x^{(2)})\right| \,\mathrm{d}x^{(2)} \\
&\qquad + \sum_{\nu=1}^{r} \binom{r}{\nu} \int_{[0,2\pi]^2} \left|\sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} \{\Lambda_3(k^{(2)})\}^\nu\right| \,\mathrm{d}x^{(2)}
\end{aligned}$$

uniformly in (integer) $r \geq 1$.

Proof. If $\langle\cdot\rangle = \{\cdot\}$ this is clear. Hence suppose that $\langle x\rangle = x - \lceil x\rceil$. Then

$$\langle x\rangle = \{x\} - 1 + \begin{cases} 1 & \text{if } x \in \mathbb{Z} \\ 0 & \text{otherwise.} \end{cases}$$

By construction $\Lambda_3(k^1,k^2)\notin\mathbb{Z}$ for $k^1,k^2\in\mathbb{Z}$. Thus, $\langle\Lambda_3(k^1,k^2)\rangle=\{\Lambda_3(k^1,k^2)\}-1$. Then

$$\begin{aligned}
&\sum_{k^1=[\lambda_1]}^{[\Lambda_1]}\sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2)e^{ik^{(2)}x^{(2)}}\left\langle\Lambda_3(k^{(2)})\right\rangle^r\\
&=\sum_{\nu=0}^{r}(-1)^{r-\nu}\binom{r}{\nu}\sum_{k^1=[\lambda_1]}^{[\Lambda_1]}\sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2)e^{ik^{(2)}x^{(2)}}\{\Lambda_3(k^{(2)})\}^\nu\\
&=(-1)^r\tilde{D}_2^j(x^{(2)})+\sum_{\nu=1}^{r}(-1)^{r-\nu}\binom{r}{\nu}\sum_{k^1=[\lambda_1]}^{[\Lambda_1]}\sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2)e^{ik^{(2)}x^{(2)}}\{\Lambda_3(k^{(2)})\}^\nu. \quad\square
\end{aligned}$$

We now bound the second summand of Lemma 3.B.6 similarly to [KL18, Lemmas 3.8 and 3.9]. We first define $\tilde{\Lambda}_3$, a rational approximation of Λ_3. Recall the definition of Λ_3 in Equation (3.B.3). By Dirichlet's approximation theorem we may for any Q_∞ find integers p,q with $1\le q\le Q_\infty$ such that

$$\gamma_3:=n_3-\frac{p}{q}\qquad\text{satisfies}\qquad|\gamma_3|<\frac{1}{qQ_\infty}.$$

We will choose $Q_\infty=Q_3\alpha_3$. Define then

$$\tilde{\Lambda}_3(k^{(2)})=\Lambda_3(k^{(2)})-\gamma_3=\frac{p}{q}-\frac{Q_1\alpha_1}{Q_3\alpha_3}k^1-\frac{Q_2\alpha_2}{Q_3\alpha_3}k^2. \tag{3.B.6}$$

Note that this takes values in $\frac{1}{qQ_\infty}\mathbb{Z}$ for integers k^1,k^2. In particular (for integers k^1,k^2) $\{\tilde{\Lambda}_3(k^{(2)})\}\in\{0,\frac{1}{qQ_\infty},\dots,\frac{qQ_\infty-1}{qQ_\infty}\}$. Thus, since $|\gamma_3|<\frac{1}{qQ_\infty}$ we have

$$\{\Lambda_3(k^{(2)})\}=\gamma_3+\{\tilde{\Lambda}_3(k^{(2)})\}+\begin{cases}1 & \text{if } \gamma_3<0 \text{ and } \tilde{\Lambda}_3(k^{(2)})\in\mathbb{Z},\\ 0 & \text{otherwise.}\end{cases} \tag{3.B.7}$$

We claim that

Lemma 3.B.7. *For N sufficiently large, we have uniformly in (integer) $r\ge1$ that*

$$\begin{aligned}
&\int_{[0,2\pi]^2}\left|\sum_{k^1=[\lambda_1]}^{[\Lambda_1]}\sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2)e^{ik^{(2)}x^{(2)}}\{\Lambda_3(k^{(2)})\}^r\right|\,\mathrm{d}x^{(2)}\\
&\lesssim\log(rQ)\int_{[0,2\pi]^2}\left|\tilde{D}_2^j(x^{(2)})\right|\,\mathrm{d}x^{(2)}\\
&\quad+\int_{[0,2\pi]^2}\left|\sum_{k^1=[\lambda_1]}^{[\Lambda_1]}\sum_{\substack{k^2=[\lambda_2(k^1)]\\ \tilde{\Lambda}_3(k^1,k^2)\in\mathbb{Z}}}^{[\Lambda_2(k^1)]} t_j(k^1,k^2)e^{ik^{(2)}x^{(2)}}\right|\,\mathrm{d}x^{(2)}+2^r
\end{aligned}$$

The proof differs from that of [KL18, Lemmas 3.8 and 3.9] in a few key location, so we give it here.

Proof. Using Equation (3.B.7) we have

$$\begin{aligned}
&\sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} \{\Lambda_3(k^{(2)})\}^r \\
&\quad = \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} \left(\gamma_3 + \{\tilde\Lambda_3(k^{(2)})\}\right)^r \\
&\qquad + \chi_{(\gamma_3<0)} \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{\substack{k^2=[\lambda_2(k^1)] \\ \tilde\Lambda_3(k^1,k^2)\in\mathbb{Z}}}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} + \text{mixed terms.}
\end{aligned}$$

All the mixed terms have at least one power of $\gamma_3 + \{\tilde\Lambda_3(k^{(2)})\} = \gamma_3$. (Indeed, in the mixed terms we have $\tilde\Lambda_3(k^{(2)}) \in \mathbb{Z}$ so $\{\tilde\Lambda_3(k^{(2)})\} = 0$.) Since $|\gamma_3| < 1/(qQ_\infty) \leq 1/Q$ the sum of all mixed terms may be bounded by $2^r R^4 Q^{-1} \lesssim 2^r$ for N sufficiently large (independent of r) by our choice of Q, see Definition 3.2.7. Similarly expanding the first summand, all the terms with at least one power of γ_3 may be bounded the same way. We thus have

$$\begin{aligned}
&\sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} \{\Lambda_3(k^{(2)})\}^r \\
&\quad = \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} \{\tilde\Lambda_3(k^{(2)})\}^r \\
&\qquad + \chi_{(\gamma_3<0)} \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{\substack{k^2=[\lambda_2(k^1)] \\ \tilde\Lambda_3(k^1,k^2)\in\mathbb{Z}}}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} + O(2^r),
\end{aligned} \tag{3.B.8}$$

where the error is $O(2^r)$ uniform in $x^{(2)}$. For the first summand we have by a simple modification of [KL18, Lemma 3.8] (including the factor t_j) that

$$\begin{aligned}
&\int_{[0,2\pi]^2} \left| \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} \{\tilde\Lambda_3(k^{(2)})\}^r \right| \,\mathrm{d}x^{(2)} \\
&\qquad\qquad \lesssim \log(rqQ_\infty) \int_{[0,2\pi]^2} \left| D_2^j(x^{(2)}) \right| \,\mathrm{d}x^{(2)}.
\end{aligned}$$

This importantly uses that $\{\tilde\Lambda_3(k^{(2)})\} \in \{0, \frac{1}{qQ_\infty}, \ldots, \frac{qQ_\infty - 1}{qQ_\infty}\}$ for integers k^1, k^2, so that on can find some smartly chosen function $h(u) \approx u^r$ on $[0,1]$ but with a smooth cut-off at 1 and $h(\{\tilde\Lambda_3(k^{(2)})\}) = \{\tilde\Lambda_3(k^{(2)})\}^r$ for which one can bound Fourier coefficients, see [KL18, Lemma 3.8].

We have $q \leq Q_\infty = Q_3\alpha_3 \leq CQ^{3/2}$. We conclude the desired. □

Next we bound the second term in Lemma 3.B.7, where $\tilde\Lambda_3$ is integer. If there are no valid choices of k^1, k^2 for which $\tilde\Lambda_3(k^1,k^2)$ is an integer, then this term is clearly zero. Otherwise we have the following.

Lemma 3.B.8. *Let N be sufficiently large and suppose that the set*

$$I_0 = \left\{(k^1,k^2) \in \mathbb{Z}^2 \,:\, [\lambda_1] \leq k^1 \leq [\Lambda_1],\, [\lambda_2(k^1)] \leq k^2 \leq [\Lambda_2(k^1)],\, \tilde\Lambda_3(k^1,k^2) \in \mathbb{Z}\right\}$$

is non-empty. Then we may find a point $k_0^{(2)} \in I_0$, a (non-zero) lattice vector $\kappa = \kappa^{(2)} \in \mathbb{Z}^2$ and an integer $h \geq 0$ with $k_0^{(2)} + h\kappa \in I_0$ (in particular $h|\kappa| \lesssim R$) such that $I_0 = \{k_0^{(2)} + \tau\kappa^{(2)} : \tau \in \{0, \ldots, h\}\}$. In particular

$$\int_{[0,2\pi]^2} \left| \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{\substack{k^2=[\lambda_2(k^1)] \\ \tilde{\Lambda}_3(k^1,k^2)\in\mathbb{Z}}}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} \right| \mathrm{d}x^{(2)} \lesssim \int_0^{2\pi} \left| \sum_{\tau=0}^{h} t_j\left(k_0^{(2)} + \tau\kappa^{(2)}\right) e^{i\tau|\kappa^{(2)}|x} \right| \mathrm{d}x. \tag{3.B.9}$$

The proof is an exercise in elementary number theory analysing the set I_0.

Proof. Define $k_0^{(2)}$ to be any point in the (non-empty) set I_0. Recall Equation (3.B.6), and that $\left|\tilde{\Lambda}_3(k^1,k^2)\right| \leq CR$ for any $k^{(2)} \in I_0$. (This follows since the relevant tetrahedron is contained in $[0, CR]^3$.) By redefining α_j as $\alpha_j / \gcd(\alpha_1, \alpha_2, \alpha_3)$ we may assume that $\alpha_1, \alpha_2, \alpha_3$ have no shared prime factors. (This only decreases their values, so that still $|\alpha_j| \leq C\sqrt{Q}$.) In case one of the α_j's is zero we will use the convention that $\gcd(\alpha, \beta, 0) = \gcd(\alpha, \beta)$ and $\gcd(\alpha, 0) = \alpha$ for $\alpha, \beta > 0$.

Solving the general problem. We first consider the general problem of finding all $k^1, k^2 \in \mathbb{Z}$ for which $\tilde{\Lambda}_3(k^1,k^2)$ is an integer. This set has the form $k_0^{(2)} + \Gamma$ for some two-dimensional lattice Γ. We now find spanning lattice vectors of Γ.

Define $\alpha_{ij} = \gcd(\alpha_i, \alpha_j)$ for $i \neq j$. (Note that the α_j's are not necessarily pairwise coprime, only all 3 α_j's have no shared factor by the reduction above. Also, since α_1 and α_2 are not both 0, we have $\alpha_{12} \neq 0$ is well-defined.) Shifting $k_0^{(2)}$ by $\kappa_0 := (Q_2 \frac{\alpha_2}{\alpha_{12}}, -Q_1 \frac{\alpha_1}{\alpha_{12}})$ we have

$$\tilde{\Lambda}_3(k_0^{(2)} + b\kappa_0) = \tilde{\Lambda}_3(k_0^{(2)}) \in \mathbb{Z}, \qquad b \in \mathbb{Z}$$

and κ_0 is the shortest lattice vector with this property. One should note here that κ_0 is not "short". Indeed $|\kappa_0| \gtrsim Q$ since both $Q_1, Q_2 \gtrsim Q$, see Definition 3.2.7, and α_1, α_2 are not both 0. We now look for the lattice vector in Γ giving the smallest possible (integer) increase of $\tilde{\Lambda}_3$. This lattice vector together with κ_0 spans Γ. Note that

$$\delta\tilde{\Lambda}_3(\kappa) := \tilde{\Lambda}_3(k_0^{(2)} + \kappa) - \tilde{\Lambda}_3(k_0^{(2)}) = \frac{-Q_1\alpha_1\kappa^1 - Q_2\alpha_2\kappa^2}{Q_3\alpha_3}. \tag{3.B.10}$$

Suppose first that either $\alpha_1 = 0$ or $\alpha_2 = 0$, say $\alpha_2 = 0$. Now, $Q_1 \neq Q_3$ and $|\alpha_j| \leq C\sqrt{Q}$ so Q_j is not a factor of α_i for any $i = 1, 3, j = 1, 2, 3$. Thus, $\gcd(Q_3\alpha_3, Q_1\alpha_1) = \gcd(\alpha_1, \alpha_3) = 1$ since $\alpha_2 = 0$. For the ratio $\delta\tilde{\Lambda}_3(\kappa)$ to be an integer we need that the numerator is some multiple of $Q_3\alpha_3$, and thus that $|\kappa| \gtrsim Q_3 \gg R$. Thus there is at most one $k_0^{(2)} \in I_0$ and the lemma is clear.

Suppose then that $\alpha_1 \neq 0$, $\alpha_2 \neq 0$. Varying $\kappa \in \mathbb{Z}^2$ we have by Bézout's lemma that the numerator in Equation (3.B.10) assumes as values all multiples of $\gcd(Q_1\alpha_1, Q_2\alpha_2)$. We have $\gcd(Q_1\alpha_1, Q_2\alpha_2) = \gcd(\alpha_1, \alpha_2) = \alpha_{12}$. For the ratio $\delta\tilde{\Lambda}_3(\kappa)$ to be an integer we need that the numerator is some multiple of $Q_3\alpha_3$. Since by assumption there are no prime factors shared by all α_j's and Q_3 is not a factor of α_{12} we have $\gcd(\alpha_{12}, Q_3\alpha_3) = 1$. Thus, the smallest integer increase of $\tilde{\Lambda}_3$ is $\alpha_{12} \geq 1$ and this happens along some lattice vector κ_1.

Immediately then $\Gamma \supset \{a\kappa_1 + b\kappa_0 : a, b \in \mathbb{Z}\}$. To see that $\Gamma \subset \{a\kappa_1 + b\kappa_0 : a, b \in \mathbb{Z}\}$ note that by Bézout's lemma the (integer) solutions to the equation

$$-Q_1\alpha_1\kappa^1 - Q_2\alpha_2\kappa^2 = Q_3\alpha_3 A,$$

for some integer $A \in \mathbb{Z}$, is exactly $(\kappa^1, \kappa^2) \in \left\{\frac{A}{\alpha_{12}}\kappa_1 + b\kappa_0 : b \in \mathbb{Z}\right\}$ if α_{12} divides A and there are no solutions otherwise. In summary then

$$\Gamma = \{a\kappa_1 + b\kappa_0 : a, b \in \mathbb{Z}\}, \qquad \tilde{\Lambda}_3(k_0^{(2)} + a\kappa_1 + b\kappa_0) = \tilde{\Lambda}_3(k_0^{(2)}) + a\alpha_{12}, \quad a, b \in \mathbb{Z}. \tag{3.B.11}$$

Moreover

$$I_0 = \left(k_0^{(2)} + \Gamma\right) \cap \left\{(k^1, k^2) \in \mathbb{Z}^2 \,:\, [\lambda_1] \leq k^1 \leq [\Lambda_1],\, [\lambda_2(k^1)] \leq k^2 \leq [\Lambda_2(k^1)]\right\}.$$

Finding the candidate for κ. We now find the candidate for the κ in the lemma. Either $I_0 = \{k_0^{(2)}\}$, in which case the lemma is clear (take $h = 0$), or there exists some (non-zero) $\kappa = a\kappa_1 + b\kappa_0 \in \Gamma$ such that $k_0^{(2)} + \kappa \in I_0$. For such κ we have (for sufficiently large N) that $a \neq 0$ as $|\kappa_0| \gtrsim Q \gg R$ and any such κ has $|\kappa| \leq CR$. Let $\kappa_2 = a_2\kappa_1 + b_2\kappa_0$ be the κ such that $k_0^{(2)} + \kappa \in I_0$ with minimal value of $|a_2|$. (κ_2 is unique up to potentially a sign if both $k_0^{(2)} - \kappa_2 \in I_0$ and $k_0^{(2)} + \kappa_2 \in I_0$.) It follows from Equation (3.B.11) that $|a_2| \leq CR/\alpha_{12} \leq CR$ since $|\delta\tilde{\Lambda}_3(\kappa_2)| \leq CR$ as the tetrahedron is contained in $[0, CR]^3$.

If $b_2 = 0$ then $a_2 = \pm 1$, else if $b_2 \neq 0$ then $\gcd(a_2, b_2) = 1$. Indeed, if a_2 and b_2 shared some common factor, we could factor this out to find a κ with smaller value $|a|$ contradicting the minimality of $|a_2|$.

Characterizing all allowed κ's. We claim that by potentially redefining $k_0^{(2)}$ to $k_0^{(2)} - a\kappa_2$ with $a \in \mathbb{Z}$ largest such that still $k_0^{(2)} - a\kappa_2 \in I_0$ we have that

$$I_0 = \{k_0^{(2)} + \tau\kappa_2 : \tau \in \{0, \ldots, h\}\}, \qquad \text{for some } h \in \mathbb{Z}, h \geq 0. \tag{3.B.12}$$

(The intuition for the remainder of the argument is as follows. Essentially, if some κ had $k_0^{(2)} + \kappa \in I_0$ but was not a multiple of κ_2, it would have to differ from some multiple of κ_2 by at least κ_0 or κ_1. Since $|\kappa_0| \gg R$ and either $\kappa_1 = \kappa_2$ or $|\kappa_1| \gg R$, this is impossible.)

To prove Equation (3.B.12) we first introduce the following notation. We view a lattice vector $\kappa \in \mathbb{Z}^2$ as a vector $\kappa \in \mathbb{R}^2$ and write $\kappa^\parallel$ for its component parallel to κ_0. Note that $\kappa^\parallel$ need not have integer coordinates. Define the constant A such that $\kappa_1^\parallel = A\kappa_0$. (Note that A need not be an integer.) Let $0 \neq \kappa = a\kappa_1 + b\kappa_0 \in \Gamma$ with $k_0^{(2)} + \kappa \in I_0$. We have

$$\kappa^\parallel = a\kappa_1^\parallel + b\kappa_0 = (aA + b)\kappa_0.$$

Thus, since $|\kappa_0| \gtrsim Q$, $|\kappa| \lesssim CR$ and $|a| \geq 1$ (since $\kappa \neq 0$) we have $\left|\frac{b}{a} + A\right| \leq \frac{CR}{Q}$.

Using this also for $\kappa_2 = a_2\kappa_1 + b_2\kappa_0$ we get

$$|ba_2 - b_2a| = \left|\frac{b}{a} - \frac{b_2}{a_2}\right| |aa_2| \leq |aa_2| \left(\left|\frac{b}{a} + A\right| + \left|-\frac{b_2}{a_2} - A\right|\right) \leq CR^2\frac{R}{Q} \ll 1.$$

But $ba_2 - b_2a$ is an integer. Hence (for N sufficiently large) we have $ba_2 = b_2a$. Now, if $b_2 = 0$ then $b = 0$ and so $a_2 = \pm 1$ is a divisor of a so $\kappa = \pm a\kappa_2$. If $b_2 \neq 0$ then $\gcd(a_2, b_2) = 1$ and thus a_2 is again a divisor of a and $a/a_2 = b/b_2$. Then $\kappa = \frac{a}{a_2}\kappa_2$ is a multiple of κ_2. This shows the desired.

Integral form. To prove Equation (3.B.9) we do the following. Define $e_2 = \kappa_2/|\kappa_2|$ as the unit vector parallel to κ_2 and $e_2^\perp$ as the unit vector perpendicular to κ_2. Then define the domain

$$S_0 := \left\{x^{(2)} \in \mathbb{R}^2 : \left|x^{(2)} \cdot e_2\right| \le 4\pi, \left|x^{(2)} \cdot e_2^\perp\right| \le 4\pi\right\}$$

and note that $[0, 2\pi]^2 \subset S_0$. Thus, using Equation (3.B.12)

$$\int_{[0,2\pi]^2} \left|\sum_{k \in I_0} t_j(k^1, k^2) e^{ik^{(2)}x^{(2)}}\right| \mathrm{d}x^{(2)} \le \int_{S_0} \left|\sum_{\tau=0}^{h} t_j\left(k_0^{(2)} + \tau\kappa^{(2)}\right) e^{i\tau\kappa^{(2)}x^{(2)}}\right| \mathrm{d}x^{(2)}.$$

The integrand is constant in the $e_2^\perp$-direction, and 2π-periodic in the e_2-direction. Thus, computing the integral in these coordinates we have

$$\int_{S_0} \left|\sum_{\tau=0}^{h} t_j\left(k_0^{(2)} + \tau\kappa^{(2)}\right) e^{i\tau\kappa^{(2)}x^{(2)}}\right| \mathrm{d}x^{(2)} = 32\pi \int_0^{2\pi} \left|\sum_{\tau=0}^{h} t_j\left(k_0^{(2)} + \tau\kappa^{(2)}\right) e^{i\tau|\kappa^{(2)}|x}\right| \mathrm{d}x.$$

This concludes the proof. □

Combining Lemmas 3.B.5, 3.B.6, 3.B.7 and 3.B.8 the r- and ν-sums in Lemmas 3.B.5 and 3.B.6 are readily bounded because of the factor $1/r!$ from Lemma 3.B.5. We conclude that

$$\int_{[0,2\pi]^3} \left|F_3^j(x)\right| \mathrm{d}x \lesssim \log Q \int_{[0,2\pi]^2} \left|\tilde{D}_2^j(x)\right| \mathrm{d}x + 1 + \int_0^{2\pi} \left|\sum_{\tau=0}^{h} t_j\left(k_0^{(2)} + \tau\kappa^{(2)}\right) e^{i\tau|\kappa^{(2)}|x^1}\right| \mathrm{d}x^1,$$

where $k_0^{(2)}$ and $\kappa^{(2)}$ are as in Lemma 3.B.8. If the set I_0 from Lemma 3.B.8 is empty, then the bound is valid without the last term. In particular it is valid with any $k_0^{(2)} \in [0, CR]^2$, (non-zero) $\kappa = \kappa^{(2)} \in \mathbb{Z}^2$ and $h = 0$. Thus, by Lemma 3.B.4 and Equation (3.B.5) we prove the desired bound, Lemma 3.B.3.

3.B.3 Reduction from $d = 2$ to $d = 1$

For $j = 1, 2$ we will do one more step reducing the dimension. The argument is basically the same as for going from dimension $d = 3$ to $d = 2$ in Section 3.B.2. We sketch the main differences.

As we did in Section 3.B.1 for $d = 3$ by adding and subtracting the lower tail of the sum, we may assume that the k^2-sum is $\sum_{k^2=0}^{[\Lambda_2(k^1)]}$.

Remark 3.B.9. It is valid here to make the k^2-sum go from 0, since now the k^2-sum is the innermost sum and we do not risk values of k^3 much larger that R by doing so (as in Remark 3.B.2). Indeed, we already computed the sum over the relevant k^3. We could at this point also do the same splitting of the k^1-sum, but we would have the same problems that $\Lambda_2(k^1)$ or $\lambda_2(k^1)$ might be much larger than R for $k^1 \le \lambda_1$ as in Remark 3.B.2.

Additionally, by splitting the k^1-sum into at most 2 parts, we may assume that Λ_2 is just the equation for a line. Here again one needs to be careful with what to do with the boundary terms. This gives some sums over 1-dimensional tetrahedra (i.e. line segments), which we can write as differences of sums over 2-dimensional tetrahedra exactly as for the 3-dimensional case. We are led to define the quantities

$$
\begin{aligned}
D_2^j(x) &:= \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} t_j(k^1) \sum_{k^2=0}^{[\Lambda_2(k^1)]} e^{ik^{(2)}x^{(2)}}, \\
\tilde{D}_1^j(x) &:= \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} t_j(k^1) e^{ik^1x^1}, \\
G_2^j(x) &:= \frac{1}{e^{ix^2}-1}\left(e^{i(n_2+1)x^2}\tilde{D}_1^j(x^1-m_1x^2) - \tilde{D}_1^j(x^1)\right), \\
F_2^j(x) &:= \frac{e^{i(n_2+1)x^2}}{e^{ix^2}-1}\sum_{k^1=[\lambda_1]}^{[\Lambda_1]} t_j(k^1)e^{ik^1(x^1-m_1x^2)}\left(e^{-i\langle \Lambda_2(k^1)\rangle x^2}-1\right).
\end{aligned}
$$

We claim the following inductive bound.

Lemma 3.B.10. *For $j=1,2$ we have for N sufficiently large that*

$$
\int_{[0,2\pi]^2}\left|D_2^j(x^{(2)})\right| \,\mathrm{d}x^{(2)} \lesssim (\log R + \log Q)\int_{[0,2\pi]}\left|\tilde{D}_1^j(x^1)\right| \,\mathrm{d}x^1 + \begin{cases} R & j=1, \\ R^2 & j=2. \end{cases}
$$

Proof. As for Λ_3, we have that the equation of a line between any two points $(p_i^1/Q_1, p_i^2/Q_2)$, $i=1,2$ is given by

$$
\frac{p_1^1-p_2^1}{Q_2}k^1 + \frac{p_2^2-p_1^2}{Q_1}k^2 = \text{const}\,.
$$

If we choose the points to be either corners of RP or the central point Rz we get the equation

$$
\frac{\alpha_1}{Q_2}k^1 + \frac{\alpha_2}{Q_1}k^2 = R\sigma\gamma \notin \mathbb{Q}.
$$

Here we might have that $\alpha_1 = 0$ or $\alpha_2 = 0$.

If $\alpha_2 = 0$ this line is parallel to the k^2-axis and so does not give rise to a bound for the k^2-sum. Thus $\alpha_2 \neq 0$. If $\alpha_1 = 0$ the sum in $D_2^j(x)$ and integral thereof factorizes, and hence by [KL18, Lemma 3.2] we have that

$$
\int_{[0,2\pi]^2}\left|D_2^j(x^{(2)})\right| \,\mathrm{d}x^{(2)} \le C\log R\int_0^{2\pi}\left|\tilde{D}_1^j(x^1)\right| \,\mathrm{d}x^1.
$$

Hence, this case yields the desired inductive bound, Lemma 3.B.10. Suppose then $\alpha_1, \alpha_2 \neq 0$.

Then

$$
\Lambda_2(k^1) = n_2 - m_1k^1 = n_2 - \frac{Q_1\alpha_1}{Q_2\alpha_2}k^1, \qquad n_2 \notin \mathbb{Q}, \qquad |\alpha_j| \le CQ^{1/4}, \quad j=1,2.
$$

Lemmas 3.B.4, 3.B.5 and 3.B.6 are readily adapted and proven as before. The adaptation of Lemma 3.B.7 is then mostly analogous. One chooses $Q_\infty = Q_2\alpha_2$ and finds the rational approximation of Λ_2 as

$$
\tilde{\Lambda}_2(k^1) = \Lambda_2(k^1) - \gamma_2 = \frac{p}{q} - \frac{Q_1\alpha_1}{Q_2\alpha_2}k^1, \qquad |\gamma_2| < \frac{1}{qQ_\infty} \le Q^{-1}.
$$

The rest of the argument follows exactly as for $d = 3$ only that the extra term of the sum where $\tilde{\Lambda}_2(k^1) \in \mathbb{Z}$ may be bounded as follows.

$$\left| \sum_{\substack{k^1=[\lambda_1] \\ \tilde{\Lambda}_2(k^1)\in\mathbb{Z}}}^{[\Lambda_1]} t_j(k^1) e^{ik^1x^1} \right| \leq \begin{cases} R & j=1 \\ R^2 & j=2 \end{cases}$$

since there is at most one k^1 such that $\tilde{\Lambda}_2(k^1)$ is an integer. To see this note that $\gcd(\alpha_1, Q_2) = 1$ since $|\alpha_1| \leq CQ^{1/4} \ll Q_2$, hence the change in k^1 to change $\tilde{\Lambda}_2(k^1)$ by an integer is at least $Q_3 \gg R$. We thus conclude the desired bound. □

3.B.4 Bounding the one-dimensional integrals

Now we bound $\int |\tilde{D}_1^j|$ and $\int \left|\sum_{\tau=0}^{h} t_j\left(k_0^{(2)} + \tau\kappa\right) e^{i\tau|\kappa|x}\right| \mathrm{d}x$ from the right-hand-sides of Lemmas 3.B.3 and 3.B.10. For $\tilde{D}_1^j$ we may assume that the lower bound of the summations are at 0 by the same procedure as in Section 3.B.1. Expanding $t_j\left(k_0^{(2)} + \tau\kappa\right)$ we see that $j = 1$ gives an affine expression in τ and $j = 2, 3$ give quadratic expressions in τ. For instance,

$$t_2\left(k_0^{(2)} + \tau\kappa\right) = (k_0^1)^2 + 2k_0^1\kappa^1\tau + (\kappa^1)^2\tau^2.$$

Thus, bounding both the integrals amounts to bounding the following:

Lemma 3.B.11. *Let $M \geq 2$ be an integer. Then*

(1) $\displaystyle\int_0^{2\pi} \left|\sum_{k=0}^{M} e^{ikx}\right| \mathrm{d}x \leq C\log M$*,*

(2) $\displaystyle\int_0^{2\pi} \left|\sum_{k=0}^{M} ke^{ikx}\right| \mathrm{d}x \leq CM\log M$*,*

(3) $\displaystyle\int_0^{2\pi} \left|\sum_{k=0}^{M} k^2e^{ikx}\right| \mathrm{d}x \leq CM^2\log M$*.*

Proof. The bound (1) is elementary, see also [KL18, Lemma 3.2]. For any $M \in \mathbb{N}$ and $q \in \mathbb{C} \setminus \{1\}$ we have

$$\begin{aligned} \sum_{k=0}^{M} q^k &= \frac{q^{M+1}-1}{q-1} \\ \sum_{k=0}^{M} kq^k &= \frac{q}{(q-1)^2}\left[q^M(Mq-M-1)+1\right] \\ \sum_{k=0}^{M} k^2q^k &= \frac{q}{(q-1)^3}\left[q^M\left(M^2(q-1)^2-2M(q-1)+q+1\right)-q-1\right]. \end{aligned} \tag{3.B.13}$$

Consider now the integrals (2) and (3). By symmetry of complex conjugation $\int_0^{2\pi} = 2\int_0^{\pi}$. We split the integrals according according to whether $x \leq 1/M$ or $x \geq 1/M$. For $x \leq 1/M$ we have

$$\int_0^{1/M} \left|\sum_{k=0}^{M} ke^{ikx}\right| \mathrm{d}x \lesssim \int_0^{1/M} M^2\,\mathrm{d}x \lesssim M,$$

$$\int_0^{1/M} \left|\sum_{k=0}^{M} k^2e^{ikx}\right| \mathrm{d}x \lesssim \int_0^{1/M} M^3\,\mathrm{d}x \lesssim M^2.$$

For $x \geq 1/M$ we use Equation (3.B.13) and note that $|e^{ix} - 1| \geq cx$ for $x \leq \pi$. Expanding the exponentials $e^{ix} = 1 + O(x)$ we thus have

$$\begin{aligned}\int_{1/N}^{\pi} \left| \sum_{k=0}^{M} k e^{ikx} \right| \mathrm{d}x &\lesssim \int_{1/M}^{\pi} \frac{1}{x^2} \left[M e^{iMx}(e^{ix} - 1) + 1 - e^{iMx} \right] \mathrm{d}x \\ &\lesssim \int_{1/M}^{\pi} \left(\frac{M}{x} + \frac{1}{x^2} \right) \mathrm{d}x \lesssim M \log M\end{aligned}$$

and

$$\begin{aligned}&\int_{1/N}^{\pi} \left| \sum_{k=0}^{M} k^2 e^{ikx} \right| \mathrm{d}x \\ &\lesssim \int_{1/M}^{\pi} \frac{1}{x^3} \left[e^{iMx} \left(M^2 (e^{ix} - 1)^2 - 2M(e^{ix} - 1) + e^{ix} + 1 \right) - e^{ix} - 1 \right] \mathrm{d}x \\ &\lesssim \int_{1/M}^{\pi} \left(\frac{M^2}{x} + \frac{M}{x^2} + \frac{1}{x^3} \right) \mathrm{d}x \lesssim M^2 \log M.\end{aligned}$$

This concludes the proof. □

With this we may thus bound for ($j = 2$, say)

$$\begin{aligned}&\int_0^{2\pi} \left| \sum_{\tau=0}^{h} t_2 \left(k_0^{(2)} + \tau\kappa \right) e^{i\tau|\kappa|x} \right| \mathrm{d}x \\ &= \int_0^{2\pi} \left| \sum_{\tau=0}^{h} \left((k_0^1)^2 + 2k_0^1 \kappa^1 \tau + (\kappa^1)^2 \tau^2 \right) e^{i\tau|\kappa|x} \right| \mathrm{d}x \\ &\leq CR^2 \int_0^{2\pi} \left| \sum_{\tau=0}^{h} e^{i\tau|\kappa|x} \right| \mathrm{d}x + CR|\kappa| \int_0^{2\pi} \left| \sum_{\tau=0}^{h} \tau e^{i\tau|\kappa|x} \right| \mathrm{d}x + C|\kappa|^2 \int_0^{2\pi} \left| \sum_{\tau=0}^{h} \tau^2 e^{i\tau|\kappa|x} \right| \mathrm{d}x\,.\end{aligned}$$

Substituting $y = |\kappa|x$, using Lemma 3.B.11 and recalling that $h|\kappa| \lesssim R$ and $|\kappa| \geq 1$ by Lemma 3.B.8 we may bound this by $R^2 \log R$. An analoguous bound holds for $j = 1$. This takes care of all the one-dimensional integrals. In combination with Lemmas 3.B.3 and 3.B.10 we get the bounds for $j = 1, 2$ of Equation (3.B.2). It remains to consider the two-dimensional integral for $j = 3$.

3.B.5 Bounding the $j = 3$ two-dimensional integral

We are left with bounding the integral $\int |\tilde{D}_2^3|$ on the right-hand-side of Lemma 3.B.3. We first reduce to the case of a simpler tetrahedron (triangle). By shifting the sums by a fixed $\kappa = (\kappa^1, 0) \in \mathbb{Z}^2$ and using the bounds in Lemma 3.B.11 to evaluate the extra contributions of the shift, we may assume that the k^1-sum starts at 0. By splitting the k^2-sum as in Section 3.B.1 we may assume that that k^2-sum also starts at 0. That is, we need to evaluate the integral

$$\iint_{[0,2\pi]^2} \left| \sum_{k=0}^{[\Lambda_1]} \sum_{\ell=0}^{[\Lambda_2(k)]} k\ell e^{ikx} e^{i\ell y} \right| \mathrm{d}x\, \mathrm{d}y,$$

where $\Lambda_2(k) = n_2 - \frac{Q_1\alpha_1}{Q_2\alpha_2} k$ for an irrational n_2. Recall that $|\Lambda_1| \leq CR$ and for any $0 \leq k \leq [\Lambda_1]$ we have $|\Lambda_2(k)| \leq CR$.

The analysis given here is in spirit the same as given in Sections 3.B.2, 3.B.3 and 3.B.4. It is sufficiently different that we find it easier to do the arguments separately. We shall show the following.

Lemma 3.B.12. *We have the following bound*

$$\iint_{[0,2\pi]^2} \left| \sum_{k=0}^{[\Lambda_1]} \sum_{\ell=0}^{[\Lambda_2(k)]} k\ell e^{ikx} e^{i\ell y} \right| \mathrm{d}x\, \mathrm{d}y \le CR^2 (\log R)^2 \log Q.$$

Combining then Lemmas 3.B.3, 3.B.10, 3.B.11 and 3.B.12 and choosing Q some sufficiently large power of N as required in Definition 3.2.7 we conclude the proof of Equation (3.B.2) and thus of Lemma 3.4.9. It remains to give the proof of Lemma 3.B.12.

Proof. Denote $M = [\Lambda_1]$ and recall $\Lambda_2(k) = n_2 - m_1 k = n_2 - \frac{Q_1\alpha_1}{Q_2\alpha_2} k$. First note that by mapping $\ell \mapsto [\Lambda_2(k)] - \ell$ we may assume that $m_1 \ge 0$. If $m_1 = 0$ the sum factors, and so does the integral into two one-dimensional sums/integrals. These may be bounded using Lemma 3.B.11. In this case we get the bound $\le CR^2(\log R)^2$ as desired. Hence assume that $m_1 > 0$. Moreover, if $n_2 > m_1 M$ we may split the (k,ℓ)-sum into two parts,

$$\sum_{k=0}^{M} \sum_{\ell=0}^{[\Lambda_2(k)]} = \sum_{k=0}^{M} \sum_{\ell=0}^{[n_2 - m_1 M]} + \sum_{k=0}^{M} \sum_{\ell=[n_2-m_1M]+1}^{[\Lambda_2(k)]} .$$

The first sum factors into one-dimensional integrals which we may bound using Lemma 3.B.11 again. The second we may shift by a constant ℓ (again then using Lemma 3.B.11 to evaluate the contribution of the shift) and assume that the lower limit of the ℓ-sum is 0. The upper limit then becomes $[\Lambda(k)]$, where

$$\Lambda(k) = n_2 - ([n_2 - m_1 M] + 1) - m_1 k := n - mk\,.$$

Geometrically, this means that the domain of the (k,ℓ)-sum is a triangle with two sides along the axes. We thus need to bound

$$\iint_{[0,2\pi]^2} \left| \sum_{k=0}^{M} \sum_{\ell=0}^{[\Lambda(k)]} k\ell e^{ikx} e^{i\ell y} \right| \mathrm{d}x\, \mathrm{d}y,$$

where

$$\Lambda(k) = n - mk, \qquad M \le R, \qquad mM = n + O(1), \qquad n \le R.$$

By the symmetries of translation invariance and complex conjugation we may integrate over the domain $[-\pi,\pi] \times [0,\pi]$ instead. We evaluate the ℓ-sum using Equation (3.B.13). Recall that $[\Lambda(k)] = \Lambda(k) - \langle \Lambda(k) \rangle$. We thus have

$$\begin{aligned}
\sum_{\ell=0}^{[\Lambda(k)]} \ell e^{i\ell y} &= \frac{e^{iy}}{(e^{iy}-1)^2} \left[e^{i[\Lambda(k)]y}([\Lambda(k)]e^{iy} - [\Lambda(k)] - 1) + 1 \right] \\
&= \frac{e^{iy}}{(e^{iy}-1)^2} \Big[\Big(e^{i\Lambda(k)y}(\Lambda(k)e^{iy} - \Lambda(k) - 1) + 1 \Big) \\
&\qquad + \Big(e^{-i\langle\Lambda(k)\rangle y} - 1 \Big) \Big(e^{i\Lambda(k)y}(\Lambda(k)e^{iy} - \Lambda(k) - 1) + 1 \Big) \\
&\qquad - \Big(\langle\Lambda(k)\rangle\, e^{i(\Lambda(k) - \langle\Lambda(k)\rangle)y}(e^{iy} - 1) + (e^{-i\langle\Lambda(k)\rangle y} - 1) \Big) \Big] \\
&=: (\mathrm{I}) + (\mathrm{II}) + (\mathrm{III}).
\end{aligned}$$

The third summand (III) may be calculated as

$$\frac{-e^{iy}}{(e^{iy}-1)^2}\left[\langle\Lambda(k)\rangle\left(e^{i[\Lambda(k)]y}-1\right)iy+O(y^2)\right].$$

The factor $\frac{-e^{iy}}{(e^{iy}-1)^2}$ may be bounded by $1/y^2$. For this term we split the y-integral according to whether $y\leq 1/n$ or $y\geq 1/n$. For $y\leq 1/n$ we expand additionally $e^{i[\Lambda(k)]y}-1=O(ny)$. We get the contribution

$$\int_{-\pi}^{\pi}\mathrm{d}x\int_0^{1/n}\mathrm{d}y\frac{1}{y^2}\left|\sum_{k=0}^{M}ke^{ikx}\left[\langle\Lambda(k)\rangle\left(e^{i[\Lambda(k)]y}-1\right)y+O(y^2)\right]\right|\lesssim\frac{1}{n}M^2n+\frac{1}{n}M^2\lesssim R^2.$$

For $y\geq 1/n$ we bound $e^{i[\Lambda(k)]y}-1=O(1)$. We get

$$\begin{aligned}\int_{-\pi}^{\pi}\mathrm{d}x\int_{1/n}^{\pi}\mathrm{d}y\frac{1}{y^2}\left|\sum_{k=0}^{M}ke^{ikx}\left[\langle\Lambda(k)\rangle\left(e^{i[\Lambda(k)]y}-1\right)y+O(y^2)\right]\right|&\lesssim(\log n)M^2+M^2\\&\lesssim R^2\log R.\end{aligned}$$

For the second summand (II) we again split the integral according to whether $y\leq 1/n$ or $y\geq 1/n$. If $y\leq 1/n$ we have

$$\frac{e^{iy}}{(e^{iy}-1)^2}\left(e^{-i\langle\Lambda(k)\rangle y}-1\right)\left(e^{i\Lambda(k)y}(\Lambda(k)e^{iy}-\Lambda(k)-1)+1\right)=O(\Lambda(k)^2y)=O(n).$$

Hence this contributes the term

$$\int_{-\pi}^{\pi}\mathrm{d}x\int_0^{1/n}\mathrm{d}y\left|\sum_{k=0}^{M}ke^{ikx}O(\Lambda(k)^2y)\right|\lesssim\frac{1}{n}M^2n\lesssim R^2.$$

For $y\geq 1/n$ we write

$$\begin{aligned}&\frac{e^{iy}}{(e^{iy}-1)^2}\left(e^{-i\langle\Lambda(k)\rangle y}-1\right)\left(e^{i\Lambda(k)y}(\Lambda(k)e^{iy}-\Lambda(k)-1)+1\right)\\&\quad=\frac{e^{iy}}{(e^{iy}-1)^2}\sum_{\nu=1}^{\infty}\frac{(-iy)^\nu}{\nu!}\langle\Lambda(k)\rangle^\nu\left(e^{i\Lambda(k)y}(\Lambda(k)e^{iy}-\Lambda(k)-1)+1\right).\end{aligned}$$

Again we bound the factor $\frac{e^{iy}}{(e^{iy}-1)^2}$ as $1/y^2$. We treat each summand similarly as in Lemmas 3.B.6 and 3.B.7 (or rather, the 2-dimensional version of these as used in Section 3.B.3.) Completely analogously to Lemma 3.B.6 we see that for any integer $r\geq 1$ we have

$$\begin{aligned}&\iint\left|\sum_{k=0}^{M}ke^{ikx}\frac{e^{i\Lambda(k)y}(\Lambda(k)e^{iy}-\Lambda(k)-1)+1}{y^2}\langle\Lambda(k)\rangle^r\right|\mathrm{d}x\,\mathrm{d}y\\&\leq\iint\left|\sum_{k=0}^{M}ke^{ikx}\frac{e^{i\Lambda(k)y}(\Lambda(k)e^{iy}-\Lambda(k)-1)+1}{y^2}\right|\mathrm{d}x\,\mathrm{d}y\\&\quad+\sum_{\nu=1}^{r}\binom{r}{\nu}\iint\left|\sum_{k=0}^{M}ke^{ikx}\frac{e^{i\Lambda(k)y}(\Lambda(k)e^{iy}-\Lambda(k)-1)+1}{y^2}\{\Lambda(k)\}^\nu\right|\mathrm{d}x\,\mathrm{d}y,\end{aligned}$$

for either definition of $\langle\cdot\rangle$ (i.e. either $\langle\cdot\rangle=\{\cdot\}$ or $\langle\cdot\rangle=\cdot-\lceil\cdot\rceil$). Also the application of Lemma 3.B.7 is analogous to its use in Section 3.B.3. There is at most one k such that

$\tilde{\Lambda}(k) \in \mathbb{Z}$ for the appropriate rational approximation $\tilde{\Lambda}$ of Λ. Using that $e^{iy} = 1 + O(y)$ we obtain the bound

$$\left| ke^{ikx} \frac{e^{i\Lambda(k)y}(\Lambda(k)e^{iy} - \Lambda(k) - 1) + 1}{y^2} \right| \lesssim M \frac{ny+1}{y^2} \lesssim \frac{R^2}{y} + \frac{R}{y^2},$$

valid for any k. Hence this error term contributes at most

$$\int_{-\pi}^{\pi} \mathrm{d}x \int_{1/n}^{\pi} \mathrm{d}y \left(\frac{R^2}{y} + \frac{R}{y^2} \right) \lesssim R^2 \log n + Rn \lesssim R^2 \log R.$$

The rest of the argument in Lemma 3.B.7 is the same. We conclude that we may bound the contribution of the term (II) by that of (I) up to a factor of $\log Q$ and an error $R^2 \log R$, i.e.

$$\iint \left| \sum_k ke^{ikx}(\mathrm{II}) \right| \mathrm{d}x\,\mathrm{d}y \lesssim \log Q \iint \left| \sum_k ke^{ikx}(\mathrm{I}) \right| \mathrm{d}x\,\mathrm{d}y + R^2 \log R.$$

In particular

$$\begin{aligned} &\iint_{[0,2\pi]^2} \left| \sum_{k=0}^{M} \sum_{\ell=0}^{[\Lambda(k)]} k\ell e^{ikx} e^{i\ell y} \right| \mathrm{d}x\,\mathrm{d}y \\ &\quad\lesssim \log Q \int_{-\pi}^{\pi} \mathrm{d}x \int_0^{\pi} \mathrm{d}y \left| \sum_{k=0}^{M} ke^{ikx} \frac{e^{i\Lambda(k)y}(\Lambda(k)e^{iy} - \Lambda(k) - 1) + 1}{y^2} \right| + R^2 \log R. \end{aligned} \tag{3.B.14}$$

In order to evaluate the integral on the right-hand side, we split the integration domain into 5 regions, see Figure 3.B.1.

$$\begin{aligned} &I_1 = \{|x| \le 2/M, y \le 2/n\}, && I_2 = \{|x| \le 1/M, y \ge 2/n\}, \\ &I_3 = \{y \le 1/n, |x| \ge 2/M\}, && I_4 = \{y \ge 1/n, |x| \ge 1/M, |x - my| \ge 1/M\} \\ &I_5 = \{|x - my| \le 1/M, (x,y) \notin I_1\}. \end{aligned}$$

We will be a bit sloppy with notation and refer to both the domain of integration and the value of the integration over that domain by I_j.

(I_1). We expand

$$(*) := \sum_{k=0}^{M} ke^{ikx} \frac{e^{i\Lambda(k)y}(\Lambda(k)e^{iy} - \Lambda(k) - 1) + 1}{y^2}$$

(or rather the numerator) to second order in y. Using that $\Lambda(k) = O(n)$ we get that $(*) \lesssim M^2 n^2$. Thus the integral gives

$$I_1 \lesssim \int_{-2/M}^{2/M} \mathrm{d}x \int_0^{2/n} \mathrm{d}y M^2 n^2 \lesssim Mn \lesssim R^2.$$

(I_2). We expand $e^{iy} = 1 + O(y)$ in $(*)$. Then $(*) \lesssim \frac{M^2 n}{y} + \frac{M^2}{y^2}$. The integral is then $I_2 \lesssim R^2 \log R$.

(I_3, I_4, I_5). For the remaining integrals we use the explicit formula for $\Lambda(k) = n - mk$. Then

$$\begin{aligned} (*) &= \frac{1}{y^2} \sum_{k=0}^{M} ke^{ikx}(e^{i\Lambda(k)y}(\Lambda(k)e^{iy} - \Lambda(k) - 1) + 1) \\ &= \frac{1}{y^2} \sum_{k=0}^{M} \left(ke^{ikx} + ke^{ik(x-my)} e^{iny}(ne^{iy} - n - 1) + k^2 e^{ik(x-my)} e^{iny}(m - me^{iy}) \right) \\ &= \frac{1}{y^2} \left(-i\partial D(x) - ie^{iny}(ne^{iy} - n - 1)\partial D(x - my) + me^{iny}(e^{iy} - 1)\partial^2 D(x - my) \right), \end{aligned} \tag{3.B.15}$$

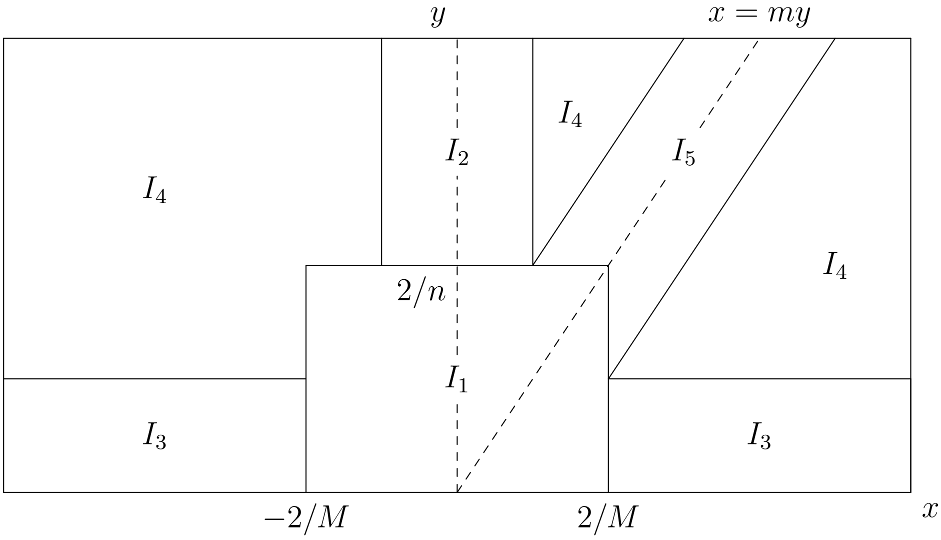


Figure 3.B.1: Decomposition of the domain $[-\pi, \pi] \times [0, \pi]$ into different regions.

where we introduced $D(z) = \sum_{k=0}^{M} e^{ikz} = \frac{e^{i(M+1)z}-1}{e^{iz}-1}$. From Equation (3.B.13) we conclude that we may bound derivatives of D as

$$|\partial D(z)| \lesssim \frac{M}{z} + \frac{1}{z^2}, \quad |\partial^2 D(z)| \lesssim \frac{M^2}{z} + \frac{M}{z^2} + \frac{1}{z^3}, \quad |\partial^3 D(z)| \lesssim \frac{M^3}{z} + \ldots + \frac{1}{z^4}. \tag{3.B.16}$$

(I_3). We have $y \leq 1/n$ and $|x| \geq 2/M$. We expand Equation (3.B.15) to second order in y. Expanding first the exponentials and then derivatives of D where needed we get

$$\begin{aligned}
\text{(3.B.15)} = \frac{1}{y^2}\Big(& - i\partial D(x) + i\partial D(x - my) + imy\partial^2 D(x - my) \\
& + O(n^2 y^2 \partial D(x - my)) + O(nmy^2 \partial^2 D(x - my))\Big) \\
\lesssim\ & n^2 \sup_y |\partial D(x - my)| + nm \sup_y |\partial^2 D(x - my)| + m^2 \sup_y |\partial^3 D(x - my)|.
\end{aligned}$$

Now we use the bounds Equation (3.B.16) and use that $z := x - my$ has $|z| \geq |x| - m/n = |x| - 1/M + O(1/(Mn))$ (recall that $mM = n + O(1)$) and $|x| \geq 2/M$. Thus

$$I_3 \lesssim \frac{1}{n} \int_{1/M}^{\pi} \mathrm{d}z \left(n^2 |\partial D(z)| + nm|\partial^2 D(z)| + m^2 |\partial^3 D(z)|\right) \lesssim R^2 \log R.$$

(I_4). We expand the exponentials $e^{iy} = 1 + O(y)$. Then

$$|\text{(3.B.15)}| \leq \frac{|\partial D(x)|}{y^2} + \frac{n|\partial D(x - my)|}{y} + \frac{|\partial D(x - my)|}{y^2} + \frac{m|\partial^2 D(x - my)|}{y}.$$

Using the bounds Equation (3.B.16) as before and noting that $|x| \geq 2/M$ and $z = x - my$ has $|z| \geq 1/M$ one easily sees that $I_4 \lesssim R^2 (\log R)^2$.

(I_5). Again, expanding the exponentials $e^{iy} = 1 + O(y)$ we have as for I_4 that

$$|\text{(3.B.15)}| \leq \frac{|\partial D(x)|}{y^2} + \frac{n|\partial D(x - my)|}{y} + \frac{|\partial D(x - my)|}{y^2} + \frac{m|\partial^2 D(x - my)|}{y}.$$

We use the bounds

$$|\partial D(z)| = \left|\sum_{k=0}^{M} k e^{ikz}\right| \leq M^2, \qquad |\partial^2 D(z)| = \left|\sum_{k=0}^{M} k^2 e^{ikz}\right| \leq M^3.$$

Thus

$$I_5 \lesssim \frac{1}{M}\int_{1/n}^{\pi} \frac{M^2}{y^2} + \frac{nM^2 + mM^3}{y}\, \mathsf{d}y \lesssim R^2 \log R.$$

We conclude that

$$\int_{-\pi}^{\pi} \mathsf{d}x \int_{0}^{\pi} \mathsf{d}y \left|\sum_{k=0}^{M} k e^{ikx} \frac{e^{i\Lambda(k)y}(\Lambda(k)e^{iy} - \Lambda(k) - 1) + 1}{y^2}\right| \lesssim R^2(\log R)^2.$$

Together with Equation (3.B.14) this concludes the proof. $\square$

Chapter 4

Ground state energy of the dilute spin-polarized Fermi gas: Lower bound

This chapter contains the paper

[GSELow] A. B. Lauritsen and R. Seiringer. "Ground state energy of the dilute spin-polarized Fermi gas: Lower bound". arXiv: 2402.17558 [math-ph]. 2024. DOI: 10.48550/arXiv.2402.17558.

Abstract. We prove a lower bound on the ground state energy of the dilute spin-polarized Fermi gas capturing the leading correction to the kinetic energy resulting from repulsive interactions. This correction depends on the p-wave scattering length of the interaction and matches the corresponding upper bound in Chapter 3

Contents

4.1 Introduction and Main Results

In recent years much effort in mathematical physics has been devoted towards establishing the validity of asymptotic formulas for the ground state energy (and the free energy at non-zero temperature) of dilute quantum gases, motivated in part by the advances in the physics of cold atoms. The validity of leading order terms was proved for bosons at zero [Dys57; LY98; LY01] and positive [DMS20; MS20; Sei08; Yin10] temperature, as well as for fermions with $q \geq 2$ spin components [FGHP21; LSS05; Sei06b], in dimensions $d \geq 2$. For bosons, even the next-order term (the Lee–Huang–Yang correction) has been established [BCS21; FGJMO24; FS20; FS23; HHNST23; YY09]. In all these cases, the strength of the interparticle interaction is quantified by the s-wave scattering length. In the special case of one dimension, both bosonic and fermionic gases were recently studied in [ARS22].

Notably absent from this list is the spinless Fermi gas in dimensions $d \geq 2$. At low density, the effect of the interactions (quantified by the p-wave scattering length in this case) is significantly smaller than for bosons or for fermions with spin, due to the vanishing of the wave functions at spatial coincidences of the particles as a consequence of the Pauli principle. This makes the mathematical analysis much more subtle. In Chapter 3, an asymptotically correct upper bound on the ground state energy of a dilute spinless Fermi gas was obtained, by developing a cluster expansion technique (see also Chapter 6 for a version of this technique applicable at non-zero temperature). In this paper, we prove a corresponding lower bound. Our method is inspired by [FGHP21], and utilizes a suitable unitary transformation implementing the relevant correlations when two particles are at close distances.

To formulate our result more precisely, consider a gas of N indistinguishable fermions in a d-dimensional box $\Lambda = [-L/2, L/2]^d$ of side length $L > 0$ interacting through a repulsive pair potential V, meaning that $V \geq 0$. Our main focus will be on the physically most relevant case $d = 3$. The Hamiltonian of such a system is given by (in units where $\hbar = 1$ and the particle mass is $m = 1/2$)

$$H_N = \sum_{j=1}^{N} -\Delta_{x_j} + \sum_{j<k} V(x_j - x_k) \tag{4.1.1}$$

and is defined on (an appropriate domain in) $L^2_a(\Lambda^N; \mathbb{C}^q) := \bigwedge^N L^2(\Lambda; \mathbb{C}^q)$ with $q \in \mathbb{N}$ the number of spin states. We consider such a system in the regime where the particle density $\rho = N/L^d$ is small compared to the length scale set by the interaction potential V. The particles being fermions, an important role is played by the spin: The interactions between fermions in different spin states gives a much larger contribution to the energy than the interactions between fermions in the same spin state. This is due to the Pauli exclusion principle suppressing the probability of two fermions of equal spin being close. For fermions of different spin there is no such suppression.

In this paper we study the setting of spinless (or, equivalently, fully spin-polarized) fermions, meaning that $q = 1$. In the physics literature, one finds the following conjecture for the ground state energy $E_N = \inf \operatorname{spec} H_N$ [AE68; DZ19; Efi66; EA65] (see also the numerics in [BTP23]): for small ak_F

$$E_N^{d=3} = Nk_F^2 \left[\frac{3}{5} + \frac{2}{5\pi} a^3 k_F^3 - \frac{1}{35\pi} a^6 R_{\text{eff}}^{-1} k_F^5 + \frac{2066 - 312 \log 2}{10395\pi^2} a^6 k_F^6 + o(a^6 k_F^6) \right] \tag{4.1.2}$$

with $k_F = (6\pi^2\rho)^{1/3}$ the Fermi momentum, a the p-*wave scattering length* and R_{eff} the p-*wave effective range*. The first term $\frac{3}{5}Nk_F^2$ is the (kinetic) energy of the free (i.e., non-interacting) Fermi gas. In Chapter 3 the validity of the first three terms was proved as an upper bound. In this paper we shall prove the validity of the first two terms as a lower bound. In particular, in combination with the result in Chapter 3 we establish the validity of Equation (4.1.2) to order $Na^3k_F^5$.

For comparison, let us consider the case of fermions with spin $\geq 1/2$, where there are $q \geq 2$ spin states. To leading order, one only sees the interaction between fermions of different spins. In this case it is known [FGHP21; Gia23a; LSS05], [Chapter 5] that, for a gas with $N_\sigma = \rho_\sigma L^3$ fermions of spin σ,

$$E^{d=3}_{\{N_\sigma\}} = \sum_\sigma \frac{3}{5} N_\sigma (6\pi^2 \rho_\sigma)^{2/3} + \sum_{\sigma \neq \sigma'} 4\pi a_s N_\sigma N_{\sigma'} L^{-3} + o(N a_s \rho) \tag{4.1.3}$$

with a_s the s-*wave scattering length* of the interaction V. The first term $\sum_\sigma \frac{3}{5} N_\sigma (6\pi^2\rho_\sigma)^{2/3}$ is again the energy of a free Fermi gas. We note that the second term, of order $Na_s\rho$, is much larger than the corresponding second term for the spin-polarized fermions in Equation (4.1.2). The next term in the expansion Equation (4.1.3) is conjectured to be of order $Na_s^2\rho^{4/3}$ [Gia23a; Gia23b; HY57]. Also this term arises from interactions of fermions with different spin and is still much larger than the largest term coming from the same-spin interaction in Equation (4.1.2) above.

Finally, we consider also the lower-dimensional cases $d \leq 2$. Here the expected formulas for the spin-polarized gas read [ARS22] (and Chapter 3)

$$E_N^{d=2} = Nk_F^2 \left[\frac{1}{2} + \frac{1}{4} a^2 k_F^2 + o(a^2 k_F^2) \right], \qquad E_N^{d=1} = Nk_F^2 \left[\frac{1}{3} + \frac{2}{3\pi} a k_F + o(a k_F) \right]$$

with $k_F = (4\pi\rho)^{1/2}$ for $d = 2$ and $k_F = \pi\rho$ for $d = 1$, and a the p-*wave scattering length* in the respective dimension. In Chapter 3 we proved the validity of both of these formulas as upper bounds, and in [ARS22] the one-dimensional formula is proved both as an upper and a lower bound. In this paper, we shall also prove the formula for $d = 2$ as a lower bound.

4.1.1 Precise statement of results

We shall now give a precise statement of our main results, given in Theorem 4.1.2 below. To do this, we first define the Hamiltonian H_N and its ground state energy E_N properly.

We shall work with periodic boundary conditions on $\Lambda = [-L/2, L/2]^3$. In particular we replace the interaction V by its periodization $\sum_{n\in\mathbb{Z}^3} V(x+nL)$, which we will with a slight abuse of notation continue to denote by V. We assume that V has compact support, so for L large enough at most one of the summands in $\sum_{n\in\mathbb{Z}^3} V(x+nL)$ is non-zero and no confusion should arise. The Hamiltonian H_N is then defined as in Equation (4.1.1) with Δ denoting the Laplacian with periodic boundary conditions on the box Λ and realized as a self-adjoint operator on (an appropriate domain in) the fermionic space $L^2_a(\Lambda^N) = \bigwedge^N L^2(\Lambda)$. The ground state energy E_N is then given by

$$E_N = \inf_{\psi\in L^2_a(\Lambda^N)} \frac{\langle\psi|H_N|\psi\rangle}{\langle\psi|\psi\rangle}.$$

The p-*wave scattering length* of the interaction potential V is defined as follows (a different-looking but equivalent definition is given in [SY20] and Chapters 3 and 6).

Definition 4.1.1. Let φ_0 be the solution of the p-*wave scattering equation*

$$x\Delta\varphi_0 + 2\nabla\varphi_0 + \frac{1}{2}xV(1-\varphi_0) = 0 \tag{4.1.4}$$

on $\mathbb{R}^3$, with $\varphi_0(x) \to 0$ for $|x| \to \infty$. Then $\varphi_0(x) = a^3/|x|^3$ for $x \notin \operatorname{supp} V$ for some constant a called the p-*wave scattering length*.

With these definitions we can formulate our main theorem:

Theorem 4.1.2. *Let $V \in L^1$ be non-negative, radial and compactly supported. Then for ak_F small enough and N large enough we have*

$$\frac{E_N}{N} \geq k_F^2 \left[\frac{3}{5} + \frac{2}{5\pi}a^3k_F^3 + O((ak_F)^{3+3/10}\,|\log ak_F|) + O(N^{-1/3})\right].$$

Remark 4.1.3. The appearance of the scattering length a in the error term is for dimensional consistency. The error term $O((ak_F)^{3+3/10}\,|\log ak_F|)$ really depends on the range R_0 of V and on $\|V\|_{L^1}$ (both of dimension length). We think of a as a constant of dimension length and thus use the bounds

$$R_0 \leq Ca, \qquad \|V\|_{L^1} \leq Ca$$

with the constants C then being dimensionless.

Remark 4.1.4 (Extension to less regular V)**.** A posteriori we can extend Theorem 4.1.2 to less regular V (and, in particular, to the case of hard spheres where, formally, $V_{\mathsf{hs}}(x) = \infty$ for $|x| \leq R_0$ and $V_{\mathsf{hs}}(x) = 0$ otherwise). Indeed, any positive radial and compactly supported measurable function V can be approximated from below by some (positive radial compactly supported) $\widetilde{V} \in L^1$. Then we can apply the theorem for $\widetilde{V}$ and note that $E_N \geq \widetilde{E}_N$ with $\widetilde{E}_N$ the ground state energy with interaction $\widetilde{V}$. The error bounds in the theorem, being dependent on $\|\widetilde{V}\|_{L^1}$, necessarily blow up when $\widetilde{V}$ converges to V. However, choosing $\widetilde{V}$ to converge to V slowly enough we may achieve $a(\widetilde{V}) = a(V)(1+o(1))$ with the error-terms of Theorem 4.1.2 still being small. Then

$$\frac{E_N}{N} \geq k_F^2 \left[\frac{3}{5} + \frac{2}{5\pi}a^3k_F^3 + o(a^3k_F^3) + O(N^{-1/3})\right].$$

In the same way, also the restriction to V having compact support can be lifted. For finiteness of the p-wave scattering length it is only needed that $x \mapsto |x|^2 V(x)$ is integrable outside some ball.

While the main focus of this paper is a *lower* bound on the ground state energy, our method can also be applied to obtain a corresponding *upper* bound. In fact, we shall show the following.

Proposition 4.1.5 (Upper bound)**.** *Let $V \in L^1$ be positive, radial and compactly supported. Then for ak_F small enough and N large enough we have*

$$\frac{E_N}{N} \leq k_F^2 \left[\frac{3}{5} + \frac{2}{5\pi} a^3 k_F^3 + O(a^4 k_F^4 \left|\log ak_F\right|) + O(N^{-1/3})\right].$$

We remark, however, that in Theorem 3.1.3, using a very different method, a significantly stronger upper bound was shown (capturing also the next term of order $(ak_F)^5$) under weaker assumptions on the interaction V (in particular, allowing also for hard spheres).

In the proof of Theorem 4.1.2 and Proposition 4.1.5 we will consider particle numbers N arising from a "filled Fermi ball". This is done for convenience. We shall discuss in Remark 4.1.7 below why this is in fact not a restriction on N to the precision given in Theorem 4.1.2. Concretely this means the following.

Definition 4.1.6. For $k_F > 0$ the *Fermi ball* is defined as $B_F = \{k \in \frac{2\pi}{L}\mathbb{Z}^3 : |k| \leq k_F\}$. We then take $N = \#B_F$.

In this case there are two variables, which we are free to choose: The side-length of the box L and the Fermi momentum k_F. The particle number N and density $\rho = N/L^3$ then depend on the values of L, k_F. Any constraint on N (that it is sufficiently large, say) should thus more precisely be written as a constraint on $k_F L \sim N^{1/3}$. Counting the number of lattice points inside a ball of a given radius we see that $\rho = N/L^3$ and k_F are related by $k_F = (6\pi^2\rho)^{1/3}(1 + O(N^{-1/3}))$.

Remark 4.1.7. The choice of $N = \#B_F$ puts a restriction on which values N may assume — not all integers arise as $\#B_F$ for some L and k_F. To the precision given in Theorem 4.1.2 and Proposition 4.1.5, however, it suffices to consider N arising as $N = \#B_F$. To see this, assume that Theorem 4.1.2 and Proposition 4.1.5 hold for integers N arising as $N = \#B_F$.

For a general integer N and length L define $k_F^{\leq}$ and $k_F^{\geq}$ as the largest, respectively smallest, k_F such that $N^< = \#B_F^{\leq} \leq N \leq \#B_F^{\geq} = N^>$ with $B_F^{\leq}, B_F^{\geq}$ defined using the Fermi momenta $k_F^{\leq}$ and $k_F^{\geq}$. Then $N^<, N^> = N + O(N^{2/3})$ since $k_F^{\leq} + \frac{2\pi}{L} \geq k_F^{\geq}$. Moreover, $k_F^{\leq}, k_F^{\geq} = (6\pi^2\rho)^{1/3}(1 + O(N^{-1/3}))$. We may apply Theorem 4.1.2 and Proposition 4.1.5 for particle numbers $N^>$ and $N^<$. By positivity of the interaction we have $E_{N^<} \leq E_N \leq E_{N^>}$. Thus,

$$\begin{aligned}
\frac{E_N}{N} &\geq \frac{E_{N^<}}{N^<}(1 + O(N^{-1/3})) \\
&\geq (k_F^{\leq})^2 \left[\frac{3}{5} + \frac{2}{5\pi} a^3 (k_F^{\leq})^3 + O((ak_F^{\leq})^{3+3/10} \left|\log ak_F^{\leq}\right|) + O(N^{-1/3})\right] \\
&= k_F^2 \left[\frac{3}{5} + \frac{2}{5\pi} a^3 k_F^3 + O((ak_F)^{3+3/10} \left|\log ak_F\right|) + O(N^{-1/3})\right]
\end{aligned}$$

and similarly for the upper bound.

4.1.1.1 Two dimensions

We consider next the analogous problem in two dimensions. The scattering length is defined as in Definition 4.1.1, with the only difference that now one has $\varphi_0(x) = a^2/|x|^2$ outside the support of V. The two-dimensional analogue of Theorem 4.1.2 is as follows.

Theorem 4.1.8 (Two dimensions)**.** *Let $V \in L^1$ be positive, radial and compactly supported. Then for ak_F small enough and N large enough we have*

$$\frac{E_N}{N} \geq k_F^2 \left[\frac{1}{2} + \frac{1}{4}a^2k_F^2 + O((ak_F)^{2+1/4}|\log ak_F|) + O(N^{-1/2})\right].$$

Remark 4.1.9. Theorem 4.1.8 matches the upper bound of Theorem 3.1.10 to order $Na^2k_F^4$. Indeed, k_F and ρ are related by $k_F = (4\pi\rho)^{1/2}(1 + O(N^{-1/2}))$.

We sketch in Section 4.A how to adapt the proof of Theorem 4.1.2 to the two-dimensional setting.

4.1.2 Second quantization

An important step in the proof is to write the Hamiltonian in second quantization and analyse it using an appropriate unitary transformation. The choice of the unitary can be motivated by a suitable version of second order perturbation theory, as we shall discuss in the next subsection.

We will here only briefly describe the central concepts of second quantization. A detailed introduction to second quantization in general can be found in [Sol14]. Moreover, the specific case of a Fermi gas in a periodic box $\Lambda = [-L/2, L/2]^3$ is discussed in detail in [FGHP21; Gia23a], see also [Gia23b].

Since we consider the box Λ with periodic boundary conditions, a natural basis for the one-body space $L^2(\Lambda)$ is given by the plane waves $f_k(x) = L^{-3/2}e^{ikx}$ with momenta $k \in \frac{2\pi}{L}\mathbb{Z}^3$. We will denote the creation and annihilation operators in the state f_k by $a_k^* = a^*(f_k)$ and $a_k = a(f_k)$, respectively. They satisfy the canonical anti-commutation relations $\{a_k^*, a_{k'}\} = \delta_{k,k'}$ and $\{a_k, a_{k'}\} = \{a_k^*, a_{k'}^*\} = 0$. In second quantization the Hamiltonian is then given by

$$\mathcal{H} = \mathrm{d}\Gamma(-\Delta) + \mathrm{d}\Gamma(V) = \sum_k |k|^2 a_k^* a_k + \frac{1}{2L^3}\sum_{p,k,k'} \hat{V}(p) a_{k+p}^* a_{k'-p}^* a_{k'} a_k \tag{4.1.5}$$

and defined on the Fock space $\mathcal{F} = \bigoplus_{n=0}^\infty L_a^2(\Lambda^n) = \bigoplus_{n=0}^\infty \bigwedge^n L^2(\Lambda)$. Here we have adopted the notation

Notation 4.1.10. The Fourier transform of a function g (on Λ) is given by $\hat{g}(k) = \int g(x)e^{-ikx}\,\mathrm{d}x$.

Notation 4.1.11. For any sum the variables are summed over $\frac{2\pi}{L}\mathbb{Z}^3$ unless otherwise noted. That is, $\sum_k = \sum_{k\in\frac{2\pi}{L}\mathbb{Z}^3}$.

We will consider N-particle states ψ, meaning that $\mathcal{N}\psi = N\psi$ with $\mathcal{N} = \sum_k a_k^* a_k$ the number operator. To extract the leading contribution to the ground state energy it is convenient to introduce the particle-hole transformation R, satisfying

$$R^* a_k R = \begin{cases} a_k^* & k \in B_F, \\ a_k & k \notin B_F, \end{cases} \qquad R\Omega = \left[\prod_{k\in B_F} a_k^*\right]\Omega = \psi_F. \tag{4.1.6}$$

Here Ω denotes the vacuum and the free Fermi state ψ_F is given by

$$\psi_F(x_1,\ldots,x_N) = \frac{1}{\sqrt{N!}} \det\left[f_k(x_j)\right]_{\substack{k\in B_F\\ 1\le j\le N}},$$

with $N = \#B_F$. The state ψ_F is the ground state of the corresponding non-interacting system. For later use we introduce the following convenient notation.

Notation 4.1.12. The expectation of an operator A in the free Fermi state ψ_F is denoted by $\langle A\rangle_F$.

It will prove helpful to distinguish between creation and annihilation operators for momenta inside and outside the Fermi ball. Moreover, it will sometimes be convenient to consider operators written in configuration space, i.e., using the operator-valued distributions a_x, a_x^* given by $a_x = L^{-3/2}\sum_k e^{ikx}a_k$. For instance we have

$$\mathrm{d}\Gamma(V) = \frac{1}{2}\iint V(x-y)a_x^*a_y^*a_ya_x \,\mathrm{d}x\,\mathrm{d}y.$$

Also for the operator-valued distributions a_x, a_x^* we wish to be able to distinguish whether they arise from particles inside or outside the Fermi ball. This leads to the following definition.

Definition 4.1.13. Define

$$c_k = a_k\chi_{(k\in B_F)}, \qquad b_k = a_k\chi_{(k\notin B_F)},$$

with χ denoting the characteristic function. Define further the operator-valued distributions

$$b_x = \frac{1}{L^{3/2}}\sum_k e^{ikx}b_k = \frac{1}{L^{3/2}}\sum_{k\notin B_F} e^{ikx}a_k, \qquad c_x = \frac{1}{L^{3/2}}\sum_k e^{-ikx}c_k = \frac{1}{L^{3/2}}\sum_{k\in B_F} e^{-ikx}a_k. \tag{4.1.7}$$

Note the different choice of signs in the exponents. This is done for convenience, so that the particle-hole transformation satisfies

$$R^*a_xR = b_x + c_x^*. \tag{4.1.8}$$

Note that c_x and c_x^* are in fact bounded operators with $\|c_x\| = \|c_x^*\| \le Ck_F^{3/2}$. Moreover, since their supports (in momentum-space) are disjoint we have that b_x and c_y^* anti-commute.

For later use we define the operators u, v as follows.

Definition 4.1.14. Define the operators u, v as the projection outside and inside the Fermi ball, respectively. That is, their kernels are given by (with a slight abuse of notation)

$$\begin{aligned}
v(x;y) = v(x-y) &= \frac{1}{L^3}\sum_k \hat{v}(k)e^{ikx} = \frac{1}{L^3}\sum_{k\in B_F} e^{ikx},\\
u(x;y) = u(x-y) &= \frac{1}{L^3}\sum_k \hat{u}(k)e^{ikx} = \frac{1}{L^3}\sum_{k\notin B_F} e^{ikx} = \delta(x-y) - v(x-y).
\end{aligned}$$

Remark 4.1.15. The operator-valued distributions b_x and c_x are denoted $a(u_x) = a(u(\cdot;x))$ and $a(\overline{v}_x) = a(\overline{v}(\cdot;x))$, respectively, in [FGHP21; Gia23a]. The different signs in the exponents in Equation (4.1.7) above reflect the $^-$ in $a(\overline{v}_x)$.

4.1.3 Heuristics

Conceptually, the strategy of the proof of Theorem 4.1.2 can be motivated via (a suitable version of) second order perturbation theory, where one treats only the "off-diagonal" parts of the interaction as the perturbation and includes the "diagonal" part in the unperturbed operator. This is similar to the method of [FGHP21; Gia23a], which itself is inspired by Bogoliubov transformations in the case of bosons; the latter effectively appear as pairs of fermions with opposite spin. This (bosonic) picture does not apply in the spinless case, but the method can be applied nonetheless, as we shall show below.

Before we explain this is more details we first recall second order perturbation theory in general.

4.1.3.1 General second order perturbation theory

Consider a generic perturbed Hamiltonian $H = H_0 + \lambda V$ and write $V = V_{\mathsf{D}} + V_{\mathsf{OD}}$ with V_{D} the part of V diagonal in a basis where H_0 is diagonal. We use a formulation of second order perturbation theory using a unitary operator $e^{\lambda B}$ with B chosen appropriately such that $e^{-\lambda B} H e^{\lambda B}$ is (approximately) diagonal. Using the Baker–Campbell–Hausdorff formula $e^{-X} Y e^{X} \approx Y + [Y,X] + \frac{1}{2}[[Y,X],X] + \ldots$ we have

$$
\begin{aligned}
&e^{-\lambda B} H e^{\lambda B} \\
&\quad = H_0 + \lambda\left([H_0, B] + V\right) + \lambda^2 \left(\frac{1}{2}[[H_0,B],B] + [V,B]\right) + O(\lambda^3) \\
&\quad = H_0 + \lambda\left([H_0 + \lambda V_{\mathsf{D}}, B] + V\right) + \lambda^2 \left(\frac{1}{2}[[H_0 + \lambda V_{\mathsf{D}},B],B] + [V_{\mathsf{OD}},B]\right) + O(\lambda^3).
\end{aligned}
$$

Since H_0 and V_{D} are both diagonal operators, $[H_0 + \lambda V_{\mathsf{D}}, B]$ is off-diagonal for any B. We choose B to (approximately) cancel the off-diagonal part of V, i.e., such that $[H_0 + \lambda V_{\mathsf{D}}, B] \approx -V_{\mathsf{OD}}$. Then

$$
e^{-\lambda B} H e^{\lambda B} \approx H_0 + \lambda V_{\mathsf{D}} + \frac{1}{2}\lambda^2 [V_{\mathsf{OD}}, B] \tag{4.1.9}
$$

is diagonal to order λ. With $e_n^{(0)} = \langle n | H_0 + \lambda V_{\mathsf{D}} | n \rangle$ the eigenvalues of $H_0 + \lambda V_{\mathsf{D}}$ the equation for B reads $\langle n|B|m\rangle \,(e_n^{(0)} - e_m^{(0)}) = \langle n|V|m\rangle$. Thus, we find the well-known formula for the eigenvalues e_n of H as the diagonal matrix-elements of $e^{-\lambda B} H e^{\lambda B}$

$$
e_n \approx e_n^{(0)} + \lambda^2 \sum_{m : m \neq n} \frac{|\langle n|V|m\rangle|^2}{e_n^{(0)} - e_m^{(0)}} \approx \langle n|H_0|n\rangle + \lambda \langle n|V|n\rangle + \lambda^2 \sum_{m : m\neq n} \frac{|\langle n|V|m\rangle|^2}{\langle n|H_0|n\rangle - \langle m|H_0|m\rangle}
$$

valid to order λ^2.

If one is only interested in the ground state energy, one can simplify the computation above. Decompose the Hilbert space as $\operatorname{span}\{|0\rangle\} \oplus \operatorname{span}\{|0\rangle\}^\perp$ with $|0\rangle$ being the ground state of H_0. We then instead take V_{D} as the part of V *block* diagonal in this decomposition and choose B to only cancel the *block* off-diagonal part of V. (This is in general a considerably simpler choice of B.) The formula in Equation (4.1.9) then still applies, being however only (approximately) *block* diagonal, and we find the ground state energy as

$$
e_0 \approx e_0^{(0)} + \lambda^2 \sum_{m\neq 0} \frac{|\langle 0|V|m\rangle|^2}{e_0^{(0)} - e_m^{(0)}}. \tag{4.1.10}
$$

In our case of interest, there is no small coupling parameter λ. Nevertheless, the relevance of (4.1.10) is suggested by the following observation. If one integrates Equation (4.1.4) against

x, one finds via an integration by parts that

$$12\pi a^3 = \frac{1}{2}\int V(x)|x|^2(1-\varphi_0(x))\,\mathrm{d}x. \tag{4.1.11}$$

Equation (4.1.4) can be rewritten as $(-x\Delta - 2\nabla + \frac{1}{2}xV)\varphi_0 = \frac{1}{2}xV$, hence (4.1.11) is reminiscent of (4.1.10), only that it is actually exact!

4.1.3.2 Application to the many-body setting

Our goal is to apply the formula in Equation (4.1.9) to the Hamiltonian H_N, with $\lambda = 1$. This is not a small parameter — the potential V is not assumed to be small. For Equation (4.1.9) to still be a good approximation, it is essential that the "diagonal" part of V is taken as part of the unperturbed Hamiltonian. Indeed, the formula in Theorem 4.1.2 is non-perturbative and *does not* arise from any finite order "standard" perturbation theory, where all of V is taken as the perturbation.

First, we need to define what we mean by "diagonal" and "off-diagonal". Recall from Definition 4.1.14 that v and $u = \mathbb{1} - v$ are the projections inside, respectively outside, the Fermi ball. For the two-body operator V we then have

$$V \approx V_{\mathsf{D}} + V_{\mathsf{OD}}, \qquad V_{\mathsf{D}} = vvVvv + uuVuu, \qquad V_{\mathsf{OD}} = vvVuu + uuVvv.$$

(By an expression like vv we mean the two-body operator $v \otimes v$.) Here we have neglected terms with a factor uv or vu. These will turn out to be small. The ground state of the free Hamiltonian $\sum_{j=1}^N -\Delta_{x_j}$ is the free Fermi state ψ_F. Hence the calculation above suggests that the ground state of H_N is roughly $e^{\widetilde{B}}\psi_F$ with $\widetilde{B}$ the analogue of the operator B from above.

To compute $\left\langle e^{\widetilde{B}}\psi_F \middle| H_N \middle| e^{\widetilde{B}}\psi_F \right\rangle$ it is convenient to first conjugate the Hamiltonian H_N by the particle-hole transformation R, defined in Equation (4.1.6) above. Define also $B = R^*\widetilde{B}R$. Then the ground state of H_N is expected to be roughly $e^{\widetilde{B}}\psi_F = RT\Omega$ with $T = e^B$. Our choice of B will be of the form

$$B = \frac{1}{2L^3}\sum_{p,k,k'} \hat{\varphi}(p) b_{k+p} b_{k'-p} c_{k'} c_k - \text{h.c.} = \frac{1}{2}\iint \varphi(z-z') b_z b_{z'} c_{z'} c_z \,\mathrm{d}z\,\mathrm{d}z' - \text{h.c.}$$

for $\varphi \approx \varphi_0$. This particular choice of B will be justified by the validity of Equation (4.1.16) below.

Remark 4.1.16. The form of the operator B is (up to the spin dependence) the same as for the operator $B - B^*$ considered in [FGHP21; Gia23a]. Furthermore, we note that $\widetilde{B}$ is closely related to the *transfer operator* M_2 considered in [AE68]. In [AE68] it is claimed that the ground state is (up to normalization) approximately given by $(1 + M_2)\psi_F$. Pretending that $\widetilde{B} \sim M_2$ is small we find that the ground state is roughly $e^{\widetilde{B}}\psi_F = RT\Omega$ as claimed.

To compute the expectation of H_N in the state $\psi \approx RT\Omega$ we first compute the conjugation of the Hamiltonian $\mathcal{H}$ by the particle-hole transformation R. (Recall that $\mathcal{H}$, defined in Equation (4.1.5), is the second quantized analogue of H_N.) To calculate $R^*\mathcal{H}R$ we use Equation (4.1.8) and normal order. This is a straightforward calculation which we omit. The details of the calculation can for instance be found in [HPR20, Proposition 4.1]. We have for the kinetic energy (on the space of states of the form $R^*\psi$ with ψ an N-particle state, see [HPR20, Proposition 4.1])

$$R^* \, \mathrm{d}\Gamma(-\Delta)R = E_F + \mathbb{H}_0, \qquad E_F = \sum_{k\in B_F} |k|^2, \qquad \mathbb{H}_0 = \sum_k \Big| |k|^2 - k_F^2 \Big| a_k^* a_k \tag{4.1.12}$$

and for the interaction (in the second $\approx$ by neglecting the quadratic terms)

$$R^* \mathrm{d}\Gamma(V)R \approx R^* \mathrm{d}\Gamma(V_{\mathsf{D}} + V_{\mathsf{OD}})R \approx \langle \mathrm{d}\Gamma(V)\rangle_F + \mathbb{Q}_2 + \mathbb{Q}_4$$

with $\mathbb{Q}_2$ and $\mathbb{Q}_4$ given by

$$\mathbb{Q}_2 = \frac{1}{2L^3}\sum_{p,k,k'} \hat{V}(p) b_{k+p}^* b_{k'-p}^* c_{k'}^* c_k^* + \text{h.c.} = \frac{1}{2}\iint V(x-y) b_x^* b_y^* c_y^* c_x^* \, \mathrm{d}x \, \mathrm{d}y + \text{h.c.}, \tag{4.1.13}$$

$$\mathbb{Q}_4 = \frac{1}{2L^3}\sum_{p,k,k'} \hat{V}(p) b_{k+p}^* b_{k'-p}^* b_{k'} b_k \qquad = \frac{1}{2}\iint V(x-y) b_x^* b_y^* b_y b_x \, \mathrm{d}x \, \mathrm{d}y. \tag{4.1.14}$$

Here $\langle \mathrm{d}\Gamma(V)\rangle_F + \mathbb{Q}_4$ is the operator corresponding to the "diagonal" part $vvVvv + uuVuu$ and $\mathbb{Q}_2$ is the operator corresponding to the "off-diagonal" part $vvVuu + uuVvv$.

Remark 4.1.17 (Comparison to [FGHP21; Gia23a])**.** The analogues of the operators $\mathbb{Q}_2$ and $\mathbb{Q}_4$ above are denoted by $\mathbb{Q}_4$ and $\mathbb{Q}_1$, respectively, in [FGHP21; Gia23a].

The calculation of general second order perturbation theory above then translates to the calculation

$$T^*(\mathbb{H}_0 + \mathbb{Q}_2 + \mathbb{Q}_4)T \approx \mathbb{H}_0 + \mathbb{Q}_4 + [\mathbb{H}_0 + \mathbb{Q}_4, B] + \mathbb{Q}_2 + \frac{1}{2}[[\mathbb{H}_0 + \mathbb{Q}_4, B], B] + [\mathbb{Q}_2, B]. \tag{4.1.15}$$

The operator B is chosen such that

$$[\mathbb{H}_0 + \mathbb{Q}_4, B] + \mathbb{Q}_2 \approx 0, \tag{4.1.16}$$

which constrains the function φ in the definition of B to (roughly) satisfy the p-wave scattering equation (4.1.4). Then,

$$T^*(\mathbb{H}_0 + \mathbb{Q}_2 + \mathbb{Q}_4)T \approx \mathbb{H}_0 + \mathbb{Q}_4 + \frac{1}{2}[\mathbb{Q}_2, B].$$

Next, one computes that $\langle [\mathbb{Q}_2, B]\rangle_\Omega \approx -2 \langle \mathrm{d}\Gamma(V\varphi)\rangle_F$. We then find

$$E_N \approx E_F + \langle \mathbb{H}_0 + \mathbb{Q}_4\rangle_\Omega + \langle \mathrm{d}\Gamma(V)\rangle_F + \frac{1}{2}\langle [\mathbb{Q}_2, B]\rangle_\Omega \approx E_F + \langle \mathrm{d}\Gamma(V(1-\varphi))\rangle_F .$$

Finally, we compute that $E_F \approx \frac{3}{5}Nk_F^2$ and $\langle \mathrm{d}\Gamma(V(1-\varphi))\rangle_F \approx \frac{2}{5\pi}Na^3k_F^5$ (see Equation (4.2.13) below). This recovers the formula of Theorem 4.1.2.

4.2 Rigorous Analysis

In this section we shall describe how to rigorously implement the heuristic computation above in order to prove Theorem 4.1.2. A first step is the precise definition of the operators B and T.

4.2.1 Regularizing the operators

For technical reasons, we need to regularize the operator(-valued distribution)s b_k and b_x. We introduce regularized b_k-operators using a smooth radial function $\hat{u}^r : \mathbb{R}^3 \to [0,1]$ with

$$\hat{u}^r(k) = \begin{cases} 0 & |k| \le 2k_F, \\ 1 & |k| \ge 3k_F. \end{cases}$$

Let

$$b_k^r = \hat{u}^r(k) a_k, \qquad b_x^r = \frac{1}{L^{3/2}} \sum_k e^{ikx} b_k^r. \tag{4.2.1}$$

The function $\hat{u}^r$ defines an operator u^r on $L^2(\Lambda)$ with kernel (with slight abuse of notation) $u^r(x;y) = u^r(x-y)$. As an operator $0 \le u^r \le \mathbb{1}$. Moreover, by proceeding as in [FGHP21, Proposition 4.2] one easily checks that $u^r - \delta \in L^1$. More precisely:

Lemma 4.2.1. *Write $u^r = \delta - v^r$. Then $\|v^r\|_{L^1} \le C$ for large $k_F L$.*

4.2.2 The scattering function

We shall now define the function φ appearing in the operator B. Since φ_0 is not integrable at infinity (it decays like $a^3/|x|^3$) it will be necessary to introduce a cut-off for technical reasons. Moreover, we need to periodize to define φ on the torus.

Let $\chi_\varphi : [0,\infty) \to [0,1]$ be a smooth function with

$$\chi_\varphi(t) = \begin{cases} 1 & t \le 1, \\ 0 & t \ge 2. \end{cases}$$

Then we choose the function φ as

$$\varphi(x) = \varphi_0(x) \chi_\varphi(k_F|x|) \tag{4.2.2}$$

with φ_0 the p-wave scattering function defined in Definition 4.1.1. To be more precise, we choose φ to be the periodization of $\varphi_0 \chi_\varphi(k_F|\cdot|)$. We shall always assume that $L > 4k_F^{-1}$ so that $\operatorname{supp} \varphi_0 \chi_\varphi(k_F|\cdot|) \subset \Lambda$, in which case no confusion should arise.

To measure the error in φ not exactly satisfying the scattering equation (4.1.4) we define

$$\begin{aligned} \mathcal{E}_\varphi(x) &= x\Delta\varphi(x) + 2\nabla\varphi(x) + \frac{1}{2} x V(x)(1-\varphi(x)) \\ &= 2k_F x \nabla^\mu \varphi_0(x) \nabla^\mu \chi_\varphi(k_F x) + k_F^2 x \varphi_0(x) \Delta\chi_\varphi(k_F x) + 2k_F \varphi_0(x) \nabla\chi_\varphi(k_F x). \end{aligned} \tag{4.2.3}$$

Again, $\mathcal{E}_\varphi$ is more precisely the periodization of the expression in the second line. Here we have used the notation:

Notation 4.2.2. We adopt the Einstein summation convention of summing over repeated indices denoting components of a vector, i.e., $x^\mu y^\mu = \sum_{\mu=1}^3 x^\mu y^\mu = x \cdot y$ for vectors $x, y \in \mathbb{R}^3$.

Remark 4.2.3. We will in general abuse notation slightly and refer to any (compactly supported) function and its periodization by the same name. For sufficiently large L at most one summand in the periodization is non-zero and so no issue will arise.

Remark 4.2.4. Any derivative of $\chi_\varphi(t)$ is supported in $1 \le t \le 2$. In particular $\mathcal{E}_\varphi$ is supported in the annulus $k_F^{-1} \le |x| \le 2k_F^{-1}$. For ak_F small enough such x are outside the support of V and hence $\varphi_0(x) = a^3/|x|^3$ there. In particular

$$|\mathcal{E}_\varphi(x)| \le Ck_F \frac{a^3}{|x|^3} \chi_{k_F^{-1} \le |x| \le 2k_F^{-1}} \le Ck_F \varphi(x/2). \tag{4.2.4}$$

4.2.3 The transformation T

The operators B and T are defined as

$$T = e^{B}, \qquad B = \frac{1}{2L^3}\sum_{p,k,k'} \hat{\varphi}(p) b^r_{k+p} b^r_{k'-p} c_{k'} c_k - \text{h.c.} = \frac{1}{2}\iint \varphi(z-z') b^r_z b^r_{z'} c_{z'} c_z \, \mathrm{d}z \, \mathrm{d}z' - \text{h.c.}. \tag{4.2.5}$$

with φ given in Equation (4.2.2) and b^r_k the regularized operators in (4.2.1).

Remark 4.2.5 (Comparison to [FGHP21; Gia23a])**.** Compared to the analogous construction of an operator T in [FGHP21; Gia23a] we avoid regularizing the operators c_x and we do not have an ultraviolet regularization of the operators b_x. This simplifies much of the analysis below, since we do not have to treat the errors arising from such a regularization.

4.2.4 Implementation

We shall describe now how to rigorously implement the heuristic calculation in the previous section. The main step is the calculation in Equation (4.1.15), which uses the Baker–Campbell–Hausdorff expansion. We give a rigorous implementation of this calculation using a Duhamel expansion as follows.

As discussed in the heuristic analysis above, we expect the ground state to be roughly $RT\Omega$. Thus define (for some ψ)

$$\xi_\lambda = T^{-\lambda} R^* \psi \ , \quad \text{where } T^{-\lambda} := e^{-\lambda B}, \quad \lambda \in [0,1]. \tag{4.2.6}$$

Then $\psi = R\xi_0 = RT\xi_1$. We will consider the following ψ's:

Definition 4.2.6. Let ψ be an N-particle state. Then ψ is called an *approximate ground state* if

$$\left| \langle H_N \rangle_\psi - \sum_{k\in B_F} |k|^2 \right| \leq C N a^3 k_F^5.$$

for some $C > 0$ (independent of N and ak_F).

Remark 4.2.7 (Existence of approximate ground states)**.** Note that the free Fermi state ψ_F is an approximate ground state. Indeed, we show in the proof of Lemma 4.3.3 below that $\langle \mathrm{d}\Gamma(V)\rangle_F \leq C N a^3 k_F^5$. In particular, the ground state is an approximate ground state.

Motivated by the discussion above we write

$$\langle H_N \rangle_\psi = E_F + \langle \mathrm{d}\Gamma(V)\rangle_F + \langle \mathbb{H}_0 + \mathbb{Q}_2 + \mathbb{Q}_4 \rangle_{\xi_0} + \mathcal{E}_V(\psi) \tag{4.2.7}$$

with $\mathcal{E}_V(\psi)$ defined so that this holds, i.e., $\mathcal{E}_V(\psi) = \langle \mathrm{d}\Gamma(V)\rangle_\psi - \langle \mathrm{d}\Gamma(V)\rangle_F - \langle \mathbb{Q}_2 + \mathbb{Q}_4 \rangle_{\xi_0}$. We shall show in Proposition 4.2.8 below that $\mathcal{E}_V(\psi)$ is small for an approximate ground state ψ, i.e., it is negligible compared to $Na^3k_F^5$. To compute $\langle \mathbb{H}_0 + \mathbb{Q}_2 + \mathbb{Q}_4 \rangle_{\xi_0}$ we note that for any operator A we have

$$\langle \xi_\lambda | A | \xi_\lambda \rangle = \langle \xi_1 | A | \xi_1 \rangle - \int_\lambda^1 \mathrm{d}\lambda' \, \frac{\mathrm{d}}{\mathrm{d}\lambda'} \langle \xi_{\lambda'} | A | \xi_{\lambda'} \rangle = \langle \xi_1 | A | \xi_1 \rangle + \int_\lambda^1 \mathrm{d}\lambda' \, \langle \xi_{\lambda'} | [A, B] | \xi_{\lambda'} \rangle \, .$$

Using this for $\mathbb{H}_0$ and $\mathbb{Q}_4$ we find

$$\begin{aligned}&\langle \mathbb{H}_0 + \mathbb{Q}_4 \rangle_{\xi_0} \\ &\quad = \langle \xi_1 | \mathbb{H}_0 + \mathbb{Q}_4 | \xi_1 \rangle + \int_0^1 \mathrm{d}\lambda \, \langle \xi_\lambda | [\mathbb{H}_0 + \mathbb{Q}_4, B] + \mathbb{Q}_2 | \xi_\lambda \rangle - \int_0^1 \mathrm{d}\lambda \, \langle \xi_\lambda | \mathbb{Q}_2 | \xi_\lambda \rangle \,.\end{aligned}$$

Similarly, for $\mathbb{Q}_2$ we find

$$\begin{aligned}\langle \mathbb{Q}_2 \rangle_{\xi_0} &= \langle \xi_1 | \mathbb{Q}_2 | \xi_1 \rangle + \int_0^1 \mathrm{d}\lambda \, \langle \xi_\lambda | [\mathbb{Q}_2, B] | \xi_\lambda \rangle \,, \\ \int_0^1 \mathrm{d}\lambda \, \langle \xi_\lambda | \mathbb{Q}_2 | \xi_\lambda \rangle &= \langle \xi_1 | \mathbb{Q}_2 | \xi_1 \rangle + \int_0^1 \mathrm{d}\lambda \int_\lambda^1 \mathrm{d}\lambda' \, \langle \xi_{\lambda'} | [\mathbb{Q}_2, B] | \xi_{\lambda'} \rangle \,.\end{aligned}$$

In conclusion then

$$\begin{aligned}\langle \xi_0 | \mathbb{H}_0 + \mathbb{Q}_2 + \mathbb{Q}_4 | \xi_0 \rangle = &\int_0^1 \mathrm{d}\lambda \, \langle \xi_\lambda | [\mathbb{Q}_2, B] | \xi_\lambda \rangle - \int_0^1 \mathrm{d}\lambda \int_\lambda^1 \mathrm{d}\lambda' \, \langle \xi_{\lambda'} | [\mathbb{Q}_2, B] | \xi_{\lambda'} \rangle \\ &+ \langle \xi_1 | \mathbb{H}_0 + \mathbb{Q}_4 | \xi_1 \rangle + \int_0^1 \mathrm{d}\lambda \, \langle \xi_\lambda | [\mathbb{H}_0 + \mathbb{Q}_4, B] + \mathbb{Q}_2 | \xi_\lambda \rangle \,.\end{aligned}$$

The two terms with $[\mathbb{Q}_2, B]$ are the leading terms. To leading order they are given by the constant (i.e. fully contracted) contribution from $[\mathbb{Q}_2, B]$ obtained after normal ordering. This constant term is (approximately) given by $-2 \langle \mathrm{d}\Gamma(V\varphi) \rangle_F$. This motivates to write

$$[\mathbb{Q}_2, B] = -2 \langle \mathrm{d}\Gamma(V\varphi) \rangle_F + \mathbb{Q}_{2;B}^{\mathcal{E}}. \tag{4.2.8}$$

The last term, with $[\mathbb{H}_0 + \mathbb{Q}_4, B] + \mathbb{Q}_2$, is an error term. It is small by virtue of φ (almost) satisfying the p-wave scattering equation. The third term $\langle \xi_1 | \mathbb{H}_0 + \mathbb{Q}_4 | \xi_1 \rangle$ is positive. We thus find

$$\langle \xi_0 | \mathbb{H}_0 + \mathbb{Q}_2 + \mathbb{Q}_4 | \xi_0 \rangle = - \langle \mathrm{d}\Gamma(V\varphi) \rangle_F + \langle \xi_1 | \mathbb{H}_0 + \mathbb{Q}_4 | \xi_1 \rangle + \mathcal{E}_{\mathbb{Q}_2}(\psi) + \mathcal{E}_{\mathsf{scat}}(\psi),$$

where

$$\mathcal{E}_{\mathbb{Q}_2}(\psi) = \int_0^1 \mathrm{d}\lambda \, \left\langle \xi_\lambda \middle| \mathbb{Q}_{2;B}^{\mathcal{E}} \middle| \xi_\lambda \right\rangle - \int_0^1 \mathrm{d}\lambda \int_\lambda^1 \mathrm{d}\lambda' \left\langle \xi_{\lambda'} \middle| \mathbb{Q}_{2;B}^{\mathcal{E}} \middle| \xi_{\lambda'} \right\rangle, \tag{4.2.9}$$

$$\mathcal{E}_{\mathsf{scat}}(\psi) = \int_0^1 \mathrm{d}\lambda \, \langle \xi_\lambda | [\mathbb{H}_0 + \mathbb{Q}_4, B] + \mathbb{Q}_2 | \xi_\lambda \rangle \,. \tag{4.2.10}$$

We will derive bounds on these terms in Propositions 4.2.9 and 4.2.10 below. In conclusion then (for any N-particle state ψ)

$$\langle H_N \rangle_\psi = E_F + \langle \mathrm{d}\Gamma(V(1-\varphi)) \rangle_F + \langle \xi_1 | \mathbb{H}_0 + \mathbb{Q}_4 | \xi_1 \rangle + \mathcal{E}_V(\psi) + \mathcal{E}_{\mathbb{Q}_2}(\psi) + \mathcal{E}_{\mathsf{scat}}(\psi). \tag{4.2.11}$$

With this formula we give the

Proof of Theorem 4.1.2. First, we calculate that $E_F = \frac{3}{5} N k_F^2 (1 + O(N^{-1/3}))$ by viewing the sum $E_F = \sum_{k \in B_F} |k|^2$ as a Riemann-sum for the corresponding integral $\frac{L^3}{(2\pi)^3} \int_{|k| \le k_F} |k|^2 \, \mathrm{d}k$. Next, we calculate $\langle \mathrm{d}\Gamma(V(1-\varphi)) \rangle_F$. With the aid of Equation (4.1.11) we find (since V has compact support) that

$$\int V(1-\varphi)|x|^2 \, \mathrm{d}x = \int_{|x| \le k_F^{-1}} V(1-\varphi_0)|x|^2 \, \mathrm{d}x = 24\pi a^3$$

for small k_F. Moreover, the two-particle reduced density of the free Fermi state satisfies Lemma 3.2.14

$$\rho^{(2)}(x,y) = \frac{1}{5(6\pi^2)^2} k_F^8 |x-y|^2 \left(1 + O(k_F^2|x-y|^2) + O(N^{-1/3})\right) \tag{4.2.12}$$

(with $|x-y|$ denoting the metric on the torus.) Thus,

$$\begin{aligned} \langle \mathrm{d}\Gamma(V(1-\varphi))\rangle_F &= \frac{1}{2}\iint V(x-y)(1-\varphi(x-y))\rho^{(2)}(x,y)\,\mathrm{d}x\,\mathrm{d}y \\ &= \frac{2}{5\pi} N a^3 k_F^5 (1 + O((ak_F)^2) + O(N^{-1/3})). \end{aligned} \tag{4.2.13}$$

For the third term in Equation (4.2.11), we can simply use $\mathbb{H}_0 + \mathbb{Q}_4 \geq 0$. Bounding the error terms $\mathcal{E}_V(\psi), \mathcal{E}_{\mathbb{Q}_2}(\psi)$ and $\mathcal{E}_{\mathsf{scat}}(\psi)$ occupies the main part of this paper. We shall show that they are bounded as follows.

Proposition 4.2.8. *Let ψ be an approximate ground state. Then*

$$|\mathcal{E}_V(\psi)| \leq C N a^3 k_F^5 (ak_F)^{3/4}.$$

Proposition 4.2.9. *Let ψ be an approximate ground state. Then*

$$|\mathcal{E}_{\mathbb{Q}_2}(\psi)| \leq C N a^3 k_F^5 (ak_F)^{3/2}.$$

Proposition 4.2.10. *Let ψ be an approximate ground state. Then*

$$|\mathcal{E}_{\mathsf{scat}}(\psi)| \leq C N a^3 k_F^5 (ak_F)^{3/10} \left|\log ak_F\right|.$$

Noting that the ground state is in particular an approximate ground state, we conclude the proof of Theorem 4.1.2. □

The remainder of the paper deals with the proofs of Propositions 4.2.8, 4.2.9 and 4.2.10.

Structure of the paper

First, in Section 4.3, we prove some useful a priori bounds and give the proof of Proposition 4.2.8. Next, in Section 4.4, we calculate the commutators $[\mathbb{H}_0, B]$, $[\mathbb{Q}_4, B]$ and $[\mathbb{Q}_2, B]$ and extract the claimed leading terms. Then, in Section 4.5, we bound the error terms arising from the commutators in a general state ξ. Finally, in Section 4.6, we use the bounds of Section 4.5 for the particular states ξ_λ to prove Propositions 4.2.9 and 4.2.10. Additionally we shall give the proof of Proposition 4.1.5.

In Section 4.A we sketch how to adapt the proof to the two-dimensional setting.

4.3 A Priori Bounds

We begin our analysis with some a priori bounds on the operators $\mathcal{N}, \mathbb{H}_0, \mathbb{Q}_2$ and $\mathbb{Q}_4$ (defined in Equations (4.1.12), (4.1.13) and (4.1.14) above) and on the scattering function φ in Equation (4.2.2).

4.3.1 A priori analysis of the kinetic energy

We may bound $\langle \mathcal{N} \rangle_{R^*\psi}$ and $\langle \mathbb{H}_0 \rangle_{R^*\psi}$ for an approximate ground state ψ exactly as in [FGHP21, Lemma 3.5 and Corollary 3.7] using the positivity of the interaction. We give the arguments here for completeness.

Lemma 4.3.1 (A priori bound on $\mathbb{H}_0$)**.** *Let ψ be an approximate ground state. Then*

$$\langle \mathbb{H}_0 \rangle_{R^*\psi} \leq C N a^3 k_F^5.$$

Proof. By the positivity of the interaction we have (recalling Equation (4.1.12))

$$\langle H_N \rangle_\psi = \langle \mathcal{H} \rangle_\psi \geq \langle \mathrm{d}\Gamma(-\Delta) \rangle_\psi = \langle R^* \mathrm{d}\Gamma(-\Delta) R \rangle_{R^*\psi} = E_F + \langle \mathbb{H}_0 \rangle_{R^*\psi}.$$

Then,

$$\langle \mathbb{H}_0 \rangle_{R^*\psi} \leq \langle H_N \rangle_\psi - E_F \leq C N a^3 k_F^5$$

by assumption of ψ being an approximate ground state. □

Lemma 4.3.2 (A priori bound on $\mathcal{N}$)**.** *Let ψ be an approximate ground state. Then*

$$\langle \mathcal{N} \rangle_{R^*\psi} \leq C N (a k_F)^{3/2}.$$

Proof. For any $\lambda > 0$ we can bound

$$\begin{aligned} \mathcal{N} = \sum_k a_k^* a_k &\leq \sum_{k:||k|^2 - k_F^2| \leq \lambda} 1 + \lambda^{-1} \sum_{k:||k|^2 - k_F^2| > \lambda} ||k|^2 - k_F^2| a_k^* a_k \\ &\leq C N \lambda k_F^{-2} + \lambda^{-1} \mathbb{H}_0. \end{aligned}$$

Using the bound on $\mathbb{H}_0$ from Lemma 4.3.1 and choosing the optimal $\lambda = k_F^2 (a k_F)^{3/2}$ we conclude the desired bound. □

4.3.2 A priori analysis of the interaction

Next, we study the interaction V and prove a priori bounds on the operators $\mathbb{Q}_2$ and $\mathbb{Q}_4$ (defined in Equations (4.1.13) and (4.1.14)) and bound the error-term $\mathcal{E}_V(\psi)$ from Equation (4.2.7).

Lemma 4.3.3. *Let $\psi \in \mathcal{F}$ be any state. Then*

$$\langle \mathrm{d}\Gamma(V) \rangle_\psi = \langle \mathrm{d}\Gamma(V) \rangle_F + \langle \mathbb{Q}_2 + \mathbb{Q}_4 \rangle_{R^*\psi} + \mathcal{E}_V(\psi),$$

with

$$|\mathcal{E}_V(\psi)| \lesssim \varepsilon N a^3 k_F^5 + \varepsilon \langle \mathbb{Q}_4 \rangle_{R^*\psi} + \varepsilon^{-1} a^3 k_F^5 \langle \mathcal{N} \rangle_{R^*\psi} + \varepsilon^{-1} a^3 k_F^3 \langle \mathbb{H}_0 \rangle_{R^*\psi}$$

for any $0 < \varepsilon < 1$.

Proof. Recall Definition 4.1.14 and the short-hand notation uu for $u \otimes u$. Viewing V as a two-particle operator, we can write

$$V = [vv + vu + uv + uu] V [vv + vu + uv + uu]$$

and expand the product. Since $V \geq 0$ we may bound the cross-terms as

$$\begin{aligned} \pm(uuV(vu + uv) + \text{h.c.}) &\leq \varepsilon uuVuu + \frac{1}{\varepsilon}(vu + uv)V(vu + uv) \\ \pm(vvV(vu + uv) + \text{h.c.}) &\leq \varepsilon vvVvv + \frac{1}{\varepsilon}(vu + uv)V(vu + uv) \end{aligned}$$

for any $\varepsilon > 0$. Then we have the bound

$$V \geq (1-\varepsilon)vvVvv+vvVuu+uuVvv+(1-\varepsilon)uuVuu+\left(1-\frac{2}{\varepsilon}\right)(vu+uv)V(vu+uv). \quad (4.3.1)$$

(An analogous upper bound on V holds if the signs in front of all ε-dependent terms are reversed.) Next, we shall write (4.3.1) in second quantization, conjugate by the particle-hole transformation R in (4.1.6), use Equation (4.1.8) and normal order the terms. We leave out the details of the computations; they can be found for instance in [HPR20, Proposition 4.1]. The result is

$$R^*\mathrm{d}\Gamma(V)R \geq (1-\varepsilon)\left\langle \mathrm{d}\Gamma(V)\right\rangle_F + \mathbb{Q}_2 + (1-\varepsilon)\mathbb{Q}_4 + \mathbb{X}_\varepsilon + \mathbb{Q}_\varepsilon. \quad (4.3.2)$$

(Again, an analogous upper bound holds reversing the sign of ε.) Here $\mathbb{Q}_2, \mathbb{Q}_4$ are as in Equations (4.1.13) and (4.1.14) and

$$\begin{aligned}
\mathbb{X}_\varepsilon &= \frac{1-\varepsilon}{L^3}\sum_{\substack{p,q \\ p,q\in B_F}}[\hat{V}(p-q)-\hat{V}(0)]c_q^*c_q - \frac{1-2/\varepsilon}{L^3}\sum_{\substack{p,q\\ p\in B_F\\ q\notin B_F}}[\hat{V}(p-q)-\hat{V}(0)]b_q^*b_q,\\
\mathbb{Q}_\varepsilon &= \frac{1-\varepsilon}{2}\iint V(x-y)c_x^*c_y^*c_yc_x\,\mathrm{d}x\,\mathrm{d}y\\
&\quad+\left(\frac{1}{2}-\frac{1}{\varepsilon}\right)\iint V(x-y)[b_x^*c_x^*c_yb_y + b_y^*c_y^*c_xb_x - b_x^*c_y^*c_yb_x - b_y^*c_x^*c_xb_y]\,\mathrm{d}x\,\mathrm{d}y. \quad (4.3.3)
\end{aligned}$$

In particular, for any $\varepsilon > 0$

$$|\mathcal{E}_V(\psi)| \leq \varepsilon\left\langle \mathrm{d}\Gamma(V)\right\rangle_F + \varepsilon\left\langle \mathbb{Q}_4\right\rangle_{R^*\psi} + \left|\left\langle \mathbb{X}_{\pm\varepsilon}\right\rangle_{R^*\psi}\right| + \left|\left\langle \mathbb{Q}_{\pm\varepsilon}\right\rangle_{R^*\psi}\right|$$

(where the $\pm\varepsilon$ has to be interpreted as taking the maximum over the two terms, either with ε or $-\varepsilon$). To bound this we first note that $\left\langle \mathrm{d}\Gamma(V)\right\rangle_F \leq CNa^3k_F^5$. Indeed, by a simple Taylor-expansion, the two-particle density of the free Fermi gas is bounded by $\rho^{(2)}(x,y) \leq Ck_F^8|x-y|^2$, see Lemma 3.2.14 or Equation (4.2.12) above. Hence

$$\left\langle \mathrm{d}\Gamma(V)\right\rangle_F = \frac{1}{2}\iint V(x-y)\rho^{(2)}(x,y)\,\mathrm{d}x\,\mathrm{d}y \leq Ck_F^8\iint V(x-y)|x-y|^2\,\mathrm{d}x\,\mathrm{d}y \leq CNa^3k_F^5.$$

(Here $\int |x|^2V\,\mathrm{d}x$ is a finite constant of dimension (length)^3 and hence we write it as Ca^3, as discussed in Remark 4.1.3.) We are left with bounding the operators $\mathbb{X}_{\pm\varepsilon}$ and $\mathbb{Q}_{\pm\varepsilon}$.

To bound $\mathbb{X}_{\pm\varepsilon}$ view $\hat{V}(k) = \int_\Lambda V(x)e^{-ikx}\,\mathrm{d}x = \int_{\mathbb{R}^3} V(x)e^{-ikx}$ (for L sufficiently large, by the compact support of V) as defined on all of $\mathbb{R}^3$ (i.e., not just on $\frac{2\pi}{L}\mathbb{Z}^3$) and Taylor expand. We find $\hat{V}(k) = \hat{V}(0) + O(|k|^2\int_{\mathbb{R}^3}|x|^2V(x)\,\mathrm{d}x) = \hat{V}(0) + O(a^3|k|^2)$ since V is a real-valued radial function. Thus, for any state $\xi \in \mathcal{F}$,

$$\begin{aligned}
\left|\left\langle \mathbb{X}_{\pm\varepsilon}\right\rangle_\xi\right| &\lesssim \frac{a^3}{L^3}\sum_{k\in B_F}\sum_{\ell\in B_F}|k-\ell|^2\left\langle c_\ell^*c_\ell\right\rangle_\xi\\
&\qquad+\varepsilon^{-1}\frac{a^3}{L^3}\left[\sum_{k\in B_F}|k|^2\sum_\ell\left\langle b_\ell^*b_\ell\right\rangle_\xi + \sum_{k\in B_F}\sum_\ell|\ell|^2\left\langle b_\ell^*b_\ell\right\rangle_\xi\right]\\
&\lesssim \varepsilon^{-1}a^3k_F^5\left\langle \mathcal{N}\right\rangle_\xi + \varepsilon^{-1}a^3k_F^3\left\langle \mathbb{H}_0\right\rangle_\xi
\end{aligned}$$

(for any $0 < \varepsilon < 1$) by noting that $\sum_k |k|^2a_k^*a_k \leq \mathbb{H}_0 + k_F^2\mathcal{N}$.

Finally, we shall show that $\mathbb{Q}_{\pm\varepsilon}$ is suitably small. Note that the first term in Equation (4.3.3) is actually non-negative for $0 \le \varepsilon \le 1$ and could be dropped for a lower bound; since we will also derive an upper bound with our method, however, we shall not do this and estimate it instead. The main idea is to "Taylor expand in $x-y$". More precisely, for the first term in Equation (4.3.3) we write

$$c_y = c_x + (y-x) \cdot \int_0^1 \nabla c_{x+t(y-x)} \, \mathrm{d}t. \tag{4.3.4}$$

The integration has to be understood as connecting the two points x and y by the shortest line on the torus. We apply this to the factors c_y^* and c_y. Noting that $c_x^2 = 0$ (recall that c_x is in fact a bounded operator) and changing variables to $z = y - x$ we then find (recalling that V is even)

$$\iint V(x-y) c_x^* c_y^* c_y c_x \,\mathrm{d}x\,\mathrm{d}y = \iint V(z) z^\mu z^\nu \int_0^1 \mathrm{d}t \int_0^1 \mathrm{d}s\, c_x^* \nabla^\mu c_{x+tz}^* \nabla^\nu c_{x+sz} c_x \,\mathrm{d}x\,\mathrm{d}z.$$

In norm we have $\|\nabla c_x\| \le C k_F^{3/2+1}$. Thus, the expectations value of the first term in Equation (4.3.3) in any state ξ is bounded by

$$\left| \frac{1 \mp \varepsilon}{2} \iint V(x-y) \left\langle c_x^* c_y^* c_y c_x \right\rangle_\xi \mathrm{d}x\,\mathrm{d}y \right| \le C k_F^5 \int |z|^2 V(z) \,\mathrm{d}z \int \|c_x \xi\|^2 \,\mathrm{d}x.$$

Furthermore,

$$\int \|c_x \xi\|^2 \,\mathrm{d}x = \sum_{k \in B_F} \langle \xi | a_k^* a_k | \xi \rangle \le \langle \mathcal{N} \rangle_\xi \,.$$

Denote the second term of Equation (4.3.3) by $\mathbb{Q}_{\varepsilon,2}$ and define for any state ξ the function $\phi(x,y) = \left\langle b_x^* c_x^* c_y b_y + b_y^* c_y^* c_x b_x - b_x^* c_y^* c_y b_x - b_y^* c_x^* c_x b_y \right\rangle_\xi$. We note that $\phi(y,x) = \phi(x,y)$ and $\phi(x,x) = 0$. Thus, by Taylor-expansion in y around $y = x$ the zeroth and first orders vanish, and hence

$$\phi(x,y) = (y-x)^\mu (y-x)^\nu \int_0^1 \mathrm{d}t\, (1-t) [\nabla_2^\mu \nabla_2^\nu \phi](x, x + t(y-x)).$$

(Here ∇_2^μ denotes a derivative in the second variable.) Thus (changing variables to $z = x - y$ and using that V is even) we have

$$\langle \mathbb{Q}_{\pm\varepsilon,2} \rangle_\xi = \left(\frac{1}{2} \mp \frac{1}{\varepsilon} \right) \int_0^1 \mathrm{d}t\, (1-t) \int \mathrm{d}z\, z^\mu z^\nu V(z) \int \mathrm{d}x\, [\nabla_2^\mu \nabla_2^\nu \phi](x, x+tz).$$

The x-integral is given by (with the derivatives now being with respect to x)

$$\begin{aligned}
&\int \mathrm{d}x \Big\langle b_x^* c_x^* [\nabla^\mu \nabla^\nu c_{x+tz} b_{x+tz}] + [\nabla^\mu \nabla^\nu b_{x+tz}^* c_{x+tz}^*] c_x b_x - b_x^* [\nabla^\mu \nabla^\nu c_{x+tz}^* c_{x+tz}] b_x \\
&\quad - [\nabla^\mu \nabla^\nu b_{x+tz}^*] c_x^* c_x b_{x+tz} - b_{x+tz}^* c_x^* c_x [\nabla^\mu \nabla^\nu b_{x+tz}] \\
&\quad - ([\nabla^\mu b_{x+tz}^*] c_x^* c_x [\nabla^\nu b_{x+tz}] + (\mu \leftrightarrow \nu)) \Big\rangle_\xi \\
&= \int \mathrm{d}x \Big\langle -[\nabla^\mu b_x^* c_x^*][\nabla^\nu c_{x+tz} b_{x+tz}] - [\nabla^\mu b_{x+tz}^* c_{x+tz}^*][\nabla^\nu c_x b_x] - b_x^* [\nabla^\mu \nabla^\nu c_{x+tz}^* c_{x+tz}] b_x \\
&\quad + [\nabla^\mu b_{x+tz}^*][\nabla^\nu c_x^* c_x b_{x+tz}] + [\nabla^\mu b_{x+tz}^* c_x^* c_x][\nabla^\nu b_{x+tz}] \\
&\quad - ([\nabla^\mu b_{x+tz}^*] c_x^* c_x [\nabla^\nu b_{x+tz}] + (\mu \leftrightarrow \nu)) \Big\rangle_\xi
\end{aligned}$$

by integration by parts. Using the norm estimate $\|\nabla^n c_x\| \leq C k_F^{3/2+n}$ with ∇^n denoting any n'th derivative we thus bound the x-integral with the aid of Cauchy–Schwarz as

$$\lesssim k_F^3 \int \mathrm{d}x \, \|\nabla b_x \xi\|^2 + k_F^5 \int \mathrm{d}x \, \|b_x \xi\|^2 .$$

Noting that

$$\int \|b_x \xi\|^2 \, \mathrm{d}x = \sum_{k \notin B_F} \langle \xi | a_k^* a_k | \xi \rangle \leq \langle \mathcal{N} \rangle_\xi ,$$

$$\int \|\nabla b_x \xi\|^2 \, \mathrm{d}x = \sum_{k \notin B_F} |k|^2 \langle \xi | a_k^* a_k | \xi \rangle \leq \langle \mathbb{H}_0 \rangle_\xi + k_F^2 \langle \mathcal{N} \rangle_\xi$$

we thus obtain

$$\left| \langle \mathbb{Q}_{\pm\varepsilon,2} \rangle_\xi \right| \lesssim \varepsilon^{-1} a^3 k_F^5 \langle \mathcal{N} \rangle_\xi + \varepsilon^{-1} a^3 k_F^3 \langle \mathbb{H}_0 \rangle_\xi .$$

Together with the bounds above, this concludes the proof of the lemma. □

Additionally, we need a priori bounds on $\mathbb{Q}_2$ and $\mathbb{Q}_4$ (defined in Equations (4.1.13) and (4.1.14)). These follow from arguments similar to the analogous bounds in [FGHP21, Proposition 3.3(e) and Lemma 3.9].

Lemma 4.3.4 (A priori bound for $\mathbb{Q}_2$)**.** *For suitable $C > 0$ we have*

$$\left| \langle \mathbb{Q}_2 \rangle_\xi \right| \leq \delta \langle \mathbb{Q}_4 \rangle_\xi + C \delta^{-1} N a^3 k_F^5 .$$

for any $\delta > 0$ and any state $\xi \in \mathcal{F}$.

Proof. By Cauchy–Schwarz we have for any $\delta > 0$

$$\begin{aligned} 2 \left| \langle \mathbb{Q}_2 \rangle_\xi \right| &\leq \iint V(x-y) \left| \left\langle b_x^* b_y^* c_y^* c_x^* + \text{h.c.} \right\rangle_\xi \right| \mathrm{d}x \, \mathrm{d}y \\ &\leq \iint V(x-y) \left(\delta \|b_y b_x \xi\|^2 + \delta^{-1} \left\| c_y^* c_x^* \xi \right\|^2 \right) \mathrm{d}x \, \mathrm{d}y \\ &\leq 2\delta \langle \mathbb{Q}_4 \rangle_\xi + \delta^{-1} \iint V(x-y) \left\| c_y^* c_x^* \right\|^2 \mathrm{d}x \, \mathrm{d}y. \end{aligned}$$

We Taylor expand c_y^* as in Equation (4.3.4) above. Being fermionic operators $(c_x^*)^2 = 0$. In particular we have $\left\| c_y^* c_x^* \right\| \leq C k_F^4 |x-y|$ since $\|c_x^*\| \leq C k_F^{3/2}$ and $\|\nabla c_x^*\| \leq C k_F^{3/2+1}$. With $\int |x|^2 V \, \mathrm{d}x \leq C a^3$ we conclude the proof of the lemma. □

Lemma 4.3.5 (A priori bound for $\mathbb{Q}_4$)**.** *Let ψ be an approximate ground state. Then*

$$\langle \mathbb{Q}_4 \rangle_{R^*\psi} \leq C N a^3 k_F^5 .$$

Proof. Recalling Equation (4.1.12), applying Lemma 4.3.3 and Lemma 4.3.4 with $\delta = 1/2$, and using $\langle \mathrm{d}\Gamma(V) \rangle_F \geq 0$ we find

$$\begin{aligned} \langle H_N \rangle_\psi \geq E_F + \langle \mathbb{H}_0 \rangle_{R^*\psi} + \left(\frac{1}{2} - \varepsilon \right) \langle \mathbb{Q}_4 \rangle_{R^*\psi} - C N a^3 k_F^5 \\ - C \varepsilon^{-1} a^3 k_F^5 \langle \mathcal{N} \rangle_{R^*\psi} - C \varepsilon^{-1} a^3 k_F^3 \langle \mathbb{H}_0 \rangle_{R^*\psi} . \end{aligned}$$

Using the a priori bounds of Lemmas 4.3.1 and 4.3.2 and noting that $\mathbb{H}_0 \geq 0$ we obtain the desired result (by taking $\varepsilon = 1/4$, say). □

With the results of this section we can give the

Proof of Proposition 4.2.8. Combining Lemmas 4.3.1, 4.3.2, 4.3.3 and 4.3.5 and choosing the optimal $\varepsilon = (ak_F)^{3/4}$ we conclude the proof of Proposition 4.2.8. $\square$

4.3.3 The scattering function

We now prove some a priori bounds on the scattering function φ defined in Equation (4.2.2) above.

Lemma 4.3.6 (Properties of φ)**.** *The scattering function φ satisfies*

$$\begin{aligned} &\| |\cdot|^n \varphi \|_{L^1} \le C a^3 k_F^{-n}, \quad n = 1,2, && \| |\cdot|^n \nabla^n \varphi \|_{L^1} \le C a^3 \left|\log a k_F\right|, \quad n = 0,1,2 \\ &\| |\cdot| \varphi \|_{L^2} \le C a^{3/2+1}, && \| |\cdot|^n \nabla^n \varphi \|_{L^2} \le C a^{3/2}, \qquad\qquad n = 0,1. \end{aligned}$$

Here ∇^n represents any combination of n derivatives and $|\cdot|$ denotes the metric on the torus in the sense that $|x|$ is the distance between x and the point 0.

Remark 4.3.7. Recalling the bound in Equation (4.2.4) for $\mathcal{E}_\varphi$ we see that $\mathcal{E}_\varphi$ satisfies the same bounds as φ only with an additional power k_F.

Proof. Recall that the scattering function is given by (the periodization of) $\varphi = \varphi_0 \chi_\varphi(k_F |\cdot|)$. Since φ_0 is a radial function, so is φ (rather, $\varphi_0 \chi_\varphi(k_F|\cdot|)$ is). In particular, for the bounds we may replace ∇^n by ∂_r^n, with ∂_r the derivative in the radial direction.

We first establish the bound

$$|\partial_r \varphi_0(x)| \le \frac{C a^3}{|x|(a^3 + |x|^3)}, \qquad \text{for all } x \in \mathbb{R}^3. \tag{4.3.5}$$

To prove this, we note that, in radial coordinates, the scattering equation (4.1.4) reads

$$r \partial_r^2 \varphi_0 + 4 \partial_r \varphi_0 + \frac{1}{2} r V (1 - \varphi_0) = 0.$$

Further, we recall that $0 \le \varphi_0(x) \le \min\{1, a^3/|x|^3\}$ for all x and that φ_0 is a radially decreasing function, which follows from [LY01, Lemma A.1] applied to 5 dimensions. Using the scattering equation we then compute

$$\partial_r \left[\partial_r \varphi_0 + \frac{4}{r} \varphi_0 \right] = \partial_r^2 \varphi_0 + \frac{4}{r} \partial_r \varphi_0 - \frac{4}{r^2} \varphi_0 = -\frac{4}{r^2} \varphi_0 - \frac{1}{2} V (1 - \varphi_0) \le 0.$$

Integrating and recalling that $\varphi_0(x) = a^3/|x|^3$ outside the support of V we find

$$\partial_r \varphi_0 + \frac{4}{r} \varphi_0 \ge 0.$$

Since $\partial_r \varphi_0 \le 0$ this proves Equation (4.3.5). From Equation (4.3.5) and the scattering equation (4.1.4) we immediately find

$$\left| \partial_r^2 \varphi_0 \right| \lesssim \frac{a^3}{|x|^2 (a^3 + |x|^3)} + V.$$

To extract the bounds on φ we note that $\|\partial^n \chi_\varphi\|_{L^\infty} \le C$ for any n, since χ_φ is smooth by assumption. Furthermore, also by assumption, $V \in L^1$. Finally, φ is supported only for $|x| \le 2k_F^{-1}$ since $\chi_\varphi(t) = 0$ for $t > 2$. The bounds immediately follow. $\square$

4.4 Calculation of Commutators

In this section we shall calculate the commutators $[\mathbb{H}_0, B]$, $[\mathbb{Q}_4, B]$ and $[\mathbb{Q}_2, B]$ and find formulas for the error-terms $\mathcal{E}_{\mathbb{Q}_2}(\psi)$ and $\mathcal{E}_{\mathsf{scat}}(\psi)$ in Equations (4.2.9) and (4.2.10). The computations of the commutators are analogous to those in [FGHP21; Gia23a], where similar commutators are computed.

4.4.1 $[\mathbb{H}_0, B]$:

We have (recalling the formula for $\mathbb{H}_0$ in Equation (4.1.12) and using the representation of B in momentum-space in Equation (4.2.5))

$$[\mathbb{H}_0, B] = \frac{1}{2L^3} \sum_{p,q,k,k'} ||q|^2 - k_F^2| \hat{\varphi}(p) [a_q^* a_q, b_{k+p}^r b_{k'-p}^r c_{k'} c_k] + \text{h.c.}.$$

To compute the commutator we note that $[a_q^* a_q, a_k] = -\delta_{q,k} a_k$, hence

$$[a_q^* a_q, b_{k+p}^r b_{k'-p}^r c_{k'} c_k] = -(\delta_{q,k+p} + \delta_{q,k'-p} + \delta_{q,k'} + \delta_{q,k}) b_{k+p}^r b_{k'-p}^r c_{k'} c_k.$$

Next, for $k+p, k'-p \notin B_F$ and $k, k' \in B_F$ we have

$$\begin{aligned} &||k+p|^2 - k_F^2| + ||k'-p|^2 - k_F^2| + ||k|^2 - k_F^2| + ||k'|^2 - k_F^2| \\ &\quad = |k+p|^2 + |k'-p|^2 - |k|^2 - |k'|^2 \\ &\quad = 2|p|^2 + 2p \cdot (k - k'). \end{aligned}$$

We conclude that

$$[\mathbb{H}_0, B] = -\frac{1}{L^3} \sum_{p,k,k'} \left(|p|^2 + p \cdot (k - k') \right) \hat{\varphi}(p) b_{k+p}^r b_{k'-p}^r c_{k'} c_k + \text{h.c.}.$$

By the symmetry $k \leftrightarrow k'$ and $p \to -p$ we may write the second summand as

$$-\frac{2}{L^3} \sum_{p,k,k'} p \cdot k \hat{\varphi}(p) b_{k+p}^r b_{k'-p}^r c_{k'} c_k + \text{h.c.}.$$

Writing then in configuration space we get (recall the Einstein summation convention, introduced in Notation 4.2.2.)

$$[\mathbb{H}_0, B] = \iint \left(\Delta\varphi(x-y) b_x^r b_y^r c_y c_x + 2\nabla^\mu \varphi(x-y) b_x^r b_y^r c_y \nabla^\mu c_x \right) \mathrm{d}x \, \mathrm{d}y + \text{h.c.}.$$

We first replace the b's by their non-regularized counterparts. That is, we write

$$[\mathbb{H}_0, B] = \iint (\Delta\varphi(x-y) b_x b_y c_y c_x + 2\nabla^\mu \varphi(x-y) b_x b_y c_y \nabla^\mu c_x) \, \mathrm{d}x \, \mathrm{d}y + \text{h.c.} + \mathbb{H}_{0;B}^{\div r} \quad (4.4.1)$$

with $\mathbb{H}_{0;B}^{\div r}$ defined so that this holds. Write now (similarly as in Equation (4.3.4))

$$\begin{aligned} c_x &= c_y + (x-y)^\mu \int_0^1 \mathrm{d}t \, \nabla^\mu c_{y+t(x-y)} \\ &= c_y + (x-y)^\mu \nabla^\mu c_x - (x-y)^\mu (x-y)^\nu \int_0^1 \mathrm{d}t \, (1-t) \nabla^\mu \nabla^\nu c_{x+t(y-x)}. \end{aligned} \quad (4.4.2)$$

Note that the first order term $\nabla^\mu c_x$ is evaluated at x and not at y. We apply Equation (4.4.2) to the factor c_x in the first term in Equation (4.4.1) above. Being a fermionic operator $c_y^2 = 0$. Thus, we have

$$\begin{aligned} [\mathbb{H}_0, B] = \iint & \left[(x-y)^\mu \Delta\varphi(x-y) + 2\nabla^\mu \varphi(x-y)\right] b_x b_y c_y \nabla^\mu c_x \,\mathsf{d}x\,\mathsf{d}y + \text{h.c.} \\ & + \mathbb{H}_{0;B}^{\text{Taylor}} + \mathbb{H}_{0;B}^{\div r}, \end{aligned} \tag{4.4.3}$$

with $\mathbb{H}_{0;B}^{\text{Taylor}}$ as in the first term of Equation (4.4.1) only with the factor c_x replaced by the last term of Equation (4.4.2). It is an error term.

4.4.2 $[\mathbb{Q}_4, B]$:

Recall the definition of $\mathbb{Q}_4$ from Equation (4.1.14) and of B from Equation (4.2.5). We compute

$$[\mathbb{Q}_4, B] = \frac{1}{4} \iiiint \mathsf{d}x\,\mathsf{d}y\,\mathsf{d}z\,\mathsf{d}z'\, V(x-y)\varphi(z-z')[b_x^* b_y^* b_y b_x, b_z^r b_{z'}^r c_{z'} c_z] + \text{h.c.}$$

The commutator is (using that b's and c's have disjoint support in momentum-space so they anti-commute: $\{b_x^*, c_y\} = 0$)

$$[b_x^* b_y^* b_y b_x, b_z^r b_{z'}^r c_{z'} c_z] = [b_x^* b_y^*, b_z^r b_{z'}^r] b_y b_x c_{z'} c_z.$$

Using that

$$\{b_x^*, b_y^r\} = \frac{1}{L^3} \sum_k \hat{u}^r(k) e^{ik(y-x)} = u^r(y-x) = u^r(x-y)$$

one computes

$$\begin{aligned} [b_x^* b_y^*, b_z^r b_{z'}^r] &= u^r(x-z) u^r(y-z') - u^r(y-z) u^r(x-z') \\ &\quad + u^r(y-z) b_x^* b_{z'}^r + u^r(x-z') b_y^* b_z^r - u^r(x-z) b_y^* b_{z'}^r - u^r(y-z') b_x^* b_z^r \end{aligned} \tag{4.4.4}$$

The two first terms, respectively the four last terms, give the same contributions to $[\mathbb{Q}_4, B]$ when the integration is performed by the symmetries $x \leftrightarrow y$ and $z \leftrightarrow z'$. We write the u^r's as $u^r = \delta - v^r$. The quartic term with two δ's is the main term. In conclusion then

$$[\mathbb{Q}_4, B] = -\frac{1}{2} \iint V(x-y)\varphi(x-y) b_x b_y c_y c_x \,\mathsf{d}x\,\mathsf{d}y + \text{h.c.} + \mathbb{Q}_{4;B}^{\mathcal{E}} \tag{4.4.5}$$

with

$$\begin{aligned} \mathbb{Q}_{4;B}^{\mathcal{E}} = \frac{1}{2} \iiiint & V(x-y)\varphi(z-z') \Big[\Big(2\delta(y-z) v^r(x-z') - v^r(x-z') v^r(y-z) \Big) b_y b_x c_{z'} c_z \\ & - 2(\delta(x-z) - v^r(x-z)) b_y^* b_{z'}^r b_y b_x c_{z'} c_z \Big] \,\mathsf{d}x\,\mathsf{d}y\,\mathsf{d}z\,\mathsf{d}z' + \text{h.c.}. \end{aligned} \tag{4.4.6}$$

In the first term we rewrite c_x using Equation (4.4.2) as for the case of $\mathbb{H}_0$. Then we find

$$[\mathbb{Q}_4, B] = -\frac{1}{2} \iint (x-y)^\mu V(x-y)\varphi(x-y) b_x b_y c_y \nabla^\mu c_x \,\mathsf{d}x\,\mathsf{d}y + \text{h.c.} + \mathbb{Q}_{4;B}^{\text{Taylor}} + \mathbb{Q}_{4;B}^{\mathcal{E}} \tag{4.4.7}$$

and $\mathbb{Q}_{4;B}^{\text{Taylor}}$ as in the first term of (4.4.5) only with c_x replaced by the last term of Equation (4.4.2).

4.4.3 $[\mathbb{Q}_2, B]$:

Recall the definition of $\mathbb{Q}_2$ from Equation (4.1.13) and of B from Equation (4.2.5). We have

$$[\mathbb{Q}_2, B] = \frac{1}{4} \iiiint V(x-y)\varphi(z-z')[b_x^* b_y^* c_y^* c_x^*, b_z^r b_{z'}^r c_{z'} c_z] \,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z' + \text{h.c.}.$$

The commutator is given by (recall again that b's and c's anti-commute)

$$\begin{aligned}[b_x^* b_y^* c_y^* c_x^*, b_z^r b_{z'}^r c_{z'} c_z] = -[b_x^* b_y^*, b_z^r b_{z'}^r][c_y^* c_x^*, c_{z'} c_z] + b_x^* b_y^* b_z^r b_{z'}^r [c_y^* c_x^*, c_{z'} c_z] \\ + c_y^* c_x^* c_{z'} c_z [b_x^* b_y^*, b_z^r b_{z'}^r].\end{aligned} \tag{4.4.8}$$

The b-commutator is as in Equation (4.4.4). Similarly

$$\begin{aligned}[c_y^* c_x^*, c_{z'} c_z] &= v(x-z)v(y-z') - v(y-z)v(x-z') \\ &\quad + v(y-z)c_x^* c_{z'} + v(x-z')c_y^* c_z - v(x-z)c_y^* c_{z'} - v(y-z')c_x^* c_z\end{aligned} \tag{4.4.9}$$

The leading term is the constant (i.e. fully contracted) one. All other terms contribute to the error. Furthermore, in the constant term we write $u^r = \delta - v^r$. Then the term with all δ's is the main one and the remainder are errors. We conclude

$$\begin{aligned}[\mathbb{Q}_2, B] &= -\frac{1}{2} \iiiint V(x-y)\varphi(z-z')\left[\delta(x-z)\delta(y-z') - \delta(x-z')\delta(y-z)\right] \\ &\qquad \times \left[v(x-z)v(y-z') - v(x-z')v(y-z)\right] \,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z' + \mathbb{Q}_{2;B}^{\mathcal{E}} \\ &= -\iint V(x-y)\varphi(x-y)\rho^{(2)}(x,y)\,\mathrm{d}x\,\mathrm{d}y + \mathbb{Q}_{2;B}^{\mathcal{E}} = -2\left\langle \mathrm{d}\Gamma(V\varphi)\right\rangle_F + \mathbb{Q}_{2;B}^{\mathcal{E}}\end{aligned} \tag{4.4.10}$$

using that the two-particle density of the free Fermi state is given by $\rho^{(2)}(x,y) = |v(0)|^2 - |v(x-y)|^2$.

4.5 Bounding Error Terms

To prove the bounds in Propositions 4.2.9 and 4.2.10 we first bound $[\mathbb{H}_0+\mathbb{Q}_4, B]+\mathbb{Q}_2$ and $\mathbb{Q}_{2;B}^{\mathcal{E}}$. Then in Section 4.6 we use these bounds for the particular states ξ_λ from Equation (4.2.6) with ψ an approximate ground state to conclude the proofs of Propositions 4.2.9 and 4.2.10.

To bound $[\mathbb{H}_0 + \mathbb{Q}_4, B] + \mathbb{Q}_2$ we first recall the definition of $\mathbb{Q}_2$ in Equation (4.1.13)

$$\mathbb{Q}_2 = \frac{1}{2} \iint V(x-y) b_x b_y c_y c_x \,\mathrm{d}x\,\mathrm{d}y + \text{h.c.}.$$

Rewriting the factor c_x as in Equation (4.4.2) we thus have

$$\mathbb{Q}_2 = \frac{1}{2} \iint (x-y)^\mu V(x-y) b_x b_y c_y \nabla^\mu c_x \,\mathrm{d}x\,\mathrm{d}y + \text{h.c.} + \mathbb{Q}_2^{\text{Taylor}}$$

with $\mathbb{Q}_2^{\text{Taylor}}$ appropriately defined. Then, recalling Equations (4.4.3) and (4.4.7), we have

$$[\mathbb{H}_0 + \mathbb{Q}_4, B] + \mathbb{Q}_2 = \mathbb{Q}_{\text{scat}} + \mathbb{H}_{0;B}^{\text{Taylor}} + \mathbb{H}_{0;B}^{\div r} + \mathbb{Q}_{4;B}^{\text{Taylor}} + \mathbb{Q}_{4;B}^{\mathcal{E}} + \mathbb{Q}_2^{\text{Taylor}} \tag{4.5.1}$$

with (recalling Equation (4.2.3))

$$\mathbb{Q}_{\text{scat}} = \iint \mathcal{E}_\varphi^\mu(x-y) b_x b_y c_y \nabla^\mu c_x \,\mathrm{d}x\,\mathrm{d}y + \text{h.c.}. \tag{4.5.2}$$

Below we bound separately each of the operators

$$\mathbb{T} := \mathbb{H}_{0;B}^{\text{Taylor}} + \mathbb{Q}_{4;B}^{\text{Taylor}} + \mathbb{Q}_{2}^{\text{Taylor}}, \quad \mathbb{Q}_{\text{scat}}, \quad \mathbb{H}_{0;B}^{\div r}, \quad \mathbb{Q}_{4;B}^{\mathcal{E}} \quad \text{and} \quad \mathbb{Q}_{2;B}^{\mathcal{E}}$$

with $\mathbb{Q}_{2;B}^{\mathcal{E}}$ from Equation (4.4.10). We shall show that

Lemma 4.5.1. *For any state $\xi \in \mathcal{F}$, and any $\alpha > 0$, we have*

$$\begin{aligned}
\left|\langle\mathbb{T}\rangle_\xi\right| + \left|\langle\mathbb{Q}_{\text{scat}}\rangle_\xi\right| &\lesssim N^{1/2}a^3k_F^5(ak_F)^{-3\alpha/2}\left|\log ak_F\right|\langle\mathcal{N}\rangle_\xi^{1/2} + N^{1/2}ak_F^2(ak_F)^{1/2+\alpha}\langle\mathbb{H}_0\rangle_\xi^{1/2},\\
\left|\left\langle\mathbb{H}_{0;B}^{\div r}\right\rangle_\xi\right| &\lesssim N^{1/2}a^3k_F^4\left|\log ak_F\right|\langle\mathbb{H}_0\rangle_\xi^{1/2} + N^{1/2}a^3k_F^5\left|\log ak_F\right|\langle\mathcal{N}\rangle_\xi^{1/2},\\
\left|\left\langle\mathbb{Q}_{4;B}^{\mathcal{E}}\right\rangle_\xi\right| &\lesssim N^{1/2}a^3k_F^4(ak_F)^{1/2}\langle\mathbb{Q}_4\rangle_\xi^{1/2} + a^3k_F^4\langle\mathcal{N}\rangle_\xi^{1/2}\langle\mathbb{Q}_4\rangle_\xi^{1/2},\\
\left|\left\langle\mathbb{Q}_{2;B}^{\mathcal{E}}\right\rangle_\xi\right| &\lesssim a^2k_F^2\langle\mathbb{H}_0\rangle_\xi^{1/2}\langle\mathbb{Q}_4\rangle_\xi^{1/2} + a^3k_F^5\langle\mathcal{N}\rangle_\xi + Na^5k_F^7\left|\log ak_F\right|.
\end{aligned}$$

The rest of this section deals with the proof of Lemma 4.5.1. We first give some preliminary bounds.

4.5.1 Technical lemmas

In the proof of Lemma 4.5.1 below we shall need a bound on integrals of the form $\int F(y)b_yc_y\,\mathrm{d}y$ and similar. The following lemma will turn out to be very helpful.

Lemma 4.5.2. *Let F be a compactly supported function with $F(x) = 0$ for $|x| \geq Ck_F^{-1}$. Then, uniformly in $x \in \Lambda$ and $t \in [0,1]$, (with ∇^n denoting any n'th derivative)*

$$\left\|\int F(x-y)a_yc_y\,\mathrm{d}y\right\| \lesssim k_F^{3/2}\left\|F\right\|_{L^2}, \tag{4.5.3}$$

$$\left\|\int F(x-y)a_yc_y\nabla^n c_{ty+(1-t)x}\,\mathrm{d}y\right\| \lesssim k_F^{3+n}\left\|F\right\|_{L^2}. \tag{4.5.4}$$

Remark 4.5.3. Recall that $\int F(y)a_y\,\mathrm{d}y = a(\overline{F})$ has norm $\left\|a(\overline{F})\right\| = \left\|F\right\|_{L^2}$. The lemma shows that for certain bounded operators A_y (being either c_y or $c_y\nabla^n c_{ty+(1-t)x}$) $\left\|\int F(y)a_yA_y\,\mathrm{d}y\right\|$ can be bounded by (a constant times) $\left\|F\right\|_{L^2}\sup_y\left\|A_y\right\|$.

Remark 4.5.4. A similar bound is given in [Gia23a, Lemma 4.8]. There, however, the right-hand side depends on $\left\|F\right\|_{L^1}, \left\|\nabla F\right\|_{L^1}$ and $\left\|\Delta F\right\|_{L^1}$. In Lemma 4.5.2 we do not require any smoothness on F. This translates to having no smoothness assumptions on V in Theorem 4.1.2.

Remark 4.5.5. Applying Equation (4.5.3) for $F = \varphi$ we find (by writing $b_{z'}^r = a_{z'} - (a_{z'} - b_{z'}^r)$ and noting that $\left\|a_{z'} - b_{z'}^r\right\| \leq Ck_F^{3/2}$ since both operators agree for momenta $|k| \geq 3k_F$)

$$\left\|\int \varphi(z-z')b_{z'}^rc_{z'}\,\mathrm{d}z'\right\| \lesssim k_F^3\left\|\varphi\right\|_{L^1} + k_F^{3/2}\left\|\varphi\right\|_{L^2} \leq C(ak_F)^{3/2} \tag{4.5.5}$$

where we have used Lemma 4.3.6 to bound the norms of φ. Moreover, by Taylor-expanding as in Equation (4.3.4) we have

$$\int \varphi(z-z')b_{z'}^rc_{z'}c_z\,\mathrm{d}z' = \int (z-z')^\mu\varphi(z-z')b_{z'}^rc_{z'}\int_0^1\mathrm{d}t\,\nabla^\mu c_{z'+t(z-z')}\,\mathrm{d}z'.$$

Thus, by Equation (4.5.4), we conclude in a similar way the bound

$$\left\|\int \varphi(z-z')b_{z'}^rc_{z'}c_z\,\mathrm{d}z'\right\| \lesssim k_F^{4+3/2}\left\||\cdot|\varphi\right\|_{L^1} + k_F^4\left\||\cdot|\varphi\right\|_{L^2} \leq Ck_F^{3/2}(ak_F)^{5/2}. \tag{4.5.6}$$

Proof of Lemma 4.5.2. The main ingredient in the proof is a result of Birman and Solomjak [BS69; BS80], stated in [Sim05, Theorem 4.5]. We start with Equation (4.5.3) and write the integral as

$$\int F(x-y)a_y c_y \,\mathrm{d}y = \iint F^x(y)v(y-z)a_y a_z \,\mathrm{d}y\,\mathrm{d}z, \qquad F^x(y) = F(x-y).$$

We write the operator K^x with integral kernel $K^x(y,z) = F^x(y)v(y-z)$ in terms of its singular value decomposition. That is, for some orthonormal systems $\{\phi_i^x\}$ and $\{\psi_i^x\}$ we have

$$F^x(y)v(y-z) = \sum_i \mu_i \phi_i^x(y)\psi_i^x(z) \tag{4.5.7}$$

with $\mu_i \geq 0$ the singular values. (Note that the singular values do not depend on x since K^x is unitarily equivalent to the translated operator with $x = 0$; moreover, $\phi_i^x(y) = \phi_i^0(y-x)$ and likewise for ψ_i^x.) Thus

$$\int F(x-y)a_y c_y \,\mathrm{d}y = \sum_i \mu_i \iint \phi_i^x(y)\psi_i^x(z)a_y a_z \,\mathrm{d}y\,\mathrm{d}z = \sum_i \mu_i a(\overline{\phi_i^x})a(\overline{\psi_i^x}).$$

In norm this is thus bounded by $\sum \mu_i = \|K^x\|_{\mathfrak{S}_1}$, the trace-norm of K^x. Furthermore, K^x is unitarily equivalent to the dilated operator with kernel $k_F^{-3}F^x(k_F^{-1}y)v(k_F^{-1}(y-z))$. Since the functions $F^x(k_F^{-1}\cdot)$ and $k_F^{-3}\widehat{v(k_F^{-1}\cdot)} = \widehat{v}(k_F\cdot)$ are compactly supported (in configuration and momentum-space, respectively) with diameter of support of order 1, we can apply [Sim05, Theorem 4.5][1] and conclude that

$$\left\| \int F(x-y)a_y c_y \right\| \leq \sum_i \mu_i = \|K^x\|_{\mathfrak{S}_1} \leq C \left\| F^x(k_F^{-1}\cdot) \right\|_{L^2} \|\widehat{v}(k_F\cdot)\|_{\ell^2} \leq C k_F^{3/2} \|F\|_{L^2},$$

where we introduced the notation $\|f\|_{\ell^2} = L^{-3/2}(\sum_k |f(k)|^2)^{1/2}$.

In order to prove Equation (4.5.4) we similarly write

$$\int F(x-y)a_y c_y \nabla^n c_{ty+(1-t)x} \,\mathrm{d}y = \iiint F^x(y)v(y-z)\nabla^n v^{(1-t)x}(ty-w)a_y a_z a_w \,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}w$$

with $v^x(y) = v(y+x)$. Using again (4.5.7),

$$\int F(x-y)a_y c_y \nabla^n c_{ty+(1-t)x} \,\mathrm{d}y = -\sum_i \mu_i a(\overline{\psi_i^x}) \iint \phi_i^x(y)\nabla^n v^{(1-t)x}(ty-w)a_y a_w \,\mathrm{d}y\,\mathrm{d}w.$$

We do one more singular value decomposition, this time for the operators $\widetilde{K}_i^{x,t}$ with kernels $\widetilde{K}_i^{x,t}(y,w) = \phi_i^x(y)\nabla^n v^{(1-t)x}(ty-w) = \sum_j \widetilde{\mu}_{ij}^{x,t}\widetilde{\phi}_{ij}^{x,t}(y)\widetilde{\psi}_{ij}^{x,t}(w)$. In combination we thus obtain the bound

$$\left\| \int F(x-y)a_y c_y \nabla^n c_{ty+(1-t)x} \,\mathrm{d}y \right\| \leq \sum_i \mu_i \sum_j \widetilde{\mu}_{ij}^{x,t}.$$

Similarly as above, observe that $\widetilde{K}_i^{x,t}$ has the same trace norm as the dilated operator with integral kernel $\phi_i^x(k_F^{-1}y)k_F^{-3}t^{3/2}\nabla^n v^{(1-t)x}(tk_F^{-1}(y-w))$. Each ϕ_i^x has compact support of diameter $\lesssim k_F^{-1}$ (since F^x has). Furthermore, the Fourier transform of $k_F^{-3}t^{3/2}\nabla^n v^{(1-t)x}(tk_F^{-1}\cdot)$

[1][Sim05, Theorem 4.5] is stated only for Euclidean space but can be extended to the torus Λ without much difficulty.

has compact support of diameter $t \leq 1$. Thus we can again apply [Sim05, Theorem 4.5] to conclude

$$\sum_j \widetilde{\mu}_{ij}^{x,t} = \left\|\widetilde{K}_i^{x,t}\right\|_{\mathfrak{S}_1} \leq C \left\|\phi_i^x(k_F^{-1}\cdot)\right\|_{L^2} \left\|t^{-3/2}(|\cdot|^n\widehat{v})(t^{-1}k_F\cdot)\right\|_{\ell^2} \leq Ck_F^{3/2+n}$$

uniformly in i, x and t. In combination with the bound $\sum_i \mu_i \leq Ck_F^{3/2}\|F\|_{L^2}$ from above, this concludes the proof of Equation (4.5.4). □

In order to state some of the intermediary bounds in the proof of Lemma 4.5.1, we introduce the following operators.

Definition 4.5.6 (Highly excited particles)**.** For $\alpha > 0$ we define

$$\mathcal{N}_{>\alpha} = \sum_{|k|>k_F(ak_F)^{-\alpha}} a_k^* a_k, \qquad \mathcal{N}_{>} = \sum_{|k|>2k_F} a_k^* a_k.$$

Remark 4.5.7 (see also [Gia23a, Proposition 4.15])**.** For any $|k| > 2k_F$ we have $||k|^2 - k_F^2| \geq k_F^2$, and for any $|k| > k_F(ak_F)^{-\alpha}$ with $\alpha > 0$ we have $||k|^2 - k_F^2| \geq Ck_F^2(ak_F)^{-2\alpha}$ for small ak_F. Hence

$$\mathcal{N}_{>} \leq Ck_F^{-2}\mathbb{H}_0, \qquad \mathcal{N}_{>\alpha} \leq Ck_F^{-2}(ak_F)^{2\alpha}\mathbb{H}_0. \tag{4.5.8}$$

Before giving the proof of Lemma 4.5.1 we first explain some intuition behind the proof.

Remark 4.5.8 (Intuition behind the bounds)**.** Conceptually, the main difficulty is "how to deal with the b_x's". The operator-valued distribution b_x is *not* a bounded operator, so we cannot bound it in norm. Essentially we have 3 different methods of treating a factor b_x.

- We can bound one factor b_x in terms of $\mathcal{N}$ via a computation similar to

  $$\int \|b_x\xi\| \,\mathrm{d}x \leq L^{3/2}\left(\int \|b_x\xi\|^2 \,\mathrm{d}x\right) \leq L^{3/2}\langle\mathcal{N}\rangle_\xi^{1/2} \leq CN^{1/2}k_F^{-3/2}\langle\mathcal{N}\rangle_\xi^{1/2}.$$

  Analogously, the regularized operator b_x^r can be bounded in terms of $\mathcal{N}_{>}$ and the operator $b_x^{>}$ (introduced in Equation (4.5.10) below) can be bounded in terms of $\mathcal{N}_{>\alpha}$.

- We can bound two factors of b_x in terms of $\mathbb{Q}_4$ using a factor $V(x-y)$ via a computation similar to

  $$\begin{aligned}&\iint V(x-y)\|b_xb_y\xi\| \,\mathrm{d}x\,\mathrm{d}y \\ &\leq \left(\iint V(x-y)\,\mathrm{d}x\,\mathrm{d}y\right)^{1/2}\left(\iint V(x-y)\|b_xb_y\xi\|^2 \,\mathrm{d}x\,\mathrm{d}y\right)^{1/2} \\ &= L^{3/2}\|V\|_{L^1}^{1/2}\langle 2\mathbb{Q}_4\rangle_\xi^{1/2} \leq CN^{1/2}a^{1/2}k_F^{-3/2}\langle\mathbb{Q}_4\rangle_\xi^{1/2}.\end{aligned}$$

- Finally, we can bound one factor b_x "in norm" using any appropriate (compactly supported) function F and a factor c_x (or two) via an application of Lemma 4.5.2.

Factors of c_x are not problematic. These we either bound in norm as $\|c_x\| \leq Ck_F^{3/2}$ or Taylor expand and bound the resulting ∇c_x in norm as $\|\nabla c_x\| \leq Ck_F^{3/2+1}$. Similarly, factors of $v(x-y)$ can either be bounded by $\|v\|_{L^2} \leq Ck_F^{3/2}$ or $\|v\|_{L^\infty} \leq Ck_F^3$. Finally, for factors $u^r(x-y)$ we either use $0 \leq u^r \leq \mathbb{1}$ as operators or write $u^r(x-y) = \delta(x-y) - v^r(x-y)$ and compute separately the terms with δ and v^r. Here we note that $\|v^r\|_{L^1} \leq C$ by Lemma 4.2.1.

The remainder of this section gives the proof of Lemma 4.5.1. We prove each of the bounds separately.

4.5.2 Taylor-expansion errors

We bound all error-terms with a superscript "Taylor" in Equation (4.5.1), resulting from the remainder term in the expansion (4.4.2). Together they are of the form

$$\mathbb{T} = \iint F^{\mu\nu}(x-y) b_x b_y c_y \int_0^1 \mathrm{d}t\,(1-t)\nabla^\mu \nabla^\nu c_{x+t(y-x)} \,\mathrm{d}x\,\mathrm{d}y + \text{h.c.} \tag{4.5.9}$$

for the function(s) (using Equation (4.2.3))

$$F^{\mu\nu}(x) = -\left[x^\mu x^\nu \Delta\varphi(x) + \frac{1}{2} x^\mu x^\nu V(x)(1-\varphi(x))\right] = 2x^\mu \nabla^\nu \varphi(x) - x^\mu \mathcal{E}_\varphi^\nu(x).$$

We note that by Lemma 4.3.6 and Remark 4.3.7 we have (with $\|F\|_{L^1} = \sum_{\mu,\nu} \|F^{\mu\nu}\|_{L^1}$ and similarly for the L^2 norm)

$$\|F\|_{L^1} \le Ca^3 |\log ak_F|, \qquad \|F\|_{L^2} \le Ca^{3/2}.$$

To bound $\langle \mathbb{T} \rangle_\xi$ we write

$$b_x = b_x^< + b_x^>, \qquad b_x^> = \frac{1}{L^{3/2}} \sum_{|k| > k_F (ak_F)^{-\alpha}} e^{ikx} a_k \tag{4.5.10}$$

for some $\alpha > 0$. Note that $\mathcal{N}_{>\alpha} = \int (b_x^>)^* b_x^> \,\mathrm{d}x$ with $\mathcal{N}_{>\alpha}$ from Definition 4.5.6. For the term with $b_x^<$ we bound $\|b_x^<\| \le Ck_F^{3/2}(ak_F)^{-3\alpha/2}$ and $\left\|\nabla^\mu\nabla^\nu c_{x+t(y-x)}\right\| \le Ck_F^{3/2+2}$. Then by Cauchy–Schwarz

$$\begin{aligned} &\left|\left\langle \iint F^{\mu\nu}(x-y) b_x^< b_y c_y \int_0^1 \mathrm{d}t\,(1-t)\nabla^\mu\nabla^\nu c_{x+t(y-x)}\,\mathrm{d}x\,\mathrm{d}y \right\rangle_\xi\right| \\ &\quad \le C\|F\|_{L^1} k_F^{5+3/2}(ak_F)^{-3\alpha/2} \int \|b_y \xi\| \,\mathrm{d}y \le CN^{1/2} a^3 k_F^5 |\log ak_F| (ak_F)^{-3\alpha/2} \langle \mathcal{N} \rangle_\xi^{1/2}. \end{aligned}$$

Here we used that b_x and c_y anti-commute to reorder the annihilation operators such that b_y is the last operator and we can bound all others in norm, while b_y yields the bound $\|b_y\xi\|$. For the terms with $b_x^>$ we use Equation (4.5.4) to bound the y-integral. To do this we write $b_y = a_y - c_{-y}$. The term with c_{-y} can be bounded in the same way as the term with $b_x^<$ above. For the term with a_y we obtain

$$\begin{aligned} &\left|\left\langle \iint F^{\mu\nu}(x-y) b_x^> a_y c_y \int_0^1 \mathrm{d}t\,(1-t)\nabla^\mu\nabla^\nu c_{x+t(y-x)}\,\mathrm{d}x\,\mathrm{d}y \right\rangle_\xi\right| \\ &\quad \le Ck_F^5 \|F\|_{L^2} \int \|b_x^> \xi\| \,\mathrm{d}x \le CN^{1/2} a k_F^3 (ak_F)^{1/2} \langle \mathcal{N}_{>\alpha} \rangle_\xi^{1/2}. \end{aligned}$$

We conclude the bound

$$\left|\langle \mathbb{T} \rangle_\xi\right| \lesssim N^{1/2} a^3 k_F^5 |\log ak_F| (ak_F)^{-3\alpha/2} \langle \mathcal{N} \rangle_\xi^{1/2} + N^{1/2} a k_F^3 (ak_F)^{1/2} \langle \mathcal{N}_{>\alpha} \rangle_\xi^{1/2}$$

for any $\alpha > 0$. Using the bound on $\mathcal{N}_{>\alpha}$ in Equation (4.5.8) we conclude the desired.

4.5.3 Scattering equation cancellation

We proceed with bounding $\mathbb{Q}_{\mathsf{scat}}$ in Equation (4.5.2). This bound is analogous to that of $\mathbb{T}$ above, only $F^{\mu\nu}$ is replaced by $\mathcal{E}_\varphi^\mu$ and $\nabla^\mu\nabla^\nu c$ is replaced by $\nabla^\mu c$. That is, the bound for $\mathbb{Q}_{\mathsf{scat}}$ is as for $\mathbb{T}$, only we have one fewer power of k_F (from $\|\nabla c\|$ instead of $\|\nabla^2 c\|$) and norms of F are replaced by norms of $\mathcal{E}_\varphi$. We conclude the bound

$$\begin{aligned}\left|\langle \mathbb{Q}_{\mathsf{scat}}\rangle_\xi\right| &\leq CN^{1/2}k_F^4(ak_F)^{-3\alpha/2}\|\mathcal{E}_\varphi\|_{L^1}\langle\mathcal{N}\rangle_\xi^{1/2} + CN^{1/2}k_F^{3/2+1}\|\mathcal{E}_\varphi\|_{L^2}\langle\mathcal{N}_{>\alpha}\rangle_\xi^{1/2} \\ &\leq CN^{1/2}a^3k_F^5(ak_F)^{-3\alpha/2}|\log ak_F|\langle\mathcal{N}\rangle_\xi^{1/2} + CN^{1/2}ak_F^3(ak_F)^{1/2}\langle\mathcal{N}_{>\alpha}\rangle_\xi^{1/2}\end{aligned}$$

for any $\alpha > 0$, where we have used Lemma 4.3.6 and Remark 4.3.7 for the bound on the norms of $\mathcal{E}_\varphi$. Again, using the bound on $\mathcal{N}_{>\alpha}$ in Equation (4.5.8) we conclude the desired.

4.5.4 (Non-)regularization of $[\mathbb{H}_0, B]$

Next we bound $\mathbb{H}_{0;B}^{\div r}$ defined in Equation (4.4.1), given by

$$\mathbb{H}_{0;B}^{\div r} = \iint (\Delta\varphi(x-y)c_yc_x + 2\nabla^\mu\varphi(x-y)c_y\nabla^\mu c_x)\left(b_x^rb_y^r - b_xb_y\right)\,\mathrm{d}x\,\mathrm{d}y + \text{h.c.}. \tag{4.5.11}$$

To bound this, write $b_x = b_x^r + c_x^r$ with the latter operator satisfying $\|c_x^r\| \leq Ck_F^{3/2}$ since b_k and b_k^r agree for all momenta $|k| > 3k_F$. Further, we Taylor expand the factor c_y in the first term as in Equation (4.3.4). Then we have (changing variables to $z = y - x$)

$$\begin{aligned}\left\langle\mathbb{H}_{0;B}^{\div r}\right\rangle_\xi &= -2\operatorname{Re}\iint z^\mu\Delta\varphi(z)\int_0^1\mathrm{d}t\left\langle\nabla^\mu c_{x+tz}c_x(c_x^rb_{x+z}^r + b_x^rc_{x+z}^r + c_x^rc_{x+z}^r)\right\rangle_\xi\,\mathrm{d}x\,\mathrm{d}z \\ &\quad + 2\operatorname{Re}\iint\nabla^\mu\varphi(z)\left\langle c_{x+z}\nabla^\mu c_x(c_x^rb_{x+z}^r + b_x^rc_{x+z}^r + c_x^rc_{x+z}^r)\right\rangle_\xi\,\mathrm{d}x\,\mathrm{d}z.\end{aligned} \tag{4.5.12}$$

The two terms are treated similarly. We start with the first. Define for any state ξ the function $\phi(x,z) = \left\langle\nabla^\mu c_{x+tz}c_x(c_x^rb_{x+z}^r + b_x^rc_{x+z}^r + c_x^rc_{x+z}^r)\right\rangle_\xi$ and note that it vanishes at $z = 0$. Thus we Taylor expand: (with ∇_2^μ denoting a derivative in the second argument)

$$\phi(x,z) = z^\nu\int_0^1\mathrm{d}s\,[\nabla_2^\nu\phi](x,sz).$$

The derivative hits either a factor c or c^r or a factor b^r. In the terms where the derivative hits a factor c or c^r we bound the c's and c^r's in norm. (Apart from the term with only c's and c^r's, where we keep one factor c^r without a derivative.) Recall that $\|\nabla^n c\| \leq Ck_F^{3/2+n}$ for any n. Similarly $\|\nabla^n c_x^r\| \leq Ck_F^{3/2+n}$. Thus, the terms where the derivative hits a factor c or c^r are bounded by

$$k_F^{3/2+5}\left\||\cdot|^2\Delta\varphi\right\|_{L^1}\int(\|b_x^r\xi\| + \|c_x^r\xi\|)\,\mathrm{d}x \leq CN^{1/2}a^3k_F^5|\log ak_F|\langle\mathcal{N}\rangle_\xi^{1/2}$$

using the bounds of Lemma 4.3.6. For the term where the derivative hits a factor b^r we again bound the c's and c^r's in norm. These terms are then bounded by

$$\begin{aligned}&k_F^{3/2+4}\left\||\cdot|^2\Delta\varphi\right\|_{L^1}\int\|\nabla b_x^r\xi\|\,\mathrm{d}x \\ &\qquad\leq CN^{1/2}a^3k_F^4|\log ak_F|\langle\mathbb{H}_0\rangle_\xi^{1/2} + CN^{1/2}a^3k_F^5|\log ak_F|\langle\mathcal{N}\rangle_\xi^{1/2}\end{aligned}$$

since $\int\|\nabla b_x^r\xi\|^2\,\mathrm{d}x \leq \langle\mathbb{H}_0\rangle_\xi + k_F^2\langle\mathcal{N}\rangle_\xi$. The second term in Equation (4.5.12) is treated analogously, only the bound has a factor $\||\cdot|\nabla\varphi\|_{L^1}$ instead of $\||\cdot|^2\Delta\varphi\|_{L^1}$. Collecting all the terms, we conclude the desired bound on $\mathbb{H}_{0;B}^{\div r}$.

4.5.5 Error terms from $[\mathbb{Q}_4, B]$

We now bound $\mathbb{Q}_{4;B}^{\mathcal{E}}$, given in Equation (4.4.6). We split the operator into 4 terms and bound each separately:

1. The quartic term with one δ and one v^r,
2. The quartic term with two v^r's,
3. The order 6 term with δ, and
4. The order 6 term with v^r.

4.5.5.1 Quartic term with one δ and one v^r:

This term is of the form

$$\mathbb{A}_1 = \iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z'\, V(x-y)\varphi(y-z')v^r(z'-x)b_y b_x c_{z'} c_y + \text{h.c.}.$$

We bound $\|c_{z'}c_y\| \le C|y-z'|k_F^4$ and $\|v^r\|_{L^\infty} \le Ck_F^3$. Then by Cauchy–Schwarz we get (using Lemma 4.3.6 to bound the norm of φ)

$$\begin{aligned}\left|\langle \mathbb{A}_1\rangle_\xi\right| &\le Ck_F^7 \,\||\cdot|\varphi\|_{L^1} \iint V(x-y)\,\|b_x b_y \xi\|\,\mathrm{d}x\,\mathrm{d}y \le Ck_F^7\,\||\cdot|\varphi\|_{L^1}\,\|V\|_{L^1}^{1/2} L^{3/2}\,\langle \mathbb{Q}_4\rangle_\xi^{1/2} \\ &\le CN^{1/2}a^{3+1/2}k_F^{4+1/2}\,\langle \mathbb{Q}_4\rangle_\xi^{1/2}.\end{aligned}$$

(Here we reordered the annihilation operators such that $b_x b_y$ is last so we can bound $c_{z'}c_y$ in norm and get the factor $\|b_x b_y \xi\|$.)

4.5.5.2 Quartic term with two v^r's:

This term is of the form

$$\mathbb{A}_2 = -\frac{1}{2}\iiiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\, V(x-y)\varphi(z-z')v^r(z'-x)v^r(z-y)b_y b_x c_{z'} c_z + \text{h.c.}.$$

As above, we bound $\|c_{z'}c_z\| \le C|z-z'|k_F^4$. By Cauchy–Schwarz the z, z' integrals are then bounded as

$$\iint \mathrm{d}z\,\mathrm{d}z'\,|\varphi(z-z')||z-z'||v^r(z'-x)||v^r(z-y)| \le \||\cdot|\varphi\|_{L^1}\,\|v^r\|_{L^2}^2 \le Ca^3k_F^2.$$

Then by Cauchy–Schwarz as above we obtain

$$\left|\langle \mathbb{A}_2\rangle_\xi\right| \le Ca^3k_F^6 \iint V(x-y)\,\|b_x b_y\xi\|\,\mathrm{d}x\,\mathrm{d}y \le CN^{1/2}a^{3+1/2}k_F^{4+1/2}\,\langle \mathbb{Q}_4\rangle_\xi^{1/2}.$$

4.5.5.3 Order 6 term with δ:

This term is of the form

$$\mathbb{A}_3 = -\iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z'\, V(x-y)\varphi(x-z')b_y^* b_{z'}^r b_y b_x c_{z'} c_x + \text{h.c.}.$$

Computing the expectation in some state ξ we bound the z'-integral as

$$\left| \int \mathrm{d}z'\, \varphi(x-z') \left\langle b_y^* b_{z'}^r b_y b_x c_{z'} c_x \right\rangle_\xi \right| \le \left\| \int \mathrm{d}z'\, \varphi(x-z') b_{z'}^r c_{z'} c_x \right\| \|b_y \xi\| \, \|b_x b_y \xi\| \,.$$

Using Equation (4.5.6) to bound the first factor we get by Cauchy–Schwarz

$$\begin{aligned} \left| \langle \mathbb{A}_3 \rangle_\xi \right| &\le C (a k_F)^{5/2} k_F^{3/2} \iint V(x-y) \, \|b_y \xi\| \, \|b_x b_y \xi\| \, \mathrm{d}x \, \mathrm{d}y \\ &\le C (a k_F)^{5/2} k_F^{3/2} \|V\|_{L^1}^{1/2} \langle \mathcal{N} \rangle_\xi^{1/2} \langle \mathbb{Q}_4 \rangle_\xi^{1/2} \\ &\le C a^3 k_F^4 \langle \mathcal{N} \rangle_\xi^{1/2} \langle \mathbb{Q}_4 \rangle_\xi^{1/2} \,. \end{aligned}$$

4.5.5.4 Order 6 term with v^r:

This term is of the form

$$\mathbb{A}_4 = - \iiiint \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z \, \mathrm{d}z' \, V(x-y) \varphi(z-z') v^r(z-x) b_y^* b_{z'}^r b_y b_x c_{z'} c_z + \text{h.c.}.$$

Computing the expectation in some state ξ we bound the z, z'-integrals, again using Equation (4.5.6), as

$$\begin{aligned} &\left| \iint \mathrm{d}z \, \mathrm{d}z' \, \varphi(z-z') v^r(z-x) \left\langle b_y^* b_{z'}^r b_y b_x c_{z'} c_z \right\rangle_\xi \right| \\ &\le \int \mathrm{d}z \, |v^r(z-x)| \left\| \int \mathrm{d}z' \, \varphi(z-z') b_{z'}^r c_{z'} c_z \right\| \|b_y \xi\| \, \|b_x b_y \xi\| \\ &\le C (a k_F)^{5/2} k_F^{3/2} \|v^r\|_{L^1} \|b_y \xi\| \, \|b_x b_y \xi\| \,. \end{aligned}$$

Recall that $\|v^r\|_{L^1} \le C$ by Lemma 4.2.1. Using then Cauchy–Schwarz as above we find

$$\left| \langle \mathbb{A}_4 \rangle_\xi \right| \le C a^3 k_F^4 \langle \mathcal{N} \rangle_\xi^{1/2} \langle \mathbb{Q}_4 \rangle_\xi^{1/2} \,.$$

This gives the desired bound on $\mathbb{Q}_{4;B}^{\mathcal{E}}$.

4.5.6 Error terms from $[\mathbb{Q}_2, B]$

Finally we bound $\mathbb{Q}_{2;B}^{\mathcal{E}}$. Recalling Equations (4.4.8) and (4.4.10), it is given by

$$\begin{aligned} \mathbb{Q}_{2;B}^{\mathcal{E}} = \frac{1}{4} \iiiint & \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z \, \mathrm{d}z' \, V(x-y) \varphi(z-z') \Big\{ b_x^* b_y^* b_z^r b_{z'}^r [c_y^* c_x^*, c_{z'} c_z] + c_y^* c_x^* c_{z'} c_z [b_x^* b_y^*, b_z^r b_{z'}^r] \\ & + \Big((\delta(x-z)\delta(y-z') - \delta(x-z')\delta(y-z)) \\ & \times (v(x-z)v(y-z') - v(x-z')v(y-z)) \\ & - [b_x^* b_y^*, b_z^r b_{z'}^r][c_y^* c_x^*, c_{z'} c_z] \Big) \Big\} + \text{h.c.}. \end{aligned}$$

We split the terms into three groups:

1. The terms with only the c-commutator (i.e. of the form $b^* b^* b b [c^* c^*, cc]$),
2. The terms with only the b-commutator, and
3. The rest, involving terms with both commutators, with the leading term [of the form $\delta\delta vv$] subtracted.

4.5.6.1 Terms with only the c-commutator:

Recalling the formula for the commutator in Equation (4.4.9) all terms with c^*c give the same contribution, so do all the constant terms. That is, we need to bound terms of the form

$$\begin{aligned}\mathbb{A}_{1a} &= -\iiiint V(x-y)\varphi(z-z')v(x-z)b_x^*b_y^*b_z^rb_{z'}^rc_y^*c_{z'}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z' + \text{h.c.},\\ \mathbb{A}_{1b} &= \frac{1}{2}\iiiint V(x-y)\varphi(z-z')v(x-z)v(y-z')b_x^*b_y^*b_z^rb_{z'}^r\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z' + \text{h.c.}.\end{aligned}$$

For $\mathbb{A}_{1a}$ we note that as an operator $0 \le v \le \mathbb{1}$. Then by Cauchy–Schwarz we have for any $\varepsilon > 0$ (recall that $\{b_x, c_y^*\} = 0$)

$$\begin{aligned}\pm\mathbb{A}_{1a} &= \mp\iint \mathrm{d}x\,\mathrm{d}z\,v(x-z)\left[\int \mathrm{d}y\,V(x-y)b_x^*b_y^*c_y^*\right]\left[\int \mathrm{d}z'\,\varphi(z-z')b_z^rb_{z'}^rc_{z'}\right] + \text{h.c.}\\ &\le \varepsilon k_F^{-2}\iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,V(x-y)V(x-z)b_x^*b_z^*c_z^*c_yb_yb_x\\ &\quad + \varepsilon^{-1}k_F^2\iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\varphi(x-y)\varphi(x-z)c_z^*(b_z^r)^*(b_x^r)^*b_x^rb_y^rc_y\\ &=: \varepsilon\mathbb{A}_{1a}^V + \varepsilon^{-1}\mathbb{A}_{1a}^\varphi.\end{aligned}$$

For $\mathbb{A}_{1a}^V$ we bound c_z^*, c_y in norm. Then by Cauchy–Schwarz we have

$$\begin{aligned}\left|\left\langle\mathbb{A}_{1a}^V\right\rangle_\xi\right| &\le Ck_F\iiint V(x-y)V(x-z)\left\|b_zb_x\xi\right\|\left\|b_yb_x\xi\right\|\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\\ &\le Ck_F\iiint V(x-y)V(x-z)\left\|b_yb_x\xi\right\|^2\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \le Cak_F\left\langle\mathbb{Q}_4\right\rangle_\xi.\end{aligned}$$

For $\mathbb{A}_{1a}^\varphi$ we use Equation (4.5.5) to bound the y- and z-integrations. We find

$$\left|\langle\mathbb{A}_{1a}^\varphi\rangle_\xi\right| \le k_F^2\int \mathrm{d}x\left\|\int \mathrm{d}y\,\varphi(x-y)b_y^rc_y\right\|^2\left\|b_x^r\xi\right\|^2 \le Ck_F^2(ak_F)^3\left\langle\mathcal{N}_>\right\rangle_\xi.$$

Optimising in ε we thus obtain the bound

$$\left|\langle\mathbb{A}_{1a}\rangle_\xi\right| \le Ca^2k_F^3\left\langle\mathcal{N}_>\right\rangle_\xi^{1/2}\left\langle\mathbb{Q}_4\right\rangle_\xi^{1/2}. \tag{4.5.13}$$

Next, we bound $\mathbb{A}_{1b}$ as

$$\left|\langle\mathbb{A}_{1b}\rangle_\xi\right| \le \iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,V(x-y)|v(x-z)|\left\|\int \mathrm{d}z'\,\varphi(z-z')v(y-z')b_{z'}^r\right\|\left\|b_z^r\xi\right\|\left\|b_yb_x\xi\right\|.$$

Since $0 \le \hat{u}^r \le 1$, we have

$$\left\|\int \mathrm{d}z'\,\varphi(z-z')v(y-z')b_{z'}^r\right\| \le \left\|\int \mathrm{d}z'\,\varphi(z-z')v(y-z')a_{z'}\right\| = \left(\varphi^2 * v^2(y-z)\right)^{1/2}$$

(with $*$ denoting convolution) and hence, by Cauchy–Schwarz,

$$\begin{aligned}\left|\langle\mathbb{A}_{1b}\rangle_\xi\right| &\le \left[\iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,V(x-y)|v(x-z)|^2\left\|b_yb_x\xi\right\|^2\right]^{1/2}\\ &\quad\times\left[\iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,V(x-y)\varphi^2 * v^2(y-z)\left\|b_z^r\xi\right\|^2\right]^{1/2}\\ &\le \|v\|_{L^2}^2\left\langle\mathbb{Q}_4\right\rangle_\xi^{1/2}\|V\|_{L^1}^{1/2}\|\varphi\|_{L^2}\left\langle\mathcal{N}_>\right\rangle_\xi^{1/2} \le Ca^2k_F^3\left\langle\mathbb{Q}_4\right\rangle_\xi^{1/2}\left\langle\mathcal{N}_>\right\rangle_\xi^{1/2},\end{aligned} \tag{4.5.14}$$

where we have used Lemma 4.3.6 to bound the L^2-norm of φ in the final step.

4.5.6.2 Terms with only the b-commutator:

Recalling the formula for the commutator in Equation (4.4.4) all terms with b^*b give the same contribution, so do all the constant terms. That is, we need to bound terms of the forms

$$\begin{aligned}\mathbb{A}_{2a} &= -\iiiint V(x-y)\varphi(z-z')u^r(x-z)b_y^* b_{z'}^r c_y^* c_x^* c_{z'} c_z \,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z' + \text{h.c.},\\ \mathbb{A}_{2b} &= \frac{1}{2}\iiiint V(x-y)\varphi(z-z')u^r(x-z)u^r(y-z')c_y^* c_x^* c_{z'} c_z \,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z' + \text{h.c.}.\end{aligned}$$

For $\mathbb{A}_{2a}$ we use that $0 \le u^r \le \mathbb{1}$ as an operator. Thus, for any $\varepsilon > 0$,

$$\begin{aligned}\pm\mathbb{A}_{2a} &= \mp \iint \mathrm{d}x\,\mathrm{d}z\, u^r(x-z)\left[\int \mathrm{d}y\, V(x-y)b_y^* c_y^* c_x^*\right]\left[\int \mathrm{d}z'\,\varphi(z-z')b_{z'}^r c_{z'} c_z\right] + \text{h.c.}\\ &\le \varepsilon k_F^{-2}\iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\, V(x-y)V(x-z)b_z^* c_z^* c_x^* c_x c_y b_y\\ &\quad + \varepsilon^{-1}k_F^2 \iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\varphi(x-y)\varphi(x-z)c_x^* c_z^* (b_z^r)^* b_y^r c_y c_x\\ &=: \varepsilon\mathbb{A}_{2a}^V + \varepsilon^{-1}\mathbb{A}_{2a}^\varphi.\end{aligned}$$

For $\mathbb{A}_{2a}^V$ we bound $\|c_x c_y\| \le C|x-y|k_F^4$. Then by Cauchy–Schwarz we have

$$\begin{aligned}\left|\left\langle \mathbb{A}_{2a}^V\right\rangle_\xi\right| &\le Ck_F^6 \iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\, V(x-y)V(x-z)|x-y||x-z|\,\|b_z\xi\|\,\|b_y\xi\|\\ &\le Ck_F^6\, \||x|V\|_{L^1}^2 \langle\mathcal{N}\rangle_\xi \le Ca^4k_F^6\langle\mathcal{N}\rangle_\xi.\end{aligned}$$

Analogously

$$\left|\langle \mathbb{A}_{2a}^\varphi\rangle_\xi\right| \le Ck_F^{10}\,\||x|\varphi\|_{L^1}^2 \langle\mathcal{N}_>\rangle_\xi \le Ca^6k_F^8\langle\mathcal{N}_>\rangle_\xi.$$

Optimising in ε we find

$$\left|\langle\mathbb{A}_{2a}\rangle_\xi\right| \le Ca^5k_F^7\langle\mathcal{N}\rangle_\xi^{1/2}\langle\mathcal{N}_>\rangle_\xi^{1/2} \le Ca^5k_F^7\langle\mathcal{N}\rangle_\xi. \tag{4.5.15}$$

For $\mathbb{A}_{2b}$ we write $u^r = \delta - v^r$. The term with both factors δ is

$$\mathbb{A}_{2b}^{\delta\delta} = -\iint V(x-y)\varphi(x-y)c_x^* c_y^* c_y c_x\,\mathrm{d}x\,\mathrm{d}y.$$

By Taylor expanding c_y and c_y^* as in Equation (4.3.4) and bounding $\varphi \le 1$ we have

$$\left|\left\langle\mathbb{A}_{2b}^{\delta\delta}\right\rangle_\xi\right| \le Ck_F^5\left\||\cdot|^2 V\right\|_{L^1}\langle\mathcal{N}\rangle_\xi \le Ca^3k_F^5\langle\mathcal{N}\rangle_\xi.$$

Both terms with one factor δ and one factor v^r can be treated the same way. They are of the form

$$\mathbb{A}_{2b}^{v\delta} = \frac{1}{2}\iiint V(x-y)\varphi(z-y)v^r(x-z)c_y^* c_x^* c_y c_z\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z + \text{h.c.}.$$

Thus, by Cauchy–Schwarz and Taylor-expanding c_y as in Equation (4.3.4)

$$\begin{aligned}\left|\left\langle\mathbb{A}_{2b}^{v\delta}\right\rangle_\xi\right| &\le \left[\iiint V(x-y)v^r(x-z)^2\|c_x c_y\xi\|^2\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\right]^{1/2}\\ &\qquad\times\left[\iiint V(x-y)\varphi(z-y)^2\|c_y c_z\xi\|^2\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\right]^{1/2}\\ &\le Ck_F^5\left\||\cdot|^2V\right\|_{L^1}^{1/2}\|v^r\|_{L^2}\|V\|_{L^1}^{1/2}\||\cdot|\varphi\|_{L^2}\langle\mathcal{N}\rangle_\xi \le Ca^4k_F^6(ak_F)^{1/2}\langle\mathcal{N}\rangle_\xi.\end{aligned}$$

Finally, we bound the term $\mathbb{A}_{2b}^{vv}$ with two factors v^r by Cauchy–Schwarz as

$$\begin{aligned}\left|\langle \mathbb{A}_{2b}^{vv}\rangle_\xi\right| &\leq \left[\iiiint V(x-y)\varphi(z-z')v^r(x-z)^2 \left\|c_x c_y \xi\right\|^2 \,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\right]^{1/2} \\ &\quad\times\left[\iiiint V(x-y)\varphi(z-z')v^r(y-z')^2 \left\|c_{z'} c_z \xi\right\|^2 \,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\right]^{1/2} \\ &\leq Ck_F^5 \left\||\cdot|^2 V\right\|_{L^1}^{1/2} \|\varphi\|_{L^1}^{1/2} \|V\|_{L^1}^{1/2} \left\||\cdot|^2\varphi\right\|_{L^1}^{1/2} \|v^r\|_{L^2}^2 \langle\mathcal{N}\rangle_\xi \\ &\leq Ca^5 k_F^7 \left|\log ak_F\right|^{1/2} \langle\mathcal{N}\rangle_\xi .\end{aligned}$$

We conclude that

$$\left|\langle\mathbb{A}_{2b}\rangle_\xi\right| \leq Ca^3 k_F^5 \langle\mathcal{N}\rangle_\xi . \tag{4.5.16}$$

4.5.6.3 Terms with both commutators:

Recalling the formulas for the commutators in Equations (4.4.4) and (4.4.9) we split the terms into four groups

a. Terms of the form b^*bc^*c,

b. Terms of the form b^*b,

c. Terms of the form c^*c, and

d. The constant (i.e. fully contracted) terms.

—Terms of the form b^*bc^*c: These terms have one factor u^r and one factor v. The factors u^r and v can either have both different arguments, share one variable or have the same argument. That is, we have the different types of terms

$$\begin{aligned}\mathbb{A}_{3a,1} &= -\frac{1}{4}\iiiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\, V(x-y)\varphi(z-z')u^r(x-z)v(y-z')b_y^* c_x^* c_z b_{z'}^r + \text{h.c.}, \\ \mathbb{A}_{3a,2} &= \frac{1}{4}\iiiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\, V(x-y)\varphi(z-z')u^r(x-z)v(y-z)b_y^* c_x^* c_{z'} b_{z'}^r + \text{h.c.}, \\ \mathbb{A}_{3a,3} &= -\frac{1}{4}\iiiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\, V(x-y)\varphi(z-z')u^r(x-z)v(x-z)b_y^* c_y^* c_{z'} b_{z'}^r + \text{h.c.}.\end{aligned}$$

We consider the term $\mathbb{A}_{3a,1}$ and write $u^r(x-z) = \delta(x-z) - v^r(x-z)$. For the term with δ we bound $\|v\|_{L^\infty} \leq Ck_F^3$ and $\|c_x\| \leq Ck_F^{3/2}$. Then by Cauchy–Schwarz the expectation value of this term in a state ξ is bounded by

$$\begin{aligned}Ck_F^6 \iiint V(x-y)\varphi(x-z')\left\|b_y\xi\right\|\left\|b_{z'}^r\xi\right\| \,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z' &\leq Ck_F^6 \|V\|_{L^1}\|\varphi\|_{L^1} \langle\mathcal{N}\rangle_\xi^{1/2}\langle\mathcal{N}_>\rangle_\xi^{1/2} \\ &\leq Ca^4 k_F^6 \left|\log ak_F\right| \langle\mathcal{N}\rangle_\xi^{1/2}\langle\mathcal{N}_>\rangle_\xi^{1/2} .\end{aligned}$$

Similarly we bound the term with v^r by

$$\begin{aligned}
&Ck_F^3 \iiiint V(x-y)\varphi(z-z')|v^r(x-z)||v(y-z')| \, \|b_y\xi\| \, \|b^r_{z'}\xi\| \, \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z' \\
&\quad\le Ck_F^3 \left[\iiiint V(x-y)\varphi(z-z')v(y-z')^2 \, \|b_y\xi\|^2 \, \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\right]^{1/2} \\
&\qquad\times \left[\iiiint V(x-y)\varphi(z-z')v^r(x-z)^2 \, \|b^r_{z'}\xi\|^2 \, \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\right]^{1/2} \\
&\quad\le Ca^4k_F^6 |\log ak_F| \left\langle \mathcal{N} \right\rangle_\xi^{1/2} \left\langle \mathcal{N}_> \right\rangle_\xi^{1/2}
\end{aligned}$$

using that $\|v\|_{L^2}, \|v^r\|_{L^2} \le Ck_F^{3/2}$. The terms $\mathbb{A}_{3a,2}$ and $\mathbb{A}_{3a,3}$ can be bounded in the same way. We conclude that

$$\begin{aligned}
\left|\langle \mathbb{A}_{3a,1}\rangle_\xi\right| + \left|\langle \mathbb{A}_{3a,2}\rangle_\xi\right| + \left|\langle \mathbb{A}_{3a,3}\rangle_\xi\right| &\le Ca^4k_F^6 |\log ak_F| \left\langle \mathcal{N} \right\rangle_\xi^{1/2} \left\langle \mathcal{N}_> \right\rangle_\xi^{1/2} \\
&\le Ca^4k_F^6 |\log ak_F| \left\langle \mathcal{N} \right\rangle_\xi .
\end{aligned} \tag{4.5.17}$$

—Terms of the form b^*b: These may be dealt with as the terms $\mathbb{A}_{3a,1}$, $\mathbb{A}_{3a,2}$ and $\mathbb{A}_{3a,3}$ only we bound $\|v\|_{L^\infty} \le Ck_F^3$ instead of $\|c\|^2 \le Ck_F^3$.

—Terms of the form c^*c: For these terms it is important to take into account the cancellations between different terms. Recalling the formulas for the commutators in Equations (4.4.4) and (4.4.9) and noting the symmetries $x \leftrightarrow y$ and $z \leftrightarrow z'$ we find that together all terms of this form are given by

$$\begin{aligned}
\mathbb{A}_{3c} = 2 \iiiint &V(x-y)\varphi(z-z')[u^r(x-z')u^r(y-z) - u^r(x-z)u^r(y-z')]v(y-z) \\
&\times c_x^* c_{z'} \, \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'.
\end{aligned}$$

Writing the term in momentum-space we find

$$\mathbb{A}_{3c} = \frac{2}{L^6} \sum_{\substack{k,\ell,\ell' \\ \ell,\ell' \in B_F}} \hat{V}(k) \left[\hat\varphi(k) - \hat\varphi(k+\ell-\ell')\right] \hat{u}^r(k-\ell)\hat{u}^r(k+\ell')c_\ell^* c_\ell.$$

We view $\hat\varphi$ as being defined on all of $\mathbb{R}^3$ (as opposed to just on $\frac{2\pi}{L}\mathbb{Z}^3$) and Taylor expand. Noting that φ is a real radial function the first order vanishes. That is,

$$\hat\varphi(k+\ell-\ell') = \hat\varphi(k) + (\ell-\ell')^\mu(\ell-\ell')^\nu \int_0^1 \mathrm{d}t\,(1-t)\nabla^\mu\nabla^\nu\hat\varphi(k+t(\ell-\ell')).$$

We write $\hat{u}^r(k) = 1 - \hat{v}^r(k)$ and observe that $\hat{v}^r$ is supported for $|k| \le 3k_F$. Since further $\ell,\ell' \in B_F$ we have $\hat{v}^r(k+\ell'), \hat{v}^r(k-\ell) \le \chi_{|k|\le 4k_F}$. The terms with at least one factor $\hat{v}^r$ we then bound by

$$\begin{aligned}
&2\int_0^1 \mathrm{d}t\,(1-t)\frac{1}{L^6}\sum_{\ell,\ell'\in B_F} |\ell-\ell'|^2 \left\langle c_\ell^* c_\ell\right\rangle_\xi \sum_{|k|\le 4k_F} |\hat{V}(k)||\nabla^2\hat\varphi(k+t(\ell-\ell'))| \\
&\quad\le Ck_F^8 \|V\|_{L^1} \left\| |\cdot|^2\varphi\right\|_{L^1} \sum_\ell \left\langle c_\ell^* c_\ell\right\rangle_\xi \le Ca^4k_F^6 \left\langle \mathcal{N}\right\rangle_\xi .
\end{aligned}$$

We compute the term with both factors 1 using Parseval's theorem. It is given by

$$-2\int_0^1 \mathrm{d}t\,(1-t)\frac{1}{L^3}\sum_{\ell,\ell'\in B_F}(\ell-\ell')^\mu(\ell-\ell')^\nu\left\langle c_\ell^* c_\ell\right\rangle_\xi \int V(x)x^\mu x^\nu e^{-it(\ell-\ell')x}\varphi(x)\,\mathrm{d}x.$$

Using $\varphi\leq 1$ we bound this by $Ck_F^5\,\| |\cdot|^2 V\|_{L^1}\left\langle\mathcal{N}\right\rangle_\xi \leq Ca^3k_F^5\left\langle\mathcal{N}\right\rangle_\xi$. We conclude that

$$\left|\left\langle\mathbb{A}_{3c}\right\rangle_\xi\right| \leq Ca^3k_F^5\left\langle\mathcal{N}\right\rangle_\xi. \tag{4.5.18}$$

—Constant terms: The constant term is given by

$$\begin{aligned}\mathbb{A}_{3d} = \frac{1}{2}\iiiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\,V(x-y)\varphi(z-z')\Big[&\delta(x-z)\delta(y-z')-\delta(x-z')\delta(y-z)\\ &- u^r(x-z)u^r(y-z')+u^r(x-z')u^r(y-z)\Big]\\ &\times\left(v(x-z)v(y-z')-v(x-z')v(y-z)\right).\end{aligned}$$

We write $u^r=\delta-v^r$ and expand everything. The terms with one factor v^r and one factor δ together give

$$\mathbb{A}_{3d,1} = 2\iiint V(x-y)\varphi(x-z)v^r(y-z)\left(v(0)v(y-z)-v(x-z)v(y-x)\right)\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z.$$

Noting that the last factor vanishes for $x=y$ we Taylor expand and bound it as

$$|v(0)v(y-z)-v(x-z)v(y-x)| \leq Ck_F^7|x-y|$$

using that $\|\nabla v\|_{L^\infty}\leq Ck_F^4$. Then

$$\begin{aligned}|\mathbb{A}_{3d,1}| &\leq Ck_F^7\iiint |x-y|V(x-y)\varphi(x-z)|v^r(y-z)|\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\\ &\leq CL^3k_F^7\,\||\cdot|V\|_{L^1}\|\varphi\|_{L^1}\|v^r\|_{L^\infty}\leq CNa^5k_F^7\left|\log ak_F\right|.\end{aligned}$$

Similarly all terms with two factors v^r are together bounded by

$$CL^3k_F^7\,\||\cdot|V\|_{L^1}\|\varphi\|_{L^1}\|v^r\|_{L^2}^2 \leq CNa^5k_F^7\left|\log ak_F\right|.$$

In particular, we conclude that

$$|\mathbb{A}_{3d}| \lesssim Na^5k_F^7\left|\log ak_F\right|. \tag{4.5.19}$$

Combining then Equations (4.5.13)–(4.5.19) we find

$$\left|\left\langle\mathbb{Q}_{2;B}^{\mathcal{E}}\right\rangle_\xi\right| \lesssim a^2k_F^3\left\langle\mathcal{N}_>\right\rangle_\xi^{1/2}\left\langle\mathbb{Q}_4\right\rangle_\xi^{1/2} + a^3k_F^5\left\langle\mathcal{N}\right\rangle_\xi + Na^5k_F^7\left|\log ak_F\right|.$$

Finally, using (4.5.8) to bound $\mathcal{N}_>$ we conclude the desired.

4.6 Finalizing the Proof

In this section, we use the bounds of Lemma 4.5.1 to prove Propositions 4.2.9 and 4.2.10. We shall also give the proof of Proposition 4.1.5.

4.6.1 Propagation of a priori estimates

To use the bounds of Lemma 4.5.1 we need bounds for the expectation value of $\mathcal{N}$, $\mathbb{H}_0$ and $\mathbb{Q}_4$ in the states ξ_λ. These states do not necessarily arise from approximate ground states, so we cannot just use the a priori bounds of Lemmas 4.3.1, 4.3.2 and 4.3.5. We show (as in [Gia23a, Proposition 4.11])

Lemma 4.6.1 (Propagation of $\mathcal{N}$)**.** *Let $\psi \in \mathcal{F}$ be any state and let ξ_λ be as in Equation* (4.2.6)*. Then, for any $0 \leq \lambda, \lambda' \leq 1$,*

$$\langle \mathcal{N} \rangle_{\xi_\lambda} \leq C \langle \mathcal{N} \rangle_{\xi_{\lambda'}} + CN(ak_F)^5.$$

Proof. This is an application of Grönwall's lemma. We compute

$$\frac{\mathrm{d}}{\mathrm{d}\lambda} \langle \mathcal{N} \rangle_{\xi_\lambda} = - \langle \xi_\lambda | [\mathcal{N}, B] | \xi_\lambda \rangle = -4 \operatorname{Re} \iint \varphi(z - z') \langle \xi_\lambda | b_z^r b_{z'}^r c_{z'} c_z | \xi_\lambda \rangle \, \mathrm{d}z \, \mathrm{d}z'.$$

Using Equation (4.5.6) to bound the integral in z' we find

$$\left| \frac{\mathrm{d}}{\mathrm{d}\lambda} \langle \mathcal{N} \rangle_{\xi_\lambda} \right| \leq C k_F^{3/2} (ak_F)^{5/2} \int \| b_z^r \xi_\lambda \| \, \mathrm{d}z \leq C N^{1/2} (ak_F)^{5/2} \langle \mathcal{N} \rangle_{\xi_\lambda}^{1/2}.$$

By Grönwall's lemma we conclude the desired. ☐

Remark 4.6.2. Using Lemma 4.6.1 for an approximate ground state ψ for $\lambda' = 0$ we find (for any $0 \leq \lambda \leq 1$)

$$\langle \mathcal{N} \rangle_{\xi_\lambda} \leq C \langle \mathcal{N} \rangle_{\xi_0} + CN(ak_F)^5 \leq CN(ak_F)^{3/2} \tag{4.6.1}$$

by Lemma 4.3.2.

Lemma 4.6.3 (Propagation of $\mathbb{H}_0, \mathbb{Q}_4$)**.** *Let $\psi \in \mathcal{F}$ be any state and let ξ_λ be as in Equation* (4.2.6)*. Then, for any $\alpha > 0$ and any $0 \leq \lambda, \lambda' \leq 1$,*

$$\begin{aligned} \langle \mathbb{H}_0 + \mathbb{Q}_4 \rangle_{\xi_\lambda} \lesssim \langle \mathbb{H}_0 + \mathbb{Q}_4 \rangle_{\xi_{\lambda'}} + Na^3 k_F^5 \left[1 + (ak_F)^{5/2 - 3\alpha/2} |\log ak_F| \right] \\ + k_F^2 (ak_F)^6 \langle \mathcal{N} \rangle_{\xi_{\lambda'}} + N^{1/2} k_F^2 (ak_F)^{3 - 3\alpha/2} |\log ak_F| \langle \mathcal{N} \rangle_{\xi_{\lambda'}}^{1/2}, \end{aligned}$$

the implicit constants depending only on α.

Remark 4.6.4. We apply Lemma 4.6.3 for an approximate ground state ψ and choose $\alpha < 1/2$ and $\lambda' = 0$. Noting that both $\mathbb{H}_0$ and $\mathbb{Q}_4$ are positive operators we find (for any $0 \leq \lambda \leq 1$)

$$\langle \mathbb{H}_0 \rangle_{\xi_\lambda} \leq CNa^3 k_F^5, \qquad \langle \mathbb{Q}_4 \rangle_{\xi_\lambda} \leq CNa^3 k_F^5 \tag{4.6.2}$$

by Lemmas 4.3.1, 4.3.2 and 4.3.5.

Proof. Again, this is an application of Grönwall's lemma. We have

$$\frac{\mathrm{d}}{\mathrm{d}\lambda} \langle \xi_\lambda | \mathbb{H}_0 + \mathbb{Q}_4 | \xi_\lambda \rangle = - \langle \xi_\lambda | [\mathbb{H}_0 + \mathbb{Q}_4, B] | \xi_\lambda \rangle = - \langle \xi_\lambda | [\mathbb{H}_0 + \mathbb{Q}_4, B] + \mathbb{Q}_2 | \xi_\lambda \rangle + \langle \xi_\lambda | \mathbb{Q}_2 | \xi_\lambda \rangle.$$

We may bound the first term using Equation (4.5.1) and the bounds of Lemma 4.5.1. This way we obtain

$$\begin{aligned}
&|\langle\xi_\lambda|[\mathbb{H}_0+\mathbb{Q}_4,B]+\mathbb{Q}_2|\xi_\lambda\rangle| \\
&\quad\lesssim N^{1/2}k_F^2(ak_F)^{3-3\alpha/2}\left|\log ak_F\right|\langle\mathcal{N}\rangle_{\xi_\lambda}^{1/2}+N^{1/2}k_F[(ak_F)^{3/2+\alpha}+(ak_F)^3\left|\log ak_F\right|]\langle\mathbb{H}_0\rangle_{\xi_\lambda}^{1/2} \\
&\qquad+N^{1/2}k_F(ak_F)^{3+1/2}\langle\mathbb{Q}_4\rangle_{\xi_\lambda}^{1/2}+a^3k_F^4\langle\mathcal{N}\rangle_{\xi_\lambda}^{1/2}\langle\mathbb{Q}_4\rangle_{\xi_\lambda}^{1/2} \\
&\quad\lesssim \langle\mathbb{Q}_4\rangle_{\xi_\lambda}+\langle\mathbb{H}_0\rangle_{\xi_\lambda}+Nk_F^2\left[(ak_F)^{3+2\alpha}+(ak_F)^{3+5/2-3\alpha/2}\left|\log ak_F\right|\right] \\
&\qquad+k_F^2(ak_F)^6\langle\mathcal{N}\rangle_{\xi_{\lambda'}}+N^{1/2}k_F^2(ak_F)^{3-3\alpha/2}\left|\log ak_F\right|\langle\mathcal{N}\rangle_{\xi_{\lambda'}}^{1/2}
\end{aligned}$$

for any $\alpha>0$ and $0\leq\lambda,\lambda'\leq 1$, where we have used Lemma 4.6.1 in the last step. Bounding $\left|\langle\mathbb{Q}_2\rangle_{\xi_\lambda}\right|\leq\langle\mathbb{Q}_4\rangle_{\xi_\lambda}+CNa^3k_F^5$ by Lemma 4.3.4 we obtain

$$\begin{aligned}
|\langle\xi_\lambda|[\mathbb{H}_0+\mathbb{Q}_4,B]|\xi_\lambda\rangle| &\lesssim \langle\mathbb{H}_0+\mathbb{Q}_4\rangle_{\xi_\lambda}+Na^3k_F^5\left[1+(ak_F)^{5/2-3\alpha/2}\left|\log ak_F\right|\right] \\
&\qquad+k_F^2(ak_F)^6\langle\mathcal{N}\rangle_{\xi_{\lambda'}}+N^{1/2}k_F^2(ak_F)^{3-3\alpha/2}\left|\log ak_F\right|\langle\mathcal{N}\rangle_{\xi_{\lambda'}}^{1/2}.
\end{aligned}$$

By Grönwall's lemma we conclude the desired. □

4.6.2 Lower bound

We now give the proof of Propositions 4.2.9 and 4.2.10, therefore concluding the proof of Theorem 4.1.2.

Proof of Proposition 4.2.9. Combining Lemma 4.5.1 with the bounds on $\mathcal{N},\mathbb{H}_0$ and $\mathbb{Q}_4$ from Equations (4.6.1) and (4.6.2) we find for any approximate ground state ψ that

$$\left|\left\langle\mathbb{Q}_{2;B}^{\mathcal{E}}\right\rangle_{\xi_\lambda}\right|\lesssim Na^4k_F^6(ak_F)^{1/2}$$

with ξ_λ as in Equation (4.2.6). Recalling Equation (4.2.9), this concludes the proof of Proposition 4.2.9. □

Proof of Proposition 4.2.10. As in the proof of Proposition 4.2.9 above we find for any approximate ground state ψ and any $\alpha>0$

$$\begin{aligned}
\left|\langle\mathbb{T}\rangle_{\xi_\lambda}\right|+\left|\langle\mathbb{Q}_{\mathsf{scat}}\rangle_{\xi_\lambda}\right| &\lesssim Na^3k_F^5\left[(ak_F)^{3/4-3\alpha/2}\left|\log ak_F\right|+(ak_F)^\alpha\right], \\
\left|\left\langle\mathbb{H}_{0;B}^{\div r}\right\rangle_{\xi_\lambda}\right| &\lesssim Na^3k_F^5(ak_F)^{3/4}\left|\log ak_F\right|, \\
\left|\left\langle\mathbb{Q}_{4;B}^{\mathcal{E}}\right\rangle_{\xi_\lambda}\right| &\lesssim Na^3k_F^5(ak_F)^2.
\end{aligned}$$

In particular, recalling Equations (4.2.10) and (4.5.1), we have the bound

$$|\mathcal{E}_{\mathsf{scat}}(\psi)|\leq CNa^3k_F^5\left[(ak_F)^{3/4-3\alpha/2}\left|\log ak_F\right|+(ak_F)^\alpha\right]$$

for any $\alpha>0$. Choosing the optimal $\alpha=3/10$ we conclude the proof of Proposition 4.2.10. □

4.6.3 Upper bound

Finally, we prove the upper bound stated in Proposition 4.1.5. The starting point is again Equation (4.2.11). To obtain an upper bound, we need to choose some trial state ψ and compute the energy. For the lower bound we used that $\mathbb{H}_0 + \mathbb{Q}_4 \geq 0$, whereas in general we can only bound $\langle \mathbb{H}_0 + \mathbb{Q}_4 \rangle_{\xi_1} \leq CNa^3k_F^5$ for an approximate ground state ψ (recall the definition of ξ_λ in Equation (4.2.6)). This bound is not good enough for our purposes. We can, however, choose the specific trial state $\psi = RT\Omega$, satisfying $\xi_1 = T^{-1}R^*\psi = \Omega$ and thus $\langle \mathbb{H}_0 + \mathbb{Q}_4 \rangle_{\xi_1} = 0$. However, it is not a priori clear whether or not this trial state is an approximate ground state. Thus, we cannot just apply the bounds on the error terms $\mathcal{E}_V(\psi), \mathcal{E}_{\mathbb{Q}_2}(\psi)$ and $\mathcal{E}_{\mathsf{scat}}(\psi)$ from Propositions 4.2.8, 4.2.9 and 4.2.10. Instead, we bound these error terms as follows.

We first note the bounds (for any $0 \leq \lambda \leq 1$)

$$\langle \mathcal{N} \rangle_{\xi_\lambda} \leq CNa^5k_F^5, \qquad \langle \mathbb{H}_0 \rangle_{\xi_\lambda} \leq CNa^3k_F^5, \qquad \langle \mathbb{Q}_4 \rangle_{\xi_\lambda} \leq CNa^3k_F^5 \tag{4.6.3}$$

by applying Lemmas 4.6.1 and 4.6.3 for $\lambda' = 1$ and using that $\xi_1 = \Omega$. Using these bounds, Lemma 4.3.3 reads

$$|\mathcal{E}_V(\psi)| \lesssim \varepsilon Na^3k_F^5 + \varepsilon^{-1}Na^6k_F^8 \leq CNa^4k_F^6(ak_F)^{1/2}$$

by choosing the optimal $\varepsilon = (ak_F)^{3/2}$. Next, using Lemma 4.5.1 and the bounds in Equation (4.6.3) we find the bounds (recall Equations (4.2.9) and (4.2.10))

$$\begin{aligned}
|\mathcal{E}_{\mathbb{Q}_2}(\psi)| &\leq CNa^5k_F^7 \left|\log ak_F\right|, \\
|\mathcal{E}_{\mathsf{scat}}(\psi)| &\leq CNa^5k_F^7(ak_F)^{1/2-3\alpha/2} \left|\log ak_F\right| + CNa^3k_F^5(ak_F)^{\alpha} \\
&\quad + CNa^4k_F^6(ak_F)^{1/2} \left|\log ak_F\right|
\end{aligned}$$

for any $\alpha > 0$. Choosing the optimal $\alpha = 1$ we find $|\mathcal{E}_{\mathsf{scat}}(\psi)| \leq CNa^4k_F^6 \left|\log ak_F\right|$. Together with the computation of $\langle \mathrm{d}\Gamma(V(1-\varphi)) \rangle_F$ in Equation (4.2.13), this concludes the proof of Proposition 4.1.5.

4.A The Two-Dimensional Case

We sketch here how to adapt the proof of Theorem 4.1.2 to the two-dimensional setting. The structure is the same as in the case $d = 3$. The main step in the proof of Theorem 4.1.8 is proving the two-dimensional analogue of Lemma 4.5.1. This reads

Lemma 4.A.1. *For any state $\xi \in \mathcal{F}$, and any $\alpha > 0$, we have*

$$\begin{aligned}
\left|\langle \mathbb{T} \rangle_\xi\right| + \left|\langle \mathbb{Q}_{\mathsf{scat}} \rangle_\xi\right| &\lesssim N^{1/2}a^2k_F^4(ak_F)^{-\alpha} \left|\log ak_F\right| \langle \mathcal{N} \rangle_\xi^{1/2} \\
&\quad + N^{1/2}ak_F^2(ak_F)^{\alpha} \left|\log ak_F\right|^{1/2} \langle \mathbb{H}_0 \rangle_\xi^{1/2}, \\
\left|\left\langle \mathbb{H}_{0;B}^{\div r} \right\rangle_\xi\right| &\lesssim N^{1/2}a^2k_F^4 \left|\log ak_F\right| \langle \mathcal{N} \rangle_\xi^{1/2} + N^{1/2}a^2k_F^3 \left|\log ak_F\right| \langle \mathbb{H}_0 \rangle_\xi^{1/2}, \\
\left|\left\langle \mathbb{Q}_{4;B}^{\mathcal{E}} \right\rangle_\xi\right| &\lesssim N^{1/2}a^2k_F^3 \left|\log ak_F\right| \langle \mathbb{Q}_4 \rangle_\xi^{1/2} + a^2k_F^3 \left|\log ak_F\right|^{1/2} \langle \mathcal{N} \rangle_\xi^{1/2} \langle \mathbb{Q}_4 \rangle_\xi^{1/2}, \\
\left|\left\langle \mathbb{Q}_{2;B}^{\mathcal{E}} \right\rangle_\xi\right| &\lesssim ak_F \langle \mathbb{H}_0 \rangle_\xi^{1/2} \langle \mathbb{Q}_4 \rangle_\xi^{1/2} + a^2k_F^4 \left|\log ak_F\right| \langle \mathcal{N} \rangle_\xi + Na^3k_F^5 \left|\log ak_F\right|.
\end{aligned}$$

Further, as in 3 dimensions, we have the a priori bounds

$$\langle \mathcal{N} \rangle_{\xi_0} \leq CNak_F, \qquad \langle \mathbb{H}_0 \rangle_{\xi_0} \leq CNa^2k_F^4, \qquad \langle \mathbb{Q}_4 \rangle_{\xi_0} \leq CNa^2k_F^4$$

for an approximate ground state ψ (recall the definition of ξ_λ in Equation (4.2.6)). Using Lemma 4.A.1 and these a priori bounds we give the

Proof of Theorem 4.1.8. Propagating the a priori bounds as in Section 4.6, using Lemma 4.A.1 and choosing the optimal $\alpha = 1/4$ we conclude the proof of Theorem 4.1.8. $\square$

To prove Lemma 4.A.1 we note the bounds on norms of φ: (being the analogue of Lemma 4.3.6)

Lemma 4.A.2. *The scattering function φ satisfies*

$$\begin{aligned} &\| |\cdot|^n \varphi \|_{L^1} \leq Ca^2 k_F^{-n}, && n = 1,2, && \| |\cdot|^n \nabla^n \varphi \|_{L^1} \leq Ca^2 \left| \log ak_F \right|, && n = 0,1,2 \\ &\| |\cdot| \varphi \|_{L^2} \leq Ca^2 \left| \log ak_F \right|^{1/2}, && && \| |\cdot|^n \nabla^n \varphi \|_{L^2} \leq Ca, && n = 0,1. \end{aligned}$$

Further, we have the analogue of Lemma 4.5.2: (which we state in general dimension d)

Lemma 4.A.3. *Let F be a compactly supported function with $F(x) = 0$ for $|x| \geq Ck_F^{-1}$. Then, uniformly in $x \in \Lambda$ and $t \in [0,1]$, (with ∇^n denoting any n'th derivative)*

$$\left\| \int F(x-y) a_y c_y \, \mathrm{d}y \right\| \lesssim k_F^{d/2} \|F\|_{L^2}, \qquad \left\| \int F(x-y) a_y c_y \nabla^n c_{ty+(1-t)x} \, \mathrm{d}y \right\| \lesssim k_F^{d+n} \|F\|_{L^2}.$$

We then sketch the

Proof of Lemma 4.A.1. The proof is the same as that of Lemma 4.5.1 only with trivial changes. We here just state all the intermediate bounds. We state these in general dimension d, to make clear the changes needed to extend the proof also to the one-dimensional setting.

We may bound $\mathbb{T}, \mathbb{Q}_{\mathsf{scat}}$ and $\mathbb{H}_{0;B}^{\div r}$ by

$$\begin{aligned} \left| \langle \mathbb{T} \rangle_\xi \right| &\leq CN^{1/2} k_F^{d+2} (ak_F)^{-d\alpha/2} \|F\|_{L^1} \langle \mathcal{N} \rangle_\xi^{1/2} + CN^{1/2} k_F^{d/2+2} \|F\|_{L^2} \langle \mathcal{N}_{>\alpha} \rangle_\xi^{1/2}. \\ \left| \langle \mathbb{Q}_{\mathsf{scat}} \rangle_\xi \right| &\leq CN^{1/2} k_F^{d+1} (ak_F)^{-d\alpha/2} \|\mathcal{E}_\varphi\|_{L^1} \langle \mathcal{N} \rangle_\xi^{1/2} + CN^{1/2} k_F^{d/2+1} \|\mathcal{E}_\varphi\|_{L^2} \langle \mathcal{N}_{>\alpha} \rangle_\xi^{1/2}. \\ \left| \left\langle \mathbb{H}_{0;B}^{\div r} \right\rangle_\xi \right| &\leq CN^{1/2} \left[\left\| |\cdot|^2 \Delta\varphi \right\|_{L^1} + \| |\cdot| \nabla\varphi \|_{L^1} \right] \left[k_F^{d+2} \langle \mathcal{N} \rangle_\xi^{1/2} + k_F^{d+1} \langle \mathbb{H}_0 \rangle_\xi^{1/2} \right]. \end{aligned}$$

For the error terms from $[\mathbb{Q}_4, B]$ we have the bounds

$$\begin{aligned} \left| \langle \mathbb{A}_1 \rangle_\xi \right| + \left| \langle \mathbb{A}_2 \rangle_\xi \right| &\leq CN^{1/2} k_F^{d+d/2+1} \| |\cdot| \varphi \|_{L^1} \|V\|_{L^1}^{1/2} \langle \mathbb{Q}_4 \rangle_\xi^{1/2} \\ \left| \langle \mathbb{A}_3 \rangle_\xi \right| + \left| \langle \mathbb{A}_4 \rangle_\xi \right| &\leq Ck_F^{d+1} \| |\cdot| \varphi \|_{L^2} \|V\|_{L^1} \langle \mathcal{N} \rangle_\xi^{1/2} \langle \mathbb{Q}_4 \rangle_\xi^{1/2}. \end{aligned}$$

Finally, the error terms from $[\mathbb{Q}_2, B]$ are bounded as follows.

$$\begin{aligned}
\left|\langle \mathbb{A}_{1a}\rangle_\xi\right| + \left|\langle \mathbb{A}_{1b}\rangle_\xi\right| &\leq Ck_F^d \left\|\varphi\right\|_{L^2} \left\|V\right\|_{L^1}^{1/2} \langle \mathcal{N}_> \rangle_\xi^{1/2} \langle \mathbb{Q}_4\rangle_\xi^{1/2} \\
\left|\langle \mathbb{A}_{2a}\rangle_\xi\right| &\leq Ck_F^{2d+2} \left\||\cdot|\varphi\right\|_{L^1} \left\||\cdot|V\right\|_{L^1} \langle \mathcal{N}\rangle_\xi \\
\left|\langle \mathbb{A}_{2b}\rangle_\xi\right| &\leq Ck_F^{d+2} \left\||\cdot|^2 V\right\|_{L^1} \langle \mathcal{N}\rangle_\xi + Ck_F^{d+d/2+2} \left\||\cdot|^2 V\right\|_{L^1}^{1/2} \left\|V\right\|_{L^1}^{1/2} \left\||\cdot|\varphi\right\|_{L^2} \langle \mathcal{N}\rangle_\xi \\
&\quad + Ck_F^{2d+2} \left\||\cdot|^2 V\right\|_{L^1}^{1/2} \left\|V\right\|_{L^1}^{1/2} \left\||\cdot|^2 \varphi\right\|_{L^1}^{1/2} \left\|\varphi\right\|_{L^1}^{1/2} \langle \mathcal{N}\rangle_\xi \\
\left|\langle \mathbb{A}_{3a}\rangle_\xi\right| + \left|\langle \mathbb{A}_{3b}\rangle_\xi\right| &\leq Ck_F^{2d} \left\|\varphi\right\|_{L^1} \left\|V\right\|_{L^1} \langle \mathcal{N}\rangle_\xi \\
\left|\langle \mathbb{A}_{3c}\rangle_\xi\right| &\leq Ck_F^{2d+2} \left\|V\right\|_{L^1} \left\||\cdot|^2 \varphi\right\|_{L^1} \langle \mathcal{N}\rangle_\xi + Ck_F^{d+2} \left\||\cdot|^2 V\right\|_{L^1} \langle \mathcal{N}\rangle_\xi \\
\left|\langle \mathbb{A}_{3d}\rangle_\xi\right| &\leq CNk_F^{2d+1} \left\||\cdot|V\right\|_{L^1} \left\|\varphi\right\|_{L^1}.
\end{aligned}$$

Bounding $\mathcal{N}_>$ and $\mathcal{N}_{>\alpha}$ as in Equation (4.5.8) and using the bounds on norms of φ above we conclude the proof of Lemma 4.A.1. □

Remark 4.A.4 (Possible extension to the one-dimensional case)**.** In dimension $d = 1$ the analogous bounds on norms of φ read

$$\begin{aligned}
&\left\||\cdot|^n \varphi\right\|_{L^1} \leq Cak_F^{-n}, \quad n = 1, 2, \qquad &&\left\||\cdot|^n \nabla^n \varphi\right\|_{L^1} \leq Ca\left|\log ak_F\right|, \quad n = 0, 1, 2 \\
&\left\||\cdot|\varphi\right\|_{L^2} \leq Cak_F^{-1/2}, &&\left\||\cdot|^n \nabla^n \varphi\right\|_{L^2} \leq Ca^{1/2}, \qquad n = 0, 1.
\end{aligned}$$

Further $\left\||\cdot|^n V\right\|_{L^1} \leq Ca^{n-1}$. Using these bounds and bounding $\langle \mathcal{N}\rangle_\xi \leq CN(ak_F)^{1/2}$, $\langle \mathbb{H}_0\rangle_\xi \leq CNak_F^3$ and $\langle \mathbb{Q}_4\rangle_\xi \leq CNak_F^3$ (as is appropriate for relevant ξ by the propagation of the a priori bounds) we see that only the estimates of the error terms $\mathbb{T}, \mathbb{Q}_{\mathsf{scat}}, \mathbb{H}_{0;B}^{\div r}, \mathbb{A}_{2a}$ and $\mathbb{A}_{2b}$ in the proof or Lemma 4.A.1 are smaller than Nak_F^3. The estimates of the (many) remaining error-terms are too big. One would have to improve these remaining estimates in order to extend our proof of Theorems 4.1.2 and 4.1.8 also to the one-dimensional setting. We do not pursue this. As already mentioned, the one-dimensional analogue of Theorems 4.1.2 and 4.1.8 is proved in [ARS22].

Chapter 5

Almost optimal upper bound for the ground state energy of a dilute Fermi gas via cluster expansion

This chapter contains the paper

[Spin-1/2] A. B. Lauritsen. "Almost Optimal Upper Bound for the Ground State Energy of a Dilute Fermi Gas via Cluster Expansion", *Ann. Henri Poincaré* (2024).
DOI: 10.1007/s00023-024-01450-1.

Abstract. We prove an upper bound on the energy density of the dilute spin-$\frac{1}{2}$ Fermi gas capturing the leading correction to the kinetic energy $8\pi a\rho_\uparrow\rho_\downarrow$ with an error of size smaller than $a\rho^2(a^3\rho)^{1/3-\varepsilon}$ for any $\varepsilon > 0$, where a denotes the scattering length of the interaction. The result is valid for a large class of interactions including interactions with a hard core. A central ingredient in the proof is a rigorous version of a fermionic cluster expansion adapted from the formal expansion of Gaudin, Gillespie and Ripka (Nucl. Phys. A, 176.2 (1971), pp. 237–260).

Contents

5.1 Introduction and main results

We consider an interacting Fermi gas of N particles interacting via a two-body interaction v which we assume to be non-negative, radial and of compact support. In units where $\hbar = 1$ and the particle mass is $m = 1/2$ the Hamiltonian is given by

$$H_N = \sum_{j=1}^{N} -\Delta_j + \sum_{i<j} v(x_i - x_j),$$

where Δ_j denotes the Laplacian on the j'th coordinate. For spin-$\frac{1}{2}$ fermions in some domain $\Lambda = \Lambda_L = [-L/2, L/2]^3$ one realises the Hamiltonian on the space $L^2_a(\Lambda^N, \mathbb{C}^2) = \bigwedge^N L^2(\Lambda, \mathbb{C}^2)$. Since the Hamiltonian is spin-independent we can specify definite values for the number of particles with each spin, i.e. N_σ particles of spin $\sigma \in \{\uparrow, \downarrow\}$ and $N_\uparrow + N_\downarrow = N$. In this setting the Hamiltonian is realized on the space $\mathcal{H}_{N_\uparrow, N_\downarrow} = L^2_a(\Lambda^{N_\uparrow}) \otimes L^2_a(\Lambda^{N_\downarrow})$. The ground state energy on the space $L^2_a(\Lambda^N, \mathbb{C}^2)$ is then given by minimizing in N_σ (satisfying $N_\uparrow + N_\downarrow = N$) the ground state energies on the spaces $\mathcal{H}_{N_\uparrow, N_\downarrow}$.

This system was previously studied in [FGHP21; Gia23a; LSS05] where it is shown that for a dilute system in the thermodynamic limit

$$e(\rho_\uparrow, \rho_\downarrow) = \lim_{\substack{L\to\infty \\ N_\sigma/L^3 \to \rho_\sigma}} \inf_{\substack{\psi \in \mathcal{H}_{N_\uparrow, N_\downarrow} \\ \|\psi\|_{L^2}=1}} \frac{\langle \psi | H_N | \psi \rangle}{L^3} = \frac{3}{5}(6\pi^2)^{2/3}(\rho_\uparrow^{5/3} + \rho_\downarrow^{5/3}) + 8\pi a \rho_\uparrow \rho_\downarrow + a\rho^2 \varepsilon(a^3\rho),$$

where $\rho = \rho_\uparrow + \rho_\downarrow$, a is the *(s-wave) scattering length* of the interaction v and $\varepsilon(a^3\rho) = o(1)$ in the limit $a^3\rho \ll 1$. The existence of the thermodynamic limit follows from [Rob71]. Moreover the limit doesn't depend on the boundary conditions.

The leading term $\frac{3}{5}(6\pi^2)^{2/3}(\rho_\uparrow^{5/3} + \rho_\downarrow^{5/3})$ is the kinetic energy of a free Fermi gas. The next term $8\pi a \rho_\uparrow \rho_\downarrow$ is the leading correction coming from the interaction. This term may be understood as coming from the energy of a pair of opposite-spin fermions times the number of such pairs. The energy correction arising from interactions between fermions of the same spin is of order $a_p^3 \rho^{8/3}$, where a_p denotes the *p-wave scattering length* (see Chapter 3) and so much smaller.

The first proof of this result was given by Lieb, Seiringer and Solovej [LSS05]. Their proof gives the explicit error bounds $-C(a^3\rho)^{1/39} \le \varepsilon(a^3\rho) \le C(a^3\rho)^{2/27}$ for some constant $C > 0$. These error bounds were later improved in [FGHP21] and very recently in [Gia23a], where in particular the "optimal" upper bound $\varepsilon(a^3\rho) \le C(a^3\rho)^{1/3}$ is shown. The works [FGHP21; Gia23a] however deal with more regular potentials than the quite general setting studied in [LSS05], where it is assumed that the interaction is non-negative, radial and compactly supported. In [FGHP21; Gia23a] the interaction is additionally assumed to be smooth. In particular interactions with a hard core are not treated in [FGHP21; Gia23a].

The upper bound of order $a\rho^{1/3}$ is optimal in the sense that this is the order of the conjectured next term in the expansion. Namely the Huang–Yang term [HY57], see [Gia23a; Gia23b].

Our main theorem is the "almost optimal" upper bound $\varepsilon(a^3\rho) \leq C_\delta(a^3\rho)^{1/3-\delta}$ for any $\delta > 0$ for some δ-dependent constant $C_\delta > 0$ under the same assumptions as in [LSS05], i.e. weaker than that of [FGHP21; Gia23a]. In particular we allow for v to have a hard core. A central ingredient in the proof is to prove a rigorous version of a fermionic cluster expansion adapted from [GGR71]. This is analogous to what is done in Chapter 3 for spin-polarized fermions. (See also Chapter 6 for the application to spin-polarized fermions at positive-temperature.)

5.1.1 Precise statements of results

To give the statement of our main theorem, we first define the *scattering length(s)* of the interaction v.

Definition 5.1.1 ([LY01, Appendix A; SY20, Section 4])**.** The s- and p-*wave scattering lengths* a and a_p are defined by

$$4\pi a = \inf\left\{\int \left(|\nabla f|^2 + \frac{1}{2}v|f|^2\right) \mathrm{d}x : f(x) \to 1 \text{ for } |x| \to \infty\right\},$$
$$12\pi a_p^3 = \inf\left\{\int \left(|\nabla f|^2 + \frac{1}{2}v|f|^2\right) |x|^2 \,\mathrm{d}x : f(x) \to 1 \text{ for } |x| \to \infty\right\}.$$

The minimizing f's are the s- and p-*wave scattering functions*. They are denoted f_{s0} and f_{p0} respectively.

The minimizing functions f_{s0} and f_{p0} are real-valued. We collect properties of them in Lemma 5.2.5.

With this we may then state our main theorem.

Theorem 5.1.2. *Let $0 \leq v \leq +\infty$ be radial and of compact support. Then for any $\delta > 0$ and for sufficiently small $a^3\rho$ we have*

$$e(\rho_\uparrow, \rho_\downarrow) \leq \frac{3}{5}(6\pi^2)^{2/3}(\rho_\uparrow^{5/3} + \rho_\downarrow^{5/3}) + 8\pi a \rho_\uparrow\rho_\downarrow + O_\delta\left(a\rho^2(a^3\rho)^{1/3-\delta}\right).$$

The subscript δ in O_δ denotes that the implicit constant depends on δ. Further, the v-dependence of the error-term $O_\delta\left(a\rho^2(a^3\rho)^{1/3-\delta}\right)$ is only via the scattering lengths a and a_p (meaning that the implicit constant depends on the ratio a_p/a but otherwise not on v). In particular we note that v is allowed to have a hard core, meaning $v(x) = +\infty$ for $|x| \leq r_0$ for some $r_0 > 0$.

The essential steps of the proof are

(1) Show the absolute convergence of a fermionic cluster expansion adapted from the formal calculations of [GGR71]. For this we need the "Fermi polyhedron", a polyhedral approximation to the Fermi ball, described in Section 3.2.2. The calculation of the fermionic cluster expansion is given in Section 5.3 and the absolute convergence in shown in Section 5.4.

(2) Bound the energy of a Jastrow-type trial state. For this step, the central part is computing the values of all diagrams of a certain type exactly and using these exact values up to some arbitrary high order. This is somewhat similar to the approach in [BCGOPS23] for the dilute Bose gas. This calculation is part of the proof of Lemma 5.5.1.

Remark 5.1.3 (Higher spin)**.** With not much difficulty one can extend the result to higher spin and with a spin-dependent interaction $v_{\sigma\sigma'} = v_{\sigma'\sigma}$. The result for $S \geq 2$ spin values $\{1, \ldots, S\}$ is

$$e(\rho_1, \ldots, \rho_S) \leq \frac{3}{5}(6\pi^2)^{2/3} \sum_{\sigma=1}^{S} \rho_\sigma^{5/3} + 8\pi \sum_{1\leq\sigma<\sigma'\leq S} a_{\sigma\sigma'}\rho_\sigma\rho_{\sigma'} + O_\delta\left(a\rho^2(a^3\rho)^{1/3-\delta}\right),$$

where $a_{\sigma\sigma'}$ is the s-wave scattering length of the spin σ – spin σ' interaction $v_{\sigma\sigma'}$ and $a = \sup_{\sigma<\sigma'} a_{\sigma\sigma'}$. For conciseness of the proof we will only give it for $S = 2$, i.e. for spin-$\frac{1}{2}$ fermions. We will however give comments on how to adapt the individual (non-trivial) steps of the proof to the higher spin setting. These comments are given in Remarks 5.3.3, 5.4.2, 5.5.4 and 5.5.6.

Remark 5.1.4 (Comparison with [FGHP21; Gia23a; LSS05])**.** The trial state we consider, $\psi_{N_\uparrow,N_\downarrow}$ (defined in Equation (5.2.5) below), is in spirit the same as that considered in [LSS05]. They differ only in technical aspects (discussed in Remark 5.2.1 below). The reason we are able to improve on the bound in [LSS05] is that we treat the cancellations between $\langle\psi|H_N|\psi\rangle$ and $\langle\psi|\psi\rangle$ more precisely (for the [non-normalized] trial state ψ being defined as $\psi_{N_\uparrow,N_\downarrow}$ in Equation (5.2.5) only without the normalization constant $C_{N_\uparrow,N_\downarrow}$).

In [FGHP21; Gia23a] a completely different method is employed. There the system is studied using a method inspired by Bogoliubov theory for dilute Bose gases. (The "bosons" appearing here as pairs of opposite-spin fermions.)

The paper is structured as follows. In Section 5.2 we give some preliminary computations and recall some properties of the scattering functions and Fermi polyhedron from [LY01] and Chapter 3. Next, in Section 5.3 we give the calculation of a fermionic cluster expansion adapted from [GGR71]. Subsequently, in Section 5.4 we find conditions for the absolute convergence of the cluster expansion formulas of Section 5.3. Finally, in Section 5.5 we use the formulas of Section 5.3 to bound the energy of a Jastrow-type trial state.

5.2 Preliminary computations

We first give a few preliminary computations. We will construct a trial state using a box method of glueing trial states in smaller boxes together in Section 5.5.4. In the smaller boxes we will need to use Dirichlet boundary conditions, however in Section 5.5.4 we will construct trial states with Dirichlet boundary conditions out of trial states with periodic boundary conditions. (See also Chapter 3.) Thus, we will use periodic boundary conditions in the box $\Lambda = \Lambda_L = [-L/2, L/2]^3$.

First we establish some notation.

5.2.1 Notation

- We write x_i and y_j for the spatial coordinates of particle i of spin $\uparrow$ respectively particle j of spin $\downarrow$.

We write z_i to mean either x_i or y_i if the spin is not important.

We write additionally $z_{(i,\uparrow)} = x_i$ and $z_{(i,\downarrow)} = y_i$.

- We write $[n,m] = \{n, n+1, \ldots, m\}$ for integers $n \le m$. If $n > m$ then $[n,m] = \varnothing$.
- For a set A we write $Z_A = (z_a)_{a\in A}$ for the coordinates of the vertices with labels in A. (Similarly for X_A and Y_A.)

  In particular we write $Z_{[n,m]} = (z_n, \ldots, z_m)$ for the coordinates of particles $n, n+1, \ldots, m$.

  If $n = 1$ we simply write $Z_m = Z_{[1,m]} = (z_1, \ldots, z_m)$.
- We write C for a generic (positive) constant, whose value may change line by line. If we want to emphasize the dependence on some parameter A we will denote this by C_A.

We consider the indices of the coordinates as vertices $\mu = (i,\sigma) \in V_{\infty,\infty} := \mathbb{N} \times \{\uparrow,\downarrow\}$. Here $\sigma \in \{\uparrow,\downarrow\}$ labels the spin of the particle. Then we define

$$V_{n,m} := V_n^{\uparrow} \cup V_m^{\downarrow}, \qquad V_p^{\sigma} := \{(1,\sigma), \ldots, (p,\sigma)\} \subset V_{\infty,\infty}, \quad \sigma \in \{\uparrow,\downarrow\}, \quad p \in \mathbb{N} \cup \{\infty\}.$$

(We mean $V_\infty^\sigma = \mathbb{N} \times \{\sigma\}$ for $p = \infty$.) On the vertices $V_{\infty,\infty}$ we define the ordering $<$ as follows.

$$\mu = (i,\sigma) < (j,\sigma') = \nu \qquad \overset{\text{def}}{\iff} \qquad (\sigma = \uparrow \text{ and } \sigma' = \downarrow) \text{ or } (\sigma = \sigma' \text{ and } i < j)\,.$$

Define the rescaled and cut-off scattering functions f_s and f_p as

$$f_s(x) = \begin{cases} \frac{1}{1-a/b} f_{s0}(|x|) & |x| \le b, \\ 1 & |x| \ge b, \end{cases} \qquad f_p(x) = \begin{cases} \frac{1}{1-a_p^3/b^3} f_{p0}(|x|) & |x| \le b, \\ 1 & |x| \ge b, \end{cases} \tag{5.2.1}$$

where $|\cdot| := \inf_{n\in\mathbb{Z}^3} |\cdot - nL|_{\mathbb{R}^3}$ (with $|\cdot|_{\mathbb{R}^3}$ denoting the norm on $\mathbb{R}^3$), $b = \rho^{-1/3}$ and the scattering function f_{s0} and f_{p0} are defined in Definition 5.1.1. (They are radial functions, see Lemma 5.2.5, so f_s and f_p are well-defined.) We prefer to write b instead of its value $\rho^{-1/3}$ to keep apparent dependences on b. For $b = \rho^{-1/3}$ we have $b > R_0$, the range of v, for sufficiently small $a^3\rho$. Hence, f_s and f_p are continuous for sufficiently small $a^3\rho$. (Note that the metric on the torus Λ is given by $d(x,y) = |x-y|$. We will abuse notation slightly and denote by $|\cdot|$ also the absolute value of some number or the norm on $\mathbb{R}^3$.)

To simplify notation we write for $\mu, \nu \in V_{\infty,\infty}$

$$f_{\mu\nu} := \begin{cases} f_p(x_i - x_j) & \mu = (i,\uparrow), \nu = (j,\uparrow), \\ f_s(x_i - y_j) & \mu = (i,\uparrow), \nu = (j,\downarrow), \\ f_s(y_i - x_j) & \mu = (i,\downarrow), \nu = (j,\uparrow), \\ f_p(y_i - y_j) & \mu = (i,\downarrow), \nu = (j,\downarrow), \end{cases} \tag{5.2.2}$$

and similar for all quantities derived from f_s and f_p. In particular $\nabla f_{\mu\nu} = \nabla f_{s/p}(z_\mu - z_\nu)$ with s/p meaning s if the spins of μ and ν are different and p if they are the same.

Next, we introduce the (non-normalized) Slater determinants $D_{N_\uparrow}$ and $D_{N_\downarrow}$ as

$$D_{N_\sigma}(Z_{N_\sigma}) = \det\left[u_k(z_i)\right]_{\substack{k\in P_F^\sigma \\ i=1,\ldots,N_\sigma}}, \qquad N_\sigma = \# P_F^\sigma, \qquad u_k(z) = L^{-3/2} e^{ikz},$$

where P_F^σ is the "Fermi polyhedron", a polyhedral approximation to the Fermi ball described in Section 5.2.3, see also Section 3.2.2, and $\#P_F^\sigma$ denotes the number of points in P_F^σ.

Further, we denote for $\mu, \nu \in V_{\infty,\infty}$

$$\gamma_{\mu\nu} := \begin{cases} \gamma_{N_\uparrow}^{(1)}(x_i; x_j) & \mu = (i,\uparrow), \nu = (j,\uparrow), \\ 0 & \mu = (i,\uparrow), \nu = (j,\downarrow), \\ 0 & \mu = (i,\downarrow), \nu = (j,\uparrow), \\ \gamma_{N_\downarrow}^{(1)}(y_i; y_j) & \mu = (i,\downarrow), \nu = (j,\downarrow), \end{cases} \tag{5.2.3}$$

where $\gamma_{N_\sigma}^{(1)}$ are the one-particle density matrices of $\frac{1}{\sqrt{N_\uparrow!}} D_{N_\uparrow}$ and $\frac{1}{\sqrt{N_\downarrow!}} D_{N_\downarrow}$.

Finally, for any (normalized) state $\psi \in L_a^2(\Lambda^{N_\uparrow}) \otimes L_a^2(\Lambda^{N_\downarrow})$ we will normalize reduced densities as follows (for $n + m \geq 1$).

$$\begin{aligned} \rho_\psi^{(n,m)} &= N_\uparrow(N_\uparrow - 1)\cdots(N_\uparrow - n + 1) N_\downarrow(N_\downarrow - 1)\cdots(N_\downarrow - m + 1) \\ &\quad \times \int\!\!\cdots\!\!\int |\psi|^2 \, \mathrm{d}X_{[n+1,N_\uparrow]} \, \mathrm{d}Y_{[m+1,N_\downarrow]}. \end{aligned} \tag{5.2.4}$$

For a (normalized) Slater determinant $\psi = \psi(X_{N_\uparrow}, Y_{N_\downarrow}) = \frac{1}{\sqrt{N_\uparrow! N_\downarrow!}} D_{N_\uparrow}(X_{N_\uparrow}) D_{N_\downarrow}(Y_{N_\downarrow})$ we write $\rho^{(n,m)} = \rho_\psi^{(n,m)}$ and for the trial state $\psi_{N_\uparrow,N_\downarrow}$ we write $\rho_{\text{Jas}}^{(n,m)} = \rho_{\psi_{N_\uparrow,N_\downarrow}}^{(n,m)}$.

We will fix the Fermi momenta k_F^σ such that the ratio $k_F^\uparrow / k_F^\downarrow$ is rational, see Remark 5.2.3. This is a restriction on which densities ρ_σ can arise from the trial state $\psi_{N_\uparrow,N_\downarrow}$, see Remark 5.2.4. We extend to all densities in Section 5.5.4. The dilute limit will be realized as $(k_F^\uparrow + k_F^\downarrow)a \to 0$.

5.2.2 Computation of the energy

We consider the trial state

$$\begin{aligned} \psi_{N_\uparrow,N_\downarrow}(X_{N_\uparrow}, Y_{N_\downarrow}) &= \frac{1}{\sqrt{C_{N_\uparrow,N_\downarrow}}} \left[\prod_{\substack{\mu,\nu \in V_{N_\uparrow,N_\downarrow} \\ \mu<\nu}} f_{\mu\nu} \right] D_{N_\uparrow}(X_{N_\uparrow}) D_{N_\downarrow}(Y_{N_\downarrow}) \\ &= \frac{1}{\sqrt{C_{N_\uparrow,N_\downarrow}}} \left[\prod_{\substack{1\leq i\leq N_\uparrow \\ 1\leq j\leq N_\downarrow}} f_s(x_i - y_j) \prod_{1\leq i<j\leq N_\uparrow} f_p(x_i - x_j) \prod_{1\leq i<j\leq N_\downarrow} f_p(y_i - y_j) \right] \\ &\qquad \times D_{N_\uparrow}(X_{N_\uparrow}) D_{N_\downarrow}(Y_{N_\downarrow}), \end{aligned} \tag{5.2.5}$$

where $C_{N_\uparrow,N_\downarrow}$ is a normalization constant such that $\int \left|\psi_{N_\uparrow,N_\downarrow}\right|^2 \mathrm{d}X_{N_\uparrow} \, \mathrm{d}Y_{N_\downarrow} = 1$.

Remark 5.2.1 (Comparison to [LSS05])**.** As mentioned in Remark 5.1.4 the trial state $\psi_{N_\uparrow,N_\downarrow}$ is mostly the same as that of [LSS05]. They differ in two technical aspects:

1. The choice of function implementing the correlations between particles of the same spin.

   The exact function used is not particularly important since the same-spin interactions give rise to a much smaller energy correction (than that of different-spin interactions). The function f_p is a natural choice.

2. The choice of Slater determinant.

   Our choice of Slater determinants with momenta in the Fermi polyhedron (as opposed to the Fermi ball, which is what is used in [LSS05]) is a technical necessity as we discuss in Section 5.2.3 below.

We compute the energy of the trial state $\psi_{N_\uparrow,N_\downarrow}$

$$\left\langle \psi_{N_\uparrow,N_\downarrow} \middle| H_N \middle| \psi_{N_\uparrow,N_\downarrow} \right\rangle = \int\!\cdots\!\int \Bigg[\sum_{\mu\in V_{N_\uparrow,N_\downarrow}} \left|\nabla_{z_\mu}\psi_{N_\uparrow,N_\downarrow}\right|^2 + \sum_{\substack{\mu,\nu\in V_{N_\uparrow,N_\downarrow}\\ \mu<\nu}} v(z_\mu - z_\nu)\left|\psi_{N_\uparrow,N_\downarrow}\right|^2 \Bigg] \mathrm{d}X_{N_\uparrow}\,\mathrm{d}Y_{N_\downarrow}.$$

Note that for (real-valued) functions F,G we have

$$\int |\nabla(FG)|^2 = -\int G\Delta G |F|^2 + \int |G|^2\,|\nabla F|^2. \tag{5.2.6}$$

By symmetries of the Fermi polyhedron, see Definition 5.2.2, we have that $D_{N_\uparrow}$ and $D_{N_\downarrow}$ are real-valued. Thus, using Equation (5.2.6) for $F=\prod_{\mu<\nu} f_{\mu\nu}$ and $G = D_{N_\uparrow}D_{N_\downarrow}$ for each of the derivatives ∇_{x_i}, ∇_{y_j} we get (recall that $\nabla f_{\mu\nu} = \nabla f_{s/p}(z_\mu - z_\nu)$)

$$\begin{aligned}
&\sum_{\mu\in V_{N_\uparrow,N_\downarrow}} \int\!\cdots\!\int \left|\nabla_{z_\mu}\psi_{N_\uparrow,N_\downarrow}\right|^2 \mathrm{d}X_{N_\uparrow}\,\mathrm{d}Y_{N_\downarrow} \\
&= E_0^\uparrow + E_0^\downarrow + \int\!\cdots\!\int \mathrm{d}X_{N_\uparrow}\,\mathrm{d}Y_{N_\downarrow} \left|\psi_{N_\uparrow,N_\downarrow}\right|^2 \Bigg[2\sum_{\mu\in V^\uparrow_{N_\uparrow}}\sum_{\nu\in V^\downarrow_{N_\downarrow}} \left|\frac{\nabla f_{\mu\nu}}{f_{\mu\nu}}\right|^2 \\
&\quad + 2\sum_{\sigma\in\{\uparrow,\downarrow\}} \sum_{\substack{\mu,\nu\in V^\sigma_{N_\sigma}\\ \mu<\nu}} \left|\frac{\nabla f_{\mu\nu}}{f_{\mu\nu}}\right|^2 + \sum_{\sigma\in\{\uparrow,\downarrow\}}\sum_{\mu\in V^\sigma_{N_\sigma}} \sum_{\substack{\nu,\lambda\in V^{-\sigma}_{N_{-\sigma}}\\ \nu\neq\lambda}} \frac{\nabla f_{\mu\nu}\nabla f_{\mu\lambda}}{f_{\mu\nu}f_{\mu\lambda}} \\
&\quad + \sum_{\sigma\in\{\uparrow,\downarrow\}} \sum_{\substack{\mu,\nu\in V^\sigma_{N_\sigma}\\ \mu\neq\nu}} \sum_{\lambda\in V^{-\sigma}_{N_{-\sigma}}} \frac{\nabla f_{\mu\nu}\nabla f_{\mu\lambda}}{f_{\mu\nu}f_{\mu\lambda}} - \sum_{\sigma\in\{\uparrow,\downarrow\}} \sum_{\substack{\mu,\nu,\lambda\in V^\sigma_{N_\sigma}\\ \mu,\nu,\lambda \text{ distinct}}} \frac{\nabla f_{\mu\nu}\nabla f_{\nu\lambda}}{f_{\mu\nu}f_{\nu\lambda}} \Bigg],
\end{aligned}$$

where $E_0^\sigma = \sum_{k\in P_F^\sigma} |k|^2$ is the kinetic energy of the Slater determinants $\frac{1}{\sqrt{N_\sigma!}}D_{N_\sigma}$ and $-\sigma$ is the "other spin", i.e. $-\uparrow=\downarrow$ and $-\downarrow=\uparrow$. (The factor 2 in the term $2\sum_{\mu\in V^\uparrow_{N_\uparrow}}\sum_{\nu\in V^\downarrow_{N_\downarrow}} \left|\frac{\nabla f_{\mu\nu}}{f_{\mu\nu}}\right|^2$ arises as $2=\sum_{\sigma\in\{\uparrow,\downarrow\}} 1$.) The terms are grouped according to how many s-wave f's appear.

In terms of the reduced densities we thus get

$$\begin{aligned}
&\left\langle \psi_{N_\uparrow,N_\downarrow} \middle| H_N \middle| \psi_{N_\uparrow,N_\downarrow} \right\rangle \\
&= E_0^\uparrow + E_0^\downarrow + 2 \iint \rho_{\mathsf{Jas}}^{(1,1)} \left[\left| \frac{\nabla f_s(x_1 - y_1)}{f_s(x_1 - y_1)} \right|^2 + \frac{1}{2} v(x_1 - y_1) \right] \mathrm{d}x_1 \, \mathrm{d}y_1 \\
&\quad + \iint \rho_{\mathsf{Jas}}^{(2,0)} \left[\left| \frac{\nabla f_p(x_1 - x_2)}{f_p(x_1 - x_2)} \right|^2 + \frac{1}{2} v(x_1 - x_2) \right] \mathrm{d}x_1 \, \mathrm{d}x_2 \\
&\quad + \iiint \rho_{\mathsf{Jas}}^{(2,1)} \left[\frac{\nabla f_s(x_1 - y_1) \nabla f_s(x_2 - y_1)}{f_s(x_1 - y_1) f_s(x_2 - y_1)} + \frac{\nabla f_s(x_1 - y_1) \nabla f_p(x_1 - x_2)}{f_s(x_1 - y_1) f_p(x_1 - x_2)} \right] \mathrm{d}x_1 \, \mathrm{d}x_2 \, \mathrm{d}y_1 \\
&\quad - \iiint \rho_{\mathsf{Jas}}^{(3,0)} \frac{\nabla f_p(x_1 - x_2) \nabla f_p(x_2 - x_3)}{f_p(x_1 - x_2) f_p(x_2 - x_3)} \, \mathrm{d}x_1 \, \mathrm{d}x_2 \, \mathrm{d}x_3 + \text{terms with } \rho_{\mathsf{Jas}}^{(0,2)}, \rho_{\mathsf{Jas}}^{(1,2)}, \rho_{\mathsf{Jas}}^{(0,3)}.
\end{aligned} \tag{5.2.7}$$

We find formulas for the reduced densities in Section 5.3. Before doing so, we first recall some properties on the "Fermi polyhedron" P_F^σ and the scattering functions f_s, f_p.

5.2.3 Properties of the "Fermi polyhedron" and the scattering functions

In this section we recall a few properties of the "Fermi polyhedron" from Section 3.2.2 and Lemma 3.4.9 and scattering functions from [LY01, Appendix A].

The reason for introducing the "Fermi polyhedron" is that for the analysis of the absolute convergence of the Gaudin–Gillespie–Ripka expansion we need good control over

$$\int_\Lambda \left| \gamma_{N_\sigma}^{(1)}(x;0) \right| \mathrm{d}x = \int_\Lambda \left| \frac{1}{L^3} \sum_{k \in P_F^\sigma} e^{ikx} \right| \mathrm{d}x.$$

By Equation (5.2.9a) below (coming from Lemma 3.2.12 and [KL18]) this is bounded by $s(\log N)^3$. If we had instead chosen the Slater determinants in the trial state $\psi_{N_\uparrow,N_\downarrow}$ to have momenta in the Fermi ball $B_F^\sigma = \{k \in \frac{2\pi}{L}\mathbb{Z}^3 : |k| \le k_F^\sigma\}$ we would have [GL19; Lif06]

$$\int_\Lambda \left| \gamma_{N_\sigma}^{(1)}(x;0) \right| \mathrm{d}x = \int_\Lambda \left| \frac{1}{L^3} \sum_{k \in B_F^\sigma} e^{ikx} \right| \mathrm{d}x \sim N^{1/3}.$$

This N-dependence would prevent us from achieving that both the Gaudin–Gillespie–Ripka expansion converges absolutely and that the finite-size error from the kinetic energy is negligible. See also Remark 5.3.4 and Remark 3.3.5.

The "Fermi polyhedron" is defined in Definition 3.2.7. We give here only a sketch of the definition and state a few properties needed for our purposes. For a full discussion with proofs we refer to Sections 3.B and 3.2.2.

Definition 5.2.2 (Sketch, see Definition 3.2.7)**.** For each spin $\sigma \in \{\uparrow, \downarrow\}$ define the (convex) polyhedron P^σ with s_σ "corners" (extremal points) as follows. All "corners" $\kappa_1^\sigma, \ldots, \kappa_{s_\sigma}^\sigma$ are chosen of the form $\kappa_j^\sigma = \zeta_\sigma(\frac{p_j^1}{Q_1^\sigma}, \frac{p_j^2}{Q_2^\sigma}, \frac{p_j^3}{Q_3^\sigma})$, where $\zeta_\sigma \in \mathbb{R}$, $p_j^i \in \mathbb{Z}$ for $i = 1,2,3$, $j = 1, \ldots, s_\sigma$ and $Q_1^\sigma, Q_2^\sigma, Q_3^\sigma$ are large distinct primes. Then P^σ is the convex hull of these "corners" and ζ_σ is chosen such that $\operatorname{Vol} P^\sigma = \frac{4\pi}{3}$.

The polyhedron P^σ approximates the unit ball in the sense that any point on the surface ∂P^σ has radial coordinate $1 + O(s_\sigma^{-1})$. The polyhedron P^σ is moreover symmetric under the maps $(k^1, k^2, k^3) \mapsto (\pm k^1, \pm k^2, \pm k^3)$ and "almost symmetric" under the maps $(k^1, k^2, k^3) \mapsto (k^a, k^b, k^c)$ for $(a, b, c) \neq (1, 2, 3)$, see Lemma 3.2.11.

The *Fermi polyhedron* P_F^σ is then defined as $P_F^\sigma := k_F^\sigma P^\sigma \cap \frac{2\pi}{L}\mathbb{Z}^3$.

Moreover, L is chosen large such that $\frac{k_F^\sigma L}{2\pi}$ is rational and large for $\sigma \in \{\uparrow, \downarrow\}$.

Remark 5.2.3. We choose k_F^σ such that $k_F^\uparrow / k_F^\downarrow$ is rational since we need L with $\frac{k_F^\sigma L}{2\pi}$ rational for both values of $\sigma \in \{\uparrow, \downarrow\}$.

Remark 5.2.4. The free parameters are the *Fermi momenta* k_F^σ, the length of the box L and the number of corners of the polyhedra s_σ. The particle numbers are then $N_\sigma = \# P_F^\sigma$ and the particle densities are $\rho_\sigma = N_\sigma / L^3 = \frac{1}{6\pi^2}(k_F^\sigma)^3 \left(1 + O(N_\sigma^{-1/3})\right)$. Not all densities $\rho_{\sigma 0}$ arise this way. We need some argument to consider general densities $\rho_{\sigma 0}$. This is discussed in Section 5.5.4. Essentially by continuity and density of the rationals in the reals we can extend results for the densities arising as $\rho_\sigma = N_\sigma / L^3$ to general densities $\rho_{\sigma 0}$.

We will later choose L, s_σ depending on $a^3\rho$, meaning more precisely on $(k_F^\uparrow + k_F^\downarrow)a$, such that $L, s_\sigma \to \infty$ as $a^3\rho \to 0$. Concretely we will choose $s_\sigma \sim (a^3\rho)^{-1/3+\varepsilon}$ for some small $\varepsilon > 0$.

Next, we recall some properties of the Fermi polyhedron from Chapter 3. For the kinetic energy (density) of the Slater determinants we have by Lemma 3.2.13

$$\frac{1}{L^3} \sum_{k \in P_F^\sigma} |k|^2 = \frac{3}{5}(6\pi^2)^{2/3} \rho_\sigma^{5/3} (1 + O(s_\sigma^{-2}) + O(N_\sigma^{-1/3})). \tag{5.2.8}$$

Here the s_σ-dependent error is only negligible if we take s_σ large enough — we need that the Fermi polyhedron approximates the Fermi ball well in order for the kinetic energies (of the associated Slater determinants) to be close. (Recall that the Slater determinant with momenta in the Fermi ball is the ground state of the non-interacting system.)

Moreover, for $N_\sigma = \# P_F^\sigma$ sufficiently large, the Fermi polyhedron satisfies the following bounds by Lemmas 3.2.12 and 3.4.9 (see also [KL18]).

$$\int_\Lambda \left| \frac{1}{L^3} \sum_{k \in P_F^\sigma} e^{ikx} \right| \mathrm{d}x \leq C s_\sigma (\log N_\sigma)^3 \leq C s (\log N)^3, \tag{5.2.9a}$$

$$\int_\Lambda \left| \frac{1}{L^3} \sum_{k \in P_F^\sigma} k^j e^{ikx} \right| \mathrm{d}x \leq C s_\sigma \rho_\sigma^{1/3} (\log N_\sigma)^3 \leq C s \rho^{1/3} (\log N)^3, \tag{5.2.9b}$$

$$\int_\Lambda \left| \frac{1}{L^3} \sum_{k \in P_F^\sigma} k^j k^{j'} e^{ikx} \right| \mathrm{d}x \leq C s_\sigma \rho_\sigma^{2/3} (\log N_\sigma)^4 \leq C s \rho^{2/3} (\log N)^4, \tag{5.2.9c}$$

for any $j, j' = 1, 2, 3$ where $s = \max\{s_\uparrow, s_\downarrow\}$, $\rho = \rho_\uparrow + \rho_\downarrow$, $N = N_\uparrow + N_\downarrow$ and k^j denotes the j'th component of the vector $k = (k^1, k^2, k^3)$.

The first bound, Equation (5.2.9a), is needed to prove the absolute convergence of the Gaudin–Gillespie–Ripka expansion discussed in Sections 5.3 and 5.4. The second two bounds, Equations (5.2.9b) and (5.2.9c), are needed to bound the terms with $\rho_{\mathsf{Jas}}^{(2,0)}$ and $\rho_{\mathsf{Jas}}^{(0,2)}$ in

Equation (5.2.7). More precisely they are used in the proof of Lemma 5.5.5 below, but only then.

Finally, we recall that the scattering functions satisfy the scattering equations (Euler-Lagrange equations of the defining minimization problems in Definition 5.1.1)

$$-2\Delta f_{s0} + v f_{s0} = 0, \qquad -4x \cdot \nabla f_{p0} - 2|x|^2 \Delta f_{p0} + |x|^2 v f_{p0} = 0. \tag{5.2.10}$$

Moreover

Lemma 5.2.5 ([LY01, Appendix A], see also Lemma 3.2.2)**.** *The functions f_{s0} and f_{p0} are real-valued and radial. Moreover*

$$\left[1 - \frac{a}{|x|}\right]_+ \leq f_{s0}(x) \leq 1, \qquad \left[1 - \frac{a_p^3}{|x|^3}\right]_+ \leq f_{p0}(x) \leq 1.$$

For $|x| \geq R_0$, the range of v, the left-hand-sides are equalities.

5.3 Gaudin–Gillespie–Ripka expansion

In this section we calculate reduced densities of the trial state $\psi_{N_\uparrow,N_\downarrow}$. The ideas behind this calculation are mostly contained in (the formal calculations of) [GGR71]. The calculation we give here is a slight generalization thereof including the spin. Additionally, we give conditions for the final formulas (given in Theorem 5.3.2) to hold, i.e. we give conditions for their absolute convergence. The argument here is in spirit the same as that of Section 3.3. Here it is slightly more involved as we have to take into account the different spins. In Section 3.3 there is only one value of the spin.

In the calculations below one may replace the functions f_s, f_p and the one-particle density matrices $\gamma_{N_\sigma}^{(1)}$ by more general functions. We discuss this in Remark 5.3.5 below.

5.3.1 Calculation of the normalization constant

We first compute the normalization constant $C_{N_\uparrow,N_\downarrow}$. Recall the definition of the trial state $\psi_{N_\uparrow,N_\downarrow}$ in Equation (5.2.5). Write $f_{\mu\nu}^2 = 1 + g_{\mu\nu}$ for all the f-factors and factor out the product $\prod_{\mu<\nu} f_{\mu\nu}^2 = \prod_{\mu<\nu}(1 + g_{\mu\nu})$. We are then led to define the set $\mathcal{G}_{p,q}$ as the set of all graphs on p black and q white vertices such that each vertex has degree at least 1, i.e. has an incident edge. We label the black vertices as $V_p^\uparrow = \{(1,\uparrow), \ldots, (p,\uparrow)\}$ and the white vertices as $V_q^\downarrow = \{(1,\downarrow), \ldots, (q,\downarrow)\}$. For an edge $e = (\mu,\nu)$ we write $g_e = g_{\mu\nu}$ and define

$$W_{p,q} = W_{p,q}(X_p, Y_q) = \sum_{G \in \mathcal{G}_{p,q}} \prod_{e \in G} g_e.$$

Then

$$\begin{aligned}
C_{N_\uparrow,N_\downarrow} &= \int\!\!\cdots\!\!\int \prod_{\mu<\nu}(1+g_{\mu\nu})|D_{N_\uparrow}|^2|D_{N_\downarrow}|^2 \,\mathrm{d}X_{N_\uparrow}\,\mathrm{d}Y_{N_\downarrow} \\
&= \int\!\!\cdots\!\!\int \left[1+\sum_{\substack{0\le p\le N_\uparrow\\ 0\le q\le N_\downarrow\\ p+q\ge 2}} \frac{N_\uparrow(N_\uparrow-1)\cdots(N_\uparrow-p+1)N_\downarrow(N_\downarrow-1)\cdots(N_\downarrow-q+1)}{p!q!}W_{p,q}\right] \\
&\quad\times |D_{N_\uparrow}|^2|D_{N_\downarrow}|^2\,\mathrm{d}X_{N_\uparrow}\,\mathrm{d}Y_{N_\downarrow} \\
&= N_\uparrow!N_\downarrow!\left[1+\sum_{\substack{0\le p\le N_\uparrow\\ 0\le q\le N_\downarrow\\ p+q\ge 2}}\frac{1}{p!q!}\int\!\!\cdots\!\!\int W_{p,q}\rho^{(p,q)}\,\mathrm{d}X_p\,\mathrm{d}Y_q\right].
\end{aligned}$$

(Recall the definition of $\rho^{(p,q)}$ in Equation (5.2.4).) A simple calculation using the Wick rule then shows (recall the definition of $\gamma_{\mu\nu}$ in Equation (5.2.3))

$$\rho^{(p,q)}(X_p,Y_q) = \det\left[\gamma_{\mu\nu}\right]_{\mu,\nu\in V_{p,q}} = \det[\gamma^{(1)}_{N_\uparrow}(x_i;y_j)]_{1\le i,j\le p}\det[\gamma^{(1)}_{N_\downarrow}(y_i;y_j)]_{1\le i,j\le q}$$

Taking this determinantal expression as the definition we have $\rho^{(p,q)}=0$ for $p>N_\uparrow$ or $q>N_\downarrow$ since the matrices $[\gamma_{(i,\uparrow),(j,\uparrow)}]_{i,j\in\mathbb{N}}$ and $[\gamma_{(i,\downarrow),(j,\downarrow)}]_{i,j\in\mathbb{N}}$ have ranks $N_\uparrow$ and $N_\downarrow$ respectively. Thus we may extend the p- and q-sums to ∞. Now, expanding the determinant $\rho^{(p,q)}$ and the $W_{p,q}$ we group the permutations and the graph together in a diagram. We will for the calculation of the reduced densities need a slightly more general definition, which we now give.

Definition 5.3.1. The set $\mathcal{G}^{n,m}_{p,q}$ is the set of all graphs with p *internal* black vertices, n *external* black vertices, q *internal* white vertices and m *external* white vertices, such that there are no edges between *external* vertices, and such that all *internal* vertices has degree at least 1. That is, all *internal* vertices are incident to at least one edge and *external* vertices may have degree 0. As above we label the black vertices as $V^\uparrow_{p+n}=\{(1,\uparrow),\ldots,(p+n,\uparrow)\}$ where the first n are the *external* vertices. The white vertices are labelled $V^\downarrow_{q+m}=\{(1,\downarrow),\ldots,(q+m,\downarrow)\}$, where the first m are the *external* vertices. In case $n=m=0$ we recover $\mathcal{G}^{0,0}_{p,q}=\mathcal{G}_{p,q}$.

If we need the vertices to have certain labels we will write $\mathcal{G}^{B^*,W^*}_{B,W}$ (or similar with only some of p,q,n,m replaced by sets) for the set of all graphs with *internal* black vertices B, *external* black vertices B^*, *internal* white vertices W and *external* white vertices W^*, where $B,B^*\subset V^\uparrow_\infty$ and $W,W^*\subset V^\downarrow_\infty$ are all pairwise disjoint.

The set $\mathcal{D}^{n,m}_{p,q}$ is the set of all *diagrams* on p *internal* black vertices, n *external* black vertices, q *internal* white vertices and m *external* white vertices. Such a diagram is a tuple $D=(\pi,\tau,G)$ where $\pi\in\mathcal{S}_{p+n}$, $\tau\in\mathcal{S}_{q+m}$ (viewed as directed graphs on the black and white vertices respectively) and $G\in\mathcal{G}^{n,m}_{p,q}$.

We will refer to the edges in G as g-edges and the graph G as a g-graph. Moreover, we refer to the edges in both π and τ as γ-edges.

The value of the diagram $D=(\pi,\tau,G)\in\mathcal{D}^{n,m}_{p,q}$ is the function

$$\begin{aligned}
&\Gamma^{n,m}_D(X_n,Y_m) \\
&\quad= (-1)^\pi(-1)^\tau\int\!\!\cdots\!\!\int\prod_{e\in G}g_e\prod_{i=1}^{p+n}\gamma^{(1)}_{N_\uparrow}(x_i;x_{\pi(i)})\prod_{j=1}^{q+m}\gamma^{(1)}_{N_\downarrow}(y_j;y_{\tau(j)})\,\mathrm{d}X_{[n+1,n+p]}\,\mathrm{d}Y_{[m+1,m+q]}.
\end{aligned}$$

If $p = 0$ and/or $q = 0$ there are no integrations in the x_i and/or y_j variables.

A diagram $D = (\pi, \tau, G)$ is said to be *linked* if the graph $\tilde{G}$ with union all edges of π, τ and G is connected. The set of linked diagrams is denoted $\mathcal{L}_{p,q}^{n,m}$.

In case $m = n = 0$ we write $\mathcal{D}_{p,q}^{0,0} = \mathcal{D}_{p,q}, \mathcal{L}_{p,q}^{0,0} = \mathcal{L}_{p,q}$ and $\Gamma_D^{0,0} = \Gamma_D$ (i.e. without a superscript).

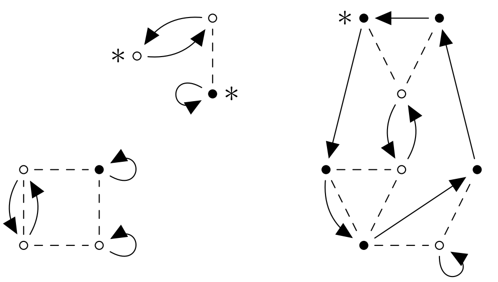


Figure 5.3.1: Example of a diagram (π, τ, G) with 3 linked components. Vertices denoted by $\bullet$ are the black vertices, i.e. of spin $\uparrow$, and vertices denoted by $\circ$ are the white vertices, i.e. of spin $\downarrow$. Moreover, vertices with label $*$ are *external*, dashed lines denote g-edges and arrows $(\mu, \nu) = ((i, \sigma), (j, \sigma'))$ denote γ-edges, i.e. that $\pi(i) = j$ if $\sigma = \sigma' = \uparrow$ or $\tau(i) = j$ if $\sigma = \sigma' = \downarrow$. Note that there are no γ-edges between vertices of different colours (i.e. with different spin).

In terms of diagrams we have

$$C_{N_\uparrow, N_\downarrow} = N_\uparrow! N_\downarrow! \left[1 + \sum_{\substack{p,q \geq 0 \\ p+q \geq 2}} \frac{1}{p!q!} \sum_{D \in \mathcal{D}_{p,q}} \Gamma_D \right]. \tag{5.3.1}$$

We may decompose any diagram $D = (\pi, \tau, G)$ into its linked components. For this, note that its value Γ_D factors over its linked components. Moreover, each linked component has at least 2 vertices, since they have degree at least one. Thus,

$$\begin{aligned} &\frac{1}{p!q!} \sum_{D \in \mathcal{D}_{p,q}} \Gamma_D \\ &= \underbrace{\sum_{k=1}^{\infty}}_{\#\text{ lnk. cps.}} \frac{1}{k!} \underbrace{\sum_{\substack{p_1,q_1 \geq 0 \\ p_1+q_1 \geq 2}} \cdots \sum_{\substack{p_k,q_k \geq 0 \\ p_k+q_k \geq 2}}}_{\text{sizes linked components}} \chi_{(\sum p_\ell = p)} \chi_{(\sum q_\ell = q)} \underbrace{\sum_{D_1 \in \mathcal{L}_{p_1,q_1}} \cdots \sum_{D_k \in \mathcal{L}_{p_k,q_k}}}_{\text{linked components}} \frac{\Gamma_{D_1}}{p_1!q_1!} \cdots \frac{\Gamma_{D_k}}{p_k!q_k!}. \end{aligned}$$

Here the factor $\frac{1}{k!}$ comes from counting the possible ways to label the k linked components and the factors $\frac{1}{p_\ell! q_\ell!}$ come from counting the possible ways of labelling the vertices in the different linked components (and using the factor $\frac{1}{p!q!}$ already present). If we assume that the sum $\sum_{p,q:p+q\geq 2} \frac{1}{p!q!} \sum_{D \in \mathcal{L}_{p,q}} \Gamma_D$ is absolutely convergent, (more precisely we assume that $\sum_{p,q:p+q\geq 2} \frac{1}{p!q!} \left| \sum_{D \in \mathcal{L}_{p,q}} \Gamma_D \right| < \infty$,) then we may interchange the p,q-sum with the p_ℓ, q_ℓ-sums. The absolute convergence is proven in Theorem 5.3.2 below. Thus, under the conditions of

Theorem 5.3.2, we have

$$\begin{aligned}
C_{N_\uparrow,N_\downarrow} &= N_\uparrow! N_\downarrow! \left[1 + \sum_{k=1}^{\infty} \frac{1}{k!} \sum_{\substack{p_1,q_1\geq 0\\ p_1+q_1\geq 2}} \cdots \sum_{\substack{p_k,q_k\geq 0\\ p_k+q_k\geq 2}} \sum_{D_1\in\mathcal{L}_{p_1,q_1}} \cdots \sum_{D_k\in\mathcal{L}_{p_k,q_k}} \frac{\Gamma_{D_1}}{p_1!q_1!} \cdots \frac{\Gamma_{D_k}}{p_k!q_k!}\right] \\
&= N_\uparrow! N_\downarrow! \left[1 + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\sum_{\substack{p,q\geq 0\\ p+q\geq 2}} \frac{1}{p!q!} \sum_{D\in\mathcal{L}_{p,q}} \Gamma_D\right)^k\right] \\
&= N_\uparrow! N_\downarrow! \exp\left[\sum_{\substack{p,q\geq 0\\ p+q\geq 2}} \frac{1}{p!q!} \sum_{D\in\mathcal{L}_{p,q}} \Gamma_D\right].
\end{aligned} \tag{5.3.2}$$

5.3.2 Calculation of the reduced densities

For the calculation of the reduced densities we need to keep track of also the external vertices. First, we have the formula (for $n+m\geq 1$)

$$\begin{aligned}
\rho^{(n,m)}_{\mathsf{Jas}} &= N_\uparrow(N_\uparrow-1)\cdots(N_\uparrow-n+1)N_\downarrow(N_\downarrow-1)\cdots(N_\downarrow-m+1) \\
&\quad\times \int\!\!\cdots\!\!\int |\psi_{N_\uparrow,N_\downarrow}(X_{N_\uparrow},Y_{N_\downarrow})|^2 \,\mathrm{d}X_{[n+1,N_\uparrow]}\,\mathrm{d}Y_{[m+1,N_\downarrow]} \\
&= \frac{N_\uparrow(N_\uparrow-1)\cdots(N_\uparrow-n+1)N_\downarrow(N_\downarrow-1)\cdots(N_\downarrow-m+1)}{C_{N_\uparrow,N_\downarrow}} \prod_{\substack{\mu<\nu\\ \mu,\nu\in V_{n,m}}} f_{\mu\nu}^2 \\
&\quad\times \int\!\!\cdots\!\!\int \prod_{\mu\in V_{n,m},\nu\notin V_{n,m}} (1+g_{\mu\nu}) \prod_{\substack{\mu<\nu\\ \mu,\nu\notin V_{n,m}}} (1+g_{\mu\nu}) \\
&\quad\quad\times D_{N_\uparrow}(X_{N_\uparrow})D_{N_\downarrow}(Y_{N_\downarrow})\,\mathrm{d}X_{[n+1,N_\uparrow]}\,\mathrm{d}Y_{[m+1,N_\downarrow]} \\
&= \frac{N_\uparrow!N_\downarrow!}{C_{N_\uparrow,N_\downarrow}} \prod_{\substack{\mu<\nu\\ \mu,\nu\in V_{n,m}}} f_{\mu\nu}^2 \left[\sum_{p,q\geq 0} \frac{1}{p!q!} \int\!\!\cdots\!\!\int \rho^{(n+p,m+q)} \sum_{G\in\mathcal{G}^{n,m}_{p,q}} \prod_{e\in G} g_e \,\mathrm{d}X_{[n+1,n+p]}\,\mathrm{d}Y_{[m+1,m+q]}\right] \\
&= \frac{N_\uparrow!N_\downarrow!}{C_{N_\uparrow,N_\downarrow}} \prod_{\substack{\mu<\nu\\ \mu,\nu\in V_{n,m}}} f_{\mu\nu}^2 \left[\rho^{(n,m)} + \sum_{\substack{p,q\geq 0\\ p+q\geq 1}} \frac{1}{p!q!} \sum_{D\in\mathcal{D}^{n,m}_{p,q}} \Gamma^{n,m}_D\right]
\end{aligned} \tag{5.3.3}$$

where we extended the p,q-sums to ∞ as in Section 5.3.1 above and used that the $p=q=0$ term gives

$$\sum_{D\in\mathcal{D}^{n,m}_{0,0}} \Gamma^{n,m}_D = \rho^{(n,m)}.$$

Note here that the p,q-sum does not require $p+q\geq 2$, since the internal vertices may connect to external ones. As for the normalization constant in Section 5.3.1 we decompose each diagram D into its linked components. Here we have to keep track of which linked components contain which external vertices. To do this we introduce the set

$$\Pi^{n,m}_\kappa := \left\{ (\mathcal{B}^*,\mathcal{W}^*) : \begin{array}{c} \mathcal{B}^* = (B^*_1,\ldots,B^*_\kappa) \text{ partition of } \{1,\ldots,n\}, \\ \mathcal{W}^* = (W^*_1,\ldots,W^*_\kappa) \text{ partition of } \{1,\ldots,m\}, \\ \text{For all } \lambda : B^*_\lambda \neq \varnothing \text{ and/or } W^*_\lambda \neq \varnothing. \end{array} \right\}. \tag{5.3.4}$$

The set $\Pi_\kappa^{n,m}$ parametrizes all possible ways for the diagram $D \in \mathcal{D}_{p,q}^{n,m}$ to have exactly κ many linked components containing at least 1 external vertex each. Note that for $\kappa > n+m$ we have $\Pi_\kappa^{n,m} = \varnothing$, since we require that for all λ we have $B_\lambda^* \neq \varnothing$ or $W_\lambda^* \neq \varnothing$. Denoting then k the number of linked components with only internal vertices we get the following.

$$
\begin{aligned}
&\frac{1}{p!q!}\sum_{D\in\mathcal{D}_{p,q}^{n,m}} \Gamma_D^{n,m} \\
&= \sum_{k=0}^{\infty}\frac{1}{k!}\sum_{\kappa=1}^{n+m}\frac{1}{\kappa!}\sum_{(\mathcal{B}^*,\mathcal{W}^*)\in\Pi_\kappa^{n,m}}\sum_{p_1^*,q_1^*\geq 0}\cdots\sum_{p_\kappa^*,q_\kappa^*\geq 0}\sum_{\substack{p_1,q_1\geq 0\\ p_1+q_1\geq 2}}\cdots\sum_{\substack{p_k,q_k\geq 0\\ p_k+q_k\geq 2}} \\
&\quad\times \chi_{(\sum_\lambda p_\lambda^*+\sum_\ell p_\ell = p)}\chi_{(\sum_\lambda q_\lambda^*+\sum_\ell q_\ell = q)} \\
&\quad\times \sum_{D_1^*\in\mathcal{L}_{p_1^*,q_1^*}^{\#B_1^*,\#W_1^*}}\cdots\sum_{D_\kappa^*\in\mathcal{L}_{p_\kappa^*,q_\kappa^*}^{\#B_\kappa^*,\#W_\kappa^*}}\frac{\Gamma_{D_1^*}^{\#B_1^*,\#W_1^*}(X_{B_1^*},Y_{W_1^*})}{p_1^*!q_1^*!}\cdots\frac{\Gamma_{D_\kappa^*}^{\#B_\kappa^*,\#W_\kappa^*}(X_{B_\kappa^*},Y_{W_\kappa^*})}{p_\kappa^*!q_\kappa^*!} \\
&\quad\times \sum_{D_1\in\mathcal{L}_{p_1,q_1}}\cdots\sum_{D_k\in\mathcal{L}_{p_k,q_k}}\frac{\Gamma_{D_1}}{p_1!q_1!}\cdots\frac{\Gamma_{D_k}}{p_k!q_k!}.
\end{aligned}
\tag{5.3.5}
$$

(Note that the linked components with external vertices may have 0 or 1 internal vertices, i.e. the p_λ^*, q_λ^*-sums do not require $p_\lambda^* + q_\lambda^* \geq 2$.) The factorial factors come from counting the different labellings: The factors $\frac{1}{k!}$ and $\frac{1}{\kappa!}$ from the labellings of the clusters and the factors $\frac{1}{p_\lambda^*!}, \frac{1}{q_\lambda^*!}, \frac{1}{p_\ell!}, \frac{1}{q_\ell!}$ from labelling the internal vertices of the different clusters exactly as in Section 5.3.1 above.

If we assume absolute convergence of all the $\Gamma^{n',m'}$-sums with $n' \leq n$ and $m' \leq m$ (i.e. that $\sum_{p,q\geq 0}\frac{1}{p!q!}\left|\sum_{D\in\mathcal{L}_{p,q}^{n',m'}}\Gamma_D^{n',m'}\right| < \infty$) then we may interchange the p,q-sum with the p_λ^*, q_λ^*- and p_ℓ, q_ℓ-sums. We then get

$$
\begin{aligned}
&\sum_{p,q\geq 0}\frac{1}{p!q!}\sum_{D\in\mathcal{D}_{p,q}^{n,m}}\Gamma_D^{n,m} \\
&\quad= \sum_{k=0}^{\infty}\frac{1}{k!}\left(\sum_{\substack{p,q\geq 0\\ p+q\geq 2}}\frac{1}{p!q!}\sum_{D\in\mathcal{L}_{p,q}}\Gamma_D\right)^k \\
&\qquad\times\sum_{\kappa=1}^{n+m}\frac{1}{\kappa!}\sum_{(\mathcal{B}^*,\mathcal{W}^*)\in\Pi_\kappa^{n,m}}\prod_{\lambda=1}^{\kappa}\left[\sum_{p_\lambda,q_\lambda\geq 0}\frac{1}{p_\lambda!q_\lambda!}\sum_{D_\lambda\in\mathcal{L}_{p_\lambda,q_\lambda}^{\#B_\lambda^*,\#W_\lambda^*}}\Gamma_{D_\lambda}^{\#B_\lambda^*,\#W_\lambda^*}(X_{B_\lambda^*},Y_{W_\lambda^*})\right].
\end{aligned}
\tag{5.3.6}
$$

Thus by Equations (5.3.2) and (5.3.3) we conclude the formula

$$
\begin{aligned}
&\rho_{\mathsf{Jas}}^{(n,m)}(X_n,Y_m) \\
&= \left[\prod_{\substack{\mu,\nu\in V_{n,m}\\ \mu<\nu}} f_{\mu\nu}^2\right]\sum_{\kappa=1}^{n+m}\frac{1}{\kappa!}\sum_{(\mathcal{B}^*,\mathcal{W}^*)\in\Pi_\kappa^{n,m}}\prod_{\lambda=1}^{\kappa}\left[\sum_{p_\lambda,q_\lambda\geq 0}\frac{1}{p_\lambda!q_\lambda!}\sum_{D_\lambda\in\mathcal{L}_{p_\lambda,q_\lambda}^{\#B_\lambda^*,\#W_\lambda^*}}\Gamma_{D_\lambda}^{\#B_\lambda^*,\#W_\lambda^*}(X_{B_\lambda^*},Y_{W_\lambda^*})\right]
\end{aligned}
$$

under the assumption of absolute convergence.

5.3.3 Summary of results

With the calculation above we may then state the following theorem.

Theorem 5.3.2. *For integers $n_0, m_0 \geq 0$ there exist constants $c_{n_0,m_0}, C_{n_0,m_0} > 0$ (small and large respectively) such that if $sab^2\rho(\log N)^3 < c_{n_0,m_0}$ then*

$$\sum_{\substack{p,q\geq 0\\ p+q\geq 2}} \frac{1}{p!q!}\left|\sum_{D\in\mathcal{L}_{p,q}} \Gamma_D\right| < \infty, \qquad \sum_{p,q\geq 0} \frac{1}{p!q!}\left|\sum_{D\in\mathcal{L}_{p,q}^{n,m}} \Gamma_D^{n,m}\right| \leq C_{n_0,m_0}\rho^{n+m} < \infty \tag{5.3.7}$$

for any $n \leq n_0$ and $m \leq m_0$ with $n+m\geq 1$. In particular, then

$$\begin{aligned}&\rho_{\mathsf{Jas}}^{(n,m)}(X_n, Y_m)\\ &= \left[\prod_{\substack{\mu,\nu\in V_{n,m}\\ \mu<\nu}} f_{\mu\nu}^2\right] \sum_{\kappa=1}^{n+m} \frac{1}{\kappa!} \sum_{(\mathcal{B}^*,\mathcal{W}^*)\in\Pi_\kappa^{n,m}} \prod_{\lambda=1}^{\kappa} \left[\sum_{p_\lambda,q_\lambda\geq 0} \frac{1}{p_\lambda! q_\lambda!} \sum_{D_\lambda\in\mathcal{L}_{p_\lambda,q_\lambda}^{\#B_\lambda^*,\#W_\lambda^*}} \Gamma_{D_\lambda}^{\#B_\lambda^*,\#W_\lambda^*}(X_{B_\lambda^*}, Y_{W_\lambda^*})\right],\end{aligned} \tag{5.3.8}$$

where $\Pi_\kappa^{n,m}$ is defined in Equation (5.3.4).

As particular cases we note that for $n+m=1$ we have by translation invariance that

$$\rho_\uparrow = \rho_{\mathsf{Jas}}^{(1,0)} = \sum_{p,q\geq 0} \frac{1}{p!q!} \sum_{D\in\mathcal{L}_{p,q}^{1,0}} \Gamma_D^{1,0}, \qquad \rho_\downarrow = \rho_{\mathsf{Jas}}^{(0,1)} = \sum_{p,q\geq 0} \frac{1}{p!q!} \sum_{D\in\mathcal{L}_{p,q}^{0,1}} \Gamma_D^{0,1}. \tag{5.3.9}$$

We give the proof of Theorem 5.3.2 below.

Remark 5.3.3 (Higher spin)**.** One may readily generalize the computation above to a general number of spins S. For this one introduces vertices of more colours and diagrams with such, i.e. the sets of graphs and diagrams $\mathcal{G}_{p_1,\ldots,p_S}^{n_1,\ldots,n_S}, \mathcal{D}_{p_1,\ldots,p_S}^{n_1,\ldots,n_S}, \mathcal{L}_{p_1,\ldots,p_S}^{n_1,\ldots,n_S}$ and the values $\Gamma_D^{n_1,\ldots,n_S}$. The condition of absolute convergence is completely analogous.

Remark 5.3.4. The condition for the absolute convergence is not uniform in the volume, hence the need for a box method as given in Section 5.5.4. The condition of absolute convergence is additionally the reason for introducing the Fermi polyhedron. This is discussed in Remark 3.3.5. If one did not introduce the Fermi polyhedron and instead used the Fermi ball the factor $s(\log N)^3$ in the assumption of Theorem 5.3.2 should be replaced by $N^{1/3}$.

Remark 5.3.5 (General f and γ)**.** In the computation above we may replace the specific functions f_s, f_p by more general functions $f_{\sigma\sigma'} = f_{\sigma'\sigma} \geq 0$. (One then introduces $g_e = f_{\sigma\sigma'}^2(z_i - z_j) - 1$ for $e = ((i,\sigma),(j,\sigma'))$.)

Moreover, for the absolute convergence we may additionally replace the one-particle densities $\gamma_{N_\sigma}^{(1)}$ by general functions $\gamma_\sigma(z_i - z_j)$. (One then defines $\gamma_{\mu\nu}$ as in Equation (5.2.3) above.) In the computation above we crucially used that $[\det \gamma_{\mu\nu}]_{\mu,\nu\in V_{p,q}} = 0$ for appropriately large p,q in order to extend the p,q-sums to ∞. If for the general γ_σ this is not valid, this step of the computation above is not valid. The rest of the calculation starting from what one gets out of this step is however still valid. That is, the calculation in Section 5.3.1 is valid starting from Equation (5.3.1) and the calculations in Equations (5.3.5) and (5.3.6) in Section 5.3.2 are valid.

The statement of the absolute convergence in this more general setting reads

Lemma 5.3.6. *Suppose there exists a constant $C_{\mathsf{TG}} \geq 1$ such that*

$$\sup_{\sigma,\sigma'} \sup_{z_1,\ldots,z_q} \prod_{1\leq i<j\leq q} f_{\sigma\sigma'}(z_i - z_j)^2 \leq (C_{\mathsf{TG}})^q \qquad \text{for any } q \in \mathbb{N}. \tag{5.3.10}$$

Then for integers $n_{1,0},\ldots,n_{S,0}$ there exists constants $c_{n_{1,0},\ldots,n_{S,0}}, C_{n_{1,0},\ldots,n_{S,0}} > 0$ such that if

$$\sup_\sigma \sum_{k\in\frac{2\pi}{L}\mathbb{Z}^3} |\hat{\gamma}_\sigma(k)| \times \sup_{\sigma,\sigma'} \int_\Lambda \left| f_{\sigma\sigma'}^2 - 1 \right| \times \left[1 + \sup_\sigma \int_\Lambda |\gamma_\sigma| \right] < c_{n_{1,0},\ldots,n_{S,0}}, \tag{5.3.11}$$

where $\hat{\gamma}_\sigma(k) = \frac{1}{L^3}\int_\Lambda \gamma_\sigma(x) e^{-ikx}\,\mathrm{d}x$ denotes the Fourier transform, then

$$\sum_{\substack{p_1,\ldots,p_S\geq 0\\ \sum_\sigma p_\sigma \geq 2}} \frac{1}{p_1!\cdots p_S!} \left| \sum_{D\in\mathcal{L}_{p_1,\ldots,p_S}} \Gamma_D \right| < \infty,$$

$$\sum_{p_1,\ldots,p_S\geq 0} \frac{1}{p_1!\cdots p_S!} \left| \sum_{D\in\mathcal{L}_{p_1,\ldots,p_S}^{n_1,\ldots,n_S}} \Gamma_D^{n_1,\ldots,n_S} \right| \leq C_{n_{1,0},\ldots,n_{S,0}} \left[\sup_\sigma \sum_{k\in\frac{2\pi}{L}\mathbb{Z}^3} |\hat{\gamma}_\sigma(k)| \right]^{\sum_\sigma n_\sigma} < \infty \tag{5.3.12}$$

for all $n_\sigma \leq n_{\sigma,0}$ with $\sum_\sigma n_\sigma \geq 1$. In particular then

$$\mathcal{Z} := 1 + \sum_{\substack{p_1,\ldots,p_S\geq 0\\ \sum_\sigma p_\sigma \geq 2}} \frac{1}{p_1!\cdots p_S!} \sum_{D\in\mathcal{D}_{p_1,\ldots,p_S}} \Gamma_D = \exp\left[\sum_{\substack{p_1,\ldots,p_S\geq 0\\ \sum_\sigma p_\sigma \geq 2}} \frac{1}{p_1!\cdots p_S!} \sum_{D\in\mathcal{L}_{p_1,\ldots,p_S}} \Gamma_D \right]$$

and

$$\begin{aligned}
&\frac{1}{\mathcal{Z}} \sum_{p_1,\ldots,p_S\geq 0} \frac{1}{\prod_\sigma p_\sigma!} \sum_{D\in\mathcal{D}_{p_1,\ldots,p_S}^{n_1,\ldots,n_S}} \Gamma_D^{n_1,\ldots,n_S}((X_{n_\sigma}^\sigma)_{\sigma=1,\ldots,S}) \\
&\quad = \sum_{\kappa=1}^{\sum_\sigma n_\sigma} \frac{1}{\kappa!} \sum_{(\mathcal{V}^{*1},\ldots,\mathcal{V}^{*S})\in\Pi_\kappa^{n_1,\ldots,n_S}} \\
&\qquad \times \prod_{\lambda=1}^{\kappa} \left[\sum_{p_\lambda^1,\ldots,p_\lambda^S\geq 0} \frac{1}{\prod_\sigma p_\lambda^\sigma!} \sum_{D_\lambda\in\mathcal{L}_{p_\lambda^1,\ldots,p_\lambda^S}^{\#V_\lambda^{*1},\ldots,\#V_\lambda^{*S}}} \Gamma_{D_\lambda}^{\#V_\lambda^{*1},\ldots,\#V_\lambda^{*S}}((X_{V_\lambda^{*\sigma}}^\sigma)_{\sigma=1,\ldots,S}) \right],
\end{aligned}$$

where

$$\Pi_\kappa^{n_1,\ldots,n_S} := \left\{ (\mathcal{V}^{*1},\ldots,\mathcal{V}^{*S}) : \begin{array}{c} \mathcal{V}^{*\sigma} = (V_1^{*\sigma},\ldots,V_\kappa^{*\sigma}) \text{ partition of } \{1,\ldots,n_\sigma\} \\ \text{For all } \lambda : V_\lambda^{*\sigma} \neq \varnothing \text{ for some } \sigma \end{array} \right\}$$

parametrizes the ways for the external vertices to lie in κ different linked components, the coordinates of each spin σ are labelled $x_j^\sigma, j \in \mathbb{N}$, and we denote by $X_A^\sigma = (x_j^\sigma)_{j\in A}$ the coordinates with labels in the set A.

The condition in Equation (5.3.10) is the "stability condition" of the tree-graph bound [PU09, Proposition 6.1; Uel18].

We give the proof of Lemma 5.3.6 in Section 5.4 below for the case $S = 2$. The proof for general S is a straightforward modification, but notationally more cumbersome. The case $S = 1$ is treated in Section 3.3.1. Theorem 5.3.2 is an immediate corollary.

Proof of Theorem 5.3.2. Note that $f_s, f_p \leq 1$ and $\hat{\gamma}_{N_\sigma}(k) := L^{-3} \int_\Lambda \gamma_{N_\sigma}^{(1)}(x;0) e^{-ikx} \,\mathrm{d}x = L^{-3}\chi_{(k\in P_F^\sigma)}$ so $\sum_{k\in\frac{2\pi}{L}\mathbb{Z}^3} \left|\hat{\gamma}_{N_\sigma}(k)\right| = \rho_\sigma \leq \rho$. Moreover, we have the bounds

$$\int |g_s| \leq Cab^2, \qquad \int |g_p| \leq Ca_p^3 \log(b/a_p) \leq Cab^2, \tag{5.3.13}$$

which follow by a simple computation using Lemma 5.2.5. Recalling also Equation (5.2.9) then Lemma 5.3.6 proves the desired. ☐

5.4 Absolute convergence of the Gaudin–Gillespie–Ripka expansion

In this section we give the proof of Lemma 5.3.6 for the case $S = 2$. The proof is similar to that of Theorem 3.3.4. We need to prove (for all n, m and uniformly in X_n, Y_m) Equation (5.3.12) if Equations (5.3.10) and (5.3.11) are satisfied. To simplify notation we define

$$\gamma_\infty := \sup_\sigma \sum_{k\in\frac{2\pi}{L}\mathbb{Z}^3} |\hat{\gamma}_\sigma(k)|, \qquad I_g := \sup_{\sigma,\sigma'} \int_\Lambda \left|f_{\sigma\sigma'}^2 - 1\right| = \sup_e \int_\Lambda |g_e|, \qquad I_\gamma := \sup_\sigma \int_\Lambda |\gamma_\sigma|,$$

where as above $\hat{\gamma}_\sigma(k) = L^{-3}\int_\Lambda \gamma_\sigma(x) e^{-ikx}\,\mathrm{d}x$. Equation (5.3.11) then reads that $\gamma_\infty I_g(1+I_\gamma)$ is sufficiently small.

We give the proof in two steps. First we consider the case $n = m = 0$.

5.4.1 Absolute convergence of the Γ-sum

In this section we show that

$$\sum_{\substack{p,q\geq 0\\ p+q\geq 2}} \frac{1}{p!q!} \left| \sum_{D\in\mathcal{L}_{p,q}} \Gamma_D \right| < \infty$$

under the relevant conditions. Defining clusters as connected components of G we split the sum into clusters as in Section 3.3.1. Denoting the sizes of the clusters by (n_ℓ, m_ℓ), $\ell = 1,\ldots,k$ (meaning that the cluster ℓ has n_ℓ black vertices and m_ℓ white vertices) we get

$$\begin{aligned}
&\frac{1}{p!q!}\sum_{D\in\mathcal{L}_{p,q}} \Gamma_D \\
&\quad = \sum_{k=1}^\infty \frac{1}{k!} \sum_{\substack{n_1,\ldots,n_k\geq 0\\ m_1,\ldots,m_k\geq 0\\ \text{For each } \ell:\ n_\ell+m_\ell\geq 2}} \chi_{(\sum_\ell n_\ell = p)}\chi_{(\sum_\ell m_\ell = q)} \frac{1}{\prod_{\ell=1}^k n_\ell! m_\ell!} \\
&\qquad \times \sum_{G_\ell\in\mathcal{C}_{n_\ell,m_\ell}} \int\!\!\cdots\!\!\int \mathrm{d}X_p\,\mathrm{d}Y_q \left[\prod_{\ell=1}^k \prod_{e\in G_\ell} g_e\right] \\
&\qquad \times \left[\sum_{\substack{\pi\in\mathcal{S}_p\\ \tau\in\mathcal{S}_q}} (-1)^\pi(-1)^\tau \chi_{((\pi,\tau,\cup_\ell G_\ell)\text{ linked})} \prod_{i=1}^p \gamma_\uparrow(x_i - x_{\pi(i)}) \prod_{j=1}^q \gamma_\downarrow(y_j - y_{\tau(j)})\right],
\end{aligned} \tag{5.4.1}$$

where $\mathcal{C}_{p,q} \subset \mathcal{G}_{p,q}$ denotes the subset of connected graphs. The factorial factors arise from counting the possible labellings exactly as in Section 5.3.

The last line of Equation (5.4.1) is what we will call the *truncated correlation*. We give a slightly more general definition for later use.

Definition 5.4.1. Let $B_1, \ldots, B_k$ and $W_1, \ldots, W_k$ be sets of distinct black and white vertices respectively, such that for each $\ell = 1, \ldots, k$ we have $B_\ell \neq \varnothing$ and/or $W_\ell \neq \varnothing$. Then the *truncated correlation*[1] is defined as follows.

$$\rho_t^{((B_1,W_1),\ldots,(B_k,W_k))} = \sum_{\substack{\pi \in \mathcal{S}_{\cup_\ell B_\ell} \\ \tau \in \mathcal{S}_{\cup_\ell W_\ell}}} (-1)^\pi (-1)^\tau \chi_{((\pi,\tau,\cup_\ell G_\ell) \text{ linked})} \prod_{i \in \cup_\ell B_\ell} \gamma_\uparrow(x_i - x_{\pi(i)}) \prod_{j \in \cup_\ell W_\ell} \gamma_\downarrow(y_j - y_{\tau(j)}) \tag{5.4.2}$$

for any connected graphs $G_\ell \in \mathcal{C}_{B_\ell, W_\ell}$. The definition does not depend on the choice of the graphs G_ℓ.

If the underlying sets $B_1, \ldots, B_k, W_1, \ldots, W_k$ are clear we will also use the notation

$$\rho_t^{((\#B_1,\#W_1),\ldots,(\#B_k,\#W_k))} = \rho_t^{((B_1,W_1),\ldots,(B_k,W_k))}.$$

The truncated correlations are studied in [GMR21, Appendix D]. To better compare to the definition in [GMR21] we note the following.

In Equation (5.4.2) we may view (π, τ) together as a permutation of all the vertices (both black and white). Moreover, if we instead sum over all permutations $\pi' \in \mathcal{S}_{\cup_\ell B_\ell \cup \cup_\ell W_\ell}$ we have that any π' not coming from two permutations π, τ on the black (respectively white) vertices contributes 0, since any γ-factor between vertices of different spins is 0. That is,

$$\rho_t^{((B_1,W_1),\ldots,(B_k,W_k))} = \sum_{\pi' \in \mathcal{S}_{\cup_\ell B_\ell \cup \cup_\ell W_\ell}} (-1)^\pi \chi_{(\pi',\cup G_\ell) \text{ linked})} \prod_{\mu \in \cup B_\ell \cup \cup W_\ell} \gamma_{\mu,\pi'(\mu)}.$$

In [GMR21, Equation (D.53)] is shown the formula for the truncated correlation

$$\rho_t^{((B_1,W_1),\ldots,(B_k,W_k))} = \sum_{A \in \mathcal{A}^{((B_1,W_1),\ldots,(B_k,W_k))}} \prod_{(\mu,\nu) \in A} \gamma_{\mu\nu} \int \mathrm{d}\mu_A(r) \det \mathcal{R}(r), \tag{5.4.3}$$

where $\mathcal{A}$ denotes the set of anchored trees, μ_A is a probability measure and $\mathcal{R}(r)$ is an explicit matrix. The set $\mathcal{A}^{((B_1,W_1),\ldots,(B_k,W_k))}$ of anchored trees is the set of all directed graphs on the vertices $\cup_\ell B_\ell \cup \cup_\ell W_\ell$ such that each vertex has at most one incoming and at most one outgoing edge, and such that upon identifying all vertices inside each cluster the resulting graph is a (directed) tree. The matrix $\mathcal{R}(r)$ satisfies the bound

$$|\det \mathcal{R}(r)| \leq \gamma_\infty^{\sum_\ell (\#B_\ell + \#W_\ell) - (k-1)}. \tag{5.4.4}$$

This follows from [GMR21, Equation (D.57)]. We give a sketch of the argument here, see also [GMR21, Lemma D.2] and Lemma 3.3.10.

[1] The truncated correlation is also sometimes referred to as the *connected correlation*. In particular, this is the terminology used in [GMR21].

Proof (sketch) of Equation (5.4.4). Write $\gamma_\sigma(z_\mu - z_\nu) = \langle \alpha_\mu | \beta_\nu \rangle_{\ell^2(\frac{2\pi}{L}\mathbb{Z}^3)}$, where for $k \in \frac{2\pi}{L}\mathbb{Z}^3$

$$\alpha_\mu(k) = e^{-ikz_\mu} \left|\hat{\gamma}_\sigma(k)\right|^{1/2} \frac{\hat{\gamma}_\sigma(k)}{\left|\hat{\gamma}_\sigma(k)\right|}, \qquad \beta_\nu(k) = e^{-ikz_\nu} \left|\hat{\gamma}_\sigma(k)\right|^{1/2},$$

with $\hat{\gamma}_\sigma(k) = L^{-3} \int_\Lambda \gamma_\sigma(x) e^{-ikx} \, \mathrm{d}x$ the Fourier coefficients. Then by the Gram-Hadamard inequality [GMR21, Lemma D.1]

$$\left|\det[\gamma_\sigma(z_\mu - z_\nu)]_{\mu,\nu \in V_p^\sigma}\right| \le \prod_{\mu \in V_p^\sigma} \|\alpha_\mu\|_{\ell^2(\frac{2\pi}{L}\mathbb{Z}^3)} \|\beta_\mu\|_{\ell^2(\frac{2\pi}{L}\mathbb{Z}^3)} \le \left[\sum_{k \in \frac{2\pi}{L}\mathbb{Z}^3} |\hat{\gamma}(k)|\right]^p.$$

It is then explained in the proof of [GMR21, Lemma D.6] how to adapt this argument to bound $\det \mathcal{R}(r)$. □

Combining Equations (5.4.3) and (5.4.4) we conclude the bound

$$\left|\rho_t^{((B_1,W_1),\ldots,(B_k,W_k))}\right| \le \gamma_\infty^{\sum_\ell (\#B_\ell + \#W_\ell) - (k-1)} \sum_{A \in \mathcal{A}^{((B_1,W_1),\ldots,(B_k,W_k))}} \prod_{(\mu,\nu) \in A} |\gamma_{\mu\nu}|. \tag{5.4.5}$$

With the truncated correlation we may write the last line of Equation (5.4.1) as $\rho_t^{(\mathcal{N},\mathcal{M})}$, where

$$\mathcal{N} = (n_1, \ldots, n_k), \qquad \mathcal{M} = (m_1, \ldots, m_k), \qquad (\mathcal{N}, \mathcal{M}) = ((n_1, m_1), \ldots, (n_k, m_k)).$$

That is,

$$\begin{aligned}\frac{1}{p!q!} \sum_{D \in \mathcal{L}_{p,q}} \Gamma_D = \sum_{k=1}^\infty \frac{1}{k!} &\sum_{\substack{n_1,\ldots,n_k \ge 0 \\ m_1,\ldots,m_k \ge 0 \\ \text{For each } \ell:\ n_\ell + m_\ell \ge 2}} \chi_{(\sum_\ell n_\ell = p)} \chi_{(\sum_\ell m_\ell = q)} \frac{1}{\prod_{\ell=1}^k n_\ell! m_\ell!} \\ &\times \int \!\!\cdots\!\! \int \mathrm{d}X_p \, \mathrm{d}Y_q \left[\prod_{\ell=1}^k \sum_{G_\ell \in \mathcal{C}_{n_\ell,m_\ell}} \prod_{e \in G_\ell} g_e\right] \rho_t^{(\mathcal{N},\mathcal{M})}.\end{aligned}$$

To bound this we use the tree-graph bound [Uel18], see also [PU09, Proposition 6.1]. By assumption Equation (5.3.10) is satisfied and thus [Uel18]

$$\left|\sum_{G \in \mathcal{C}_{p,q}} \prod_{e \in G} g_e\right| \le C_{\mathsf{TG}}^{p+q} \sum_{T \in \mathcal{T}_{p,q}} \prod_{e \in T} |g_e|, \tag{5.4.6}$$

where $\mathcal{T}_{p,q} \subset \mathcal{G}_{p,q}$ denotes the subset of trees. (To see this note that $\mathcal{C}_{p,q}$ (respectively $\mathcal{T}_{p,q}$) is the set of connected graphs (respectively trees) on $p+q$ vertices with the colours of the vertices just serving as a handy reminder of the edge-weights g_e.) By moreover using the bound on the truncated correlation in Equation (5.4.5) we conclude that

$$\begin{aligned}&\sum_{\substack{p,q \ge 0 \\ p+q \ge 2}} \frac{1}{p!q!} \left|\sum_{D \in \mathcal{L}_{p,q}} \Gamma_D\right| \\ &\le \sum_{k=1}^\infty \frac{1}{k!} \sum_{\substack{n_1,\ldots,n_k \ge 0 \\ m_1,\ldots,m_k \ge 0 \\ \text{For each } \ell:\ n_\ell + m_\ell \ge 2}} \frac{1}{\prod_{\ell=1}^k n_\ell! m_\ell!} (C_{\mathsf{TG}} \gamma_\infty)^{\sum_\ell (n_\ell + m_\ell) - (k-1)} C_{\mathsf{TG}}^{k-1} \\ &\quad \times \sum_{\substack{T_1,\ldots,T_k \\ T_\ell \in \mathcal{T}_{n_\ell,m_\ell}}} \sum_{A \in \mathcal{A}^{((n_1,m_1),\ldots,(n_k,m_k))}} \int \!\!\cdots\!\! \int \mathrm{d}X_p \, \mathrm{d}Y_q \left[\prod_{\ell=1}^k \prod_{e \in T_\ell} |g_e|\right] \prod_{(\mu,\nu) \in A} |\gamma_{\mu\nu}|.\end{aligned} \tag{5.4.7}$$

To do the integrations we note that the graph $\mathscr{T}$ with edges the union of (g-)edges in $T_1, \ldots, T_k$ and (γ-)edges in A is a tree on all the $\sum_\ell n_\ell + \sum_\ell m_\ell$ many vertices. One then integrates the coordinates one leaf at a time (meaning that the index of the corresponding coordinate is a leaf of the graph $\mathscr{T}$) and removes a vertex from the graph after integrating over its corresponding coordinate.

To be more precise suppose that ν_0 is a leaf of $\mathscr{T}$. Then the variable z_{ν_0} appears exactly once in the integrand. Either in a factor $g_{\mu\nu_0}$ (in which case the z_{ν_0}-integral gives $\int |g| \leq I_g$ by the translation invariance) or in a factor $\gamma_{\mu\nu_0}$ (in which case the z_{ν_0}-integral gives $\int |\gamma| \leq I_\gamma$ by the translation invariance). The final integral gives L^3 by the translation invariance. There are $k-1$ factors of γ and $\sum_\ell (n_\ell + m_\ell - 1) = p+q-k$ factors of g. Thus we get

$$\sum_{\substack{p,q\geq 0\\ p+q\geq 2}} \frac{1}{p!q!} \left| \sum_{D\in\mathcal{L}_{p,q}} \Gamma_D \right| \leq \sum_{k=1}^\infty \frac{1}{k!} \sum_{\substack{n_1,\ldots,n_k\geq 0\\ m_1,\ldots,m_k\geq 0\\ \text{For each } \ell\text{: } n_\ell+m_\ell\geq 2}} \frac{1}{\prod_{\ell=1}^k n_\ell! m_\ell!} \left[\prod_{\ell=1}^k \# \mathcal{T}_{n_\ell,m_\ell} \right]$$
$$\times \# \mathcal{A}^{((n_1,m_1),\ldots,(n_k,m_k))} (C_{\mathsf{TG}} I_g \gamma_\infty)^{\sum_\ell (n_\ell+m_\ell)-k} (C_{\mathsf{TG}} I_\gamma)^{k-1} C_{\mathsf{TG}} \gamma_\infty L^3.$$

In [GMR21, Appendix D.5] it is shown that

$$\# \mathcal{A}^{((n_1,m_1),\ldots,(n_k,m_k))} \leq k! C^{\sum_\ell (n_\ell+m_\ell)}.$$

Moreover, $\mathcal{T}_{n,m} = (n+m)^{n+m-2} \leq C^{n+m}(n+m)!$ by Cayley's formula. Finally, we may bound the binomial coefficients $\frac{(n+m)!}{n!m!} \leq 2^{n+m}$. Thus

$$\begin{aligned}
\sum_{\substack{p,q\geq 0\\ p+q\geq 2}} \frac{1}{p!q!} \left| \sum_{D\in\mathcal{L}_{p,q}} \Gamma_D \right| &\leq C L^3 \gamma_\infty \sum_{k=1}^\infty \left[\sum_{\substack{n,m\geq 0\\ n+m\geq 2}} \frac{(n+m)!}{n!m!} (C I_g \gamma_\infty)^{n+m-1} \right]^k (C I_\gamma)^{k-1} \\
&\leq C L^3 \gamma_\infty \sum_{k=1}^\infty \left[\sum_{\ell=2}^\infty \ell (C I_g \gamma_\infty)^{\ell-1} \right]^k (C I_\gamma)^{k-1} \\
&\leq C L^3 \gamma_\infty^2 I_g < \infty
\end{aligned}$$

for $\gamma_\infty I_g$ and $\gamma_\infty I_g I_\gamma$ small enough. This shows that $\sum_{p,q:p+q\geq 2} \frac{1}{p!q!} \sum_{D\in\mathcal{L}_{p,q}} \Gamma_D$ is absolutely convergent under this assumption. Next, we bound the $\Gamma^{n,m}$-sum for $n+m\geq 1$.

5.4.2 Absolute convergence of the $\Gamma^{n,m}$-sum

In this section we prove that (for $n+m\geq 1$ and uniformly in X_n, Y_m)

$$\sum_{p,q\geq 0} \frac{1}{p!q!} \left| \sum_{D\in\mathcal{L}_{p,q}^{n,m}} \Gamma_D^{n,m} \right| \leq C_{n,m} \gamma_\infty^{n+m} < \infty$$

if Equation (5.3.10) is satisfied and $\gamma_\infty I_g (1+I_\gamma)$ is sufficiently small.

We do the same splitting into clusters (connected components of G) as in Section 5.4.1 above. There is however a slight complication: One needs to keep track of in which clusters the external vertices lie. This is exactly parametrized by the set $\Pi_\kappa^{n,m}$ (defined in Equation (5.3.4)). Denoting the sizes (number of internal vertices) of the clusters containing external vertices by $(n_\lambda^*, m_\lambda^*)$ and the sizes of clusters only containing internal vertices by (n_ℓ, m_ℓ) and introducing

$\mathcal{C}_{p,q}^{n,m} \subset \mathcal{G}_{p,q}^{n,m}$ as the subset of connected graphs (and similarly $\mathcal{C}_{B,W}^{B^*,W^*} \subset \mathcal{G}_{B,W}^{B^*,W^*}$, recall Definition 5.3.1) we get

$$\begin{aligned}
&\frac{1}{p!q!} \sum_{D \in \mathcal{L}_{p,q}^{n,m}} \Gamma_D^{n,m} \\
&\quad = \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{\kappa=1}^{n+m} \frac{1}{\kappa!} \sum_{(\mathcal{B}^*,\mathcal{W}^*) \in \Pi_\kappa^{n,m}} \sum_{\substack{n_1^*,\ldots,n_\kappa^* \geq 0 \\ m_1^*,\ldots,m_\kappa^* \geq 0}} \sum_{\substack{n_1,\ldots,n_k \geq 0 \\ m_1,\ldots,m_k \geq 0 \\ \text{For each } \ell:\ n_\ell + m_\ell \geq 2}} \\
&\quad \times \chi_{(\sum_\ell n_\ell + \sum_\lambda n_\lambda^* = p)} \chi_{(\sum_\ell m_\ell + \sum_\lambda m_\lambda^* = q)} \frac{1}{\prod_{\lambda=1}^{\kappa} n_\lambda^*! m_\lambda^*!} \frac{1}{\prod_{\ell=1}^{k} n_\ell! m_\ell!} \\
&\quad \times \sum_{G_\lambda^* \in \mathcal{C}_{n_\lambda^*, m_\lambda^*}^{B_\lambda^*, W_\lambda^*}} \sum_{G_\ell \in \mathcal{C}_{n_\ell, m_\ell}} \int \!\cdots\! \int \mathrm{d}X_{[n+1,n+p]} \, \mathrm{d}Y_{[m+1,m+q]} \left[\prod_{\lambda=1}^{\kappa} \prod_{e \in G_\lambda^*} g_e \right] \times \left[\prod_{\ell=1}^{k} \prod_{e \in G_\ell} g_e \right] \\
&\quad \times \left[\sum_{\substack{\pi \in \mathcal{S}_{n+p} \\ \tau \in \mathcal{S}_{m+q}}} (-1)^\pi (-1)^\tau \chi_{((\pi,\tau,\cup_\lambda G_\lambda^* \cup \cup_\ell G_\ell) \text{ linked})} \prod_{i=1}^{n+p} \gamma_\uparrow(x_i - x_{\pi(i)}) \prod_{j=1}^{m+q} \gamma_\downarrow(y_j - y_{\tau(j)}) \right].
\end{aligned} \tag{5.4.8}$$

For $k = 0$ the $n_1, m_1, \ldots, n_k, m_k$-sum should be interpreted as an empty product, i.e. as a factor 1. Similarly for $p = 0$ and/or $q = 0$ the empty product of integrals should be interpreted as a factor 1.

The last line in Equation (5.4.8) is the truncated correlation

$$\rho_t^{(\mathcal{B}^*+\mathcal{N}^*, \mathcal{W}^*+\mathcal{M}^*) \oplus (\mathcal{N}, \mathcal{M})},$$

where

$$\mathcal{N}^* = (n_1^*, \ldots, n_\kappa^*), \quad \mathcal{N} = (n_1, \ldots, n_k), \quad \mathcal{M}^* = (m_1^*, \ldots, m_\kappa^*), \quad \mathcal{M} = (m_1, \ldots, m_k)$$

and $\oplus$ means concatenation of vectors, i.e.

$$\begin{aligned}
&(\mathcal{B}^* + \mathcal{N}^*, \mathcal{W}^* + \mathcal{M}^*) \oplus (\mathcal{N}, \mathcal{M}) \\
&\qquad = ((B_1^* + n_1^*, W_1^* + m_1^*), \ldots, (B_\kappa^* + n_\kappa^*, W_\kappa^* + m_\kappa^*), (n_1, m_1), \ldots, (n_k, m_k)),
\end{aligned}$$

where we abused notation slightly and wrote $B_1^* + n_1^*$ for the union of the vertices B_1^* and the n_1^* internal black vertices of the graph G_1^*. (Similarly for the other terms.)

We use as in Section 5.4.1 the tree-graph bound and the bound on the truncated correlation in Equation (5.4.5). For the clusters with external vertices we add 0-weights to the disallowed edges as in Section 3.3.1.3, i.e. for $G \in \mathcal{C}_{p,q}^{n,m}$ define

$$\tilde{g}_e = \begin{cases} 0 & e = (i,j) \text{ with } i,j \text{ external vertices} \\ g_e & \text{otherwise.} \end{cases}$$

Then we may readily apply the tree-graph bound [Uel18] with edge-weights $\tilde{g}_e$:

$$\begin{aligned}
\left| \sum_{G \in \mathcal{C}_{p,q}^{n,m}} \prod_{e \in G} g_e \right| = \left| \sum_{G \in \mathcal{C}_{p+n,q+m}} \prod_{e \in G} \tilde{g}_e \right| &\leq C_{\mathsf{TG}}^{p+q+n+m} \sum_{T \in \mathcal{T}_{p+n,q+m}} \prod_{e \in T} |\tilde{g}_e| \\
&= C_{\mathsf{TG}}^{p+q+n+m} \sum_{T \in \mathcal{T}_{p,q}^{n,m}} \prod_{e \in T} |g_e|,
\end{aligned}$$

where $\mathcal{T}_{p,q} \subset \mathcal{G}_{p,q}$ and $\mathcal{T}_{p,q}^{n,m} \subset \mathcal{C}_{p,q}^{n,m}$ denotes the subsets of trees. Thus

$$
\begin{aligned}
&\sum_{p,q\geq 0} \frac{1}{p!q!} \left| \sum_{D\in\mathcal{L}_{p,q}^{n,m}} \Gamma_D^{n,m} \right| \\
&\leq \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{\kappa=1}^{n+m} \frac{1}{\kappa!} \sum_{(\mathcal{B}^*,\mathcal{W}^*)\in\Pi_\kappa^{n,m}} \sum_{\substack{n_1^*,\ldots,n_\kappa^*\geq 0\\ m_1^*,\ldots,m_\kappa^*\geq 0}} \sum_{\substack{n_1,\ldots,n_k\geq 0\\ m_1,\ldots,m_k\geq 0\\ \text{For each } \ell\text{: } n_\ell+m_\ell\geq 2}} \frac{1}{\prod_{i=1}^{\ell} n_i^*!m_i^*!} \frac{1}{\prod_{\ell=1}^{k} n_\ell!m_\ell!} \\
&\quad\times \sum_{A\in\mathcal{A}^{(\mathcal{B}^*+\mathcal{N}^*,\mathcal{W}^*+\mathcal{M}^*)\oplus(\mathcal{N},\mathcal{M})}} \sum_{\substack{T_1^*,\ldots,T_\kappa^*\\ T_\lambda^*\in\mathcal{T}_{n_\lambda^*,m_\lambda^*}^{B_\lambda^*,W_\lambda^*}}} \sum_{\substack{T_1,\ldots,T_k\\ T_\ell\in\mathcal{T}_{n_\ell,m_\ell}}} \\
&\quad\times \int\!\!\cdots\!\!\int \mathrm{d}X_{[n+1,n+\sum_\lambda n_\lambda^*+\sum_\ell n_\ell]} \,\mathrm{d}Y_{[m+1,m+\sum_\lambda m_\lambda^*+\sum_\ell m_\ell]} \\
&\quad\times \left[\prod_{\lambda=1}^{\kappa} \prod_{e\in T_\lambda^*} |g_e| \prod_{\ell=1}^{k} \prod_{e\in T_\ell} |g_e| \prod_{(\mu,\nu)\in A} |\gamma_{\mu\nu}| \right] \\
&\quad\times (C_{\mathsf{TG}}\gamma_\infty)^{\sum_\lambda(n_\lambda^*+m_\lambda^*)+\sum_\ell(n_\ell+m_\ell)+n+m-(k+\kappa-1)} C_{\mathsf{TG}}^{k+\kappa-1}.
\end{aligned}
\tag{5.4.9}
$$

To do the integrations we bound some g- and γ-factors pointwise. Recall first, that there are κ clusters with external vertices. We split the anchored tree into pieces according to these clusters as follows.

We may view the anchored tree A as a tree on the set of clusters. If $\kappa = 1$ set $A_1 = A$. Otherwise iteratively pick a γ-edge on the path in A between any two clusters with external vertices and bound it by

$$
|\gamma_\sigma(z)| = \left| \sum_{k\in\frac{2\pi}{L}\mathbb{Z}^3} \hat{\gamma}_\sigma(k)e^{ikz} \right| \leq \gamma_\infty
$$

and remove it from A. This cuts the anchored tree A into pieces. Doing this $\kappa - 1$ many times we get κ anchored trees $A_1, \ldots, A_\kappa$ with each exactly one cluster with external vertices. That is,

$$
\prod_{(\mu,\nu)\in A} |\gamma_{\mu\nu}| \leq \gamma_\infty^{\kappa-1} \prod_{\lambda=1}^{\kappa} \prod_{(\mu,\nu)\in A_\lambda} |\gamma_{\mu\nu}|.
$$

Next, in each cluster with external vertices, say with label λ_0, we do a similar procedure of splitting the cluster into pieces according to the external vertices.

In the cluster λ_0 there are $\#B_{\lambda_0}^* + \#W_{\lambda_0}^* \geq 1$ external vertices. If $\#B_{\lambda_0}^* + \#W_{\lambda_0}^* = 1$ set $T_{\lambda_0,1}^* = T_{\lambda_0}^*$. Otherwise iteratively pick a g-edge on the path in $T_{\lambda_0}^*$ between any two external vertices and bound it by

$$
|g_e| = \left| f_e^2 - 1 \right| \leq \max\{f_e^2, 1\} \leq C_{\mathsf{TG}}^2
$$

using Equation (5.3.10) for $q = 2$. Remove the edge e from $T_{\lambda_0}^*$. This cuts the tree $T_{\lambda_0}^*$ into pieces. Doing this $\#B_{\lambda_0}^* + \#W_{\lambda_0}^* - 1$ many times we get $\#B_{\lambda_0}^* + \#W_{\lambda_0}^*$ trees $T_{\lambda_0,1}^*, \ldots, T_{\lambda_0,\#B_{\lambda_0}^*+\#W_{\lambda_0}^*}^*$ with each exactly one external vertex. That is,

$$
\prod_{e\in T_{\lambda_0}^*} |g_e| \leq C_{\mathsf{TG}}^{2(\#B_{\lambda_0}^*+\#W_{\lambda_0}^*-1)} \prod_{\nu=1}^{\#B_{\lambda_0}^*+\#W_{\lambda_0}^*} \prod_{e\in T_{\lambda_0,\nu}^*} |g_e|.
$$

We do this procedure for all the κ many clusters with external vertices. Then the graph $\mathscr{T}$ with edges the union of all (g- or γ-)edges in $T^*_{\lambda,\nu}, T_\ell, A_\lambda$ (for $\lambda \in \{1,\ldots,\kappa\}$, $\ell \in \{1,\ldots,k\}$ and $\nu \in \{1,\ldots,\#B^*_\lambda + \#W^*_\lambda - 1\}$) is a forest (disjoint union of trees) on the set of vertices $V_{n+\sum_\lambda n^*_\lambda + \sum_\ell n_\ell, m+\sum_\lambda m^*_\lambda + \sum_\ell m_\ell}$ with each connected component (tree) having exactly one external vertex. Moreover, we have the bound

$$\begin{aligned}
&\int\!\!\cdots\!\!\int \mathrm{d}X_{[n+1,n+\sum_\lambda n^*_\lambda+\sum_\ell n_\ell]}\,\mathrm{d}Y_{[m+1,m+\sum_\lambda m^*_\lambda+\sum_\ell m_\ell]}\left[\prod_{\lambda=1}^{\kappa}\prod_{e\in T^*_\lambda}|g_e|\prod_{\ell=1}^{k}\prod_{e\in T_\ell}|g_e|\prod_{(\mu,\nu)\in A}|\gamma_{\mu\nu}|\right]\\
&\quad\leq C_{\mathsf{TG}}^{2(n+m-\kappa)}\gamma_\infty^{\kappa-1}\left[\prod_{\lambda=1}^{\kappa}\prod_{\nu=1}^{\#B^*_\lambda+\#W^*_\lambda}\int\!\!\cdots\!\!\int\prod_{e\in T^*_{\lambda,\nu}}|g_e|\prod_{(\mu,\nu)\in A_\lambda}|\gamma_{\mu\nu}|\prod_{\ell:T_\ell\sim A_\lambda}\prod_{e\in T_\ell}|g_e|\right],
\end{aligned}\tag{5.4.10}$$

where $T_\ell \sim A_\lambda$ means that T_ℓ and A_λ share a vertex. (Equivalently they are part of the same connected component of $\mathscr{T}$.)

Since each connected component of $\mathscr{T}$ is a tree we may do the integrations one leaf at a time exactly as for the Γ-sum in Section 5.4.1 above. To bound the value we count the number of γ- and g-factors that are left.

The number of γ-integrations is exactly the number of γ-factors. There are $k+\kappa$ many clusters, so A has $k+\kappa-1$ many edges. In constructing $A_1,\ldots,A_\kappa$ we cut $\kappa-1$ many edges, thus there is k many γ-factors left and so there are k many γ-integrations in Equation (5.4.10). The remaining $\sum_\lambda(n^*_\lambda+m^*_\lambda)+\sum_\ell(n_\ell+m_\ell)-k$ integrations are of g-factors. The integrals may be bounded by $\int|\gamma|\leq I_\gamma$ and $\int|g|\leq I_g$ as in Section 5.4.1. Moreover, since each connected component of $\mathscr{T}$ has one external vertex, which is not integrated over, there are no volume factors from the last integrations in any of the connected components of $\mathscr{T}$. That is,

$$\begin{aligned}
&\int\!\!\cdots\!\!\int \mathrm{d}X_{[n+1,n+\sum_\lambda n^*_\lambda+\sum_\ell n_\ell]}\,\mathrm{d}Y_{[m+1,m+\sum_\lambda m^*_\lambda+\sum_\ell m_\ell]}\left[\prod_{\lambda=1}^{\kappa}\prod_{e\in T^*_\lambda}|g_e|\prod_{\ell=1}^{k}\prod_{e\in T_\ell}|g_e|\prod_{(\mu,\nu)\in A}|\gamma_{\mu\nu}|\right]\\
&\quad\leq C_{\mathsf{TG}}^{2(n+m-\kappa)}\gamma_\infty^{\kappa-1}I_g^{\sum_\lambda(n^*_\lambda+m^*_\lambda)+\sum_\ell(n_\ell+m_\ell)-k}I_\gamma^k.
\end{aligned}$$

We use this to bound the integrations in Equation (5.4.9). Additionally we need to bound the number of (anchored) tree. In [GMR21, Appendix D.5] it is shown that

$$\#\mathcal{A}^{(\mathcal{B}^*+\mathcal{N}^*,\mathcal{W}^*+\mathcal{M}^*)\oplus(\mathcal{N},\mathcal{M})}\leq(k+\kappa)!\,C^{n+m+\sum_\lambda(n^*_\lambda+m^*_\lambda)+\sum_\ell(n_\ell+m_\ell)},$$

since we have $k+\kappa$ many clusters and $n+m+\sum_\lambda(n^*_\lambda+m^*_\lambda)+\sum_\ell(n_\ell+m_\ell)$ many vertices in total. Moreover, $\#\mathcal{T}^{n,m}_{p,q}\leq\#\mathcal{T}_{p+n,q+m}=(p+q+n+m)^{p+q+n+m-2}\leq(p+q+n+m)!\,C^{p+q+n+m}$ by Cayley's formula as in Section 5.4.1. These bounds together with Equation (5.4.9) then gives

$$\begin{aligned}
&\sum_{p,q\geq0}\frac{1}{p!q!}\left|\sum_{D\in\mathcal{L}^{n,m}_{p,q}}\Gamma^{n,m}_D\right|\\
&\quad\leq(C\gamma_\infty)^{n+m}\sum_{k=0}^{\infty}\sum_{\kappa=1}^{n+m}\frac{(k+\kappa)!}{k!\kappa!}\sum_{(\mathcal{B}^*,\mathcal{W}^*)\in\Pi^{n,m}_\kappa}\ \sum_{\substack{n^*_1,\ldots,n^*_\kappa\geq0\\ m^*_1,\ldots,m^*_\kappa\geq0}}\ \sum_{\substack{n_1,\ldots,n_k\geq0\\ m_1,\ldots,m_k\geq0\\ \text{For each }\ell:\ n_\ell+m_\ell\geq2}}\\
&\qquad\times\left[\prod_{\lambda=1}^{\kappa}\frac{(n^*_\lambda+\#B^*_\lambda+m^*_\lambda+\#W^*_\lambda)!}{n^*_\lambda!m^*_\lambda!}\right]\left[\prod_{\ell=1}^{k}\frac{(n_\ell+m_\ell)!}{n_\ell!m_\ell!}\right]\\
&\qquad\times(CI_g\gamma_\infty)^{\sum_\lambda(n^*_\lambda+m^*_\lambda)+\sum_\ell(n_\ell+m_\ell-1)}(CI_\gamma)^k.
\end{aligned}\tag{5.4.11}$$

Multinomial coefficients may be bounded as $\frac{(p_1+\ldots+p_k)!}{p_1!\cdots p_k!} \le k^{p_1+\ldots+p_k}$. Moreover, $\#B_\lambda^* \le n$ and $\#W_\lambda^* \le m$. Thus we may bound

$$(n_\lambda^* + \#B_\lambda + m_\lambda^* + \#W_\lambda)! \le (n_\lambda^* + m_\lambda^* + n + m)! \le 4^{n_\lambda^* + m_\lambda^* + n + m} n! m! n_\lambda^*! m_\lambda^*!.$$

We conclude the bound

$$\begin{aligned}
&\sum_{p,q\ge 0} \frac{1}{p!q!} \left| \sum_{D\in\mathcal{L}_{p,q}^{n,m}} \Gamma_D^{n,m} \right| \\
&\le (C\gamma_\infty)^{n+m} \sum_{k=0}^{\infty} \sum_{\kappa=1}^{n+m} 2^{k+\kappa} \left[\sum_{n_0^*,m_0^*\ge 0} C_{n,m} (CI_g\gamma_\infty)^{n_0^*+m_0^*} \right]^\kappa \left[CI_\gamma \sum_{\substack{n_0,m_0\ge 0\\ n_0+m_0\ge 2}} (CI_g\gamma_\infty)^{n_0+m_0-1} \right]^k .
\end{aligned} \tag{5.4.12}$$

For some $c_{n,m} > 0$ we have that if $\gamma_\infty I_g(1+I_\gamma) < c_{n,m}$ the sums are convergent and we get

$$\sum_{p,q\ge 0} \frac{1}{p!q!} \left| \sum_{D\in\mathcal{L}_{p,q}^{n,m}} \Gamma_D^{n,m} \right| \le C_{n,m}\gamma_\infty^{n+m} < \infty.$$

This shows the desired. We conclude the proof of Lemma 5.3.6 for the case $S = 2$.

Remark 5.4.2 (Higher spin)**.** For the case of higher spin $S \ge 3$, the computations are essentially the same.

For later use we define for all diagrams some values characterising their sizes.

Definition 5.4.3. Let $D \in \mathcal{L}_{p,q}^{n,m}$. Define the number $k = k(D)$ as the number of clusters entirely within internal vertices (i.e. the same k as in the computations above) and $\kappa = \kappa(D)$ as the number of clusters containing at least one external vertex (i.e. the same κ as in the computations above). Define then $\nu^* = \nu^*(D)$ and $\nu = \nu(D)$ as

$$\nu^* = \sum_{\lambda=1}^{\kappa} (n_\lambda^* + m_\lambda^*), \qquad \nu = \sum_{\ell=1}^{k} (n_\ell + m_\ell) - 2k,$$

where $n_\lambda^*, m_\lambda^*, n_\ell, m_\ell$ are the sizes of the different clusters exactly as in the computations above. (Then $\nu + \nu^* + 2k = p + q$.)

For a diagram D the number $\nu + \nu^*$ is the "number of added vertices" in the following sense. A diagram with $n + m$ external vertices and k clusters entirely within internal vertices has at least $n + m + 2k$ many vertices, since each cluster (with only internal vertices) has at least 2 vertices. Then $\nu + \nu^*$ is the number of vertices a diagram has more than this minimal number.

Note that in the special case of consideration with the scattering functions f_s, f_p and the one-particle density matrices $\gamma_{N_\sigma}^{(1)}$ we have

$$\gamma_\infty \le \rho, \qquad I_g \le Cab^2, \qquad I_\gamma \le Cs(\log N)^3$$

by Equations (5.2.9) and (5.3.13), see also the proof of Theorem 5.3.2. Then, by following the arguments above (see in particular Equations (5.4.11) and (5.4.12)), we have (for $p + q =$

$2k_0 + \nu_0$)

$$\frac{1}{p!q!}\left|\sum_{\substack{D\in\mathcal{L}_{p,q}^{n,m}\\ k(D)=k_0\\ \nu(D)+\nu^*(D)=\nu_0}}\Gamma_D^{n,m}\right| \leq C_{n,m}\rho^{n+m}(Cab^2\rho)^{\nu_0+k_0}(Cs(\log N)^3)^{k_0} \tag{5.4.13}$$

for any n,m with $n+m\geq 1$. We think of s as $s\sim(a^3\rho)^{-1/3+\varepsilon}$ for some small $\varepsilon>0$. Thus increasing ν_0 by 1 we decrease the size of the diagram by $(a^3\rho)^{1/3}$, and increasing k_0 by 1 we decrease the size of the diagram by $(a^3\rho)^{\varepsilon}$. (Recall that $b=\rho^{-1/3}$.)

5.5 Energy of the trial state

In this section we use the formulas in Equation (5.3.8) to calculate the energy in Equation (5.2.7). We will refer to a term in Equation (5.2.7) where $\rho_{\mathsf{Jas}}^{(n,m)}$ appears as a (n,m)-type term.

5.5.1 2-body terms

In this section we consider the terms in Equation (5.2.7) where a two-particle density ($\rho_{\mathsf{Jas}}^{(n,m)}$ with $n+m=2$) appears. We consider first the term with $m=n=1$.

5.5.1.1 $(1,1)$-type terms

We consider the term

$$2\iint\rho_{\mathsf{Jas}}^{(1,1)}\left[\frac{|\nabla f_s(x_1-y_1)|^2}{f_s(x_1-y_1)^2}+\frac{1}{2}v(x_1-y_1)\right]\mathrm{d}x_1\,\mathrm{d}y_1. \tag{5.5.1}$$

The formula in Equation (5.3.8) reads for $\rho_{\mathsf{Jas}}^{(1,1)}$ as follows.

$$\begin{aligned}\rho_{\mathsf{Jas}}^{(1,1)}(x_1,y_1) &= f_s(x_1-y_1)^2\left[\rho_{\mathsf{Jas}}^{(1,0)}\rho_{\mathsf{Jas}}^{(0,1)}+\sum_{p,q\geq 0}\frac{1}{p!q!}\sum_{D\in\mathcal{L}_{p,q}^{1,1}}\Gamma_D^{1,1}\right]\\ &= f_s(x_1-y_1)^2\left[\rho_\uparrow\rho_\downarrow+\sum_{\substack{p,q\geq 0\\ p+q\geq 1}}\frac{1}{p!q!}\sum_{D\in\mathcal{L}_{p,q}^{1,1}}\Gamma_D^{1,1}\right]\end{aligned} \tag{5.5.2}$$

since $\mathcal{L}_{p,q}^{1,1}=\varnothing$ for $p=q=0$. The second summand is an error term. We bound it as follows.

Lemma 5.5.1. *There exists a constant $c>0$ such that if $sab^2\rho(\log N)^3<c$, then for any integer K there exists a constant $C_K>0$ such that*

$$\sum_{\substack{p,q\geq 0\\ p+q\geq 1}}\frac{1}{p!q!}\left|\sum_{D\in\mathcal{L}_{p,q}^{1,1}}\Gamma_D^{1,1}\right| \leq C_K ab^2\rho^3+C\rho^2(Csab^2\rho(\log N)^3)^{K+1}+Csa^3\rho^3\log(b/a)(\log N)^3.$$

We give the proof at the end of this section.

Using Equation (5.5.2) and Lemma 5.5.1 we get for any integer K

$$\begin{aligned}(5.5.1) = 2L^3 \int \left(|\nabla f_s|^2 + \frac{1}{2} v f_s^2 \right) \mathrm{d}x \Big[\rho_\uparrow \rho_\downarrow + O_K\left(ab^2\rho^3 \right) \\ + O_K\left(\rho^2 (sab^2\rho (\log N)^3)^{K+1} \right) + O\left(sa^3 \log(b/a) (\log N)^3 \right) \Big].\end{aligned}$$

By Definition 5.1.1 we have

$$\begin{aligned}\int \left(|\nabla f_s|^2 + \frac{1}{2} v f_s^2 \right) \mathrm{d}x \leq \frac{1}{(1-a/b)^2} \int \left(|\nabla f_{s0}|^2 + \frac{1}{2} v f_{s0}^2 \right) \mathrm{d}x = \frac{4\pi a}{(1-a/b)^2} \\ = 4\pi a + O(a^2/b).\end{aligned}$$

We conclude that

$$\begin{aligned}(5.5.1) \leq L^3 8\pi a \rho_\uparrow \rho_\downarrow + O(L^3 a^2 b^{-1} \rho^2) + O_K(L^3 a^2 b^2 \rho^3) + O_K\left(L^3 a \rho^2 (sab^2\rho(\log N)^3)^{K+1} \right) \\ + O(L^3 s a^3 \rho^3 \log(b/a) (\log N)^3).\end{aligned} \tag{5.5.3}$$

Finally, we give the

Proof of Lemma 5.5.1. We split the diagrams into three groups using the numbers ν^*, ν and k from Definition 5.4.3:

- (A) Diagrams with $\nu + \nu^* \geq 1$,
- (B) Diagrams with $\nu + \nu^* = 0$,
  - (B1) at least one p-wave g-factor.
  - (B2) only s-wave g-factors.

Remark 5.5.2. The diagrams of types (A) and (B1) are those for which the bound in Equation (5.4.13) is good enough to show that these diagrams give contributions to the energy density $\leq Ca^2\rho^{7/3}$. Naively using the bound in Equation (5.4.13) for the diagrams of type (B2) we only get that these are bounded by $\rho^2(a^3\rho)^\varepsilon$ with $b = \rho^{-1/3}$ and s chosen as described immediately after Equation (5.4.13). We will calculate the value of all the (infinitely many) diagrams of type (B2) below and use this exact calculation for all diagrams up to some arbitrary high order. This is an essential step in proving the "almost optimal" error bound in Theorem 5.1.2. It is similar to the approach in [BCGOPS23] for the dilute Bose gas.

The contribution of all diagrams of type (A) (with $\nu+\nu^* \geq 1$) is $\leq Cab^2\rho^3$ by Equation (5.4.13) if $sab^2(\log N)^3$ is sufficiently small (recall Theorem 5.3.2). For diagrams of type (B) note that we have $k \geq 1$, since any summand p, q has $p + q \geq 1$. Moreover, for diagrams of type (B1), at least one factor $\int |g_s| \leq Cab^2$ should be replaced by $\int |g_p| \leq Ca^3 \log b/a$ (recall the bounds in Equation (5.3.13)). Thus, again by Equation (5.4.13), we may bound the size of all diagrams of type (B1) by $Csa^3\rho^3 \log(b/a)(\log N)^3$. More precisely we have

$$\sum_{\substack{p,q\geq 0 \\ p+q\geq 1}} \frac{1}{p!q!} \left| \sum_{\substack{D \in \mathcal{L}_{p,q}^{1,1} \\ D \text{ of type (A)}}} \Gamma_D^{1,1} \right| \leq Cab^2\rho^3,$$

$$\sum_{\substack{p,q\geq 0 \\ p+q\geq 1}} \frac{1}{p!q!} \left| \sum_{\substack{D \in \mathcal{L}_{p,q}^{1,1} \\ D \text{ of type (B1)}}} \Gamma_D^{1,1} \right| \leq Csa^3\rho^3 \log(b/a)(\log N)^3$$

if $sab^2\rho(\log N)^3$ is sufficiently small. It remains to consider the diagrams of type (B2), where $\nu+\nu^*=0$ and only s-wave g-factors appear. These diagrams have g-graph as in Figure 5.5.1b. Note that in particular $p=q=k(D)$ for any such diagram.

(a) Diagram D_{small} of smallest size

(b) Graph G of general diagram, $k\geq 1$.

Figure 5.5.1: Diagrams of type (B2). In (b) only the g-graph G is drawn. The relevant diagrams (π,τ,G) have π,τ such that the diagrams are linked.

We now evaluate all these diagrams. We give an example calculation of the (unique) diagram of smallest size, and then do the computation in full generality. The diagram of smallest size is the diagram in Figure 5.5.1a. Its value is

$$
\begin{aligned}
\Gamma^{1,1}_{D_{\mathsf{small}}} &= \iint \gamma^{(1)}_{N_\uparrow}(x_1;x_2)\gamma^{(1)}_{N_\uparrow}(x_2;x_1)\gamma^{(1)}_{N_\downarrow}(y_1;y_2)\gamma^{(1)}_{N_\downarrow}(y_1;y_2)g_s(x_2-y_2)\,\mathsf{d}x_2\,\mathsf{d}y_2 \\
&= \frac{1}{L^{12}}\sum_{k_1^\uparrow,k_2^\uparrow\in P_F^\uparrow}\sum_{k_1^\downarrow,k_2^\downarrow\in P_F^\downarrow}\iint e^{ik_1^\uparrow(x_1-x_2)}e^{ik_2^\uparrow(x_2-x_1)}e^{ik_1^\downarrow(y_1-y_2)}e^{ik_2^\downarrow(y_2-y_1)}g_s(x_2-y_2)\,\mathsf{d}x_2\,\mathsf{d}y_2 \\
&= \frac{1}{L^{12}}\sum_{k_1^\uparrow,k_2^\uparrow\in P_F^\uparrow}\sum_{k_1^\downarrow,k_2^\downarrow\in P_F^\downarrow} e^{i(k_1^\uparrow-k_2^\uparrow)x_1}e^{i(k_1^\downarrow-k_2^\downarrow)y_1} \\
&\quad\times\int \mathsf{d}x_2\left[e^{i(k_2^\uparrow-k_1^\uparrow+k_2^\downarrow-k_1^\downarrow)x_2}\int \mathsf{d}y_2\left(g_s(x_2-y_2)e^{-i(k_2^\downarrow-k_1^\downarrow)(x_2-y_2)}\right)\right] \\
&= \frac{1}{L^{12}}\sum_{k_1^\uparrow,k_2^\uparrow\in P_F^\uparrow}\sum_{k_1^\downarrow,k_2^\downarrow\in P_F^\downarrow} e^{i(k_1^\uparrow-k_2^\uparrow)x_1}e^{i(k_1^\downarrow-k_2^\downarrow)y_1}L^3\chi_{(k_2^\uparrow-k_1^\uparrow=k_1^\downarrow-k_2^\downarrow)}L^3\hat{g}_s(k_2^\downarrow-k_1^\downarrow)
\end{aligned}
$$

where $\hat{g}_s(k)=L^{-3}\int g_s(x)e^{-ikx}\,\mathsf{d}x$ denotes the Fourier transform and we used the translation invariance to evaluate the g_s-integral. We have the bound (recall Equation (5.3.13))

$$
L^3\left|\hat{g}_s(k)\right|\leq\int|g(x)|\,\mathsf{d}x\leq Cab^2.
$$

The characteristic function $\chi_{(k_2^\uparrow-k_1^\uparrow=k_1^\downarrow-k_2^\downarrow)}$ effectively kills one of the four k_j^σ-sums. The remaining k_j^σ-sums have at most $N_\sigma\leq N$ many summands. We conclude the bound (uniformly in x_1,y_1)

$$
\left|\Gamma^{1,1}_{D_{\mathsf{small}}}\right|\leq Cab^2\rho^3.
$$

For the general diagram in Figure 5.5.1b we may use the same method. We then have

$$\begin{aligned}
\Gamma_D^{1,1} &= \frac{1}{L^{6+6k}} \sum_{k_1^\uparrow,\ldots,k_{k+1}^\uparrow \in P_F^\uparrow} \sum_{k_1^\downarrow,\ldots,k_{k+1}^\downarrow \in P_F^\downarrow} \int\!\!\cdots\!\!\int \mathrm{d}X_{[2,k+1]}\,\mathrm{d}Y_{[2,k+1]} \\
&\quad \times \left[\prod_{j=1}^{k+1} e^{ik_j^\uparrow(x_j - x_{\pi(j)})} e^{ik_j^\downarrow(y_j - y_{\tau(j)})}\right] \left[\prod_{j=2}^{k+1} g_s(x_j - y_j)\right] \\
&= \frac{1}{L^{6+6k}} \sum_{k_1^\uparrow,\ldots,k_{k+1}^\uparrow \in P_F^\uparrow} \sum_{k_1^\downarrow,\ldots,k_{k+1}^\downarrow \in P_F^\downarrow} e^{i\left(k_1^\uparrow - k_{\pi^{-1}(1)}^\uparrow\right)x_1} e^{i\left(k_1^\downarrow - k_{\tau^{-1}(1)}^\downarrow\right)y_1} \\
&\quad \times \prod_{j=2}^{k+1} \int \mathrm{d}x_j \left[e^{i\left(k_j^\uparrow - k_{\pi^{-1}(j)}^\uparrow + k_j^\downarrow - k_{\tau^{-1}(j)}^\downarrow\right)x_j} \int \mathrm{d}y_j \left(g_s(x_j - y_j) e^{-i\left(k_j^\downarrow - k_{\tau^{-1}(j)}^\downarrow\right)(x_j - y_j)} \right)\right] \\
&= \frac{1}{L^{6+6k}} \sum_{k_1^\uparrow,\ldots,k_{k+1}^\uparrow \in P_F^\uparrow} \sum_{k_1^\downarrow,\ldots,k_{k+1}^\downarrow \in P_F^\downarrow} e^{i\left(k_1^\uparrow - k_{\pi^{-1}(1)}^\uparrow\right)x_1} e^{i\left(k_1^\downarrow - k_{\tau^{-1}(1)}^\downarrow\right)y_1} \\
&\quad \times \left[\prod_{j=2}^{k+1} L^3 \chi_{\left(k_j^\uparrow - k_{\pi^{-1}(j)}^\uparrow = k_{\tau^{-1}(j)}^\downarrow - k_j^\downarrow\right)} L^3 \hat{g}_s\left(k_j^\downarrow - k_{\tau^{-1}(j)}^\downarrow\right)\right].
\end{aligned}$$

Again, each factor $L^3\hat{g}_s$ we may bound by Cab^2. Moreover, since the diagram is linked we have for each j that $\pi^{-1}(j) \neq j$ and/or $\tau^{-1}(j) \neq j$. (Otherwise the vertices $\{(j,\uparrow),(j,\downarrow)\}$ would be disconnected from the rest.) Thus, each characteristic function is non-trivial, and hence effectively kills one of the k_j^σ-sums. Each surviving k_j^σ-sum has at most $N_\sigma \leq N$ many summands. Thus (uniformly in x_1, y_1)

$$\left|\Gamma_D^{1,1}\right| \leq \rho^2 (Cab^2\rho)^k$$

for any diagram D of type (B2) with k clusters of internal vertices, i.e. with g-graph as in Figure 5.5.1b. For any integer K we have some finite K-dependent number of diagrams with $k \leq K$. Concretely let $M_{k_0} < \infty$ be the number of type (B2) diagrams with $k = k_0$. Thus, using Equation (5.4.13) for diagrams with $k > K$, we get

$$\begin{aligned}
\sum_{\substack{p,q\geq 0\\ p+q\geq 1}} \frac{1}{p!q!} \left| \sum_{\substack{D\in\mathcal{L}_{p,q}^{1,1}\\ D \text{ of type (B2)}}} \Gamma_D^{1,1} \right| &\leq \sum_{k=1}^{K} \frac{1}{k!^2} \sum_{\substack{D\in\mathcal{L}_{k,k}^{1,1}\\ D \text{ of type (B2)}}} \left|\Gamma_D^{1,1}\right| + \sum_{k=K+1}^{\infty} \frac{1}{k!^2} \left| \sum_{\substack{D\in\mathcal{L}_{k,k}^{1,1}\\ D \text{ of type (B2)}}} \Gamma_D^{1,1} \right| \\
&\leq \sum_{k=1}^{K} \frac{M_k}{k!^2} \rho^2 (Cab^2\rho)^k + C\rho^2 (Csab^2\rho(\log N)^3)^{K+1} \\
&\leq C_K ab^2\rho^3 + C\rho^2(Csab^2\rho(\log N)^3)^{K+1}
\end{aligned} \tag{5.5.4}$$

for some constant $C_K > 0$ if $sab^2\rho(\log N)^3$ is sufficiently small. □

Remark 5.5.3 (Upper bound on number of diagrams — why we can't pick $K = \infty$)**.** For an upper bound on the number of diagrams we first find an upper bound on the number of graphs. All the underlying graphs look like Figure 5.5.1b, but the labelling of the internal vertices may be different. We are free to choose which white (internal) vertex connects to $(2,\uparrow)$ and so on. In total there are thus $q! = k!$ many possible graphs.

Next, to bound the number of diagrams with any given g-graph we may forget the constraint that the diagram has to be linked and consider all choices of $\pi \in \mathcal{S}_{k+1}$ and $\tau \in \mathcal{S}_{k+1}$ instead of just those, for which the diagram is linked. For both π and τ there are then $(k+1)!$ many choices. Thus for each graph G there is at most $(k+1)!^2$ many linked diagrams of type (B2) with g-graph G. Thus there are at most $k!(k+1)!^2$ diagrams of type (B2) with k clusters of internal vertices. With this bound the sum

$$\sum_k \frac{1}{k!^2} \sum_{D \in \mathcal{L}_{k,k}^{1,1} \text{ of type (B2)}} \left|\Gamma_D^{1,1}\right| \leq \sum_k k!(k+1)^2 (Cab^2\rho)^k$$

is not convergent. This prevents us from taking $K = \infty$ in Equation (5.5.4) and using the exact calculations for all (infinitely many) diagrams of type (B2).

Remark 5.5.4 (Higher spin)**.** For $S \geq 3$ values of the spin the evaluation of the diagrams is the same, but the combinatorics of counting how many diagrams there are for each given size is more complicated. Still, there is only some finite K-dependent number of diagrams with $k(D) \leq K$ and thus (the appropriately modified version of) Equation (5.5.4) is valid if $sab^2\rho(\log N)^3 < c_S$ for some constant $c_S > 0$.

5.5.1.2 $(2,0)$- and $(0,2)$-type terms

We bound the term

$$\iint \rho_{\text{Jas}}^{(2,0)} \left[\left|\frac{\nabla f_p(x_1 - x_2)}{f_p(x_1 - x_2)}\right|^2 + \frac{1}{2} v(x_1 - x_2)\right] \mathrm{d}x_1 \, \mathrm{d}x_2. \tag{5.5.5}$$

The term with $\rho_{\text{Jas}}^{(0,2)}$ is completely analogous. We may bound the 2-particle density as follows.

Lemma 5.5.5. *There exist constants $c, C > 0$ such that if $N_\uparrow = \# P_F^\uparrow > C$ and $sab^2\rho(\log N)^3 < c$, then*

$$\left|\rho_{\text{Jas}}^{(2,0)}\right| \leq C f_p(x_1 - x_2)^2 \rho^2 \left[ab^2\rho + \rho^{2/3}|x_1 - x_2|^2 \left[1 + sab^2\rho(\log N)^4\right]\right].$$

This is essentially (a slightly modified version of) Lemma 3.4.1. We give the proof at the end of this section.

Using now Lemma 5.5.5 we get

$$\begin{aligned}
\text{(5.5.5)} &\leq CN\rho \int \left[|\nabla f_p|^2 + \frac{1}{2} f_p^2 v\right] \left[ab^2\rho + \rho^{2/3}|x|^2 \left[1 + sab^2\rho(\log N)^4\right]\right] \mathrm{d}x \\
&\leq CNa^2b^2\rho + CN\rho^{5/3}a^3 \left[1 + sab^2\rho(\log N)^4\right]
\end{aligned} \tag{5.5.6}$$

where we used that

$$\int \left[|\nabla f_p|^2 + \frac{1}{2} f_p^2 v\right] |x|^2 \, \mathrm{d}x \leq Ca_p^3 \leq Ca^3, \qquad \int \left[|\nabla f_p|^2 + \frac{1}{2} f_p^2 v\right] \mathrm{d}x \leq Ca_p \leq Ca.$$

The first inequality follows directly from the definition of the scattering length, Definition 5.1.1. The second inequality is a simple computation following from Lemma 5.2.5 and Equation (5.2.10): Using integration by parts and $f_{p0}(x) \geq 1 - a_p^3/|x|^3$ with equality outside the support of v we have, denoting the derivative in the radial direction by ∂_r,

$$\begin{aligned}
\int \left(|\nabla f_p|^2 + \frac{1}{2} v f_p^2\right) \mathrm{d}x &= 4\pi \int_0^b \left(|\partial_r f_p|^2 r^2 + f_p \partial_r^2 f_p r^2 + 4 f_p \partial_r f_p r\right) \mathrm{d}r \\
&= \frac{12\pi a_p^3/b^2}{1 - a_p^3/b^3} + 4\pi \left[b - 2\int_0^b f_p^2 \, \mathrm{d}r\right] \leq Ca_p.
\end{aligned}$$

Finally, we give the

Proof of Lemma 5.5.5. Equation (5.3.8) reads for $n = 2, m = 0$ (recall Equation (5.3.9))

$$\rho^{(2,0)}_{\mathsf{Jas}} = f_p(x_1 - x_2)^2 \left[\rho_\uparrow^2 + \sum_{p,q\geq 0} \frac{1}{p!q!} \sum_{D\in\mathcal{L}^{2,0}_{p,q}} \Gamma^{2,0}_D\right].$$

We split the diagrams into two types, according to whether $\nu^* = 0$ or $\nu^* \geq 1$ (ν and ν^* are defined in Definition 5.4.3). We write

$$\rho_\uparrow^2 + \sum_{p,q\geq 0} \frac{1}{p!q!} \sum_{D\in\mathcal{L}^{2,0}_{p,q}} \Gamma^{2,0}_D = \xi_0 + \xi_{\geq 1},$$

where

$$\xi_0 = \rho_\uparrow^2 + \sum_{p,q\geq 0} \frac{1}{p!q!} \sum_{\substack{D\in\mathcal{L}^{2,0}_{p,q}\\ \nu^*(D)=0}} \Gamma^{2,0}_D, \qquad \xi_{\geq 1} = \sum_{p,q\geq 0} \frac{1}{p!q!} \sum_{\substack{D\in\mathcal{L}^{2,0}_{p,q}\\ \nu^*(D)\geq 1}} \Gamma^{2,0}_D.$$

We will do a Taylor expansion of ξ_0 but not of $\xi_{\geq 1}$. This is completely analogous to what is done in the proof of Lemma 3.4.1. Consider first $\xi_{\geq 1}$. By Theorem 5.3.2 and Equation (5.4.13) we have $\xi_{\geq 1} \leq Cab^2\rho^3$ uniformly in x_1, x_2 if $sab^2\rho(\log N)^3 < c$.

Consider next ξ_0. We do a Taylor expansion to second order around the diagonal. For the zero'th order we have $\xi_0(x_1 = x_2) + \xi_{\geq 1}(x_1 = x_2) = 0$ since $\rho^{(2,0)}_{\mathsf{Jas}}(x_1, x_2)$ vanishes for $x_1 = x_2$. The first order vanishes by the symmetry in x_1 and x_2. Finally, we may bound the second derivatives $\partial^i_{x_1}\partial^j_{x_1}\xi_0$ by following the same procedure as in the proof of Lemma 3.4.1, Equation (3.4.15)–(3.4.20). This crucially uses the bounds in Equation (5.2.9). We give this argument for completeness.

Write (recalling Equation (5.4.8) and using that the $k = 0$ term together with $\rho_\uparrow^2$ give the two-particle density $\rho^{(2,0)}$ by Wick's rule)

$$\begin{aligned}\xi_0 = \rho^{(2,0)} + \sum_{k=1}^\infty \frac{1}{k!} \sum_{\substack{n_1,\ldots,n_k\geq 0\\ m_1,\ldots,m_k\geq 0\\ \text{For each } \ell: n_\ell+m_\ell\geq 2}} \frac{1}{\prod_\ell n_\ell! m_\ell!} \sum_{G_\ell\in\mathcal{C}_{n_\ell,m_\ell}} \int\cdots\int \mathrm{d}X_{[3,2+\sum_\ell n_\ell]}\, \mathrm{d}Y_{\sum_\ell m_\ell} \left[\prod_{\ell=1}^k \prod_{e\in G_\ell} g_e\right] \\ \times \left[\sum_{\substack{\pi\in\mathcal{S}_{2+\sum_\ell n_\ell}\\ \tau\in\mathcal{S}_{\sum_\ell m_\ell}}} (-1)^\pi(-1)^\tau \chi_{((\pi,\tau,\{(1,\uparrow)\}\cup\{(2,\uparrow)\}\cup\cup_\ell G_\ell)\text{ linked})} \prod_{i=1}^{2+\sum_\ell n_\ell} \gamma^{(1)}_{N_\uparrow}(x_i; x_{\pi(i)}) \prod_{j=1}^{\sum_\ell m_\ell} \gamma^{(1)}_{N_\downarrow}(y_j; y_{\tau(j)})\right].\end{aligned}$$

The only dependence on x_1 is in the γ-factors in $[\cdots]$. Computing the second derivatives $\partial^i_{x_1}\partial^j_{x_1}\xi_0$ we see that they are sums of terms where one or two of the γ-factors gain the derivatives $\partial^i_{x_1}$ and $\partial^j_{x_1}$. The term $[\cdots]$ above is the truncated correlation. So is its derivative $\partial^i_{x_1}\partial^j_{x_1}[\cdots]$ now only some of the γ-factors carry derivatives. To bound this term we do as in Section 5.4 and use the (appropriately modfied) formula in Equation (5.4.3). The γ-factors with derivative can either end up in the anchored tree, or in the matrix $\mathcal{R}(r)$. Following the argument in Section 5.4.2 to bound $\partial^i_{x_1}\partial^j_{x_1}\xi_0$ we see that we need bounds on the determinants of the matrix $\mathcal{R}(r)$, modified with the γ-factors with derivatives, and/or of the integrals of γ-factors with derivatives.

If the γ-factors with derivatives end up in the matrix $\mathcal{R}(r)$ we gain a factor $C\rho^{1/3}$ in the bound of its determinant, Equation (5.4.4). This follows from a slight modification of Equation (5.4.4) and is explained around [GMR21, Equation (D.9)]: One changes the definition of some of the functions α_μ in the proof of Equation (5.4.4) by including factors ik^i and/or ik^j. If the γ-factors with derivatives end up in the anchored tree we either have to bound them pointwise, in which case we gain a factor $C\rho^{1/3}$, or we have to bound their integrals, in which case we use Equation (5.2.9).

Following the argument in Section 5.4.2 we thus get a bound similar to Equation (5.4.12) with the following modifications: One or two factors $\int_\Lambda \left|\gamma^{(1)}_{N_\uparrow}\right|$ is replaced with factors with derivatives $\int_\Lambda \left|\partial_1\gamma^{(1)}_{N_\uparrow}\right|, \int_\Lambda \left|\partial_2\gamma^{(1)}_{N_\uparrow}\right|$, where $\partial_1, \partial_2 \in \{1, \partial^i_{x_1}, \partial^j_{x_1}, \partial^i_{x_1}\partial^j_{x_1}\}$ are the derivatives hitting γ-factors in the anchored tree that we do not bound pointwise. For diagrams with only one internal cluster (i.e. with $k=1$) there is only one such γ-factor. Moreover we gain a factor $C\rho^{(2-\#\partial_1-\#\partial_2)/3}$ where $\#\partial_j$ denotes the number of derivatives in ∂_j, i.e. $\#1 = 0, \#\partial^i_{x_1} = 1$ and $\#\partial^i_{x_1}\partial^j_{x_1} = 2$. This factor arises from the matrix $\mathcal{R}(r)$, modified to include the derivatives, and the γ-factors with derivatives we bound pointwise. The derivatives in either (the modification of) $\mathcal{R}(r)$ or on γ-factors we bound pointwise are exactly those not in ∂_1 or ∂_2. That is,

$$
\begin{aligned}
\left|\partial^i_{x_1}\partial^j_{x_1}\xi_0\right| &\leq \left|\partial^i_{x_1}\partial^j_{x_1}\rho^{(2,0)}\right| \\
&\quad + C\rho^2\Bigg[\sum_{\partial\in\{1,\partial^i_{x_1},\partial^j_{x_1},\partial^i_{x_1}\partial^j_{x_1}\}} \rho^{(2-\#\partial)/3}\int_\Lambda \left|\partial\gamma^{(1)}_{N_\uparrow}\right| \sum_{\substack{n_0,m_0\geq 0\\ n_0+m_0\geq 2}} (Cab^2\rho)^{n_0+m_0-1} \\
&\qquad + \sum_{\substack{\partial_1,\partial_2\in\{1,\partial^i_{x_1},\partial^j_{x_1},\partial^i_{x_1}\partial^j_{x_1}\}\\ \partial_1\partial_2\in\{1,\partial^i_{x_1},\partial^j_{x_1},\partial^i_{x_1}\partial^j_{x_1}\}}} \rho^{(2-\#\partial_1-\#\partial_2)/3}\int_\Lambda \left|\partial_1\gamma^{(1)}_{N_\uparrow}\right|\int_\Lambda \left|\partial_2\gamma^{(1)}_{N_\uparrow}\right| \\
&\qquad \times \sum_{k=2}^\infty \left[Cs(\log N)^3\right]^{k-1}\left[\sum_{\substack{n_0,m_0\geq 0\\ n_0+m_0\geq 2}} (Cab^2\rho)^{n_0+m_0-1}\right]^k\Bigg].
\end{aligned}
$$

Noting that $\left|\partial^i_{x_1}\partial^j_{x_1}\rho^{(2,0)}\right| \leq C\rho^{8/3}$ by a simple computation using the Wick rule and using Equation (5.2.9) to bound the integrals we conclude that

$$
\left|\partial^i_{x_1}\partial^j_{x_1}\xi_0\right| \leq C\rho^{8/3}\left[1 + sab^2\rho(\log N)^4\right]
$$

if $N_\uparrow$ is sufficiently large and $sab^2\rho(\log N)^3$ is sufficiently small. By Taylor's theorem we conclude the desired. □

5.5.2 3-body terms

In this section we bound the 3-body terms of Equation (5.2.7).

5.5.2.1 $(2,1)$- and $(1,2)$-type terms

We bound the term

$$
\iiint \rho^{(2,1)}_{\mathrm{Jas}}\left[\left|\frac{\nabla f_s(x_1-y_1)\nabla f_p(x_1-x_2)}{f_s(x_1-y_1)f_p(x_1-x_2)}\right| + \left|\frac{\nabla f_s(x_1-y_1)\nabla f_s(x_2-y_1)}{f_s(x_1-y_1)f_s(x_2-y_1}\right|\right] \mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}y_1. \tag{5.5.7}
$$

The $(1,2)$-type term is bounded analogously.

By Theorem 5.3.2 we have the bound

$$\rho^{(2,1)}_{\mathsf{Jas}} \leq C\rho^3 f_s(x_1-y_1)^2 f_s(x_2-y_1)^2 f_p(x_1-x_2)^2$$

if $sab^2\rho(\log N)^3$ is sufficiently small. In the first summand in Equation (5.5.7) we moreover bound $f_s(x_2-y_1)\leq 1$ and in the second summand we bound $f_p(x_1-x_2)\leq 1$. Then by the translation invariance we have

$$(5.5.7) \leq CN\rho^2\left[\left(\int f_s|\nabla f_s|\right)\left(\int f_p|\nabla f_p|\right)+\left(\int f_s|\nabla f_s|\right)^2\right].$$

By radiality and Lemma 5.2.5 we have

$$\begin{aligned}\frac{1}{4\pi}\int f_s|\nabla f_s| = \int_0^b r^2 f_s\partial_r f_s \,\mathrm{d}r &= \frac{1}{2}[r^2f_s^2]_0^b - \frac{1}{2}\int_0^b 2rf_s^2\,\mathrm{d}r\\ &\leq \frac{1}{2}b^2 - \frac{1}{(1-a/b)^2}\int_a^b r\left(1-\frac{a}{r}\right)^2\mathrm{d}r \leq Cab,\end{aligned}$$

where ∂_r denotes the radial derivative. Similarly by Lemma 5.2.5

$$\begin{aligned}\frac{1}{4\pi}\int f_p|\nabla f_p| = \int_0^b r^2 f_p\partial_r f_p \,\mathrm{d}r &= \frac{1}{2}[r^2f_p^2]_0^b - \frac{1}{2}\int_0^b 2rf_p^2\,\mathrm{d}r\\ &\leq \frac{1}{2}b^2 - \frac{1}{(1-a_p^3/b^3)^2}\int_a^b r\left(1-\frac{a_p^3}{r^3}\right)^2\mathrm{d}r \leq Ca_p^2.\end{aligned}$$

We conclude that (for sufficiently small $sab^2\rho(\log N)^3$)

$$(5.5.7) \leq CN\rho^2a^2b^2. \tag{5.5.8}$$

5.5.2.2 $(3,0)$- and $(0,3)$-type terms

We may bound

$$\iiint \rho^{(3,0)}_{\mathsf{Jas}}\left|\frac{\nabla f_p(x_1-x_2)\nabla f_p(x_1-x_3)}{f_p(x_1-x_2)f_p(x_1-x_3)}\right|\mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3 \leq CN\rho^2a^4 \tag{5.5.9}$$

using the same method as for the $(2,1)$-type terms. The $(0,3)$-type terms may be bounded analogously.

Remark 5.5.6 (Higher spin)**.** For higher spin we also have terms of type $(1,1,1)$. These may be bounded exactly as the $(2,1)$-type terms with two s-wave factors.

5.5.3 Putting the bounds together

Combining Equations (5.2.7), (5.2.8), (5.5.3), (5.5.6), (5.5.8) and (5.5.9) we immediately get for any integer K

$$\begin{aligned}&\frac{\left\langle\psi_{N_\uparrow,N_\downarrow}\middle|H_N\middle|\psi_{N_\uparrow,N_\downarrow}\right\rangle}{L^3}\\ &\quad= \frac{3}{5}(6\pi^2)^{2/3}\left(\rho_\uparrow^{5/3}+\rho_\downarrow^{5/3}\right)+8\pi a\rho_\uparrow\rho_\downarrow + O((s_\uparrow^{-2}+s_\downarrow^{-2})\rho^{5/3}) + O(N^{-1/3}\rho^{5/3})\\ &\qquad + O(a^2b^{-1}\rho^2) + O_K(a^2b^2\rho^3) + O_K(a\rho^2(sab^2\rho(\log N)^3)^{K+1})\\ &\qquad + O(sa^3\rho^3\log(b/a)(\log N)^3) + O(a^2b^2\rho^3) + O\left(\rho^{8/3}a^3\left[1+sab^2\rho(\log N)^4\right]\right)\end{aligned} \tag{5.5.10}$$

for $sab^2\rho(\log N)^3$ sufficiently small and $N_\sigma = \#P_F^\sigma$ sufficiently large. As in Section 3.4 we will choose N_σ some large negative power of $a^3\rho$. By choosing, say, $L \sim a(a^3\rho)^{-10}$ (still requiring that $\frac{k_F^\sigma L}{2\pi}$ is rational) we have $N \sim (a^3\rho)^{-29}$. (More precisely one chooses $L \sim a((k_F^\uparrow + k_F^\downarrow)a)^{-30}$, see Remark 5.2.4.) Additionally we choose

$$s_\sigma \sim (a^3\rho)^{-1/3+\varepsilon},$$

where $\varepsilon > 0$ is chosen as $\varepsilon = \frac{1}{K}$ for $K > 6$. Recall moreover that $b = \rho^{-1/3}$. Thus for any fixed integer $K > 6$ we have

$$\frac{\left\langle \psi_{N_\uparrow,N_\downarrow} \middle| H_N \middle| \psi_{N_\uparrow,N_\downarrow} \right\rangle}{L^3} = \frac{3}{5}(6\pi^2)^{2/3}\left(\rho_\uparrow^{5/3} + \rho_\downarrow^{5/3}\right) + 8\pi a\rho_\uparrow\rho_\downarrow + O_K\left(a\rho^2(a^3\rho)^{1/3-2/K}\right). \tag{5.5.11}$$

5.5.4 Box method

We extend to the thermodynamic limit using a box method exactly as in Section 3.4.1. We sketch the details here. Using a bound of Robinson [Rob71, Lemmas 2.1.12, 2.1.13] (more specifically the form in [MS20, Section C], see also Lemma 3.4.3) we have an isometry U such that $U\psi_{N_\uparrow,N_\downarrow}$ has Dirichlet boundary conditions in the box $\Lambda_{L+2d} = [-L/2-d, L/2+d]^3$ and

$$\left\langle U\psi_{N_\uparrow,N_\downarrow} \middle| H_{N,L+2d}^D \middle| U\psi_{N_\uparrow,N_\downarrow} \right\rangle \le \left\langle \psi_{N_\uparrow,N_\downarrow} \middle| H_{N,L}^{\mathrm{per}} \middle| \psi_{N_\uparrow,N_\downarrow} \right\rangle + \frac{6N}{d^2},$$

where $H_{N,L+2d}^D$ denotes the Hamiltonian on a box of sides $L+2d$ with Dirichlet boundary conditions, and $H_{N,L}^{\mathrm{per}}$ denotes the Hamiltonian on a box of sides L with periodic boundary conditions. We are free to choose the the parameter d. We will choose it some large negative power of $a^3\rho$.

We use this to form trial states $U\psi_{N_\uparrow,N_\downarrow}$ with Dirichlet boundary conditions in a box of sides $L+2d$. Using then a box method of glueing copies of the trial state $U\psi_{N_\uparrow,N_\downarrow}$ together (as in Section 3.4.1) with a distance b between them (same b as before) we get a trial state $\Psi_{M^3N_\uparrow,M^3N_\downarrow}$ of particle densities $\tilde\rho_\sigma = \frac{M^3N_\sigma}{M^3(L+2d+b)^3} = \rho_\sigma(1+O(b/L)+O(d/L))$. The state $\Psi_{M^3N_\uparrow,M^3N_\downarrow}$ has the energy density

$$\begin{aligned}
&\frac{\left\langle \Psi_{M^3N_\uparrow,M^3N_\downarrow} \middle| H_{M^3N,M^3(L+2d+b)}^D \middle| \Psi_{M^3N_\uparrow,M^3N_\downarrow} \right\rangle}{M^3(L+2d+b)^3} \\
&\quad = \frac{\left\langle U\psi_{N_\uparrow,N_\downarrow} \middle| H_{N,L+2d}^D \middle| U\psi_{N_\uparrow,N_\downarrow} \right\rangle}{L^3}(1+O(d/L)+O(b/L)) \\
&\quad \le \frac{\left\langle \psi_{N_\uparrow,N_\downarrow} \middle| H_{N,L}^{\mathrm{per}} \middle| \psi_{N_\uparrow,N_\downarrow} \right\rangle}{L^3}(1+O(d/L)+O(b/L)) + O(\rho d^{-2}).
\end{aligned}$$

Choosing say $d = a(a^3\rho)^{-5}$ and using Equation (5.5.11) we thus get

$$\begin{aligned}
e(\tilde\rho_\uparrow,\tilde\rho_\downarrow) &\le \limsup_{M\to\infty} \frac{\left\langle \Psi_{M^3N_\uparrow,M^3N_\downarrow} \middle| H_{M^3N,M^3(L+2d+b)}^D \middle| \Psi_{M^3N_\uparrow,M^3N_\downarrow} \right\rangle}{M^3(L+2d+b)^3} \\
&\le \frac{3}{5}(6\pi^2)^{2/3}(\rho_\uparrow^{5/3}+\rho_\downarrow^{5/3}) + 8\pi a\rho_\uparrow\rho_\downarrow + O_K\left(a\rho^2(a^3\rho)^{1/3-2/K}\right) \\
&= \frac{3}{5}(6\pi^2)^{2/3}(\tilde\rho_\uparrow^{5/3}+\tilde\rho_\downarrow^{5/3}) + 8\pi a\tilde\rho_\uparrow\tilde\rho_\downarrow + O_K\left(a\tilde\rho^2(a^3\tilde\rho)^{1/3-2/K}\right)
\end{aligned}$$

since $\tilde{\rho}_\sigma = \rho_\sigma(1 + O((a^3\rho)^{-5}))$. For any $\delta > 0$ we may take $K > (2\delta)^{-1}$. This concludes the proof of Theorem 5.1.2 for pairs of densities $(\tilde{\rho}_\uparrow, \tilde{\rho}_\downarrow)$ arising from the construction above. As noted in Remark 5.2.4 this is not all possible values of the densities ρ_σ. Finally, we extend Theorem 5.1.2 to all pairs of (sufficiently small) densities.

Consider any pair of densities $(\rho_{\uparrow 0}, \rho_{\downarrow 0})$ and define $\rho_0 = \rho_{\uparrow 0} + \rho_{\downarrow 0}$ and the Fermi momenta $k_{F0}^\sigma := (6\pi^2)^{1/3}\rho_{\sigma 0}^{1/3}$. Let $\varepsilon > 0$ be some small parameter to be chosen later and find (by density of the rationals in the reals) k_F^σ with $(1+\varepsilon)k_{F0}^\sigma \le k_F^\sigma \le (1+2\varepsilon)k_{F0}^\sigma$ and $k_F^\uparrow/k_F^\downarrow$ rational (recall Remark 5.2.3). Following the construction above we find a trial state $\psi_{N_\uparrow, N_\downarrow}$ with particle densities ρ_σ satisfying

$$(1 + 3\varepsilon + O(\varepsilon^2) + O(N_\sigma^{-1/3}))\rho_{\sigma 0} \le \rho_\sigma \le (1 + 6\varepsilon + O(\varepsilon^2) + O(N_\sigma^{-1/3}))\rho_{\sigma 0}.$$

Thus by constructing the trial states $\Psi_{M^3 N_\uparrow, M^3 N_\downarrow}$ of particle densities $\tilde{\rho}_\sigma$ as above we find

$$\left(1 + 3\varepsilon + O(\varepsilon^2) + O((a^3\rho_0)^{-5})\right)\rho_{\sigma 0} \le \tilde{\rho}_\sigma \le \left(1 + 6\varepsilon + O(\varepsilon^2) + O((a^3\rho_0)^{-5})\right)\rho_{\sigma 0}.$$

Choosing then $\varepsilon = (a^3\rho_0)^{-4}$ we have $\rho_{\sigma 0} \le \tilde{\rho}_\sigma$ and $\tilde{\rho}_\sigma = \rho_{\sigma 0}(1 + O((a^3\rho_0)^{-4}))$ for sufficiently small $a^3\rho_0$. Since $v \ge 0$ the energy is monotone increasing in the particle number, thus so is the energy density. Hence for any $\delta > 0$

$$\begin{aligned} e(\rho_{\uparrow 0}, \rho_{\downarrow 0}) &\le e(\tilde{\rho}_\uparrow, \tilde{\rho}_\downarrow) \\ &\le \frac{3}{5}(6\pi^2)^{2/3}(\tilde{\rho}_\uparrow^{5/3} + \tilde{\rho}_\downarrow^{5/3}) + 8\pi a \tilde{\rho}_\uparrow \tilde{\rho}_\downarrow + O_\delta(a\rho^2(a^3\tilde{\rho})^{1/3-\delta}) \\ &= \frac{3}{5}(6\pi^2)^{2/3}(\rho_{\uparrow 0}^{5/3} + \rho_{\downarrow 0}^{5/3}) + 8\pi a \rho_{\uparrow 0}\rho_{\downarrow 0} + O_\delta(a\rho_0^2(a^3\rho_0)^{1/3-\delta}). \end{aligned}$$

This concludes the proof of Theorem 5.1.2.

Chapter 6

Pressure of a dilute spin-polarized Fermi gas: Lower bound

This chapter contains the paper

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Abstract. We consider a dilute fully spin-polarized Fermi gas at positive temperature in dimensions $d \in \{1,2,3\}$. We show that the pressure of the interacting gas is bounded from below by that of the free gas plus, to leading order, an explicit term of order $a^d\rho^{2+2/d}$, where a is the p-wave scattering length of the repulsive interaction and ρ is the particle density. The results are valid for a wide range of repulsive interactions, including that of a hard core, and uniform in temperatures at most of the order of the Fermi temperature. A central ingredient in the proof is a rigorous implementation of the fermionic cluster expansion of Gaudin, Gillespie and Ripka (Nucl. Phys. A, 176.2 (1971), pp. 237–260).

Contents

6.1 Introduction

The study of dilute quantum gases [GPS08] has received much interest from the mathematical physics community in the recent decades. In particular much work has been done pertaining to the ground state energies of both Fermi and Bose gases in the thermodynamic limit.

For Bose gases in 3 dimensions the leading term of the ground state energy was first shown by Dyson [Dys57] as an upper bound and by Lieb–Yngvason [LY98] as a lower bound. The leading term depends only on the density and the s-wave scattering length of the interaction. More recently the second order correction, known as the Lee–Huang–Yang correction, was shown [FS20; FS23; YY09]. Also the 2-dimensional [FGJMO24; LY01] and 1-dimensional [Age23; ARS22] settings have been studied.

The fermionic setting has been similarly studied in the 3-dimensional [FGHP21; Gia23a; LSS05], [Chapters 3, 4 and 5], 2-dimensional [LSS05], [Chapters 3 and 4], and 1-dimensional [Age23; ARS22], [Chapter 3] case. For fermions the spin is important. For non-zero spin, the leading correction to the energy of the free gas is similar to the leading term for bosons and depends only on the density and the s-wave scattering length of the interaction. For fully spin-polarized (i.e., effectively spin-0) fermions the behaviour is different. By the Pauli exclusion principle the probability of two fermions of the same spin being close enough to interact is suppressed. As such, the leading correction to the energy of the free gas depends on the p-wave scattering length of the interaction instead and is much smaller for dilute gases, which makes its analysis significantly harder.

A natural question to consider is the extension of these results on the ground state energy to positive temperature. This has been done both for bosons [DMS20; HHNST23; MS20; Sei08; Yin10] and non-zero spin fermions [Sei06b]. In this paper we consider the extension for fully spin-polarized fermions. More precisely, we consider the problem of finding the pressure $\psi(\beta,\mu)$ at positive temperature $T = 1/\beta$ and chemical potential μ in the setting of a spin-polarized Fermi gas. We are interested in the dilute limit $a^d\overline{\rho} \ll 1$, where a denotes the p-*wave scattering length* of the interaction and $\overline{\rho}$ denotes the particle density. In this dilute limit we show the lower bound in dimensions $d \in \{1,2,3\}$

$$\psi(\beta,\mu) \geq \psi_0(\beta,\mu) - c_d(\beta\mu)a^d\overline{\rho}^{2+2/d}(1+o(1)) \qquad \text{as } a^d\overline{\rho} \to 0,$$

for an explicit (temperature dependent) coefficient $c_d(\beta\mu)$. Here ψ respectively ψ_0 denote the pressure of the interacting respectively non-interacting system at inverse temperature β and chemical potential μ.

As discussed in more details in Remark 6.1.6 below, the term $c_d(\beta\mu)a^d\overline{\rho}^{2+2/d}$ arises naturally from the two-body interaction and the fact that the two-body density vanishes quadratically for incident particles. In the low-temperature limit $\beta\mu \to \infty$ the coefficients $c_d(\beta\mu)$ converge to the corresponding zero-temperature constants [ARS22], [Chapters 3 and 4]. The temperature dependence of this term can then be understood via the temperature dependence of the two-particle density of the free state.

The result is valid for temperatures T at most of the order of the Fermi temperature $T_F \sim \overline{\rho}^{2/d}$ of the free gas. For larger temperatures one should expect that thermal effects become larger than quantum effects, and thus the gas should behave more like a (high temperature) classical gas. The natural parameter capturing the temperature is the *fugacity* $z = e^{\beta\mu}$. In terms of the fugacity the constraint that the temperature satisfies $T \lesssim T_F$ reads $z \gtrsim 1$.

In contrast, for non-zero spin fermions the pressure in the dilute limit is in 3 dimensions [Sei06b]

$$\psi(\beta,\mu) = \psi_0(\beta,\mu) - 4\pi\left(1-q^{-1}\right) a_s\overline{\rho}^2(1+o(1)) \qquad \text{as } a_s^3\overline{\rho} \to 0,$$

with ψ and ψ_0 the pressures of the interacting respectively non-interacting system, $q \geq 2$ the number of spin sectors and a_s the s-wave scattering length of the interaction. Notably here the coefficient $4\pi(1-q^{-1})$ does not depend on the temperature.

Our method of proof is split in two cases depending on the temperature. For sufficiently small temperatures, the result follows by a simple comparison to the zero-temperature setting and using the result of Chapter 3. In the more interesting case of higher temperatures our method of proof consists of computing the pressure of a Jastrow-type trial state using the rigorous implementation from Chapters 3 and 5 (given in Lemma 6.4.4) of the fermionic cluster expansion of Gaudin–Gillespie–Ripka [GGR71]. (More precisely in Chapters 3 and 5 we found conditions under which the formulas of [GGR71] are convergent.) A similar method was employed in the zero-temperature setting in Chapter 3, with the important difference that, because of the smoothness of the momentum distribution, the condition for convergence we obtain at positive (not too small) temperature is uniform in the volume (see Theorem 6.4.3). Thus we can compute the thermodynamic limit directly, without appealing to a box method of localizing a trial state into large but finite boxes as done in Chapter 3.

6.1.1 Precise statement

To state our main theorem precisely, define the (spin-polarized) fermionic Fock space $\mathcal{F} = \bigoplus_{n=0}^\infty L_a^2\left([0,L]^{dn};\mathbb{C}\right) = \bigoplus_{n=0}^\infty \bigwedge^n L^2\left([0,L]^d;\mathbb{C}\right)$. On this space we define the free Hamiltonian $\mathcal{H}$, the number operator $\mathcal{N}$ and interaction operator $\mathcal{V}$ as follows (in natural units where $\frac{\hbar}{2m} = 1$)

$$\begin{aligned} \mathcal{H} &= (0, H_1, \ldots, H_n, \ldots), & H_n &= \sum_{j=1}^n -\Delta_{x_j}, \\ \mathcal{N} &= (0, 1, \ldots, n, \ldots), \\ \mathcal{V} &= (0, 0, V_2, \ldots, V_n, \ldots), & V_n &= \sum_{1\leq i<j\leq n} v(x_i - x_j). \end{aligned}$$

The interacting Hamiltonian is then $\mathcal{H} + \mathcal{V}$. In the calculations below we will use periodic boundary conditions for convenience. The pressure doesn't depend on the choice of boundary conditions [Rob71] and hence we are free to choose the most convenient ones. We are interested in determining the pressure of the system described by this Hamiltonian at inverse temperature β and chemical potential μ. We denote this by

$$\psi(\beta,\mu) = \lim_{L\to\infty} \sup_{\Gamma} P[\Gamma], \qquad -L^d P[\Gamma] = \mathrm{Tr}_{\mathcal{F}}\left[(\mathcal{H} - \mu\mathcal{N} + \mathcal{V})\Gamma\right] - \frac{1}{\beta}S(\Gamma),$$

where $S(\Gamma) = -\operatorname{Tr}\Gamma\log\Gamma$ is the entropy of the state Γ and $P[\Gamma]$ is the pressure functional. By *state* we mean a density matrix, i.e., a positive trace-class operator on $\mathcal{F}$ of unit trace.

(We suppress from the notation the dependence on the dimension d and the length L.) We denote moreover by

$$\psi_0(\beta,\mu) = \lim_{L\to\infty} \sup_{\Gamma} P_0[\Gamma], \qquad -L^d P_0[\Gamma] = \mathrm{Tr}_{\mathcal{F}}\left[(\mathcal{H}-\mu\mathcal{N})\Gamma\right] - \frac{1}{\beta}S(\Gamma),$$

the pressure and pressure functional of the free gas. The supremum is a maximum and is achieved for the Gibbs state

$$\Gamma = Z^{-1}\exp\left(-\beta(\mathcal{H}-\mu\mathcal{N})\right) = Z^{-1}(\Gamma_0,\Gamma_1,\ldots,\Gamma_n,\ldots), \qquad \Gamma_n = e^{\beta\mu n}e^{-\beta H_n}. \tag{6.1.1}$$

Then [Hua87, Equation (8.63)]

$$\begin{aligned}\psi_0(\beta,\mu) &= \lim_{L\to\infty}\frac{1}{L^d}\left[-\mathrm{Tr}_{\mathcal{F}}\left[(\mathcal{H}-\mu\mathcal{N})\Gamma\right] + \frac{1}{\beta}S(\Gamma)\right] = \lim_{L\to\infty}\frac{1}{L^d\beta}\log Z \\ &= \frac{1}{\beta(2\pi)^d}\int_{\mathbb{R}^d}\log\left(1+e^{\beta\mu-\beta|k|^2}\right)\mathrm{d}k.\end{aligned} \tag{6.1.2}$$

To state our main theorem we moreover define the *p-wave scattering length* a. (See also [LY01, Appendix A] and [SY20, Equations (2.9), (4.3)].)

Definition 6.1.1 (Definitions 3.1.1, 3.1.9 and 3.1.11)**.** The *p-wave scattering length* a of the interaction v in dimension d is defined by

$$c_d a^d = \inf\left\{\int_{\mathbb{R}^d}\left(|\nabla f_0(x)|^2 + \frac{1}{2}v(x)f_0(x)^2\right)|x|^2\,\mathrm{d}x : f_0(x)\to 1 \text{ for } |x|\to\infty\right\},$$

where

$$c_d = \begin{cases} 12\pi & d=3,\\ 4\pi & d=2,\\ 2 & d=1.\end{cases} \tag{6.1.3}$$

The minimizer f_0 is the *p-wave scattering function*. (If $v(x)=+\infty$ for some x [for instance if v has a hard core, $v(x)=+\infty$ for $|x|<R_0$] we interpret $v(x)\,\mathrm{d}x$ as a measure. We suppress from the notation the dependence of a and f_0 on the dimension d.)

The dimensionless parameter measuring the diluteness is then $a^d\overline{\rho}$, with $\overline{\rho}$ the particle density[1] (in infinite volume) given by $\overline{\rho} = \partial_\mu\psi(\beta,\mu)$. We are interested in a dilute limit, meaning that $a^d\overline{\rho}\ll 1$. Moreover, we are considering temperatures $T\lesssim T_F\sim\overline{\rho}^{2/d}$ meaning that $z\gtrsim 1$. As mentioned in the introduction, small z corresponds to a (high-temperature) classical gas.

We shall prove the following theorem.

Theorem 6.1.2. *Let $v\geq 0$ be radial and of compact support. If $d=1$ assume moreover that $\int\left(|\partial f_0|^2 + \frac{1}{2}vf_0^2\right)\mathrm{d}x<\infty$. For any $z_0>0$ there exists $c>0$ such that if $a^d\overline{\rho}_0<c$ then, uniformly in $z=e^{\beta\mu}\geq z_0$, we have the lower bound*

$$\psi(\beta,\mu)\geq\psi_0(\beta,\mu) - 2\pi c_d\frac{-\mathrm{Li}_{d/2+1}(-z)}{(-\mathrm{Li}_{d/2}(-z))^{1+2/d}}a^d\overline{\rho}_0^{2+2/d}\left[1+\delta_d\right],$$

[1] For the sake of simplicity of notation we assume that the derivative $\partial_\mu\psi(\beta,\mu)$ exists. The function $\psi(\beta,\mu)$ being convex in μ always has left and right derivatives. Should these not coincide, we can just replace instances of $\partial_\mu\psi(\beta,\mu)$ with either the left or right derivative.

where $\overline{\rho}_0 = \partial_\mu \psi_0(\beta,\mu)$ is the particle density of the free gas (in infinite volume), the constants c_d are defined in Equation (6.1.3) *and*

$$|\delta_d| \leq \begin{cases} C(a^3\overline{\rho}_0)^{1/39} \left|\log a^3\overline{\rho}_0\right|^{12/13} & d=3, \\ C(a^2\overline{\rho}_0)^{1/5} \left|\log a^2\overline{\rho}_0\right|^{6/5} & d=2, \\ C(a\overline{\rho}_0)^{1/7} \left|\log a\overline{\rho}_0\right|^{12/7} & d=1. \end{cases} \tag{6.1.4}$$

Here Li_s denotes the *polylogarithm*. It satisfies [NIS, Equation 25.12.16]

$$-\mathrm{Li}_s(-e^x) = \frac{1}{\Gamma(s)} \int_0^\infty \frac{t^{s-1}}{e^{t-x}+1} \,\mathrm{d}t \tag{6.1.5}$$

with Γ the Gamma function.

We expect that the lower bound of Theorem 6.1.2 is in fact an equality (with a potentially different bound on the error term). It remains an open problem to prove this.

Remark 6.1.3. For better comparison with the zero-temperature result in Chapter 3, we find it convenient to write the correction to the pressure of the free gas in terms of the particle density (of the free gas) $\overline{\rho}_0$. The latter is given explicitly as

$$\overline{\rho}_0 = -\frac{1}{(4\pi\beta)^{d/2}} \mathrm{Li}_{d/2}(-z) \tag{6.1.6}$$

This follows from an elementary computation, which we give in Lemma 6.3.6 below.

To leading order $\overline{\rho} \simeq \overline{\rho}_0$. More precisely

Corollary 6.1.4. *Under the same assumptions as in Theorem 6.1.2 we have for the particle density*[2] $\overline{\rho} = \partial_\mu \psi(\beta,\mu)$

$$\overline{\rho} = \overline{\rho}_0 \left[1 + O((a^d\overline{\rho}_0)^{1/2})\right].$$

We shall give the proof at the end of this section. In particular the conditions of small $a^d\overline{\rho}$ and of small $a^d\overline{\rho}_0$ are equivalent. Moreover, the error terms of Theorem 6.1.2 can equally well be written with $\overline{\rho}_0$ replaced by $\overline{\rho}$.

Remark 6.1.5. The additional assumption on v in dimension $d=1$ is discussed in Remark 3.1.13. If v is either smooth or has a hard core (meaning that $v(x) = +\infty$ for $|x| \leq a_0$ for some $a_0 > 0$) this assumption is satisfied.

Remark 6.1.6. The term of order $a^d\overline{\rho}_0^{2+2/d}$ depends on the temperature. This is different to the setting of spin-$\frac{1}{2}$ fermions, where the analogous term (in 3 dimensions) is $2\pi a\overline{\rho}_0^2$ [Sei06b] uniformly in the temperature. That the term of order $a^d\overline{\rho}_0^{2+2/d}$ should depend on the temperature may be heuristically understood as follows: This term arises from the fact that the two-body density vanishes quadratically for incident particles. The rate at which it vanishes depends on the exact state, and thus the temperature. Concretely, the two-particle density of the free gas (in infinite volume) satisfies

$$\overline{\rho}^{(2)}(x_1,x_2) = 2\pi \frac{-\mathrm{Li}_{d/2+1}(-z)}{(-\mathrm{Li}_{d/2}(-z))^{1+2/d}} \overline{\rho}_0^{2+2/d} |x_1-x_2|^2 \left[1 + O\left(\overline{\rho}_0^{2/d}|x_1-x_2|^2\right)\right], \tag{6.1.7}$$

[2] Should the left and right derivatives of $\psi(\beta,\mu)$ not coincide, the statement holds for either derivative.

where $O\left(\overline{\rho}_0^{-2/d}|x_1-x_2|^2\right)$ is understood as being bounded by $C\overline{\rho}_0^{-2/d}|x_1-x_2|^2$ uniformly. This follows from an elementary computation, which we give in Lemma 6.3.6 below.

In the low-temperature limit $z\to\infty$ we recover the zero-temperature constants in the terms of order $a^d\overline{\rho}_0^{2+2/d}$. The zero-temperature results read (Theorems 3.1.3, 3.1.10 and 3.1.12)

$$e(\overline{\rho}_0) \le e_0(\overline{\rho}_0) + c_{0,d}a^d\overline{\rho}_0^{2+2/d}[1+\delta_d],$$

with $e(\overline{\rho}_0), e_0(\overline{\rho}_0)$ denoting the ground state energy density of the interacting respectively the free gas and

$$c_{0,d} = \begin{cases} \frac{12\pi}{5}(6\pi^2)^{2/3} & d=3, \\ 4\pi^2 & d=2, \\ \frac{2\pi^2}{3} & d=1, \end{cases} \qquad |\delta_d| \lesssim \begin{cases} a^2\overline{\rho}^{2/3} & d=3, \\ a^2\overline{\rho}_0\left|\log a^2\overline{\rho}_0\right|^2 & d=2, \\ (a\overline{\rho}_0)^{13/17} & d=1. \end{cases} \tag{6.1.8}$$

Indeed, we claim that

$$2\pi c_d \frac{-\operatorname{Li}_{d/2+1}(-z)}{(-\operatorname{Li}_{d/2}(-z))^{1+2/d}} = c_{0,d} + O((\log z)^{-2}) \quad \text{as } z\to\infty. \tag{6.1.9}$$

To see this write (following [Woo92])

$$\begin{aligned}
-\operatorname{Li}_s(-e^x) &= \frac{1}{\Gamma(s)}\int_0^\infty \frac{t^{s-1}}{e^{t-x}+1}\,\mathrm{d}t \\
&= \frac{1}{\Gamma(s)}\left[\int_0^x t^{s-1}\,\mathrm{d}t - \int_0^x \frac{t^{s-1}}{e^{x-t}+1}\,\mathrm{d}t + \int_x^\infty \frac{t^{s-1}}{e^{t-x}+1}\,\mathrm{d}t\right] \\
&= \frac{x^s}{\Gamma(s+1)} - \frac{1}{\Gamma(s)}\int_0^x \frac{(x-u)^{s-1}-(x+u)^{s-1}}{e^u+1}\,\mathrm{d}u - \frac{1}{\Gamma(s)}\int_x^\infty \frac{(x+u)^{s-1}}{e^u+1}\,\mathrm{d}u
\end{aligned}$$

where we changed variables $t=x\pm u$. The middle and last integrals can easily be bounded as $O(x^{s-2})$ and $O(x^se^{-x})$ respectively. Thus

$$-\operatorname{Li}_s(-e^x) = \frac{x^s}{\Gamma(s+1)} + O(x^{s-2}), \tag{6.1.10}$$

and Equation (6.1.9) follows.

Remark 6.1.7. The error bounds in Theorem 6.1.2 are uniform in z. They arise as the worst cases of two types of bounds, one good for $z\sim 1$ and one good for $z\gg 1$. In particular, for concrete values of z, the error bounds can be improved. See Propositions 6.1.8 and 6.1.9 below.

Finally we give the

Proof of Corollary 6.1.4. Note that $\psi(\beta,\mu)$ is a convex function of μ. Thus we may bound its derivative by any difference quotient. More precisely for any $\varepsilon>0$ we have

$$\overline{\rho} = \partial_\mu\psi(\beta,\mu) \le \frac{\psi(\beta,\mu+\varepsilon)-\psi(\beta,\mu)}{\varepsilon}.$$

Using the trivial upper bound $\psi(\beta,\mu+\varepsilon)\leq\psi_0(\beta,\mu+\varepsilon)$ (which is a consequence of the assumed non-negativity of the interaction potential v) and the lower bound of Theorem 6.1.2 we conclude that

$$\overline{\rho}\leq\frac{\psi_0(\beta,\mu+\varepsilon)-\psi_0(\beta,\mu)}{\varepsilon}+Ca^d\overline{\rho}_0^{2+2/d}\varepsilon^{-1}=\overline{\rho}_0+O\left(\left|\partial_\mu^2\psi_0\right|\varepsilon\right)+O\left(a^d\overline{\rho}_0^{2+2/d}\varepsilon^{-1}\right).$$

Using the explicit formula for $\overline{\rho}_0=\partial_\mu\psi_0$ and optimising in ε we get that $\overline{\rho}\leq\overline{\rho}_0(1+O((a^d\overline{\rho}_0)^{1/2}))$. For $\varepsilon<0$ the argument is analogous only the direction of the inequalities is reversed. $\square$

6.1.2 Strategy of the proof

To prove Theorem 6.1.2 we distinguish two cases. That of a "low-temperature" setting and that of a "high-temperature" setting. For sufficiently small temperatures we compare to the ground state energy studied in Chapter 3. For larger temperatures we consider a specific trial state Γ_J of Jastrow-type (defined in Equation (6.3.1) below) and compute the pressure functional evaluated on this trial state. For these computations we use the rigorous implementation from Chapters 3 and 5 of the formal cluster expansion of Gaudin–Gillespie–Ripka [GGR71].

Temperature-dependent errors naturally arise as powers of $\zeta:=1+|\log z|$. We shall prove the following propositions.

Proposition 6.1.8. *Let $v\geq 0$ be radial and of compact support. If $d=1$ assume moreover that $\int\left(|\partial f_0|^2+\frac{1}{2}vf_0^2\right)\mathrm{d}x<\infty$. Then for sufficiently small $a^d\overline{\rho}_0$ and large $z=e^{\beta\mu}$ we have*

$$\psi(\beta,\mu)\geq\psi_0(\beta,\mu)-2\pi c_d\frac{-\operatorname{Li}_{d/2+1}(-z)}{(-\operatorname{Li}_{d/2}(-z))^{1+2/d}}a^d\overline{\rho}_0^{2+2/d}\left[1+\delta_d\right] \tag{6.1.11}$$

where $\overline{\rho}_0$ is the particle density of the free gas, c_d is defined in Equation (6.1.3) *and*

$$|\delta_d|\lesssim\begin{cases}a^2\overline{\rho}_0^{2/3} & +(a^3\overline{\rho}_0)^{-1}\zeta^{-2} \quad d=3,\\ a^2\overline{\rho}_0\left|\log a^2\overline{\rho}_0\right|^2 & +(a^2\overline{\rho}_0)^{-1}\zeta^{-2} \quad d=2,\\ (a\overline{\rho}_0)^{9/13} & +(a\overline{\rho}_0)^{-1}\zeta^{-2} \quad d=1.\end{cases} \tag{6.1.12}$$

Proposition 6.1.9. *Let $v\geq 0$ be radial and of compact support. If $d=1$ assume moreover that $\int\left(|\partial f_0|^2+\frac{1}{2}vf_0^2\right)\mathrm{d}x<\infty$. Then for $z=e^{\beta\mu}$ satisfying $z\gtrsim 1$ there exists a constant $c>0$ such that if $a^d\overline{\rho}_0<c$ and $a^d\overline{\rho}_0\zeta^{d/2}\left|\log a^d\overline{\rho}_0\right|<c$ then*

$$\psi(\beta,\mu)\geq\psi_0(\beta,\mu)-2\pi c_d\frac{-\operatorname{Li}_{d/2+1}(-z)}{(-\operatorname{Li}_{d/2}(-z))^{1+2/d}}a^d\overline{\rho}_0^{2+2/d}\left[1+\delta_d\right],$$

where $\overline{\rho}_0$ is the particle density of the free gas, c_d is defined in Equation (6.1.3) *and*

$$|\delta_d|\lesssim\begin{cases}(a^3\overline{\rho}_0)^{6/15}\zeta^{-3/5}+(a^3\overline{\rho}_0)\zeta^{1/2}\left|\log a^3\overline{\rho}_0\right|^2+(a^3\overline{\rho}_0)^{7/3}\zeta^{9/2}\left|\log a^3\overline{\rho}_0\right|^3 & d=3,\\ (a^2\overline{\rho}_0)^{1/2}\zeta^{-1/2}+(a^2\overline{\rho}_0)\zeta\left|\log a^2\overline{\rho}_0\right|+(a^2\overline{\rho}_0)^2\zeta^3\left|\log a^2\overline{\rho}_0\right|^3, & d=2,\\ (a\overline{\rho}_0)^{1/2}\left|\log a\overline{\rho}_0\right|^{1/2}+a\overline{\rho}_0\zeta^{3/2}\left|\log a\overline{\rho}_0\right|^3 & d=1.\end{cases} \tag{6.1.13}$$

Proposition 6.1.8 is a simple corollary of Theorems 3.1.3, 3.1.10 and 3.1.12, extending the result to small positive temperatures. Proposition 6.1.9 is the main new result of this paper. Most of the rest of the paper is concerned with the proof of Proposition 6.1.9. Theorem 6.1.2 is an immediate consequence:

Proof of Theorem 6.1.2. We use the lower bound in Proposition 6.1.8 for

$$\zeta \geq \zeta_0 := \begin{cases} (a^3\overline{\rho}_0)^{-20/39} \left|\log a^3\overline{\rho}_0\right|^{-6/13} & d=3, \\ (a^2\overline{\rho}_0)^{-3/5} \left|\log a^2\overline{\rho}_0\right|^{-3/5} & d=2, \\ (a\overline{\rho}_0)^{-4/7} \left|\log a\overline{\rho}_0\right|^{-6/7} & d=1 \end{cases}$$

and the lower bound in Proposition 6.1.9 otherwise. Theorem 6.1.2 follows. □

We note that for $\zeta \sim \zeta_0$ the last of the summands in Equation (6.1.13) (in all dimensions) dominate the error term in Proposition 6.1.9.

Remark 6.1.10. The proof of Proposition 6.1.9 uses the Gaudin–Gillespie–Ripka expansion. This expansion consists of formulas for the normalization constant Z_J (defined in Equation (6.3.1) below) and the reduced densities of the state Γ_J, see Theorem 6.4.3. Both Z_J and the reduced densities are given as infinite series of diagrams (defined in Definition 6.4.1). Using these formulas the "smallest" diagrams give the corrections of Proposition 6.1.9 and the remaining diagrams are error terms. To bound the error terms we calculate the values of (finitely many) "small" diagrams and give crude bounds for all (infinitely many) "larger" diagrams.

Remark 6.1.11. We expect that with the method presented here one could improve the error bounds in Proposition 6.1.9 (and consequently Theorem 6.1.2) slightly by treating more diagrams in the Gaudin–Gillespie–Ripka expansion as small, i.e. calculating their values more precisely. See also Remark 3.1.8. This is similar to what is done in [BCGOPS23] and Chapter 5. (In [BCGOPS23] the hard core Bose gas is treated with a method similar to a cluster expansion. Using such an expansion to sufficiently high order proves the bounds of [BCGOPS23].)

More precisely we expect that by treating more diagrams as small one could improve the bounds in Proposition 6.1.9 to

$$|\delta_d| \lesssim O\left(\begin{cases} (a^3\overline{\rho}_0)^{6/15}\zeta^{-3/5} & d=3 \\ (a^2\overline{\rho}_0)^{1/2}\zeta^{-1/2} & d=2 \\ (a\overline{\rho}_0)^{1/2} \left|\log a\overline{\rho}_0\right|^{1/2} & d=1 \end{cases}\right) + O\left((a^d\overline{\rho}_0)^{-2/d}\left(a^d\overline{\rho}_0\zeta^{d/2}\left|\log a^d\overline{\rho}_0\right|\right)^n\right) \tag{6.1.14}$$

for any n. This would then propagate to better error terms in Theorem 6.1.2. More precisely, by using the bound in Proposition 6.1.8 for $\zeta \geq \zeta_0$ and the bound in Proposition 6.1.9 with error improved as in Equation (6.1.14) otherwise and optimising in ζ_0 one would improve the error bound in Theorem 6.1.2 to

$$|\delta_d| \lesssim \begin{cases} C_\varepsilon(a^3\overline{\rho}_0)^{1/3-\varepsilon} & d=3, \\ (a^2\overline{\rho}_0)^{1/2} & d=2, \\ (a\overline{\rho}_0)^{1/2} \left|\log a\overline{\rho}_0\right|^{1/2} & d=1 \end{cases}$$

for any $\varepsilon > 0$, where C_ε depends on ε, by taking n sufficiently large in Equation (6.1.14).

The first terms in Equation (6.1.14) come from the precise evaluation of certain small diagrams. In dimension $d = 2, 3$ one should not expect to get better bounds than this using the method presented here. In dimension $d = 1$ one might be able to do a more precise analysis, see Remark 6.5.6, and thus improve the bound.

The proof of Proposition 6.1.8 will be given in in Section 6.2. It is mostly independent of the rest of the paper (Sections 6.3, 6.4 and 6.5) which is devoted to the proof of Proposition 6.1.9.

Structure of the paper: First, in Section 6.2 we give the proof of Proposition 6.1.8. Then, in Section 6.3 we define the trial state Γ_J and give some preliminary computations. Next, in Section 6.4 we compute reduced densities of the trial state Γ_J using the (rigorous implementation of the) Gaudin–Gillespie–Ripka expansion. Finally, in Section 6.5 we calculate the individual terms in the pressure functional and prove Proposition 6.1.9. In Section 6.A we show that Γ_J has particle density $\approx \overline{\rho}_0$.

6.2 Low temperature

In this section we prove Proposition 6.1.8 by comparing to the zero-temperature problem.

Proof of Proposition 6.1.8. The pressures ψ, ψ_0 (of the interacting and non-interacting gas, respectively) are the Legendre transforms of the corresponding free energy densities ϕ, ϕ_0. That is,

$$\begin{aligned} \psi(\beta,\mu) &= \sup_{\tilde{\rho}} \left[\tilde{\rho}\mu - \phi(\beta,\tilde{\rho})\right] \geq \overline{\rho}_0\mu - \phi(\beta,\overline{\rho}_0) \\ \psi_0(\beta,\mu) &= \sup_{\tilde{\rho}} \left[\tilde{\rho}\mu - \phi_0(\beta,\tilde{\rho})\right] = \overline{\rho}_0\mu - \phi_0(\beta,\overline{\rho}_0) \end{aligned} \tag{6.2.1}$$

with $\overline{\rho}_0$ the density of the free gas at chemical potential μ and inverse temperature β, given in Equation (6.1.6). We may trivially bound the free energy density by the ground state energy density e. The latter is bounded from above in Theorems 3.1.3, 3.1.10 and 3.1.12. That is,

$$\phi(\beta,\overline{\rho}_0) \leq e(\overline{\rho}_0) \leq e_0(\overline{\rho}_0) + c_{0,d}a^d\overline{\rho}_0^{2+2/d}[1+\delta_d], \tag{6.2.2}$$

with $e_0(\overline{\rho}_0)$ denoting the ground state energy density of the free gas and $c_{0,d}$ and δ_d as in Equation (6.1.8). By a straightforward calculation, the ground state energy density of the free gas is

$$e_0(\overline{\rho}_0) = 4\pi\frac{d^{2/d}}{d+2}\left(\frac{d}{2}\right)^{2/d}\Gamma(d/2)^{2/d}\overline{\rho}_0^{1+2/d}.$$

By Equations (6.1.2), (6.1.6) and (6.1.10) we have for large $z = e^{\beta\mu}$ (see also [Hua87, Equation (11.31)])

$$\begin{aligned} \psi_0(\beta,\mu) &= \beta^{-1-d/2}\frac{\left|\mathbb{S}^{d-1}\right|\Gamma(d/2)}{2(2\pi)^d}(-\operatorname{Li}_{d/2+1}(-e^{\beta\mu})) \\ &= 4\pi\overline{\rho}_0^{1+2/d}\frac{-\operatorname{Li}_{d/2+1}(-e^{\beta\mu})}{(-\operatorname{Li}_{d/2}(-e^{\beta\mu}))^{1+2/d}} = \frac{2}{d}e_0(\overline{\rho}_0) + O\left(\overline{\rho}_0^{1+2/d}(\beta\mu)^{-2}\right) \end{aligned}$$

where $\left|\mathbb{S}^{d-1}\right| = \frac{2\pi^{d/2}}{\Gamma(d/2)}$ is the area of the $(d-1)$-sphere. Thus

$$\phi_0(\beta,\overline{\rho}_0) = \overline{\rho}_0\mu - \psi_0(\beta,\mu) = e_0 + O\left(\overline{\rho}_0^{1+2/d}(\beta\mu)^{-2}\right).$$

Combining this with Equations (6.2.1) and (6.2.2) we conclude the proof of Proposition 6.1.8. □

The rest of the paper concerns the proof of Proposition 6.1.9. We start with some preliminary computations.

6.3 Preliminaries

To prove Proposition 6.1.9 we will consider a finite system on a cubic box of side length L with periodic boundary conditions and bound $\psi(\beta,\mu)$ from below by the pressure functional evaluated on the trial state

$$\Gamma_J = \frac{Z}{Z_J} F\Gamma F, \qquad F = \bigoplus_{n=0}^{\infty} F_n, \qquad F_n = \prod_{1\le i<j\le n} f(x_i - x_j), \tag{6.3.1}$$

where f is some cut-off and rescaled scattering function defined in Equation (6.3.2) below, where Γ is defined in Equation (6.1.1), and where Z_J is such that this is normalised with $\operatorname{Tr}\Gamma_J = 1$. Concretely, on the n-particle space Γ_J acts via the kernel

$$Z_J^{-1} F_n(X_n)\Gamma_n(X_n,Y_n)F_n(Y_n).$$

(Recall that Γ acts via the kernel $Z^{-1}\Gamma_n(X_n,Y_n)$.) The function f is more precisely

$$f(x) = \begin{cases} \frac{1}{1-a^d/b^d} f_0(x) & |x|\le b \\ 1 & |x| \ge b \end{cases} \tag{6.3.2}$$

where $f_0(x)$ is the p-wave scattering function defined in Definition 6.1.1 and b is a length to be chosen later. We will choose $a \ll b \le C\rho_0^{-1/d}$. Here and in the following ρ_0 denotes the particle density of the free gas in finite volume. In particular for $a^d\rho_0$ small enough b is larger than the range of v and so f is continuous (since $f_0(x) = 1 - \frac{a^3}{|x|^3}$ for x outside the support of v).

Notation 6.3.1.

- We will denote expectation values of operators in the free state Γ by $\langle\cdot\rangle_0$ and in the trial state Γ_J by $\langle\cdot\rangle_J$. That is, $\langle\mathcal{A}\rangle_0 = \operatorname{Tr}_{\mathcal{F}}[\mathcal{A}\Gamma]$ and $\langle\mathcal{A}\rangle_J = \operatorname{Tr}_{\mathcal{F}}[\mathcal{A}\Gamma_J]$ for any operator $\mathcal{A}$ on $\mathcal{F}$.
- We denote $g(x) = f(x)^2 - 1$.
- For any function h we write $h_e = h_{ij} = h(x_i - x_j)$ for an edge $e = (i,j)$.
- Moreover we write $\gamma_e^{(1)} = \gamma_{ij}^{(1)} = \gamma^{(1)}(x_i;x_j)$ for an edge $e=(i,j)$, where $\gamma^{(1)}$ is the 1-particle density matrix of Γ defined in Equation (6.3.4) below (see also Notation 6.3.3).
- We write $X_n = (x_1,\ldots,x_n)$ and $X_{[n,m]} = (x_n,\ldots,x_m)$ if $n\le m$. For $n>m$ then $X_{[n,m]} = \varnothing$.

Remark 6.3.2. The trial state Γ_J does not have (average) particle density ρ_0. However we have that

$$\frac{1}{L^d}\langle\mathcal{N}\rangle_J = \rho_0\left(1 + O(a^d b^2 \rho_0^{1+2/d}) + O\left((a^d\rho_0)^2\zeta^d(\log b/a)^2\right)\right). \tag{6.3.3}$$

This is not needed for the proof of Proposition 6.1.9, however. We give the proof of (6.3.3) in Section 6.A.

We normalize q-particle density matrices of a general state $\tilde\Gamma = (\tilde\Gamma_0,\tilde\Gamma_1,\ldots)$ as

$$\gamma_{\tilde\Gamma}^{(q)}(X_q;Y_q) = \sum_{n=q}^{\infty}\frac{n!}{(n-q)!}\int\!\!\cdots\!\!\int \tilde\Gamma_n(X_q,X_{[q+1,n]};Y_q,X_{[q+1,n]})\,\mathrm{d}X_{[q+1,n]}. \tag{6.3.4}$$

Notation 6.3.3. For the Gibbs state $\Gamma = (Z^{-1}\Gamma_0, Z^{-1}\Gamma_1, \ldots)$ and the trial state Γ_J we denote their q-particle density matrices by $\gamma^{(q)}(X_q;Y_q) = \gamma^{(q)}_{\Gamma}(X_q;Y_q)$ and $\gamma^{(q)}_J(X_q;Y_q) = \gamma^{(q)}_{\Gamma_J}(X_q;Y_q)$ respectively. The same applies to the q-particle densities, being then denoted $\rho^{(q)}$ and $\rho^{(q)}_J$.

The Gibbs state Γ is quasi-free and particle preserving. Thus by Wick's rule (see [BR97, Section 5.2.4], [Sol14, Theorem 10.2]) we have for the q-particle density

$$\rho^{(q)}(X_q) = \gamma^{(q)}(X_q;X_q) = \det\left[\gamma^{(1)}_{ij}\right]_{1\le i,j\le q}.$$

Moreover, by translation invariance, we have that $\gamma^{(1)}(x;y)$ is a function of $x-y$ only. With a slight abuse of notation we then write

$$\gamma^{(1)}(x;y) = \gamma^{(1)}(x-y) = \frac{1}{L^d}\sum_{k\in\frac{2\pi}{L}\mathbb{Z}^d}\hat{\gamma}^{(1)}(k)e^{-ik(x-y)}.$$

A simple calculation shows that (see [Hua87, Equation (8.65)])

$$\hat{\gamma}^{(1)}(k) = \frac{ze^{-\beta|k|^2}}{1+ze^{-\beta|k|^2}} = \frac{e^{\beta\mu-\beta|k|^2}}{1+e^{\beta\mu-\beta|k|^2}}.$$

For the proof of Proposition 6.1.9 we compute the pressure of the trial state Γ_J. We have

$$\begin{aligned}\psi(\beta,\mu) &\ge \limsup_{L\to\infty}\frac{1}{L^d}\left[-\langle\mathcal{H}-\mu\mathcal{N}+\mathcal{V}\rangle_J + \frac{1}{\beta}S(\Gamma_J)\right]\\ &= \limsup_{L\to\infty}\frac{1}{L^d}\left[-\langle\mathcal{H}\rangle_J - \mu\langle\mathcal{N}\rangle_J - \frac{1}{2}\iint v_{12}\rho^{(2)}_J \,\mathrm{d}x_1\,\mathrm{d}x_2 + \frac{1}{\beta}S(\Gamma_J)\right],\end{aligned}\tag{6.3.5}$$

where $\rho^{(2)}_J$ is the two-body reduced density of the trial state Γ_J. We calculate $\rho^{(2)}_J$ in Section 6.4 using the Gaudin–Gillespie–Ripka expansion and we compute the individual terms of Equation (6.3.5) in Section 6.5 below. First, however, we need some preliminary bounds.

6.3.1 Useful bounds

We recall some useful bounds on the scattering function (defined in Equation (6.3.2)) from Chapter 3.

Lemma 6.3.4. *The scattering function f satisfies*

$$\int\left|1-f(x)^2\right||x|^n\,\mathrm{d}x \le \begin{cases} Ca^d\log b/a & n=0\\ Ca^db^n & n>0\end{cases}\tag{6.3.6}$$

$$\int\left(|\nabla f(x)|^2+\frac{1}{2}v(x)f(x)^2\right)|x|^2\,\mathrm{d}x = c_da^d\left(1+O(a^d/b^d)\right)\tag{6.3.7}$$

$$\int\left(|\nabla f(x)|^2+\frac{1}{2}v(x)f(x)^2\right)|x|^n\,\mathrm{d}x \le \begin{cases} Ca^{n+d-2} & n+d\le 2d+1\\ Ca^{n+d-2}\log b/a & n+d=2d+2\\ Ca^{2d}b^{n-d-2} & n+d\ge 2d+3\end{cases}\tag{6.3.8}$$

$$\left|\int f(x)\left|\nabla f(x)\right||x|^n\,\mathrm{d}x\right| \le \begin{cases} Ca^{d-1} & n=0\\ Ca^d\log b/a & n=1\\ Ca^db^{n-1} & n\ge 2\end{cases}\tag{6.3.9}$$

where c_d is defined in Equation (6.1.3).

Proof. Equations (6.3.6), (6.3.7), (6.3.8) and (6.3.9) all follow from the definition of the scattering length, Definition 6.1.1, and the bounds [LY01, Lemma A.1], Lemma 3.2.2

$$\left[1-\frac{a^d}{|x|^d}\right]_+ \le f_0(x) \le 1, \qquad |\nabla f_0(x)| \le \frac{da^d}{|x|^{d+1}} \quad \text{for } |x|>a$$

where the left inequality in the first inequality is an equality for x outside the support of v. We refer to (3.4.1)–(3.4.6) for a detailed proof. □

We will need the following technical lemma.

Lemma 6.3.5. *Let $\hat\gamma(k) = ze^{-\beta|k|^2}$. Let p,n,m be non-negative integers with $1\le n\le m$. Then*

$$\frac{1}{L^d}\sum_{k\in\frac{2\pi}{L}\mathbb{Z}^d}\frac{|k|^p\hat\gamma(k)^n}{(1+\hat\gamma(k))^m} = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}\frac{|k|^p\hat\gamma(k)^n}{(1+\hat\gamma(k))^m}\,\mathrm{d}k + O\left(L^{-1}\beta\max\left\{\beta^{-1},\mu\right\}^{\frac{p+d+1}{2}}\right)$$
$$\le C\max\left\{\beta^{-1},\mu\right\}^{\frac{p+d}{2}}$$

for $z=e^{\beta\mu}\gtrsim 1$ and L sufficiently large.

Note that $\hat\gamma(k)\ne\hat\gamma^{(1)}(k)$. In fact, $\hat\gamma^{(1)}(k)=\frac{\hat\gamma(k)}{1+\hat\gamma(k)}$.

Proof. We interpret the sum as a Riemann sum and compare it with its corresponding integral

$$I_{p,n,m} := \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}\frac{|k|^p\hat\gamma(k)^n}{(1+\hat\gamma(k))^m}\,\mathrm{d}k$$

Writing $F_{p,n,m}(k)=\frac{|k|^p\hat\gamma(k)^n}{(1+\hat\gamma(k))^m}$ then

$$\begin{aligned}&\frac{1}{L^d}\sum_{k\in\frac{2\pi}{L}\mathbb{Z}^d}\frac{|k|^p\hat\gamma(k)^n}{(1+\hat\gamma(k))^m}\\ &\quad= \frac{1}{(2\pi)^d}\sum_{k\in\frac{2\pi}{L}\mathbb{Z}^d}\int_{\left[-\frac{\pi}{L},\frac{\pi}{L}\right]^d}\left(F_{p,n,m}(k+\xi)-\int_0^1\partial_t F_{p,n,m}(k+t\xi)\,\mathrm{d}t\right)\mathrm{d}\xi\end{aligned}$$

The first term is the integral $I_{p,n,m}$. For the second term we may bound by direct computation (defining $F_{p,n,m}=0$ for $p<0$)

$$\begin{aligned}|\partial_t F_{p,n,m}(k+t\xi)| &\le C|\xi|\left[F_{p-1,n,m}(k+t\xi)+\beta F_{p+1,n,m}(k+t\xi)\right]\\ &\le C|\xi|e^{C\beta|\xi||k+\xi|+C\beta|\xi|^2}\left[F_{p-1,n,m}(k+\xi)+\beta F_{p+1,n,m}(k+\xi)\right].\end{aligned}$$

That is, the second term is bounded by the integral

$$CL^{-1}e^{CL^{-2}\beta}\int_{\mathbb{R}^d}e^{CL^{-1}\beta|k|}(F_{p-1,n,m}(k)+\beta F_{p+1,n,m}(k))\,\mathrm{d}k.$$

Next, to bound the integral, we note that $F_{p,n,m}\le F_{p,1,1}$. First, consider $z\ge e$, i.e. $\beta\mu\ge 1$. Then we bound

$$\begin{aligned}&\int_{\mathbb{R}^d}e^{CL^{-1}\beta|k|}F_{p,1,1}(k)\,\mathrm{d}k\\ &\quad\le C\int_0^{\sqrt{2\mu}}e^{CL^{-1}\beta k}k^{p+d-1}\,\mathrm{d}k + C\int_{\sqrt{2\mu}}^\infty e^{CL^{-1}\beta k}k^{p+d-1}e^{-\beta(k^2-\mu)}\,\mathrm{d}k\\ &\quad\le C\mu^{\frac{p+d}{2}}e^{CL^{-1}\beta\mu^{1/2}} + C\beta^{-\frac{p+d}{2}}\int_{\sqrt{\beta\mu}}^\infty t^{p+d-1}e^{-t^2+CL^{-1}\beta^{1/2}t}\,\mathrm{d}t \le C\mu^{\frac{p+d}{2}}\end{aligned}$$

for L sufficiently large.

Next, for $z < e$ we bound

$$\begin{aligned}\int_{\mathbb{R}^d} e^{CL^{-1}\beta|k|} F_{p,1,1}(k)\,\mathrm{d}k &\le C\int_0^\infty e^{CL^{-1}\beta k} k^{p+d-1} z e^{-\beta k^2}\,\mathrm{d}k \\ &\le C\beta^{-\frac{p+d}{2}} \int_0^\infty t^{p+d-1} e^{-t^2+CL^{-1}\beta^{1/2}t}\,\mathrm{d}t \le C\beta^{-\frac{p+d}{2}}\end{aligned}$$

for L sufficiently large. The equality in the lemma follows. We may bound $I_{p,n,m}$ in a similar manner and conclude the proof of the lemma. □

Finally, we have the following lemma for the reduced densities of the free state.

Lemma 6.3.6. *The reduced densities of the free Fermi gas satisfy*

$$\rho^{(1)}(x_1) = \rho_0 = \frac{1}{(4\pi)^{d/2}}\beta^{-d/2}(-\operatorname{Li}_{d/2}(-z))\left[1 + O(L^{-1}\zeta\rho_0^{-1/d})\right], \tag{6.3.10}$$

$$\begin{aligned}\rho^{(2)}(x_1,x_2) &= 2\pi\frac{-\operatorname{Li}_{d/2+1}(-z)}{(-\operatorname{Li}_{d/2}(-z))^{1+2/d}}\rho_0^{2+2/d}|x_1-x_2|^2 \\ &\quad\times\left[1 + O(\rho_0^{2/d}|x_1-x_2|^2) + O(L^{-1}\zeta\rho_0^{-1/d})\right].\end{aligned} \tag{6.3.11}$$

Equations (6.3.10) and (6.3.11) are the finite volume analogues of Equations (6.1.6) and (6.1.7).

Remark 6.3.7. Note that $\beta \sim \zeta\rho_0^{-2/d}$. (Recall that $\zeta = 1 + |\log z|$.) Indeed, for $z \le C$ this is clear from Equation (6.3.10). For $z \gg 1$ this follows from the asymptotics of the polylogarithm, Equation (6.1.10). Moreover, for $\beta\mu \ge 1$ then $\mu \sim \rho_0^{2/d}$. In particular then Lemma 6.3.5 may be reformulated as

$$\frac{1}{L^d}\sum_{k\in\frac{2\pi}{L}\mathbb{Z}^d}\frac{|k|^p\hat{\gamma}(k)^n}{(1+\hat{\gamma}(k))^m} = \frac{1}{L^d}\sum_{k\in\frac{2\pi}{L}\mathbb{Z}^d}\frac{|k|^p z^n e^{-n\beta|k|^2}}{(1+ze^{-\beta|k|^2})^m} \le C\rho_0^{1+p/d} \tag{6.3.12}$$

for $z \gtrsim 1$ and L sufficiently large. This is the form we will later use.

Proof. By translation invariance

$$\rho_0 = \frac{\langle\mathcal{N}\rangle_0}{L^d} = \frac{1}{L^d}\int \rho^{(1)}(x)\,\mathrm{d}x = \rho^{(1)}(0).$$

Moreover, by Lemma 6.3.5

$$\begin{aligned}\rho^{(1)}(0) &= \frac{1}{L^d}\sum_{k\in\frac{2\pi}{L}\mathbb{Z}^d}\frac{e^{\beta\mu-\beta|k|^2}}{1+e^{\beta\mu-\beta|k|^2}} \\ &= \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d}\frac{ze^{-\beta|k|^2}}{1+ze^{-\beta|k|^2}}\,\mathrm{d}k + O\left(L^{-1}\beta\max\left\{\beta^{-1},\mu\right\}^{\frac{d+1}{2}}\right) \\ &= \frac{\Gamma(d/2)\left|\mathbb{S}^{d-1}\right|}{2(2\pi)^d}\beta^{-d/2}(-\operatorname{Li}_{d/2}(-z))\left(1 + O\left(L^{-1}\beta\max\left\{\beta^{-1},\mu\right\}^{1/2}\right)\right)\end{aligned}$$

where $\left|\mathbb{S}^{d-1}\right| = \frac{2\pi^{d/2}}{\Gamma(d/2)}$ is the surface area of the $(d-1)$-sphere. Using that $\max\{\beta^{-1},\mu\} \sim \rho_0^{2/d}$ (which follow from this equation for L sufficiently large, see Remark 6.3.7) we conclude the proof of Equation (6.3.10).

Next, we consider the 2-particle density. By Wick's rule we have

$$\rho^{(2)}(x_1,x_2) = \rho^{(1)}(x_1)\rho^{(1)}(x_2) - \gamma^{(1)}(x_1;x_2)\gamma^{(1)}(x_2;x_1).$$

By translation invariance $\gamma^{(1)}(x_1;x_2)$ is a function of $x_1 - x_2$ only. We expand it as a Taylor series in x_1-x_2. By symmetry of reflection in any of the axes all odd orders and all off-diagonal second order terms vanish. Additionally, all second order terms are equal by the symmetry of permutation of the axes. That is,

$$\begin{aligned}
\gamma^{(1)}(x_1;x_2) &= \frac{1}{L^d}\sum_k \hat{\gamma}^{(1)}(k) e^{ik(x_1-x_2)} \\
&= \frac{1}{L^d}\sum_k \hat{\gamma}^{(1)}(k)\left[1 - \frac{1}{2d}|k|^2|x_1-x_2|^2 + O(|k|^4|x_1-x_2|^4)\right] \\
&= \rho_0 - \frac{1}{2d}\left[\frac{1}{L^d}\sum_k |k|^2\hat{\gamma}^{(1)}(k)\right]|x_1-x_2|^2 \\
&\quad + O\left(\left[\frac{1}{L^d}\sum_k |k|^4\hat{\gamma}^{(1)}(k)\right]|x_1-x_2|^4\right).
\end{aligned}$$

(Here $O(|k|^4|x_1-x_2|^4)$ means a term that is bounded by $|k|^4|x_1-x_2|^4$ uniformly in $|k|^4|x_1-x_2|^4$, even if it is large.) For the first sum we have by Lemma 6.3.5 and Equation (6.3.10) (and writing the error term in terms of ρ_0 as above)

$$\begin{aligned}
\frac{1}{L^d}\sum_{k\in\frac{2\pi}{L}\mathbb{Z}^d} |k|^2\hat{\gamma}^{(1)}(k) &= \frac{1}{(2\pi)^d}\int \frac{ze^{-\beta|k|^2}}{1+ze^{-\beta|k|^2}}|k|^2 \,\mathrm{d}k + O\left(L^{-1}\zeta\rho_0^{4/d}\right) \\
&= \frac{\Gamma(d/2+1)\left|\mathbb{S}^{d-1}\right|}{2(2\pi)^d}\beta^{-d/2-1}(-\operatorname{Li}_{d/2+1}(-z))\left(1+O(L^{-1}\zeta\rho_0^{-1/d})\right) \\
&= 2d\pi\frac{-\operatorname{Li}_{d/2+1}(-z)}{(-\operatorname{Li}_{d/2}(-z))^{1+2/d}}\rho_0^{1+2/d}\left(1+O(L^{-1}\zeta\rho_0^{-1/d})\right).
\end{aligned}$$

Using again Lemma 6.3.5 to bound the second sum we conclude that

$$\begin{aligned}
\gamma^{(1)}(x_1;x_2) &= \rho_0 - \pi\frac{-\operatorname{Li}_{d/2+1}(-z)}{(-\operatorname{Li}_{d/2}(-z))^{1+2/d}}\rho_0^{1+2/d}|x_1-x_2|^2 \\
&\quad + O\left(L^{-1}\zeta\rho_0^{1+1/d}|x_1-x_2|^2\right) + O\left(\rho_0^{1+4/d}|x_1-x_2|^4\right).
\end{aligned}$$

We conclude the proof of Equation (6.3.11). □

6.4 Gaudin–Gillespie–Ripka expansion

We use the Gaudin–Gillespie–Ripka (GGR) expansion [GGR71] to compute Z_J and $\rho_J^{(q)}$, the q-particle reduced densities of the trial state Γ_J. For this we recall some notation from Chapter 3.

Definition 6.4.1 (Definition 3.3.1). We define $\mathcal{G}_p^q$ as the set of graphs on q *external* vertices $\{1,...,q\}$ and p *internal* vertices $\{q+1,...,q+p\}$ such that there are no edges between external vertices and such that all internal vertices have degree at least 1, i.e. there is at least one edge incident to each internal vertex. We replace q and/or p with sets V^* and V respectively and write $\mathcal{G}_V^{V^*}$ if we need the external and/or internal vertices to have definite indices V^* respectively V. Concretely this means that for a set of edges $E \subset \{\{i,j\} : 1 \le i < j \le q+p\}$ the corresponding graph is in $\mathcal{G}_p^q$ if and only if

$$\forall(q+1 \le i \le q+p)\,\exists(1 \le j \le q+p) : \{i,j\} \in E, \qquad \forall(1 \le i < j \le q) : \{i,j\} \notin E.$$

Define $\mathcal{T}_p^q \subset \mathcal{C}_p^q \subset \mathcal{G}_p^q$ as the subset of trees and connected graphs respectively. (Define similarly $\mathcal{T}_V^{V^*} \subset \mathcal{C}_V^{V^*} \subset \mathcal{G}_V^{V^*}$.) Define the functions

$$W_p^q = W_p^q(x_1,\ldots,x_{p+q}) = \sum_{G\in\mathcal{G}_p^q}\prod_{e\in G} g_e.$$

A *diagram* (π, G) (on q external and p internal vertices) is a pair of a permutation $\pi \in \mathcal{S}_{p+q}$ and a graph $G \in \mathcal{G}_p^q$. We view the permutation π as a directed graph on the $p+q$ vertices. The set of all diagrams on q external and p internal vertices is denoted $\mathcal{D}_p^q$.

For a diagram (π, G) we will refer to G as the g-graph and π as the γ-graph. The value of a diagram $(\pi, G) \in \mathcal{D}_p^q$ is the function

$$\Gamma_{\pi,G}^q(x_1,\ldots,x_q) = (-1)^\pi \int\!\!\cdots\!\!\int \prod_{j=1}^{p+q} \gamma^{(1)}(x_j; x_{\pi(j)}) \prod_{e\in G} g_e \,\mathrm{d}X_{[q+1,q+p]}.$$

A diagram $(\pi, G) \in \mathcal{D}_p^q$ is *linked* if the union of π and G is a connected graph. The subset of all linked diagrams is denoted $\mathcal{L}_p^q \subset \mathcal{D}_p^q$.

For $q \ge 1$ define the set $\tilde{\mathcal{L}}_p^q \subset \mathcal{D}_p^q$ as the set of all diagrams such that each linked component contains at least one external vertex. For $q = 0$ we set $\tilde{\mathcal{L}}_p^0 = \mathcal{L}_p^0$.

A *cluster* is a connected component of the graph G.

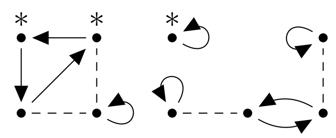


Figure 6.4.1: Example of a diagram $(\pi, G) \in \mathcal{D}_6^3$ with 3 linked components with each linked component containing 2 (left linked component), 1 (centre top linked component) and 2 (right linked component) clusters respectively. Vertices labelled with $*$ denote external vertices, dashed lines denote g-edges and arrows denote γ-edges, i.e. an arrow from i to j denotes that $\pi(i) = j$. Note that all internal vertices have at least one incident g-edge, that external vertices may have none, and that there are no g-edges between external vertices.

Notation 6.4.2. By a picture of a diagram, such as Figure 6.4.1, we will also denote the value of the pictured diagram.

We shall in the remainder of this section prove the following theorem.

Theorem 6.4.3. *For any q_0 there exists a constant $c_{q_0} > 0$ independently of L such that if $a^d \rho_0 \zeta^{d/2} \log b/a < c_{q_0}$ then*

$$Z_J = Z \exp\left[\sum_{p=2}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p} \Gamma_{\pi,G}\right], \tag{6.4.1}$$

$$\rho_J^{(q)} = \prod_{1\le i<j\le q} f_{ij}^2 \sum_{p=0}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\tilde{\mathcal{L}}_p^q} \Gamma_{\pi,G}^q. \tag{6.4.2}$$

for any $q \le q_0$.

Note that the p-sum in Equation (6.4.2) starts at $p = 0$ as opposed to that in Equation (6.4.1). This arises from the fact that diagrams with at least one external vertex may have zero internal vertices, while diagrams with no external vertices have at least 2 internal vertices.

In the proof we will use the GGR expansion as formulated in Lemma 5.3.6 and Theorem 3.3.4. For convenience we recall it here. Note that $\frac{1}{L^d}\sum_{k\in\frac{2\pi}{L}\mathbb{Z}^d}\left|\hat{\gamma}^{(1)}(k)\right| = \rho_0$. We continue to abuse notation slightly and treat $\gamma^{(1)}$ as a function and write $\left\|\gamma^{(1)}\right\|_{L^1} = \int_{[0,L]^d}\left|\gamma^{(1)}(x)\right| \,\mathrm{d}x$.

Lemma 6.4.4 (Lemma 5.3.6, Theorem 3.3.4)**.** *For any integer q_0 there exists a constant $c_{q_0} > 0$ such that if $\|g\|_{L^1}\left\|\gamma^{(1)}\right\|_{L^1}\rho_0 < c_{q_0}$ then*[3]

$$\mathcal{Z} := 1 + \sum_{p=2}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{D}_p}\Gamma_{\pi,G} = \exp\left[\sum_{p=2}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p}\Gamma_{\pi,G}\right],$$
$$\frac{1}{\mathcal{Z}}\sum_{p=0}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{D}_p^q}\Gamma_{\pi,G}^q = \sum_{p=0}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\tilde{\mathcal{L}}_p^q}\Gamma_{\pi,G}^q$$

for any $q \le q_0$, the p-sums being absolutely convergent.

We shall bound $\left\|\gamma^{(1)}\right\|_{L^1}$ and $\|g\|_{L^1}$ in Lemma 6.4.6 below.

6.4.1 Calculation of Z_J

We calculate Z_J. This is analogous to the computation in Sections 3.3.0.1 and 5.3.1 For simplicity denote the diagonal of Γ_n by $\Gamma_n = \Gamma_n(X_n) = \Gamma_n(X_n; X_n)$. Then

$$Z_J = \sum_{n=0}^{\infty}\int\!\!\cdots\!\!\int \prod_{i<j} f_{ij}^2 \Gamma_n(X_n)\,\mathrm{d}X_n = \sum_{n=0}^{\infty}\int\!\!\cdots\!\!\int \prod_{i<j}(1+g_{ij})\Gamma_n(X_n)\,\mathrm{d}X_n$$

Expanding the product and grouping all terms where p variables x_i appear in the factors g_{ij} we find the function W_p (evaluated on the respective p coordinates x_i). Noting further the permutation symmetry of the coordinates we have

$$= \sum_{n=0}^{\infty}\int\!\!\cdots\!\!\int \left[1 + \sum_{p=2}^{n}\frac{n!}{(n-p)!p!}W_p(X_p)\right]\Gamma_n(X_n)\,\mathrm{d}X_n$$

[3] In Lemma 5.3.6 and Theorem 3.3.4 the sum $\sum_{(\pi,G)\in\tilde{\mathcal{L}}_p^q}\Gamma_{\pi,G}^q$ is written by decomposing all diagrams $(\pi,G)\in\tilde{\mathcal{L}}_p^q$ into their linked components and noting that $\Gamma_{\pi,G}^q$ factorizes over linked components.

since there are $\frac{n!}{(n-p)!p!}$ many ways to choose p coordinates out of n coordinates. Now, if

$$\sum_{n=0}^{\infty}\sum_{p=2}^{n}\frac{n!}{(n-p)!p!}\int\!\!\cdots\!\!\int |W_p|\Gamma_n\,\mathrm{d}X_n<\infty$$

then we may interchange the two sums. A criterion for this is given in Lemma 6.4.5 below. Thus, if the condition of Lemma 6.4.5 is satisfied, namely that $\rho_0\left\|g\right\|_{L^1}$ is sufficiently small, we have

$$\begin{aligned}Z_J&=Z\left[1+\sum_{p=2}^{\infty}\frac{1}{p!}\int\!\!\cdots\!\!\int \mathrm{d}X_pW_p\left[\frac{1}{Z}\sum_{n=p}^{\infty}\frac{n!}{(n-p)!}\int\!\!\cdots\!\!\int \mathrm{d}X_{[p+1,n]}\Gamma_n\right]\right]\\&=Z\left[1+\sum_{p=2}^{\infty}\frac{1}{p!}\int\!\!\cdots\!\!\int \mathrm{d}X_pW_p\rho^{(p)}\right].\end{aligned}$$

The free Fermi gas is a quasi-free state, and thus by Wick's rule we have

$$Z_J=Z\left[1+\sum_{p=2}^{\infty}\frac{1}{p!}\int\!\!\cdots\!\!\int \mathrm{d}X_pW_p\det\left[\gamma^{(1)}_{ij}\right]_{1\le i,j\le p}\right]$$

Expanding W_p and the determinant we get

$$Z_J=Z\left[1+\sum_{p=2}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{D}_p}\Gamma_{\pi,G}\right].$$

Applying then Lemma 6.4.4 we conclude that, if $\rho_0\left\|g\right\|_{L^1}\left\|\gamma^{(1)}\right\|_{L^1}$ and $\rho_0\left\|g\right\|_{L^1}$ are sufficiently small, Equation (6.4.1) holds.

6.4.2 Calculation of $\rho_J^{(q)}$

Next, we calculate the reduced densities $\rho_J^{(q)}$ of the trial state Γ_J. This is analogous to the computations in Sections 3.3.0.2, 3.3.0.3, 3.3.0.4 and 5.3.2. We have

$$\rho_J^{(q)}(X_q)=\frac{1}{Z_J}\sum_{n=q}^{\infty}\frac{n!}{(n-q)!}\int\!\!\cdots\!\!\int\prod_{1\le i<j\le n}f_{ij}^2\Gamma_n(X_n)\,\mathrm{d}X_{[q+1,n]}$$

We write $f_{ij}^2=1+g_{ij}$ if at least one of i,j is an internal vertex and expand the product of the $(1+g_{ij})$'s. Grouping together those terms where p internal vertices are present we find the function W_p^q. Using additionally the symmetry of permutation of the coordinates we find

$$=\frac{1}{Z_J}\prod_{1\le i<j\le q}f_{ij}^2\sum_{n=q}^{\infty}\frac{n!}{(n-q)!}\sum_{p=0}^{n-q}\frac{(n-q)!}{p!(n-q-p)!}\int\!\!\cdots\!\!\int W_p^q(X_{p+q})\Gamma_n(X_n)\,\mathrm{d}X_{[q+1,n]}.$$

By Lemma 6.4.5 below we may interchange the sums if $\rho_0\left\|g\right\|_{L^1}$ is sufficiently small. Then

$$\begin{aligned}\rho_J^{(q)}&=\frac{Z}{Z_J}\prod_{1\le i<j\le q}f_{ij}^2\sum_{p=0}^{\infty}\frac{1}{p!}\int\!\!\cdots\!\!\int W_p^q\\&\quad\times\left[\frac{1}{Z}\sum_{n=p+q}^{\infty}\frac{n!}{(n-p-q)!}\int\!\!\cdots\!\!\int\Gamma_n\,\mathrm{d}X_{[q+p+1,n]}\right]\mathrm{d}X_{[q+1,q+p]}\\&=\frac{Z}{Z_J}\prod_{1\le i<j\le q}f_{ij}^2\sum_{p=0}^{\infty}\frac{1}{p!}\int\!\!\cdots\!\!\int W_p^q\rho^{(p+q)}\,\mathrm{d}X_{[q+1,q+p]}\end{aligned}$$

Expanding the W_p^q and using the Wick rule for the reduced densities of the free gas as above we get

$$\rho_J^{(q)} = \frac{Z}{Z_J} \prod_{1\le i<j\le q} f_{ij}^2 \sum_{p=0}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{D}_p^q} \Gamma_{\pi,G}^q.$$

As above, by Lemma 6.4.4, we get that Equation (6.4.2) holds for $\rho_0 \|g\|_{L^1} \left\|\gamma^{(1)}\right\|_{L^1}$ and $\rho_0 \|g\|_{L^1}$ small enough (dependent on q).

6.4.3 A convergence criterion

In this section we show

Lemma 6.4.5. *There exists a constant $c > 0$ such that if $\rho_0 \|g\|_{L^1} < c$ then*

$$\frac{1}{Z}\sum_{n=0}^{\infty}\sum_{p=2}^{n} \frac{n!}{(n-p)!p!} \int\!\cdots\!\int |W_p||\Gamma_n|\, \mathrm{d}X_n \le \exp(CL^d\rho_0\|g\|_{L^1}) < \infty, \tag{6.4.3}$$

and for any $q \ge 1$

$$\frac{1}{Z}\sum_{n=q}^{\infty}\sum_{p=0}^{n-q} \frac{n!}{(n-q-p)!p!} \int\!\cdots\!\int |W_p^q||\Gamma_n|\, \mathrm{d}X_{[q+1,n]} \le C_q\rho_0^q \exp(CL^d\rho_0\|g\|_{L^1}) < \infty \tag{6.4.4}$$

uniformly in $x_1, \ldots, x_q$.

Proof. Write

$$\begin{aligned}\frac{1}{Z}\sum_{n=0}^{\infty}\sum_{p=2}^{n} \frac{n!}{(n-p)!p!} \int\!\cdots\!\int |W_p||\Gamma_n|\, \mathrm{d}X_n &= \frac{1}{Z}\sum_{p=2}^{\infty}\sum_{n=p}^{\infty} \frac{n!}{(n-p)!p!} \int\!\cdots\!\int \mathrm{d}X_n|W_p|\Gamma_n \\ &= \sum_{p=2}^{\infty}\frac{1}{p!}\int\!\cdots\!\int \mathrm{d}X_p|W_p|\rho^{(p)}.\end{aligned}$$

By splitting all graphs into their connected components we have

$$\begin{aligned}&\int\!\cdots\!\int \mathrm{d}X_p\,|W_p|\rho^{(p)} \\ &\quad = \int\!\cdots\!\int \mathrm{d}X_p \left|\sum_{k=1}^{\infty}\frac{1}{k!}\sum_{n_1,\ldots,n_k\ge 2}\binom{p}{n_1,\ldots,n_k}\chi_{(\sum n_\ell = p)}\prod_{\ell=1}^{k}\left[\sum_{G_\ell\in\mathcal{C}_{n_\ell}}\prod_{e\in G_\ell} g_e\right]\right|\rho^{(p)}.\end{aligned}$$

We abused notation slightly and denote by $\mathcal{C}_{n_\ell}$ the set of connected graphs on n_ℓ specified vertices, say $\{\sum_{\ell'<\ell} n_{\ell'}+1, \ldots, \sum_{\ell'\le\ell} n_{\ell'}\}$, such that no two G_ℓ's share any vertices. Here k is the number of connected components having sizes $n_1, \ldots, n_k$. Note that $n_\ell \ge 2$ since each connected component needs at least 2 vertices since any vertex in a graph $G \in \mathcal{G}_p$ is internal and hence connected to at least one other vertex. The factor $\frac{1}{k!}$ comes from counting the possible labelings of the connected component and the factor $\binom{p}{n_1\cdots n_k}$ comes from counting the possible labelings of the vertices in the different connected components.

Next, we employ the tree-graph inequality [Uel18]. This reads (since $0 \le g \le 1$)

$$\left|\sum_{G\in\mathcal{C}_n}\prod_{e\in G} g_e\right| \le \sum_{T\in\mathcal{T}_n}\prod_{e\in T}|g_e|\,.$$

Thus,

$$\begin{aligned}
&\int\!\!\cdots\!\!\int \mathsf{d}X_p \frac{1}{p!} |W_p| \rho^{(p)} \\
&\quad \le \sum_{k=1}^{\infty} \frac{1}{k!} \sum_{n_1,\ldots,n_k \ge 2} \frac{1}{n_1! \cdots n_k!} \chi_{(\sum n_\ell = p)} \int\!\!\cdots\!\!\int \mathsf{d}X_p \prod_{\ell=1}^{k} \left[\sum_{T_\ell \in \mathcal{T}_{n_\ell}} \prod_{e \in T_\ell} |g_e| \right] \rho^{(p)}.
\end{aligned}$$

Next, we bound $\rho^{(p)}$ analogously to Lemma 3.3.10. First, $\rho^{(p)} = \det[\gamma^{(1)}_{ij}]_{1\le i,j\le p}$ by the Wick rule. Next, define $\alpha_i(k) = L^{-d/2} e^{ikx_i} \hat{\gamma}^{(1)}(k) \in \ell^2(\frac{2\pi}{L}\mathbb{Z}^d)$. Then $\gamma^{(1)}_{ij} = \langle \alpha_i | \alpha_j \rangle_{\ell^2(\frac{2\pi}{L}\mathbb{Z}^d)}$ and so by the Gram–Hadamard inequality [GMR21, Lemma D.1]

$$\rho^{(p)} = \det\left[\gamma^{(1)}_{ij}\right]_{1\le i,j\le p} \le \prod_{i=1}^{p} \|\alpha_i\|^2_{\ell^2(\frac{2\pi}{L}\mathbb{Z}^d)} = \rho_0^p.$$

Thus

$$\begin{aligned}
&\sum_{p=2}^{\infty} \frac{1}{p!} \int\!\!\cdots\!\!\int \mathsf{d}X_p |W_p| \rho^{(p)} \\
&\quad \le \sum_{k=1}^{\infty} \frac{1}{k!} \sum_{n_1,\ldots,n_k \ge 2} \frac{1}{n_1! \cdots n_k!} \rho_0^{\sum n_\ell} \prod_{\ell=1}^{k} \left[\sum_{T_\ell \in \mathcal{T}_{n_\ell}} \int\!\!\cdots\!\!\int \prod_{e \in T_\ell} |g_e| \right]
\end{aligned}$$

For each tree the integration is over all variables, thus by the translation invariance the integration over the variables in the tree T_ℓ gives $L^d (\int |g|)^{n_\ell - 1}$. Using moreover Cayley's formula $\#\mathcal{T}_n = n^{n-2} \le C^n n!$ we get

$$\begin{aligned}
&\le \sum_{k=1}^{\infty} \frac{1}{k!} \sum_{n_1,\ldots,n_k \ge 2} \frac{1}{n_1! \cdots n_k!} \rho_0^{\sum n_\ell} C^{\sum n_\ell} n_1! \cdots n_k! \left(\int |g| \right)^{\sum n_\ell - k} L^{dk} \\
&= \sum_{k=1}^{\infty} \frac{1}{k!} \left[C\rho_0 L^d \sum_{n=2}^{\infty} (C\rho_0 \|g\|_{L^1})^{n-1} \right]^k \\
&\le \exp\left(C L^d \rho_0 \|g\|_{L^1} \right) < \infty
\end{aligned}$$

if $\rho_0 \|g\|_{L^1}$ is sufficiently small.

The proof of Equation (6.4.4) is in spirit the same. Write

$$\frac{1}{Z} \sum_{n=q}^{\infty} \sum_{p=0}^{n-q} \frac{n!}{(n-q-p)!p!} \int\!\!\cdots\!\!\int |W_p^q||\mathit{\Gamma}_n| \, \mathsf{d}X_{[q+1,n]} = \sum_{p=0}^{\infty} \frac{1}{p!} \int\!\!\cdots\!\!\int \mathsf{d}X_{[q+1,q+p]} |W_p^q| \rho^{(q+p)}.$$

By decomposing the graphs into their connected components we have

$$\begin{aligned}
&\int\!\!\cdots\!\!\int \mathsf{d}X_{[q+1,q+p]} \, |W_p^q| \rho^{(q+p)} \\
&= \int\!\!\cdots\!\!\int \mathsf{d}X_{[q+1,q+p]} \Bigg| \sum_{\kappa=1}^{q} \frac{1}{\kappa!} \sum_{\substack{(V_1^*,\ldots,V_\kappa^*) \\ \text{partition of } \{1,\ldots,q\} \\ V_\lambda^* \ne \varnothing}} \sum_{n_1^*,\ldots,n_\kappa^* \ge 0} \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{n_1,\ldots,n_k \ge 2} \chi_{(\sum_\lambda n_\lambda^* + \sum_\ell n_\ell = p)} \\
&\qquad \times \binom{p}{n_1^*,\ldots,n_\kappa^*, n_1,\ldots,n_k} \prod_{\lambda=1}^{\kappa} \left[\sum_{G_\lambda^* \in \mathcal{C}_{n_\lambda^*}^{V_\lambda^*}} \prod_{e \in G_\lambda^*} g_e \right] \prod_{\ell=1}^{k} \left[\sum_{G_\ell \in \mathcal{C}_{n_\ell}} \prod_{e \in G_\ell} g_e \right] \Bigg| \rho^{(q+p)}.
\end{aligned}$$

Here κ is the number of connected components having external vertices and k is the number of connected components only with internal vertices. The partition $(V_1^*, \ldots, V_\kappa^*)$ partitions the external vertices into the κ different connected components with external vertices and the numbers $n_1^*, \ldots, n_\kappa^*$ are the number of internal vertices in the connected components with external vertices. The numbers $n_1, \ldots, n_k$ and the combinatorial factors are as above.

Using the tree-graph inequality as above we will obtain a sum of trees. (Technically we need to use a trivial modification of the tree-graph bound adapted to the setting with external vertices as in Sections 3.3.1.3 and 5.4.2. One simply defines $g_e = 0$ for a disallowed edge e between external vertices.) Namely we will have factors like

$$\sum_{T_\lambda^* \in \mathcal{T}_{n_\lambda^*}^{V_\lambda^*}} \prod_{e \in T_\lambda^*} |g_e|.$$

We bound these as follows. If $\# V_\lambda^* = 1$ we do nothing and define $T_{\lambda,1}^* = T_\lambda^*$. Otherwise iteratively pick any edge on the path between any two external vertices and bound the factor $|g_e| \leq 1$. Remove this edge from T_λ^*. Repeating this procedure $\# V_\lambda^* - 1$ many times results in $\# V_\lambda^*$ many trees all with exactly 1 external vertex. Label these as $T_{\lambda,1}^*, \ldots, T_{\lambda,\# V_\lambda^*}^*$. We then have the bound

$$\prod_{e \in T_\lambda^*} |g_e| \leq \prod_{\nu=1}^{\# V_\lambda^*} \prod_{e \in T_{\lambda,\nu}^*} |g_e|.$$

Using this bound together with the Gram–Hadamard inequality as above we get

$$\begin{aligned}
&\sum_{p=0}^\infty \frac{1}{p!} \int\!\!\cdots\!\!\int \mathrm{d}X_{[q+1,q+p]} |W_p^q| \rho^{(q+p)} \\
&\leq \sum_{\kappa=1}^q \frac{1}{\kappa!} \sum_{\substack{(V_1^*,\ldots,V_\kappa^*) \\ \text{part. of } \{1,\ldots,q\} \\ V_\lambda^* \neq \varnothing}} \sum_{n_1^*,\ldots,n_\kappa^* \geq 0} \sum_{k=0}^\infty \frac{1}{k!} \sum_{n_1,\ldots,n_k \geq 2} \frac{1}{\prod_{\lambda=1}^\kappa n_\lambda^*! \prod_{\ell=1}^k n_\ell!} \rho_0^{q + \sum_\lambda n_\lambda^* + \sum_\ell n_\ell} \\
&\quad \times \sum_{T_\lambda^* \in \mathcal{T}_{n_\lambda^*}^{V_\lambda^*}} \sum_{T_\ell \in \mathcal{T}_{n_\ell}} \left[\prod_{\lambda=1}^\kappa \prod_{\nu=1}^{\# V_\lambda^*} \int\!\!\cdots\!\!\int \prod_{e \in T_{\lambda,\nu}^*} |g_e| \right] \left[\prod_{\ell=1}^k \int\!\!\cdots\!\!\int \prod_{e \in T_\ell} |g_e| \right].
\end{aligned}$$

In the integrations each tree $T_{\lambda,\nu}^*$ is integrated over all but the one external vertex and so gives a value $(\int |g|)^{\# T_{\lambda,\nu}^* - 1}$ and each tree T_ℓ is integrated over all coordinates giving the value $(\int |g|)^{n_\ell - 1} L^d$. Moreover $\sum_\nu (\# T_{\lambda,\nu}^* - 1) = n_\lambda^*$. Thus, using additionally Cayley's formula (trivially extended to the setting with external vertices: $\# \mathcal{T}_{n_\lambda^*}^{V_\lambda^*} \leq C^{n_\lambda^* + \# V_\lambda^*} (n_\lambda^* + \# V_\lambda^*)!$),

$$\begin{aligned}
&\leq \sum_{\kappa=1}^q \frac{1}{\kappa!} \sum_{\substack{(V_1^*,\ldots,V_\kappa^*) \\ \text{part. of } \{1,\ldots,q\} \\ V_\lambda^* \neq \varnothing}} \sum_{n_1^*,\ldots,n_\kappa^* \geq 0} \sum_{k=0}^\infty \frac{1}{k!} \sum_{n_1,\ldots,n_k \geq 2} \frac{1}{\prod_{\lambda=1}^\kappa n_\lambda^*! \prod_{\ell=1}^k n_\ell!} \rho_0^{q + \sum_\lambda n_\lambda^* + \sum_\ell n_\ell} \\
&\quad \times C^{q + \sum_\lambda n_\lambda^* + \sum_\ell n_\ell} \prod_{\lambda=1}^\kappa (n_\lambda^* + \# V_\lambda^*)! \prod_{\ell=1}^k n_\ell! \left(\int |g| \right)^{\sum_\lambda n_\lambda^* + \sum_\ell n_\ell - k} L^{dk}.
\end{aligned}$$

Next, we may bound the binomial coefficients as $(n+m)! \leq 2^{n+m} n! m!$ so $\prod_{\lambda=1}^{\kappa}(n_\lambda^* + \#V_\lambda^*)! \leq 2^{\sum_\lambda n_\lambda^* + q} \prod_\lambda n_\lambda^*! (\#V_\lambda^*)!$. Thus

$$
\begin{aligned}
&\leq C^q \sum_{\kappa=1}^{q} \frac{1}{\kappa!} \sum_{\substack{(V_1^*,\ldots,V_\kappa^*) \\ \text{part. of } \{1,\ldots,q\} \\ V_\lambda^* \neq \varnothing}} \prod_{\lambda=1}^{\kappa} (\#V_\lambda^*)! \left[\sum_{n^*=0}^{\infty} (C\rho_0 \|g\|_{L^1})^{n_*} \right]^{\kappa} \\
&\quad \times \rho_0^q \sum_{k=0}^{\infty} \frac{1}{k!} \left[CL^d \rho_0 \sum_{n=2}^{\infty} (C\rho_0 \|g\|_{L^1})^{n-1} \right]^k \\
&\leq C_q \rho_0^q \exp\left(CL^d \rho_0 \|g\|_{L^1} \right) < \infty
\end{aligned}
$$

if $\rho \|g\|_{L^1}$ is small enough. $\square$

6.4.4 Calculation of $\|g\|_{L^1}, \left\|\gamma^{(1)}\right\|_{L^1}$

In this section we bound the quantities $\|g\|_{L^1}$ and $\left\|\gamma^{(1)}\right\|_{L^1} = \int \left|\gamma^{(1)}(x)\right| \mathrm{d}x$. We show (recall $\zeta = 1 + |\log z|$)

Lemma 6.4.6. *The quantities $\|g\|_{L^1}$ and $\left\|\gamma^{(1)}\right\|_{L^1}$ satisfy*

$$
\|g\|_{L^1} \leq Ca^d \log b/a, \qquad \left\|\gamma^{(1)}\right\|_{L^1} \leq C\zeta^{d/2}.
$$

Note that these bounds are uniform in the volume L^d.

Proof. The bound $\|g\|_{L^1} \leq Ca^d \log b/a$ follows from Equation (6.3.6). For $\left\|\gamma^{(1)}\right\|_{L^1}$ we have for any (length) $\lambda > 0$

$$
\begin{aligned}
\left\|\gamma^{(1)}\right\|_{L^1} &= \int_{[0,L]^d} \left|\gamma^{(1)}(x)\right| \\
&\leq \left(\int_{\mathbb{R}^d} \left|\gamma^{(1)}(x)\right|^2 (\lambda^2 + |x|^2)^2 \,\mathrm{d}x \right)^{1/2} \left(\int_{\mathbb{R}^d} \frac{1}{(\lambda^2 + |x|^2)^2} \,\mathrm{d}x \right)^{1/2} \\
&= C\lambda^{d/2-2} \left[\frac{1}{L^d} \sum_{k \in \frac{2\pi}{L}\mathbb{Z}^d} \left| (\widehat{\lambda^2 + |x|^2)\gamma^{(1)}}(k) \right|^2 \right]^{1/2}
\end{aligned}
$$

Moreover (with $\hat{\gamma}(k) = ze^{-\beta|k|^2}$ is as in Equation (6.3.12))

$$
\begin{aligned}
(\widehat{\lambda^2 + |x|^2)\gamma^{(1)}}(k) &= \left[\lambda^2 - \Delta_k \right] \hat{\gamma}^{(1)}(k) \\
&= \frac{\lambda^2 \hat{\gamma}(k)^3 + (2\lambda^2 - 4\beta^2|k|^2 - 2d\beta)\hat{\gamma}(k)^2 + (\lambda^2 + 4\beta^2|k|^2 - 2d\beta)\hat{\gamma}(k)}{(1 + \hat{\gamma}(k))^3}.
\end{aligned}
$$

Using Equation (6.3.12) we conclude that

$$
\frac{1}{L^d} \sum_{k \in \frac{2\pi}{L}\mathbb{Z}^d} \left| (\widehat{\lambda^2 + |x|^2)\gamma^{(1)}}(k) \right|^2 \leq C\rho_0 \left(\lambda^4 + \beta^4 \rho_0^{4/d} + \beta^2 \right) \leq C\rho_0 \left(\lambda^4 + \zeta^2 \beta^2 \right).
$$

Thus for $\lambda = \beta^{1/2}\zeta^{1/2}$ we have $\left\|\gamma^{(1)}\right\|_{L^1} \leq C\zeta^{d/2}$. (Recall that $\beta \sim \zeta\rho_0^{-2/d}$ by Remark 6.3.7.) $\square$

We conclude that $\rho_0 \|g\|_{L^1} \left\|\gamma^{(1)}\right\|_{L^1} \leq Ca^d \rho_0 \zeta^{d/2} \log b/a$. This concludes the proof of Theorem 6.4.3.

6.5 Calculation of terms in Equation (6.3.5)

In this section we compute and bound the different terms in Equation (6.3.5) and thereby prove Proposition 6.1.9.

6.5.1 Energy

The kinetic energy of the trial state Γ_J is

$$\begin{aligned}\langle \mathcal{H} \rangle_J &= \frac{1}{Z_J} \sum_{n=1}^{\infty} \int\!\cdots\!\int \left[(-\Delta_{X_n}) \left[F_n(X_n)\Gamma(X_n, Y_n)F_n(Y_n)\right]\right]_{Y_n = X_n} \,\mathrm{d}X_n \\ &= \frac{1}{Z_J} \sum_{n=1}^{\infty} \int\!\cdots\!\int \Big(|\nabla_{X_n} F|^2 \Gamma_n(X_n; X_n) - F_n^2 (\Delta_{X_n} \Gamma_n)(X_n; X_n) \Big) \,\mathrm{d}X_n.\end{aligned}$$

The second term may be calculated as (recall that $\langle \cdot \rangle_J$ means expectation in the state Γ_J)

$$\begin{aligned}\frac{1}{Z_J} \sum_{n=1}^{\infty} \int\!\cdots\!\int F_n^2 (-\Delta_{X_n} \Gamma_n)(X_n; X_n) \,\mathrm{d}X_n &= \frac{Z}{Z_J} \operatorname{Tr}[F^2 \mathcal{H} \Gamma] \\ &= \frac{1}{Z_J} \operatorname{Tr}[F^2(-\partial_\beta(Z\Gamma) + \mu \mathcal{N} Z \Gamma)] \\ &= -\partial_\beta \log Z_J + \mu \langle \mathcal{N} \rangle_J\end{aligned}$$

Here we used that Γ is differentiable in β in the topology of trace-class operators. This may be easily verified. For the first term we have that

$$|\nabla_{X_n} F_n|^2 = \left[2 \sum_{j<k} \left| \frac{\nabla f_{jk}}{f_{jk}} \right|^2 + \sum_{\substack{i,j,k \\ \text{all distinct}}} \frac{\nabla f_{ij} \nabla f_{jk}}{f_{ij} f_{jk}} \right] F_n^2.$$

Thus the full energy is

$$\begin{aligned}\langle \mathcal{H} - \mu \mathcal{N} + \mathcal{V} \rangle_J = -\partial_\beta \log Z_J &+ \iint \left[\left| \frac{\nabla f_{12}}{f_{12}} \right|^2 + \frac{1}{2} v_{12} \right] \rho_J^{(2)} \,\mathrm{d}x_1 \,\mathrm{d}x_2 \\ &+ \iiint \frac{\nabla f_{12} \nabla f_{13}}{f_{12} f_{13}} \rho_J^{(3)} \,\mathrm{d}x_1 \,\mathrm{d}x_2 \,\mathrm{d}x_3.\end{aligned} \tag{6.5.1}$$

6.5.2 Entropy

We note that $\Gamma_J = \frac{Z}{Z_J} F \Gamma F$ is isospectral to $\frac{Z}{Z_J} \Gamma^{1/2} F^2 \Gamma^{1/2}$. Moreover, since $F \le 1$ we have $\Gamma^{1/2} F^2 \Gamma^{1/2} \le \Gamma$ as operators. Thus by operator monotonicity of the logarithm

$$\begin{aligned}\operatorname{Tr}\left[\Gamma_J \log \Gamma_J\right] &= \frac{Z}{Z_J} \operatorname{Tr}\left[\Gamma^{1/2} F^2 \Gamma^{1/2} \left(\log \frac{Z}{Z_J} + \log \Gamma^{1/2} F^2 \Gamma^{1/2} \right) \right] \\ &\le \log \frac{Z}{Z_J} + \frac{Z}{Z_J} \operatorname{Tr}\left[\Gamma^{1/2} F^2 \Gamma^{1/2} \log \Gamma \right] \\ &= -\log Z_J - \beta \frac{Z}{Z_J} \operatorname{Tr}\left[F^2 \Gamma (\mathcal{H} - \mu \mathcal{N}) \right] \\ &= -\log Z_J + \frac{1}{Z_J} \beta \partial_\beta \operatorname{Tr}\left[F^2 Z \Gamma \right] \\ &= -\log Z_J + \beta \partial_\beta \log Z_J\end{aligned}$$

We conclude the bound on the entropy

$$-\frac{1}{\beta}S(\Gamma_J) = \frac{1}{\beta}\operatorname{Tr}[\Gamma_J \log \Gamma_J] \le -\frac{1}{\beta}\log Z_J + \partial_\beta \log Z_J. \tag{6.5.2}$$

6.5.3 Pressure

Combining Equations (6.5.1) and (6.5.2) the terms $\pm\partial_\beta \log Z_j$ cancel and we conclude the bound for the pressure

$$\begin{aligned} L^d P[\Gamma_J] &= -\langle \mathcal{H} - \mu\mathcal{N} + \mathcal{V}\rangle_J + \frac{1}{\beta}S(\Gamma_J) \\ &\ge \frac{1}{\beta}\log Z_J - \iint \left[\left|\frac{\nabla f_{12}}{f_{12}}\right|^2 + \frac{1}{2}v_{12}\right]\rho_J^{(2)}\,\mathrm{d}x_1\,\mathrm{d}x_2 - \iiint \frac{\nabla f_{12}\nabla f_{13}}{f_{12}f_{13}}\rho_J^{(3)}\,\mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3. \end{aligned}$$

Remark 6.5.1. The cancellation of the terms $\pm\partial_\beta \log Z_j$ is not essential. Namely the energy of the trial state Γ_J is the energy of the free gas plus the relevant interaction term up to small errors. And the entropy of the trial state Γ_J is bounded from above by the entropy of the free gas up to small errors. To see this write

$$-\partial_\beta \log Z_J = -\partial_\beta \log Z - \partial_\beta \log \frac{Z_J}{Z} = \langle \mathcal{H} - \mu\mathcal{N}\rangle_0 - \partial_\beta \log \frac{Z_J}{Z}.$$

One can show that $\partial_\beta \log \frac{Z_J}{Z}$ is small compared to the interaction of order $L^d a^d \rho_0^{2+2/d}$. Thus, the energy of the trial state Γ_J is

$$\langle \mathcal{H} - \mu\mathcal{N} + \mathcal{V}\rangle_J = \langle \mathcal{H} - \mu\mathcal{N}\rangle_0 + \iint \left[\left|\frac{\nabla f_{12}}{f_{12}}\right|^2 + \frac{1}{2}v_{12}\right]\rho_J^{(2)}\,\mathrm{d}x_1\,\mathrm{d}x_2 + \text{small error}.$$

Similarly for the entropy

$$\begin{aligned} -\frac{1}{\beta}\log Z_J + \partial_\beta \log Z_J &= -\frac{1}{\beta}\log Z + \partial_\beta \log Z - \frac{1}{\beta}\log\frac{Z_J}{Z} + \partial_\beta \log \frac{Z_J}{Z} \\ &= -\frac{1}{\beta}S(\Gamma) - \frac{1}{\beta}\log\frac{Z_J}{Z} + \partial_\beta \log \frac{Z_J}{Z}. \end{aligned}$$

We show below that $\frac{1}{\beta}\log\frac{Z_J}{Z}$ is small compared to the interaction term of size $L^d a^d \rho_0^{2+2/d}$. Thus the entropy of the trial state Γ_J may be bounded as

$$-\frac{1}{\beta}S(\Gamma_J) \le -\frac{1}{\beta}S(\Gamma) + \text{small error}.$$

The proof that $\partial_\beta \log \frac{Z_J}{Z}$ is small is somewhat analogous to the proof of Lemma 6.5.2 in Section 6.5.4. As we will not need it, we omit the details.

By Equation (6.4.2), we have for $a^d \rho_0 \zeta^{d/2} \log b/a$ sufficiently small that

$$\rho_J^{(2)} = f_{12}^2 \left[\rho^{(2)} + \sum_{p=1}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\tilde{\mathcal{L}}_p^2} \Gamma_{\pi,G}^2\right]$$

We may then write

$$
\begin{aligned}
L^d P[\Gamma_J] \geq{}& \frac{1}{\beta}\log Z - \iint \left[|\nabla f_{12}|^2 + \frac{1}{2}v_{12}f_{12}^2\right]\rho^{(2)}\,\mathrm{d}x_1\,\mathrm{d}x_2 + \underbrace{\frac{1}{\beta}\log\frac{Z_J}{Z}}_{\varepsilon_Z} \\
& \underbrace{- \iint \left[|\nabla f_{12}|^2 + \frac{1}{2}v_{12}f_{12}^2\right]\sum_{p=1}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\tilde{\mathcal{L}}_p^2}\Gamma_{\pi,G}^2\,\mathrm{d}x_1\,\mathrm{d}x_2}_{\varepsilon_2} \\
& \underbrace{- \iiint \frac{\nabla f_{12}\nabla f_{13}}{f_{12}f_{13}}\rho_J^{(3)}\,\mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3}_{\varepsilon_3}.
\end{aligned}
\tag{6.5.3}
$$

The first term is the pressure of the free gas (times the volume), the second term leads to the leading order correction, and the remaining terms are error terms. We shall show in Section 6.5.4 below the following bounds. (Recall that $\zeta = 1 + |\log z|$.)

Lemma 6.5.2. *For $z \gtrsim 1$ there exists a constant $c > 0$ such that if $a^d\rho_0\zeta^{d/2}\left|\log a^d\rho_0\right| < c$ then, for sufficently large L, the error terms are bounded as*

$$
\begin{aligned}
\frac{|\varepsilon_Z|}{L^d} &\leq Ca^d b^2\rho_0^{2+4/d}\zeta^{-1} + Ca^{2d}\rho_0^{3+2/d}\zeta^{d/2-1}(\log b/a)^2 \\
\frac{|\varepsilon_2|}{L^d} &\leq \begin{cases} Ca^{2d}\rho_0^{3+2/d}\log b/a + Ca^{4d-2}\rho_0^5\zeta^{3d/2}(\log b/a)^3 & d\geq 2, \\ Cab\rho_0^5\log b/a + Ca^2\rho_0^5\zeta^{3/2}(\log b/a)^3 & d = 1, \end{cases} \\
\frac{|\varepsilon_3|}{L^d} &\leq \begin{cases} Ca^{2d}b^2\rho_0^{3+4/d} + Ca^{3d-2}\rho_0^4\zeta^{d/2}\log b/a & d\geq 2, \\ Ca^2\rho_0^5\zeta(\log b/a)^2 & d = 1. \end{cases}
\end{aligned}
$$

In particular we have the bounds (recalling that $a \ll b \lesssim \rho_0^{-1/d}$)

$$
\frac{|\varepsilon_Z| + |\varepsilon_2| + |\varepsilon_3|}{L^d} \leq \begin{cases} Ca^3b^2\rho_0^{10/3}\zeta^{-1} + Ca^6\rho_0^{11/3}\zeta^{1/2}(\log b/a)^2 \\ \quad + Ca^{10}\rho_0^5\zeta^{9/2}(\log b/a)^3 & d = 3, \\ Ca^2b^2\rho_0^4\zeta^{-1} + Ca^4\rho_0^4\zeta\log b/a \\ \quad + Ca^6\rho_0^5\zeta^3(\log b/a)^3 & d = 2, \\ Cab\rho_0^5\log b/a + Ca^2\rho_0^5\zeta^{3/2}(\log b/a)^3 & d = 1. \end{cases}
\tag{6.5.4}
$$

Note that this is increasing in b. For the second term in Equation (6.5.3) above we use Equations (6.3.7), (6.3.8) and (6.3.11), thus

$$
\begin{aligned}
&\iint \left[|\nabla f_{12}|^2 + \frac{1}{2}v_{12}f_{12}^2\right]\rho^{(2)}\,\mathrm{d}x_1\,\mathrm{d}x_2 \\
&= 2\pi\frac{-\operatorname{Li}_{d/2+1}(-e^{\beta\mu})}{(-\operatorname{Li}_{d/2}(-e^{\beta\mu}))^{1+2/d}}\rho_0^{2+2/d}L^d\int\left(|\nabla f|^2 + \frac{1}{2}vf^2\right)|x|^2\,\mathrm{d}x\left(1 + O(L^{-1}\zeta\rho_0^{-1/d})\right) \\
&\quad + O\left(L^d\rho_0^{2+4/d}\int\left(|\nabla f|^2 + \frac{1}{2}vf^2\right)|x|^4\,\mathrm{d}x\right) \\
&= 2\pi c_d\frac{-\operatorname{Li}_{d/2+1}(-e^{\beta\mu})}{(-\operatorname{Li}_{d/2}(-e^{\beta\mu}))^{1+2/d}}L^d a^d\rho_0^{2+2/d}\left(1 + O(a^d/b^d) + O\left(L^{-1}\zeta\rho_0^{-1/d}\right)\right) \\
&\quad + \begin{cases} O\left(L^d a^{d+2}\rho_0^{2+4/d}\log b/a\right) & d\geq 2 \\ O\left(La^2b\rho_0^6\right) & d = 1 \end{cases}
\end{aligned}
\tag{6.5.5}
$$

where c_d is defined in Equation (6.1.3). Note that the first error term is decreasing in b. This competes with the other error terms and leads to the choice of b below. Combining Equations (6.5.3), (6.5.4) and (6.5.5) we thus conclude the bound

$$\begin{aligned}\psi(\beta,\mu) &\geq \limsup_{L\to\infty} P[\Gamma_J] \\ &\geq \lim_{L\to\infty}\left[\frac{1}{L^d\beta}\log Z\right] - 2\pi c_d \frac{-\operatorname{Li}_{d/2+1}(-e^{\beta\mu})}{(-\operatorname{Li}_{d/2}(-e^{\beta\mu}))^{1+2/d}} a^d \rho_0^{2+2/d} \\ &\quad + \begin{cases} O\left(\begin{matrix} a^6 b^{-3}\rho_0^{8/3} + a^3 b^2 \rho_0^{10/3}\zeta^{-1} \\ + a^6\rho_0^{11/3}\zeta^{1/2}(\log b/a)^2 + a^{10}\rho_0^5\zeta^{9/2}(\log b/a)^3\end{matrix}\right) & d=3, \\ O\left(\begin{matrix} a^4 b^{-2}\rho_0^3 + a^2 b^2\rho_0^4\zeta^{-1} \\ + a^4\rho_0^4\zeta\log b/a + a^6\rho_0^5\zeta^3(\log b/a)^3\end{matrix}\right) & d=2, \\ O\left(a^2 b^{-1}\rho_0^4 + ab\rho_0^5\log b/a + a^2\rho_0^5\zeta^{3/2}(\log b/a)^3\right) & d=1.\end{cases}\end{aligned}$$

Using that $\lim_{L\to\infty}\left[\frac{1}{L^d\beta}\log Z\right] = \psi_0(\beta,\mu)$ and optimising in b we find for the choices (recall that we require $b \lesssim \rho_0^{-1/d}$)

$$b = \begin{cases} \min\left\{a(a^3\rho_0)^{-2/15}\zeta^{1/5}, \rho_0^{-1/3}\right\} & d=3, \\ \min\left\{a(a^2\rho_0)^{-1/4}\zeta^{1/4}, \rho_0^{-1/2}\right\} & d=2, \\ a(a\rho_0)^{-1/2}\left|\log a\rho_0\right|^{-1/2} & d=1,\end{cases}$$

that

$$\psi(\beta,\mu) \geq \psi_0(\beta,\mu) - 2\pi c_d \frac{-\operatorname{Li}_{d/2+1}(-e^{\beta\mu})}{(-\operatorname{Li}_{d/2}(-e^{\beta\mu}))^{1+2/d}} a^d \rho_0^{2+2/d}\left[1+\delta_d\right],$$

where δ_d is as in Equation (6.1.13). The calculations above are valid as long as the conditions of Theorem 6.4.3 are satisfied. That is, if $a^d\rho_0\zeta^{d/2}\left|\log a^d\rho_0\right|$ is sufficiently small. This concludes the proof of Proposition 6.1.9. It remains to give the proof of Lemma 6.5.2.

6.5.4 Error terms (proof of Lemma 6.5.2)

In this section we give the

Proof of Lemma 6.5.2. To better illustrate where the different error terms come from we will write them in terms of the quantities $\|g\|_{L^1}$, $\left\|\gamma^{(1)}\right\|_{L^1}$ and $\||\cdot|^n g\|_{L^1} = \int_{\mathbb{R}^d}|x|^n|g(x)|\,\mathrm{d}x$, $n\geq 1$. By Lemma 6.4.6 and Equation (6.3.6) we have the bounds

$$\|g\|_{L^1} \leq Ca^d\log b/a, \quad \left\|\gamma^{(1)}\right\|_{L^1} \leq C\zeta^{d/2} = C(1+|\log z|)^{d/2}, \quad \||\cdot|^n g\|_{L^1} \leq Ca^d b^n.$$

For the analysis of the error terms we use the bounds in Equations (3.4.10), (3.4.22) and (5.4.13). To state these, we define for any diagram $(\pi,G)\in\tilde{\mathcal{L}}_p^m$ the numbers $k=k(G)=k(\pi,G)$ as the number of clusters (connected components of G, recall Definition 6.4.1) entirely with internal vertices (of sizes $n_1,\ldots,n_k$) and $\kappa=\kappa(G)=\kappa(\pi,G)$ as the number of clusters with each at least one external vertex (of sizes [meaning number of internal vertices] $n_1^*,\ldots,n_\kappa^*$). Define

$$\nu^* := \sum_{\lambda=1}^{\kappa} n_\lambda^*, \qquad \nu := \sum_{\ell=1}^{k} n_\ell - 2k.$$

As discussed around Equations (3.4.10), (3.4.22) and (5.4.13) the numbers ν^* and ν count the "number of added vertices". Concretely, a diagram with k clusters of only internal vertices has at least $2k$ internal vertices. Then ν^* is the number of additional internal vertices in clusters with external vertices and ν is the number of additional internal vertices in clusters with only internal vertices.

The bounds in Equations (3.4.10), (3.4.22) and (5.4.13) (note that there bounds on $\|g\|_{L^1}$, $\left\|\gamma^{(1)}\right\|_{L^1}$ analogous to those of Lemma 6.4.6 are already used) then read for any k_0, ν_0

$$\frac{1}{p!}\left|\sum_{\substack{(\pi,G)\in\tilde{\mathcal{L}}_p^m\\ k(\pi,G)=k_0\\ \nu(\pi,G)+\nu^*(\pi,G)=\nu_0}}\Gamma_{\pi,G}^m\right| \leq \begin{cases} CL^d\rho_0\left(C\rho_0\|g\|_{L^1}\right)^{\nu_0+k_0}\left\|\gamma^{(1)}\right\|_{L^1}^{k_0-1} & m=0,\\ C_m\rho_0^m\left(C\rho_0\|g\|_{L^1}\right)^{\nu_0+k_0}\left\|\gamma^{(1)}\right\|_{L^1}^{k_0} & m>0,\end{cases}\qquad p=2k_0+\nu_0, \tag{6.5.6}$$

where the constants C, C_m depend only on m but not on ν_0 or k_0 (in particular not on p).

Remark 6.5.3. The case $m=0$ is not included in the statement in Equations (3.4.10), (3.4.22) and (5.4.13). It follows from the analysis in Section 3.3.1 (see also Section 5.4.1), however.

More precisely the analysis in Section 3.3.1 consists of the following steps: 1. Decompose the linked diagrams in $\mathcal{L}_p$ according to the connected components of the graphs. 2. Use the tree-graph inequality [Uel18] to bound each sum over graphs by a sum over trees in each connected component of the graph. 3. Use the Brydges–Battle–Federbush formula (see [GMR21, Appendix D]) to bound the truncated correlations. 4. Compute the integrals, each being now an integral of either $|g|$ or $|\gamma^{(1)}|$.

In any of the equations in Section 3.3.1 the only effect of the p-summation is to eliminate the factor $\chi_{(\sum_\ell n_\ell=p)}$ present in the very first equation (where there is no p-summation). That is, not performing the p-summation, all equations in Section 3.3.1 remain valid, only with no p-summation on their left-hand-sides and with an additional factor $\chi_{(\sum_\ell n_\ell=p)}$ on their right-hand sides. Thus, from the analysis in Section 3.3.1, modified by not performing the p-summation, we find the following modification of the final formula in Section 3.3.1:

$$\frac{1}{p!}\left|\sum_{\substack{(\pi,G)\in\mathcal{L}_p\\ k(\pi,G)=k_0\\ \nu(\pi,G)=\nu_0}}\Gamma_{\pi,G}\right| \leq CN\left\|\gamma^{(1)}\right\|_{L^1}^{k_0-1}\sum_{\substack{n_1,\ldots,n_{k_0}\geq 2\\ \sum_\ell n_\ell=2k_0+\nu_0}}\left(\rho_0\|g\|_{L^1}\right)^{\sum_\ell(n_\ell-1)},\qquad p=2k_0+\nu_0,$$

from which Equation (6.5.6) in the case $m=0$ follows.

From this bound the natural "size" of a diagram $(\pi,G)\in\tilde{\mathcal{L}}_p^m$ is not p but rather $\nu+\nu^*+k$, since its value is (neglecting $\log$'s and dependence on z) $\lesssim \rho_0^m(a^d\rho_0)^{\nu+\nu^*+k}$. For the bounds of the terms $\varepsilon_2, \varepsilon_3, \varepsilon_Z$ we will bound sufficiently large diagrams by the bound in Equation (6.5.6) and do a more precise computation for small diagrams.

Additionally we have

Lemma 6.5.4. *The reduced densities $\rho^{(3)}$ and $\rho^{(4)}$ satisfy*

$$\rho^{(3)}(x_1,x_2,x_3) \le C\rho_0^{3+4/d}|x_1-x_2|^2|x_1-x_3|^2,$$
$$\rho^{(4)}(x_1,x_2,x_3,x_4) \le C\rho_0^{4+6/d}|x_1-x_2|^2|x_1-x_3|^2|x_1-x_4|^2.$$

Proof. Note that both $\rho^{(3)}$ and $\rho^{(4)}$ vanish whenever two particles are incident and are invariant under permutation of the particle positions. Thus, for fixed x_1 as functions of x_j, $j \neq 1$ they vanish quadratically around $x_j = x_1$. Writing $\rho^{(q)} = \det[\gamma^{(1)}_{ij}]_{1\le i,j\le q}$ using the Wick rule, Taylor expanding in x_j, $j \neq 1$ around $x_j = x_1$ and using Equation (6.3.12) to bound the derivatives we conclude the proof of the lemma. □

We first bound ε_Z.

6.5.4.1 Bound of ε_Z

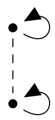
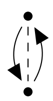
We have by Theorem 6.4.3

$$\varepsilon_Z = -\frac{1}{\beta}\log\frac{Z_J}{Z} = -\frac{1}{\beta}\sum_{p=2}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p}\Gamma_{\pi,G}.$$

We use the bound in Equation (6.5.6) above for $m=0$ and for diagrams with $\nu+k\ge 2$. These are precisely the diagrams with $p \ge 3$ (note that $k \ge 1$ for any diagram $(\pi,G)\in\mathcal{L}_p$). Thus

$$\begin{aligned}
&\sum_{p=3}^{\infty}\frac{1}{p!}\left|\sum_{(\pi,G)\in\mathcal{L}_p}\Gamma_{\pi,G}\right| \\
&\quad\le CL^d\rho_0\sum_{\substack{k_0\ge 1\\ \nu_0+k_0\ge 2}}\left(C\rho_0\left\|g\right\|_{L^1}\right)^{\nu_0+k_0}\left\|\gamma^{(1)}\right\|_{L^1}^{k_0-1} \\
&\quad= CL^d\rho_0\left[\sum_{\nu_0=1}^{\infty}\left(C\rho_0\left\|g\right\|_{L^1}\right)^{\nu_0+1}+\sum_{k_0=2}^{\infty}\sum_{\nu_0=0}^{\infty}\left(C\rho_0\left\|g\right\|_{L^1}\right)^{\nu_0+k_0}\left\|\gamma^{(1)}\right\|_{L^1}^{k_0-1}\right] \\
&\quad\le CL^d\rho_0^3\left\|g\right\|_{L^1}^2\left(1+\left\|\gamma^{(1)}\right\|_{L^1}\right)
\end{aligned}$$

for sufficiently small $\rho_0\left\|g\right\|_{L^1}$ and $\rho_0\left\|g\right\|_{L^1}\left\|\gamma^{(1)}\right\|_{L^1}$. For the diagrams with $\nu+k=1$ we do a more precise calculation. These are precisely the diagrams with $p=2$. In particular these diagrams have $\nu=0$ and $k=1$. We have then (recall that pictures of diagrams refer to their values)

$$\sum_{(\pi,G)\in\mathcal{L}_2}\Gamma_{\pi,G} =$$  $+$ 

$$\begin{aligned}
&= \iint \det\begin{bmatrix}\gamma^{(1)}(0) & \gamma^{(1)}(x-y)\\ \gamma^{(1)}(y-x) & \gamma^{(1)}(0)\end{bmatrix} g(x-y)\,\mathrm{d}x\,\mathrm{d}y \\
&= \iint \rho^{(2)}(x,y)g(x-y)\,\mathrm{d}x\,\mathrm{d}y \\
&= O\left(L^d\left\||\cdot|^2 g\right\|_{L^1}\rho_0^{2+2/d}\right)
\end{aligned}$$

using Equation (6.3.11). Thus, using Lemma 6.4.6 and recalling that $\beta \sim \zeta \rho_0^{-2/d}$ from Remark 6.3.7, we conclude that

$$\begin{aligned}\frac{1}{L^d}\left|\varepsilon_Z\right| = \frac{1}{\beta L^d}\left|\log \frac{Z_J}{Z}\right| &\leq C \left\| |\cdot|^2 g \right\|_{L^1} \rho_0^{2+4/d}\zeta^{-1} + C \left\|g\right\|_{L^1}^2 \left(\left\|\gamma^{(1)}\right\|_{L^1} + 1\right) \rho_0^{3+2/d}\zeta^{-1} \\ &\leq C a^d b^2 \rho_0^{2+4/d}\zeta^{-1} + C a^{2d}\rho_0^{3+2/d}\zeta^{d/2-1}(\log b/a)^2.\end{aligned}$$

6.5.4.2 Bound of ε_3

We have by Theorem 6.4.3

$$\rho_J^{(3)} = f_{12}^2 f_{13}^2 f_{23}^2 \left[\rho^{(3)} + \sum_{p=1}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\tilde{\mathcal{L}}_p^3}\Gamma_{\pi,G}^3\right].$$

We use the bound in Lemma 6.5.4 to bound $\rho^{(3)}$ and the bound in Equation (6.5.6) on the remaining terms. (That is, a precise calculation for diagrams with $\nu + \nu^* + k = 0$ and the bound in Equation (6.5.6) for diagrams with $\nu + \nu^* + k \geq 1$.) Thus, by a similar computation as for ε_Z

$$\begin{aligned}\left|\sum_{p=1}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\tilde{\mathcal{L}}_p^3}\Gamma_{\pi,G}^3\right| &\leq C\rho_0^3\left[\sum_{\nu_0=1}^{\infty}(C\rho_0\left\|g\right\|_{L^1})^{\nu_0} + \sum_{k_0=1}^{\infty}\sum_{\nu_0=0}^{\infty}(C\rho_0\left\|g\right\|_{L^1})^{\nu_0+k_0}\left\|\gamma^{(1)}\right\|_{L^1}^{k_0}\right] \\ &\leq C\rho_0^4\left\|g\right\|_{L^1}\left(1 + \left\|\gamma^{(1)}\right\|_{L^1}\right)\end{aligned}$$

for sufficiently small $\rho_0\left\|g\right\|_{L^1}$ and $\rho_0\left\|g\right\|_{L^1}\left\|\gamma^{(1)}\right\|_{L^1}$. Moreover, $f \leq 1$ and the support of ∇f is contained a ball of radius $\sim b$. Thus by Equation (6.3.9) and Lemma 6.4.6

$$\begin{aligned}\left|\varepsilon_3\right| &\leq CL^d\rho_0^{3+4/d}\left(\int f|\nabla f||x|^2\right)^2 + CL^d\left\|g\right\|_{L^1}(\left\|\gamma^{(1)}\right\|_{L^1}+1)\rho_0^4\left(\int f|\nabla f|\right)^2 \\ &\leq CL^d a^{2d}b^2\rho_0^{3+4/d} + CL^d a^{3d-2}\rho_0^4\zeta^{d/2}\log b/a.\end{aligned}$$

Refined analysis in dimension $d = 1$. In dimension $d = 1$ we need also to analyse diagrams with $k + \nu + \nu^* = 1$ in more detail. Intuitively this follow by "counting powers of ρ_0": The claimed leading term in Theorem 6.1.2 is of order $a\rho_0^4$. Thus, we need to compute precisely all diagrams for which the naive bound Equation (6.5.6) only gives a power ≤ 4 of ρ_0.

The diagrams with $k + \nu + \nu^* = 1$ have either $p = 1$, in which case $\nu^* = 1$, or $p = 2$, in which case $k = 1$. For the diagrams with $p = 1$ for any graph any permutation makes each linked component have at least one external vertex and thus we get

$$\sum_{(\pi,G)\in\tilde{\mathcal{L}}_1^3}\Gamma_{\pi,G}^3 = \sum_{G\in\mathcal{G}_1^3}\int \rho^{(4)}(x_1,x_2,x_3,x_4)\prod_{e\in G}g_e\,\mathrm{d}x_4.$$

Bound all but one g-factor, by symmetry say g_{14}, by $|g_{ij}| \leq 1$ and bound $\rho^{(4)}$ using Lemma 6.5.4. We conclude

$$\begin{aligned}|\cdot| &\leq C\rho_0^{10}|x_1-x_2|^2|x_1-x_3|^2\int |g(z)||z|^2\,\mathrm{d}z \\ &\leq Cab^2\rho_0^{10}|x_1-x_2|^2|x_1-x_3|^2.\end{aligned}$$

By Equation (6.3.9) this gives the contribution $La^3b^4\rho_0^{10}$ to ε_3. For $p=2$ we have the graph (recall that $*$'s label external vertices)

$$G = \begin{array}{ccc} \overset{1}{*\bullet} & \overset{2}{*\bullet} & \overset{3}{*\bullet} \\ & \overset{4}{\bullet}\text{-}\,\text{-}\,\text{-}\,\text{-}\overset{5}{\bullet} & \end{array}$$

The only π's for which $(\pi,G)\notin\tilde{\mathcal{L}}_2^3$ are those not connecting $\{4,5\}$ to $\{1,2,3\}$. Thus

$$\sum_{(\pi,G)\in\tilde{\mathcal{L}}_2^3}\Gamma^3_{\pi,G} = \int\left[\rho^{(5)}(x_1,\ldots,x_5)-\rho^{(3)}(x_1,x_2,x_3)\rho^{(2)}(x_4,x_5)\right]g_{45}\,\mathrm{d}x_4\,\mathrm{d}x_5.$$

This vanishes (quadratically) whenever any x_i and x_j, $i,j=1,2,3$ are incident. Thus, as with $\rho^{(3)}$ and $\rho^{(4)}$, we bound the derivatives and use Taylor's theorem. Denote the derivative w.r.t. x_j by ∂_{x_j}. We are thus interested in bounding $\partial_{x_2}^2\partial_{x_3}^2\Gamma^3_{\pi,G}$. By explicit computation (with the permutation denoted π^{-1} for convenience of notation) we have

$$\begin{aligned}
&\partial_{x_2}^2\partial_{x_3}^2\Gamma^3_{\pi^{-1},G}\\
&\quad=\partial_{x_2}^2\partial_{x_3}^2\left[(-1)^\pi\frac{1}{L^5}\sum_{k_1,\ldots,k_5}\hat{\gamma}^{(1)}(k_1)\cdots\hat{\gamma}^{(1)}(k_5)\iint e^{i(k_1-k_{\pi(1)})x_1}\cdots e^{i(k_5-k_{\pi(5)})x_5}g_{45}\,\mathrm{d}x_4\,\mathrm{d}x_5\right]\\
&\quad=-(-1)^\pi\frac{1}{L^4}\sum_{k_1,\ldots,k_5}(k_2-k_{\pi(2)})^2(k_3-k_{\pi(3)})^2\hat{\gamma}^{(1)}(k_1)\cdots\hat{\gamma}^{(1)}(k_5)\\
&\qquad\times e^{i(k_1-k_{\pi(1)})x_1}\cdots e^{i(k_3-k_{\pi(3)})x_3}\hat{g}(k_4-k_{\pi(4)})\chi_{(k_5-k_{\pi(5)}+k_4-k_{\pi(4)}=0)},
\end{aligned}$$

where χ denotes a characteristic function. Any permutation such that $(\pi,G)\in\tilde{\mathcal{L}}_3^2$ has $\pi(\{4,5\})\neq\{4,5\}$. In particular for the relevant permutations the characteristic function is not identically one, and thus effectively it reduces the number of k-sums by 1. More precisely we get for the permutations with $\pi(5),\pi(4)\neq 5$ (the others are similar)

$$\begin{aligned}
&=-(-1)^\pi\frac{1}{L^4}\sum_{k_1,\ldots,k_4}(k_2-k_{\pi(2)})^2(k_3-k_{\pi(3)})^2\hat{\gamma}^{(1)}(k_1)\cdots\hat{\gamma}^{(1)}(k_4)\hat{\gamma}^{(1)}(-k_4+k_{\pi(4)}+k_{\pi(5)})\\
&\qquad\times e^{i(k_1-k_{\pi(1)})x_1}\cdots e^{i(k_3-k_{\pi(3)})x_3}\hat{g}(k_4-k_{\pi(4)}).
\end{aligned}$$

Bounding $\left|\hat{\gamma}^{(1)}(-k_4+k_{\pi(4)}+k_{\pi(5)})\right|\leq 1$ and $|\hat{g}|\leq\|g\|_{L^1}\leq Ca\log b/a$ the k-sums are readily bounded by Equation (6.3.12). Thus for any valid permutation π we have

$$\left|\partial_{x_2}^2\partial_{x_3}^2\Gamma^3_{\pi,G}\right|\leq Ca\rho_0^{4+4}\log b/a.$$

By Taylor's theorem we conclude that

$$\left|\Gamma^3_{\pi,G}\right|\leq Ca\rho_0^{4+4}\log b/a|x_1-x_2|^2|x_1-x_3|^2.$$

We thus get the contribution to ε_3 of $La^3b^2\rho_0^8\log b/a$ by Equation (6.3.9). Finally, using the bound in Equation (6.5.6) for diagrams with $k+\nu+\nu^*\geq 2$ we get (again for suffiently small $\rho_0\|g\|_{L^1}$ and $\rho_0\|g\|_{L^1}\left\|\gamma^{(1)}\right\|_{L^1}$)

$$\sum_{p=2}^\infty\frac{1}{p!}\left|\sum_{\substack{(\pi,G)\in\tilde{\mathcal{L}}_p^2\\(k+\nu+\nu^*)(\pi,G)\geq 2}}\Gamma^2_{\pi,G}\right|\leq Ca^3\rho_0^5\zeta(\log b/a)^2.$$

By Equation (6.3.9) this gives a contribution to ε_3 of $La^2\rho_0^5(\log b/a)^2$. We conclude the bound

$$\begin{aligned}|\varepsilon_3| &\le CL\left(a^2b^4\rho_0^9 + a^3b^4\rho_0^{10} + a^3b^2\rho_0^8\log b/a + a^2\rho_0^5\zeta(\log b/a)^2\right)\\ &\le CLa^2\rho_0^5\zeta(\log b/a)^2\end{aligned}$$

in dimension $d = 1$.

6.5.4.3 Bound of ε_2

We use the bound in Equation (6.5.6) for diagrams with $\nu + \nu^* + k \ge 3$ and a more precise analysis for the small diagrams. Write

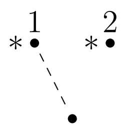
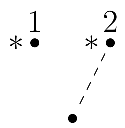
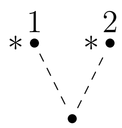
$$\sum_{p=2}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\tilde{\mathcal{L}}_p^2}\Gamma_{\pi,G}^2 = \xi_{=1} + \xi_{=2} + \xi_{\ge 3}, \tag{6.5.7}$$

where $\xi_{=j}$ is the sum of the values of all diagrams with $\nu + \nu^* + k = j$ and $\xi_{\ge 3}$ is the sum of the values of all diagrams with $\nu + \nu^* + k \ge 3$.

For the large diagrams with $\nu + \nu^* + k \ge 3$ we have similarly as above for $\rho_0\,\|g\|_{L^1}$ and $\rho_0\,\|g\|_{L^1}\left\|\gamma^{(1)}\right\|_{L^1}$ sufficiently small

$$|\xi_{\ge 3}| = \left|\sum_{p=2}^{\infty}\frac{1}{p!}\sum_{\substack{(\pi,G)\in\tilde{\mathcal{L}}_p^2\\(k+\nu+\nu^*)(\pi,G)\ge 2}}\Gamma_{\pi,G}^2\right| \le C\rho_0^5\,\|g\|_{L^1}^3\,(1 + \left\|\gamma^{(1)}\right\|_{L^1}^3). \tag{6.5.8}$$

Diagrams with $k + \nu + \nu^* = 1$. For the diagrams with $p = 1$ and $p = 2$ with $k = 1$ we do a more precise calculation. For $p = 1$ there are three possible g-graphs: (Recall that $*$'s label the external vertices)

$G =$  , $G =$  , $G =$ 

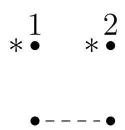
Any permutation makes any of these diagrams have at least one external vertex in each linked component and thus

$$\sum_{(\pi,G)\in\tilde{\mathcal{L}}_1^2}\Gamma_{\pi,G}^2 = \int \rho^{(3)}(x_1,x_2,x_3)\,[g_{13} + g_{23} + g_{13}g_{23}]\,\mathrm{d}x_3$$

Bounding $|g_{13}g_{23}| \le |g_{13}|$ and recalling the bound $\rho^{(3)}(x_1,x_2,x_3) \le C\rho_0^{3+4/d}|x_1-x_2|^2|x_1-x_3|^2$ from Lemma 6.5.4 we get by symmetry

$$\left|\sum_{(\pi,G)\in\tilde{\mathcal{L}}_1^2}\Gamma_{\pi,G}^2\right| \le C\rho_0^{3+4/d}|x_1-x_2|^2\int |g(z)||z|^2\,\mathrm{d}z = C\left\||\cdot|^2 g\right\|_{L^1}\rho_0^{3+4/d}|x_1-x_2|^2 \tag{6.5.9}$$

The diagrams with $p = 2$ and $k = 1$ have g-graph

$G =$  (6.5.10)

The only permutations π such that $(\pi, G) \notin \tilde{\mathcal{L}}_2^2$ are those connecting only external to external and internal to internal, i.e. those with either $\pi(3) = 3, \pi(4) = 4$ or $\pi(3) = 4, \pi(4) = 3$. Thus

$$\sum_{\substack{(\pi,G)\in\tilde{\mathcal{L}}_2^2 \\ k(\pi,G)=1}} \Gamma^2_{\pi,G} = \iint \left[\rho^{(4)}(x_1,\ldots,x_4) - \rho^{(2)}(x_1,x_2)\rho^{(2)}(x_3,x_4)\right] g_{34} \, \mathrm{d}x_3 \, \mathrm{d}x_4. \tag{6.5.11}$$

Clearly this vanishes quadratically in $x_1 - x_2$ since both determinants do, thus we bound it using Taylor's theorem, expanding in x_1 around $x_1 = x_2$ analogously to what we did for (some of the diagrams for) ε_3 above. We treat each diagram separately. (For convenience we denote the permutation π^{-1}.) Denoting the derivative with respect to x_1^μ by $\partial^\mu_{x_1}$ we have

$$\begin{aligned}
\partial^\mu_{x_1}\partial^\nu_{x_1}\Gamma^2_{\pi^{-1},G} &= -\frac{1}{L^{4d}} \sum_{k_1,\ldots,k_4} \left(k_1^\mu - k^\mu_{\pi(1)}\right)\left(k_1^\nu - k^\nu_{\pi(1)}\right) \hat\gamma^{(1)}(k_1)\hat\gamma^{(1)}(k_2)\hat\gamma^{(1)}(k_3)\hat\gamma^{(1)}(k_4) \\
&\qquad \times e^{i(k_1-k_{\pi(1)})x_1} e^{i(k_2-k_{\pi(2)})x_2} \iint e^{i(k_3-k_{\pi(3)})x_3} e^{i(k_4-k_{\pi(4)})x_4} g(x_3-x_4) \, \mathrm{d}x_3 \, \mathrm{d}x_4 \\
&= -\frac{1}{L^{3d}} \sum_{k_1,\ldots,k_4} \left(k_1^\mu - k^\mu_{\pi(1)}\right)\left(k_1^\nu - k^\nu_{\pi(1)}\right) \hat\gamma^{(1)}(k_1)\hat\gamma^{(1)}(k_2)\hat\gamma^{(1)}(k_3)\hat\gamma^{(1)}(k_4) \\
&\qquad \times \hat g(k_{\pi(3)} - k_3)\chi_{(k_4-k_{\pi(4)}=k_{\pi(3)}-k_3)}
\end{aligned}$$

The only permutations for which the characteristic function is identically 1 are those with either $\pi(3) = 3, \pi(4) = 4$ or $\pi(3) = 4, \pi(4) = 3$. These are exactly the permutations that do not appear in Equation (6.5.11) above. Thus, similarly as for (some of the diagrams for) ε_3 above the charactersitic function effectively reduces the number of k-sums by 1. Bounding $|\hat g| \le \|g\|_{L^1}$, $\hat\gamma^{(1)} \le 1$ for one of the $\gamma^{(1)}$-factors, and using Equation (6.3.12) to bound the k-sums we have for any diagram $(\pi, G) \in \tilde{\mathcal{L}}_2^2$ with G as in Equation (6.5.10)

$$\left|\partial^\mu_{x_1}\partial^\nu_{x_1}\Gamma^2_{\pi,G}\right| \le C\|g\|_{L^1}\rho_0^{3+2/d}.$$

We conclude the bound

$$\left|\sum_{\substack{(\pi,G)\in\tilde{\mathcal{L}}_2^2 \\ k(\pi,G)=1}} \Gamma^2_{\pi,G}\right| \le C\|g\|_{L^1}\rho_0^{3+2/d}|x_1-x_2|^2. \tag{6.5.12}$$

In particular, by combining Equations (6.5.9) and (6.5.12), we have

$$|\xi_{=1}| \le C\|g\|_{L^1}\rho_0^{3+2/d}|x_1-x_2|^2. \tag{6.5.13}$$

Diagrams with $k + \nu + \nu^* = 2$. Finally consider all diagrams with $k + \nu + \nu^* = 2$ more precisely. We split these into three groups.

(i) $\nu^* = 2$

(ii) $\nu^* = 1$ and vertices $\{1\}$ and $\{2\}$ are connected

(iii) Remaining diagrams

We will use a Taylor expansion to bound the values of the diagrams in group (iii). Write

$$\xi_{=2} = \xi_{\text{(i)}} + \xi_{\text{(ii)}} + \xi_{\text{(iii)}}$$

Then as $\rho_J^{(2)}(x_2; x_2) = 0$ we get from Equation (6.5.7)

$$\left|\xi_{\text{(iii)}}(x_2, x_2)\right| \le \left|\xi_{\text{(i)}}(x_2, x_2)\right| + \left|\xi_{\text{(ii)}}(x_2, x_2)\right| + \left|\xi_{=1}(x_2, x_2)\right| + \left|\xi_{\ge 3}(x_2, x_2)\right|.$$

Moreover, $\xi_{\text{(iii)}}$ is symmetric in exchange of x_1 and x_2 so the first order vanishes. We conclude by Taylor's theorem that

$$\begin{aligned}\left|\xi_{\text{(iii)}}(x_1, x_2)\right| &\le \left|\xi_{\text{(i)}}(x_2, x_2)\right| + \left|\xi_{\text{(ii)}}(x_2, x_2)\right| + \left|\xi_{=1}(x_2, x_2)\right| + \left|\xi_{\ge 3}(x_2, x_2)\right| \\ &\quad + C \sup_{\mu,\nu} \sup_{z_1,z_2} \left|\partial_{x_1}^{\mu} \partial_{x_1}^{\nu} \xi_{\text{(iii)}}(z_1, z_2)\right| |x_1 - x_2|^2,\end{aligned} \tag{6.5.14}$$

where again $\partial_{x_1}^{\mu}$ denotes the derivative w.r.t. x_1^{μ}. Bounding $\partial_{x_1}^{\mu}\partial_{x_1}^{\nu}\xi_{\text{(iii)}}$ is analogous to the argument in the proof of Lemmas 3.4.1 and 3.4.8: For diagrams with an internal vertex connected to $\{1\}$ with a g-edge we do a precise calculation as in the proof of Lemma 3.4.8. For the remaining diagrams where $\{1\}$ has no incident g-edges we modify the proof of the absolute convergence of the GGR expansion as in the proof of Lemma 3.4.1.

First, the diagrams in group (iii) with an internal vertex connected to $\{1\}$ with a g-edge all have g-graph

$$G = \begin{array}{ccc} {*}\overset{1}{\bullet}\text{-----}\overset{3}{\bullet} & & \overset{2}{\bullet}{*} \\ \\ \overset{4}{\bullet}\text{-----}\overset{5}{\bullet} & & \end{array} \tag{6.5.15}$$

since $\nu^* = 1$ and $k + \nu + \nu^* = 2$. Then

$$\begin{aligned}\Gamma^2_{\pi^{-1},G} &= (-1)^{\pi} \frac{1}{L^{5d}} \sum_{k_1,\ldots,k_5} \hat{\gamma}^{(1)}(k_1) \cdots \hat{\gamma}^{(1)}(k_5) \\ &\quad \times \iiint e^{i(k_1 - k_{\pi(1)})x_1} \cdots e^{i(k_5 - k_{\pi(5)})x_5} g_{13} g_{45} \,\mathrm{d}x_3 \,\mathrm{d}x_4 \,\mathrm{d}x_5 \\ &= (-1)^{\pi} \frac{1}{L^{4d}} \sum_{k_1,\ldots,k_5} \hat{\gamma}^{(1)}(k_1) \cdots \hat{\gamma}^{(1)}(k_5) e^{i(k_1 - k_{\pi(1)} + k_3 - k_{\pi(3)})x_1} e^{i(k_2 - k_{\pi(2)})x_2} \\ &\quad \times \hat{g}(k_3 - k_{\pi(3)}) \hat{g}(k_5 - k_{\pi(5)}) \chi_{(k_4 - k_{\pi(4)} + k_5 - k_{\pi(5)} = 0)}.\end{aligned}$$

The characteristic function χ is identically 1 only if $\pi(\{4,5\}) = \{4,5\}$, but then $(\pi, G) \notin \tilde{\mathcal{L}}_3^2$ so these permutations do not appear in $\xi_{\text{(iii)}}$. Taking the derivative, bounding $|\hat{g}| \le \|g\|_{L^1}$ and using Equation (6.3.12) to bound the k-sums we conclude as above that

$$\left|\partial_{x_1}^{\mu}\partial_{x_1}^{\nu} \Gamma^2_{\pi^{-1},G}\right| \le C \rho_0^{4+2/d} \|g\|_{L^1}^2$$

for all diagrams $(\pi, G) \in \tilde{\mathcal{L}}_3^2$ with G as in Equation (6.5.15).

Next, for the diagrams with no g-edges connected to $\{1\}$ the argument is as for the bound of $\partial_{x_1}^{\mu}\partial_{x_1}^{\nu}\xi_0$ in the proof of Lemma 3.4.1. Analogously to Equations (3.4.19) and (3.4.20) we conclude the bound (the term 1 in the factor $\left\|\gamma^{(1)}\right\|_{L^1} + 1$ arises similarly as in the bounds above from the value of diagrams with $k = 1$)

$$\begin{aligned}&\left|\partial_{x_1}^2 \sum_{\substack{(\pi,G)\in\tilde{\mathcal{L}}_3^2 \\ \text{no } g\text{-edges incident to } \{1\}}} \Gamma^2_{\pi^{-1},G}\right| \\ &\quad \le C \rho_0^4 \|g\|_{L^1}^2 \left(\left\|\gamma^{(1)}\right\|_{L^1} + 1\right) \left[\rho_0^{2/d} \left\|\gamma^{(1)}\right\|_{L^1} + \rho_0^{1/d} \left\|\partial\gamma^{(1)}\right\|_{L^1} + \left\|\partial^2\gamma^{(1)}\right\|_{L^1}\right]\end{aligned}$$

where with a similar abuse of notation

$$\left\|\partial\gamma^{(1)}\right\|_{L^1} = \max_{\mu} \int_{[0,L]^d} \left|\partial^\mu \gamma^{(1)}\right| \, \mathrm{d}x, \qquad \left\|\partial^2\gamma^{(1)}\right\|_{L^1} = \max_{\mu,\nu} \int_{[0,L]^d} \left|\partial^\mu \partial^\nu \gamma^{(1)}\right| \, \mathrm{d}x.$$

Recall that $\left\|\gamma^{(1)}\right\|_{L^1} \leq C\zeta^{d/2}$ by Lemma 6.4.6. By a simple modification of the proof of Lemma 6.4.6 we may bound $\left\|\partial\gamma^{(1)}\right\|_{L^1} \leq C\zeta^{d/2}\rho_0^{1/d}$ and $\left\|\partial^2\gamma^{(1)}\right\|_{L^1} \leq C\zeta^{d/2}\rho_0^{2/d}$. Thus

$$\left|\partial_{x_1}^2 \xi_{(\mathrm{iii})}(z_1, z_2)\right| \leq C\rho_0^{4+2/d} \left\|g\right\|_{L^1}^2 \zeta^d. \tag{6.5.16}$$

Next, we bound $\xi_{(\mathrm{i})}$. For the diagrams with $\nu^* = 2$, if G is any graph with $\nu^*(G) = 2$ then for any permutation $\pi \in \mathcal{S}_4$ we have $(\pi, G) \in \tilde{\mathcal{L}}_2^2$. Thus using Lemma 6.5.4 to bound $\rho^{(4)}$ and bounding some g-factors by 1 we get similarly to Equation (6.5.9)

$$\begin{aligned}
\xi_{(\mathrm{i})} &= \sum_{\substack{G \in \mathcal{G}_2^2 \\ \nu^*(G)=2}} \iint \rho^{(4)} \prod_{e \in G} g_e \, \mathrm{d}x_3 \, \mathrm{d}x_4 \\
\left|\xi_{(\mathrm{i})}\right| &\leq C\rho_0^{4+6/d} |x_1 - x_2|^2 \iint |g(z_1)|^2 |g(z_2)|^2 (|z_1|^2 + |z_2|^2 + |x_1 - x_2|^2)^2 \, \mathrm{d}z_1 \, \mathrm{d}z_2 \\
&\leq C \left\|g\right\|_{L^1}^2 \rho_0^{4+6/d} |x_1 - x_2|^2 (b^2 + |x_1 - x_2|^2)^2.
\end{aligned} \tag{6.5.17}$$

Finally, we bound $\xi_{(\mathrm{ii})}$. All diagrams with $\nu^* = 1$ and $\{1\}$ and $\{2\}$ connected have g-graph

$$G_0 = \begin{array}{c} * \overset{1}{\bullet} \text{-----} \overset{3}{\bullet} \text{-----} \overset{2}{\bullet} * \\[1em] \overset{4}{\bullet} \text{-----} \overset{5}{\bullet} \end{array} \tag{6.5.18}$$

For convenience of notation we denote the permutation in the diagram π^{-1}. Then

$$\begin{aligned}
\Gamma^2_{\pi^{-1}, G_0} &= (-1)^\pi \frac{1}{L^{5d}} \sum_{k_1, \ldots, k_5} \hat{\gamma}^{(1)}(k_1) \cdots \hat{\gamma}^{(1)}(k_5) \\
&\quad \times \iiint e^{i(k_1 - k_{\pi(1)})x_1} \cdots e^{i(k_5 - k_{\pi(5)})x_5} g(x_1 - x_3) g(x_2 - x_3) g(x_4 - x_5) \, \mathrm{d}x_3 \, \mathrm{d}x_4 \, \mathrm{d}x_5 \\
&= (-1)^\pi \frac{1}{L^{5d}} \sum_{k_1, \ldots, k_5} \hat{\gamma}^{(1)}(k_1) \cdots \hat{\gamma}^{(1)}(k_5) e^{i\left(k_1 - k_{\pi(1)} - \frac{k_3 - k_{\pi(3)}}{2}\right)x_1} e^{i\left(k_2 - k_{\pi(2)} - \frac{k_3 - k_{\pi(3)}}{2}\right)x_2} \\
&\quad \times \int e^{i(k_3 - k_{\pi(3)})(x_3 - \frac{x_1 + x_2}{2})} g\left(\frac{x_1 - x_2}{2} + \frac{x_1 + x_2}{2} - x_3\right) \\
&\quad \times g\left(-\frac{x_1 - x_2}{2} + \frac{x_1 + x_2}{2} - x_3\right) \mathrm{d}x_3 \\
&\quad \times \iint g(x_4 - x_5) e^{i(k_4 - k_{\pi(4)})(x_4 - x_5)} e^{i(k_5 - k_{\pi(5)} + k_4 - k_{\pi(4)})x_5} \, \mathrm{d}x_4 \, \mathrm{d}x_5 \\
&= (-1)^\pi \frac{1}{L^{4d}} \sum_{k_1, \ldots, k_5} \hat{\gamma}^{(1)}(k_1) \cdots \hat{\gamma}^{(1)}(k_5) e^{i\left(k_1 - k_{\pi(1)} - \frac{k_3 - k_{\pi(3)}}{2}\right)x_1} e^{i\left(k_2 - k_{\pi(2)} - \frac{k_3 - k_{\pi(3)}}{2}\right)x_2} \\
&\quad \times \hat{G}_1(k_3 - k_{\pi(3)}) \hat{g}(k_{\pi(4)} - k_4) \chi_{(k_5 - k_{\pi(5)} + k_4 - k_{\pi(4)} = 0)},
\end{aligned}$$

where

$$\hat{G}_1(k) := \int e^{-ikz} g\left(\frac{x_1 - x_2}{2} + z\right) g\left(-\frac{x_1 - x_2}{2} + z\right) \mathrm{d}z.$$

We group together pairs of diagrams π and (using cycle notation) $\pi \cdot (4\,5) = (\pi(4)\,\pi(5)) \cdot \pi$, meaning where $\pi(4)$ and $\pi(5)$ are swapped. These have opposite signs. Thus,

$$
\begin{aligned}
&\Gamma^2_{\pi^{-1},G_0} + \Gamma^2_{(\pi(4\,5))^{-1},G_0} \\
&= (-1)^\pi \frac{1}{L^{4d}} \sum_{k_1,\ldots,k_5} \hat{\gamma}^{(1)}(k_1)\cdots\hat{\gamma}^{(1)}(k_5) e^{i\left(k_1 - k_{\pi(1)} - \frac{k_3-k_{\pi(3)}}{2}\right)x_1} e^{i\left(k_2 - k_{\pi(2)} - \frac{k_3-k_{\pi(3)}}{2}\right)x_2} \\
&\quad \times \hat{G}_1(k_3 - k_{\pi(3)}) \chi_{(k_5 - k_{\pi(5)} + k_4 - k_{\pi(4)} = 0)} \left[\hat{g}(k_{\pi(4)} - k_4) - \hat{g}(k_{\pi(5)} - k_4)\right].
\end{aligned}
$$

We Taylor expand $\hat{g}(k_{\pi(5)} - k_4)$ in $k_{\pi(5)}$ around $k_{\pi(5)} = k_{\pi(4)}$. That is,

$$
\hat{g}(k_{\pi(5)} - k_4) = \hat{g}(k_{\pi(4)} - k_4) + O\left(\nabla \hat{g}\right) \left|k_{\pi(4)} - k_{\pi(5)}\right|,
$$

where $O\left(\nabla\hat{g}\right)$ should be interpreted as being bounded by $|\nabla \hat{g}(k)| \le \int |x||g(x)| = \| |\cdot| g\|_{L^1}$ uniformly in $k_{\pi(4)} - k_{\pi(5)}$. Moreover, $\left|\hat{G}_1\right| \le \|g\|_{L^1}$. Thus

$$
\begin{aligned}
&\left|\Gamma^2_{\pi^{-1},G_0} + \Gamma^2_{(\pi(4\,5))^{-1},G_0}\right| \\
&\le C \|g\|_{L^1} \| |\cdot| g\|_{L^1} \times \frac{1}{L^{4d}} \sum_{k_1,\ldots,k_5} \hat{\gamma}^{(1)}(k_1)\cdots\hat{\gamma}^{(1)}(k_5) \left|k_{\pi(4)} - k_{\pi(5)}\right| \chi_{(k_5 - k_{\pi(5)} + k_4 - k_{\pi(4)} = 0)}.
\end{aligned}
$$

The characteristic function is not identically 1 for linked diagrams. Indeed, if $\pi(\{4,5\}) = \{4,5\}$ then the diagram would not be linked. Thus, the characteristic function effectively reduces the number of k-sums by 1. Bounding similarly as above $\hat{\gamma}^{(1)} \le 1$ and using finally Equation (6.3.12) to bound the k-sums we conclude for any permutation π such that $(\pi, G_0) \in \tilde{\mathcal{L}}^2_3$ that

$$
\left|\Gamma^2_{\pi^{-1},G_0} + \Gamma^2_{(\pi(4\,5))^{-1},G_0}\right| \le C \rho_0^{4+1/d} \| |\cdot| g\|_{L^1} \|g\|_{L^1}.
$$

Since, π and $\pi(4\,5)$ either both give rise to linked diagrams or neither do we conclude that

$$
\left|\xi_{\text{(ii)}}\right| = \frac{1}{3!} \left| \sum_{(\pi,G_0)\in\tilde{\mathcal{L}}^2_3} \Gamma_{\pi,G_0} \right| \le C\rho_0^{4+1/d} \| |\cdot| g\|_{L^1} \|g\|_{L^1}. \tag{6.5.19}
$$

Combining then Equations (6.5.8), (6.5.13), (6.5.14), (6.5.16), (6.5.17) and (6.5.19) and using Lemma 6.4.6 we conclude the bound

$$
\left|\xi_{\text{(iii)}}\right| \le Ca^{2d} b \rho_0^{4+1/d} \log b/a + Ca^{3d}\rho_0^5 \zeta^{3d/2} (\log b/a)^3 + Ca^{2d}\rho_0^{4+2/d}\zeta^d (\log b/a)^2 |x_1 - x_2|^2.
$$

We conclude the bound

$$
\begin{aligned}
\left|\sum_{p=1}^\infty \frac{1}{p!} \sum_{(\pi,G)\in\tilde{\mathcal{L}}^2_p} \Gamma^2_{\pi,G}\right| &\le Ca^d \rho_0^{3+2/d} \log b/a |x_1 - x_2|^2 + a^d b^2 \rho_0^{3+4/d} |x_1 - x_2|^2 \\
&\quad + Ca^d\rho_0^{4+6/d} |x_1 - x_2|^2 (b^2 + |x_1 - x_2|^2)^2 (\log b/a)^2 \\
&\quad + Ca^{2d} b \rho_0^{4+1/d} \log b/a + Ca^{2d} \rho_0^{4+2/d} \zeta^d (\log b/a)^2 |x_1 - x_2|^2 \\
&\quad + Ca^{3d} \rho_0^5 \zeta^{3d/2} (\log b/a)^3.
\end{aligned}
$$

Thus, using Lemma 6.3.4 we get

$$\begin{aligned}
\frac{|\varepsilon_2|}{L^d} &\leq Ca^{2d}\rho_0^{3+2/d}\log b/a + Ca^{2d}b^2\rho_0^{3+4/d} + Ca^{4d}b^{4-d}\rho_0^{4+6/d}(\log b/a)^2 \\
&\quad + Ca^{3d-2}b\rho_0^{4+1/d}\log b/a + Ca^{3d}\rho_0^{4+2/d}\zeta^d(\log b/a)^2 + Ca^{4d-2}\rho_0^5\zeta^{3d/2}(\log b/a)^3. \\
&\leq \begin{cases} Ca^{2d}\rho_0^{3+2/d}\log b/a + Ca^{4d-2}\rho_0^5\zeta^{3d/2}(\log b/a)^3 & d \geq 2, \\ Cab\rho_0^5\log b/a + Ca^2\rho_0^5\zeta^{3/2}(\log b/a)^3 & d = 1. \end{cases}
\end{aligned}$$

This concludes the proof of Lemma 6.5.2. □

Remark 6.5.5 (Necessity of precise analysis of diagrams with $k+\nu+\nu^* = 2$)**.** For the bound of ε_2 we give here a precise analysis of the diagrams with $k+\nu+\nu^* = 2$. In general, one should not expect this to be needed in dimensions $d = 2, 3$. More precisely, by just considering powers of ρ_0, one would expect that diagrams with $k+\nu+\nu^* \geq 1$ are all subleading as they carry a higher power of ρ_0 (using Equation (6.5.6)) than the claimed leading term, with exponent $2+2/d$.

The reason we need a precise analysis here is the temperature dependence of our bounds: For some regime of temperatures the bound one would get by using Equation (6.5.6) is not good enough.

Remark 6.5.6 (Optimality of the error bounds)**.** One should not expect the bound given in Equation (6.5.19) to be optimal. More precisely in Equation (6.5.19) we only took into account the cancellations of pairs of diagrams. However, one should expect much more cancellations. We have

$$\xi_{\text{(ii)}} = \frac{1}{3!}\iiint \left[\rho^{(5)}(x_1,\ldots,x_5) - \rho^{(3)}(x_1,x_2,x_3)\rho^{(2)}(x_4,x_5)\right] g_{13}g_{23}g_{45}\,\mathrm{d}x_3\,\mathrm{d}x_4\,\mathrm{d}x_5.$$

Naively, just using that $\rho^{(5)}(x_1,\ldots,x_5) - \rho^{(3)}(x_1,x_2,x_3)\rho^{(2)}(x_4,x_5)$ vanishes whenever any two of the particles $1,2,3$ or the particles $4,5$ are incident we get by Taylor expansion

$$\left|\rho^{(5)}(x_1,\ldots,x_5) - \rho^{(3)}(x_1,x_2,x_3)\rho^{(2)}(x_4,x_5)\right| \leq C\rho_0^{5+6/d}|x_1-x_2|^2|x_1-x_3|^2|x_4-x_5|^2. \tag{6.5.20}$$

Using this bound and bounding $|g_{23}| \leq 1$ we get

$$\left|\xi_{\text{(ii)}}\right| \leq \rho_0^{5+6/d}a^{2d}b^4L^d|x_1-x_2|^2. \tag{6.5.21}$$

This bound is too large by a volume factor. (This arises since we "forget" that the relevant diagrams are linked when we do the Taylor expansion.) It however illustrates how many more cancellations between the different permutations are present than what we used in the bound Equation (6.5.19) — it carries a higher power of ρ_0. Using these cancellations but losing the information that diagrams are linked is what we did in Chapter 3.

If one could somehow see these cancellations, while still keeping the information that the diagrams have to be linked, one might be able to improve upon the bound Equation (6.5.19). In 1 dimension this error term is actually (for some regime of temperatures) the dominant error term. Thus, by improving the analysis of these diagrams, one might improve the error term in Proposition 6.1.9 in $d = 1$.

6.A Particle density of the trial state

In this section we give the

Proof of Equation (6.3.3). We calculate $\langle \mathcal{N} \rangle_J$ and compare it to $\langle \mathcal{N} \rangle_0 = \rho_0 L^d$. We have by Equation (6.4.2)

$$\langle \mathcal{N} \rangle_J = \int \rho_J^{(1)}(x)\,\mathrm{d}x = L^d \left[\rho^{(1)} + \sum_{p=1}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p^1} \Gamma_{\pi,G}^1 \right] = \langle \mathcal{N} \rangle_0 + L^d \sum_{p=1}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p^1} \Gamma_{\pi,G}^1.$$

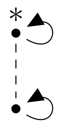
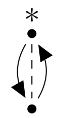
Next, we bound $\sum_{p=1}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p^1} \Gamma_{\pi,G}^1$. We use the bound in Equation (6.5.6) for diagrams with $k + \nu + \nu^* \geq 2$, i.e., for $p = 2$ with $k = 0, \nu^* = 2$ and for $p \geq 3$. That is,

$$\frac{1}{2!} \left| \sum_{\substack{(\pi,G)\in\mathcal{L}_2^1 \\ k(\pi,G)=0}} \Gamma_{\pi,G}^1 \right| \leq C \|g\|_{L^1}^2 \rho_0^3, \qquad \sum_{p=3}^{\infty} \frac{1}{p!} \left| \sum_{(\pi,G)\in\mathcal{L}_p^1} \Gamma_{\pi,G}^1 \right| \leq C \|g\|_{L^1}^2 (1 + \left\|\gamma^{(1)}\right\|_{L^1}^2) \rho_0^3$$

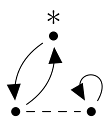
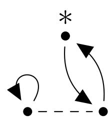
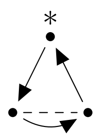
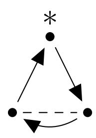
for sufficiently small $\rho_0 \|g\|_{L^1}$ and $\rho_0 \|g\|_{L^1} \left\|\gamma^{(1)}\right\|_{L^1}$. Thus, we get

$$\sum_{p=1}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p^1} \Gamma_{\pi,G}^1 = \sum_{(\pi,G)\in\mathcal{L}_1^1} \Gamma_{\pi,G}^1 + \frac{1}{2} \sum_{\substack{(\pi,G)\in\mathcal{L}_2^1 \\ k(\pi,G)=1}} \Gamma_{\pi,G}^1 + O\left(\|g\|_{L^1}^2 \left(\left\|\gamma^{(1)}\right\|_{L^1}^2 + 1 \right) \rho_0^3 \right).$$

For the $p = 1$-term there are two diagrams. Thus (where $*$ labels the external vertex)

$$\sum_{(\pi,G)\in\mathcal{L}_1^1} \Gamma_{\pi,G}^1 =$$  $$+$$  $$= \int \det \begin{bmatrix} \gamma^{(1)}(0) & \gamma^{(1)}(x) \\ \gamma^{(1)}(x) & \gamma^{(1)}(0) \end{bmatrix} g(x)\,\mathrm{d}x = O\left(\left\| |\cdot|^2 g \right\|_{L^1} \rho_0^{2+2/d} \right).$$

For the $p = 2$-term with $k = 1$ there are 4 diagrams. Thus

$$\frac{1}{2} \sum_{\substack{(\pi,G)\in\mathcal{L}_2^1 \\ k(\pi,G)=1}} \Gamma_{\pi,G}^1 = \frac{1}{2} \Bigg[$$  $$+$$  $$+$$  $$+$$  $$\Bigg]$$

$$\begin{aligned}
&= \frac{1}{L^{3d}} \sum_{k_1,k_2,k_3} \iint \mathrm{d}x_2\,\mathrm{d}x_3\, \hat{\gamma}^{(1)}(k_1)\hat{\gamma}^{(1)}(k_2)\hat{\gamma}^{(1)}(k_3) g(x_2 - x_3) \\
&\qquad \times \left[e^{i(k_1-k_2)(x_1-x_2)} - e^{ik_1(x_1-x_2)} e^{ik_2(x_2-x_3)} e^{ik_3(x_3-x_1)} \right] \\
&= \frac{1}{L^{2d}} \sum_{k_1,k_2,k_3} \hat{\gamma}^{(1)}(k_1)\hat{\gamma}^{(1)}(k_2)\hat{\gamma}^{(1)}(k_3)\hat{g}(k_1 - k_2) \left[\chi_{(k_1=k_2)} - \chi_{(k_1=k_3)} \right] \\
&= \frac{1}{L^{2d}} \sum_{k,\ell} \hat{\gamma}^{(1)}(k)^2 \hat{\gamma}^{(1)}(\ell) \left[\hat{g}(0) - \hat{g}(k - \ell) \right].
\end{aligned}$$

Taylor expanding $\hat{g}$ and using that $\int x g(x) = 0$ so $\nabla \hat{g}(0) = 0$ we get

$$\left| \frac{1}{2} \sum_{\substack{(\pi,G)\in\mathcal{L}_2^1 \\ k(\pi,G)=1}} \Gamma_{\pi,G}^1 \right| \leq C \left\| |\cdot|^2 g \right\|_{L^1} \rho_0^{2+2/d}.$$

Thus, by Lemma 6.4.6

$$\begin{aligned}\left|\sum_{p=1}^{\infty}\frac{1}{p!}\sum_{(\pi,G)\in\mathcal{L}_p^1}\Gamma_{\pi,G}^1\right| &\leq C\left\||\cdot|^2 g\right\|_{L^1}\rho_0^{2+2/d}+C\|g\|_{L^1}^2\left\|\gamma^{(1)}\right\|_{L^1}^2\rho_0^3+C\|g\|_{L^1}^2\rho_0^3 \\ &\leq Ca^d b^2\rho_0^{2+2/d}+Ca^{2d}\rho_0^3\zeta^d(\log b/a)^2.\end{aligned}$$

That is, Equation (6.3.3) is satisfied. □

CHAPTER 7

Pressure of a dilute spin-polarized Fermi gas: Upper bound

This chapter contains the paper

[PressUpp] A. B. Lauritsen and R. Seiringer. "Pressure of a dilute spin-polarized Fermi gas: Upper bound". arXiv: 2407.05990 [math-ph]. 2024. DOI: 10.48550/arXiv.2407.05990.

Abstract. We prove an upper bound on the pressure of a dilute fully spin-polarized Fermi gas capturing the leading correction to the pressure of a free gas resulting from repulsive interactions. This correction is of order $a^3\rho^{8/3}$, with a the p-wave scattering length of the interaction and ρ the particle density, depends on the temperature and matches the corresponding lower bound of Chapter 6.

Contents

7.1 Introduction

Dilute quantum gases have been the focus of much recent study in the mathematical physics literature. A natural question is the determination of asymptotic formulas for the ground state energy (at zero temperature) or the free energy or pressure (at positive temperature) valid for small particle densities. Naturally these quantities are to leading order given by the corresponding quantities for a free (i.e. non-interacting) gas, and the task is to determine the correction to the quantities for a free gas arising from repulsive interactions in such a dilute regime. The first works on such problems are the works of Dyson [Dys57] and Lieb and Yngvason [LY98], giving upper respectively lower bounds for the ground state energy of a dilute Bose gas in 3 dimensions. Here, to leading order, the ground state energy density differs from the free gas by a term of order $a_s\overline{\rho}^2$ with a_s the s-*wave scattering length* of the interaction and $\overline{\rho}$ the particle density. Similarly the spin-$\frac{1}{2}$ Fermi gas has been studied [FGHP21; Gia23a; LSS05], [Chapter 5], and also here the ground state energy density differs from that of the free gas by a term of order $a_s\overline{\rho}^2$.

We consider here a spinless Fermi gas (equivalently completely spin-polarized) with a repulsive interaction. At zero temperature, we found in Chapters 3 and 4 that the ground state energy density of the interacting gas differs from that of a free gas by a term of order $a^3\overline{\rho}^{8/3}$, with a

the p-*wave scattering length* of the interaction. We consider here the extension of this result to positive temperature and show that (at fixed $\beta\mu$)

$$\psi(\beta,\mu) \leq \psi_0(\beta,\mu) - c(\beta\mu)a^3\overline{\rho}^{8/3}[1+o(1)] \qquad \text{as } a^3\overline{\rho} \to 0, \tag{7.1.1}$$

where $\psi(\beta,\mu)$ and $\psi_0(\beta,\mu)$ are the pressures of the interacting respectively free gas at inverse temperature β and chemical potential μ, and $c(\beta\mu)$ is an explicit temperature-dependent coefficient. This upper bound matches the corresponding lower bound in Chapter 6 and we thus conclude that the asymptotic formula in (7.1.1) holds with equality.

Notably for dilute gases, where $\overline{\rho}$ is small, the correction for the spinless Fermi gas is much smaller than that for a Bose gas or spin-$\frac{1}{2}$ Fermi gas. This can be understood from the Pauli exclusion principle. For fermions of the same spin, the Pauli exclusion principle suppresses the probability of particles being close enough to interact. This has the effect that the interaction now enters through the p-wave scattering length and its effect is much smaller.

Both the dilute Bose gas and spin-$\frac{1}{2}$ Fermi gas have also been studied at positive temperature [Sei06b; Sei08; Yin10] and for the Bose gas, even the next order correction has been found at both zero [BCS21; FS20; FS23; YY09] and (suitably low) positive [HHNST23; HHST24] temperature. Also the analogous lower-dimensional problems have been studied, again both at zero [Age23; ARS22; FGJMO24; LSS05; LY01] and positive temperature [DMS20; MS20; Sei06b].

We consider here also the two-dimensional setting and prove that, for fixed $\beta\mu$,

$$\psi(\beta,\mu) \leq \psi_0(\beta,\mu) - c(\beta\mu)a^2\overline{\rho}^{3}[1+o(1)] \qquad \text{as } a^2\overline{\rho} \to 0, \tag{7.1.2}$$

with the quantities being here the two-dimensional analogues of those in (7.1.1). Again, this matches the lower bound in Chapter 6 and the asymptotic formula thus holds with equality. Our method does not directly extend to the one-dimensional case, however, and it remains an open problem to establish the validity of the analogue of (7.1.1) and (7.1.2) in one spatial dimension.

7.1.1 Precise statement of results

Consider a system of fermions confined to some large box $\Lambda = [-L/2, L/2]^3$. We impose periodic boundary conditions on the box Λ. The pressure of the gas in the thermodynamic limit $L \to \infty$ is independent of the boundary conditions [Rob71] and periodic boundary conditions is a convenient choice. Define the one-particle space $\mathfrak{h} = L^2(\Lambda;\mathbb{C})$ and the (fermionic) Fock space $\mathcal{F}(\mathfrak{h}) = \bigoplus_{n=0}^{\infty} \bigwedge^n \mathfrak{h}$. On the Fock space we consider the grand canonical interacting Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{V},$$

with the free (non-interacting) Hamiltonian $\mathcal{H}_0$ and interaction $\mathcal{V}$ given by

$$\begin{aligned} \mathcal{H}_0 &= \mathrm{d}\Gamma(-\Delta-\mu) = \sum_k (|k|^2-\mu)a_k^* a_k, \\ \mathcal{V} &= \mathrm{d}\Gamma(V) = \frac{1}{2}\iint_{\Lambda\times\Lambda} \mathrm{d}x\,\mathrm{d}y\, V(x-y)a_x^* a_y^* a_y a_x. \end{aligned} \tag{7.1.3}$$

Here $a_k^* = a^*(f_k)$ and $a_k = a(f_k)$ are the creation and annihilation operators in the one-particle state $f_k(x) = L^{-3/2}e^{ikx}$ and a_x^* and a_x are the operator-valued distributions formally given by $a_x = L^{-3/2}\sum_k e^{ikx}a_k$. Further, $\mu \in \mathbb{R}$ is the chemical potential and $V \geq 0$ is the (repulsive) two-body interaction. We assume in addition that V is radial and compactly supported. We used the notation

Notation 7.1.1. In any sum the variables are summed over $\frac{2\pi}{L}\mathbb{Z}^3$ unless otherwise noted. That is, we denote $\sum_k = \sum_{k\in\frac{2\pi}{L}\mathbb{Z}^3}$.

We consider the pressure $\psi(\beta,\mu)$ of the interacting system. It is defined as

$$\psi(\beta,\mu) = \lim_{L\to\infty} \frac{1}{\beta L^3} \operatorname{Tr}_{\mathcal{F}(\mathfrak{h})} e^{-\beta\mathcal{H}}.$$

The limit exists and is independent of the boundary conditions [Rob71]. Similarly, the pressure of the free system is given by [Hua87, (8.63)]

$$\psi_0(\beta,\mu) = \lim_{L\to\infty} \frac{1}{\beta L^3} \operatorname{Tr}_{\mathcal{F}(\mathfrak{h})} e^{-\beta\mathcal{H}_0} = \frac{1}{\beta(2\pi)^3}\int_{\mathbb{R}^3} \log\left(1+ze^{-\beta|k|^2}\right) \mathrm{d}k,$$

with $z = e^{\beta\mu}$ the *fugacity*.

To state our main theorem we first define the (p-wave) scattering length of the interaction V. We define it as in Chapter 4. Different-looking but equivalent definitions are given in Chapters 3 and 6 and [SY20].

Definition 7.1.2 (Definition 4.1.1)**.** Let φ_0 be the solution of the p*-wave scattering equation*

$$x\Delta\varphi_0 + 2\nabla\varphi_0 + \frac{1}{2}xV(1-\varphi_0) = 0 \tag{7.1.4}$$

on $\mathbb{R}^3$, with $\varphi_0(x) \to 0$ for $|x| \to \infty$. Then $\varphi_0(x) = a^3/|x|^3$ for $x \notin \operatorname{supp} V$ for some constant $a > 0$ called the p*-wave scattering length*.

The function φ_0 satisfies $0 \le \varphi_0(x) \le \min\{1, a^3|x|^{-3}\}$ for all $x \in \mathbb{R}^3$. The dimensionless quantity measuring the diluteness of the gas is given by $a^3\overline{\rho}$ with $\overline{\rho} = \partial_\mu\psi(\beta,\mu)$ the (infinite volume) particle density.[1] The density $\overline{\rho}$ is to leading order the same as that of the free gas $\overline{\rho}_0$. More precisely, $\overline{\rho} = \overline{\rho}_0(1 + O((a^3\overline{\rho}_0)^{1/2}))$ assuming that $z = e^{\beta\mu}$ is bounded away from zero by Corollary 6.1.4. We thus formulate the diluteness assumption as the assumption that $a^3\overline{\rho}_0$ is small. The density of the free gas is given by (see for instance Lemma 6.3.6)

$$\overline{\rho}_0 = \partial_\mu\psi_0(\beta,\mu) = -\frac{1}{(4\pi\beta)^{3/2}} \operatorname{Li}_{3/2}(-z),$$

with Li_s the *polylogarithm* satisfying [NIS, (25.12.16)]

$$-\operatorname{Li}_s(-e^x) = \frac{1}{\Gamma(s)}\int_0^\infty \frac{t^{s-1}}{e^{t-x}+1}\,\mathrm{d}t, \qquad s > 0,$$

with Γ the Gamma function.

The temperature is naturally measured using the dimensionless fugacity $z = e^{\beta\mu}$. A temperature on the order of the Fermi temperature (of the free gas) $T \sim T_F \sim \overline{\rho}_0^{2/3}$ corresponds to a fugacity $z \sim 1$. The relevant temperatures to consider are $T \lesssim T_F$. This corresponds to $z \gtrsim 1$. At larger temperatures thermal fluctuation dominate the quantum effects, and the gas should behave more like a (high-temperature) classical gas.

With these definitions at hand we may then formulate our main theorem:

[1]We abuse notation slightly by assuming that the derivative $\partial_\mu\psi(\beta,\mu)$ exists. The function $\psi(\beta,\mu)$, being convex in μ, has both left and right derivatives. Should these not coincide we may replace instances of $\overline{\rho}$ with either.

Theorem 7.1.3. *Let $V \in L^1(\mathbb{R}^3)$ be non-negative, radial and compactly supported. Then, for any $\varepsilon > 0$ there exist a function $C(z) > 0$ bounded uniformly on any compact subset of $(0, \infty)$ such that if $a^3\overline{\rho}_0$ is sufficiently small, then*

$$\psi(\beta, \mu) \le \psi_0(\beta, \mu) - 24\pi^2 \frac{-\operatorname{Li}_{5/2}(-z)}{(-\operatorname{Li}_{3/2}(-z))^{5/3}} a^3 \overline{\rho}_0^{8/3} \left[1 + C(z)(a^3\overline{\rho}_0)^{1/16-\varepsilon}\right]. \qquad (7.1.5)$$

Remark 7.1.4. The appearance of the scattering length in the error term is for dimensional consistency. This error term depends on the interaction V also through its range and L^1-norm, both of dimension length. We think of the scattering length as a constant of dimension length, and so write $\operatorname{range}(V) \le Ca$ and $\|V\|_{L^1} \le Ca$ with the constants $C > 0$ being then dimensionless. The function $C(z)$ in (7.1.5) depends only on these constants C.

Remark 7.1.5. The upper bound in Theorem 7.1.3 matches the corresponding lower bound in Chapter 6. Contrary to the lower bound in Chapter 6, however, Theorem 7.1.3 is not uniform in temperatures $T \lesssim T_F$. We discuss the reason for this in detail in Remark 7.7.3 below. One should rather expect the formula in Theorem 7.1.3 to hold uniformly in temperatures $T \lesssim T_F$, meaning that we expect that $C(z)$ is bounded uniformly in $z \ge z_0 > 0$ for any fixed $z_0 > 0$. It remains an open problem to prove this.

Remark 7.1.6 (Extension to less regular V)**.** We can a posteriori extend Theorem 7.1.3 to less regular V as in Chapter 4. (In particular to the case of hard spheres, where formally $V(x) = \infty$ for $|x| \le a$ and $V(x) = 0$ otherwise.) Indeed, any non-negative radial measurable function V can be approximated from below by a (non-negative, radial and compactly supported) L^1-function $\widetilde{V}$. Then clearly $\psi(\beta, \mu) \le \widetilde{\psi}(\beta, \mu)$ with $\widetilde{\psi}(\beta, \mu)$ the pressure with interaction $\widetilde{V}$. Assume in addition that $x \mapsto |x|^2 V(x)$ is integrable outside some ball. Then the p-wave scattering length of V is well-defined. If V is not of finite range or L^1-norm, the error term in Theorem 7.1.3 necessarily blows up when $\widetilde{V} \to V$. Choosing $\widetilde{V}$ converging to V slowly enough (as $a^3\overline{\rho}_0 \to 0$) however, we may achieve that $a(\widetilde{V}) = a(V)(1 + o(1))$, while still keeping the error term in Theorem 7.1.3 small. That is, we conclude for any such V that

$$\psi(\beta, \mu) \le \psi_0(\beta, \mu) - 24\pi^2 \frac{-\operatorname{Li}_{5/2}(-z)}{(-\operatorname{Li}_{3/2}(-z))^{5/3}} a^3 \overline{\rho}_0^{8/3} \left[1 + o_z(1)\right],$$

where $o_z(1)$ vanishes as $a^3\overline{\rho}_0 \to 0$ uniformly for z in compact subsets of $(0, \infty)$.

7.1.1.1 Two dimensions

Consider now the two-dimensional setting. The scattering length is defined as in Definition 7.1.2, only in this case $\varphi_0(x) = a^2/|x|^2$ outside the support of V, with $a > 0$ then the two-dimensional p-wave scattering length. The two-dimensional analogue of Theorem 7.1.3 reads

Theorem 7.1.7 (Two dimensions)**.** *Let $V \in L^1(\mathbb{R}^2)$ be non-negative, radial and compactly supported. Then, for any $\varepsilon > 0$ there exist a function $C(z) > 0$ bounded uniformly on any compact subset of $(0, \infty)$ such that if $a^2\overline{\rho}_0$ is sufficiently small, then*

$$\psi(\beta, \mu) \le \psi_0(\beta, \mu) - 8\pi^2 \frac{-\operatorname{Li}_2(-z)}{(-\operatorname{Li}_1(-z))^2} a^2 \overline{\rho}_0^3 \left[1 + C(z)(a^2\overline{\rho}_0)^{1/8-\varepsilon}\right].$$

Theorem 7.1.7 matches the lower bound of Chapter 6. Again, the upper bound in Theorem 7.1.7 is not uniform in temperatures $T \lesssim T_F$, though one should expect a uniform bound to hold.

7.2 Overview of the proof

To prove Theorem 7.1.3 we introduce a unitary operator $e^{\mathcal{B}}$ implementing the correlations between the particles arising from the interaction. This is analogous to the strategy in Chapter 4 and [FGHP21; Gia23a], see also [Gia23b]. We first introduce the variational formulation of the pressure, however.

7.2.1 Variational formulation

The pressure $\psi(\beta,\mu)$ may be characterized variationally. We define the pressure functional $\mathcal{P}$ of a state Γ by

$$-L^3\mathcal{P}(\Gamma) = \langle \mathcal{H}\rangle_\Gamma - \frac{1}{\beta}S(\Gamma) = \operatorname{Tr}_{\mathcal{F}(\mathfrak{h})} \mathcal{H}\Gamma + \frac{1}{\beta}\operatorname{Tr}_{\mathcal{F}(\mathfrak{h})} \Gamma\log\Gamma.$$

By a *state* we mean a positive trace-class operator on $\mathcal{F}(\mathfrak{h})$ of unit trace. Here we introduced the entropy $S(\Gamma) = -\operatorname{Tr}_{\mathcal{F}(\mathfrak{h})}\Gamma\log\Gamma$ and used the notation

Notation 7.2.1. We denote by $\langle\mathcal{A}\rangle_\Gamma = \operatorname{Tr}_{\mathcal{F}(\mathfrak{h})}\mathcal{A}\Gamma$ the expectation of an operator $\mathcal{A}$ in a state Γ.

The pressure $\psi(\beta,\mu)$ at inverse temperature $\beta>0$ and chemical potential $\mu\in\mathbb{R}$ then satisfies

$$\psi(\beta,\mu) = \lim_{L\to\infty}\sup_{\Gamma}\mathcal{P}(\Gamma).$$

Similarly, the pressure of the free system satisfies

$$\psi_0(\beta,\mu) = \lim_{L\to\infty}\sup_{\Gamma}\mathcal{P}_0(\Gamma) = \lim_{L\to\infty}\mathcal{P}_0(\Gamma_0) = \lim_{L\to\infty}\frac{1}{\beta L^3}\log Z_0 \tag{7.2.1}$$

with $\mathcal{P}_0$ the pressure functional of the free system (defined as $\mathcal{P}$ above only with $\mathcal{H}$ replaced by $\mathcal{H}_0$), $\Gamma_0 = \frac{1}{Z_0}e^{-\beta\mathcal{H}_0}$ the free Gibbs state and $Z_0 = \operatorname{Tr}_{\mathcal{F}(\mathfrak{h})} e^{-\beta\mathcal{H}_0}$ the free partition function.

7.2.2 Momentum cut-offs

As in the zero-temperature setting with or without spin [FGHP21; Gia23a], [Chapter 4] we wish to distinguish between small and large momenta. At zero temperature a natural cut-off is the Fermi momentum. At positive temperature there is no clearly defined Fermi momentum since the temperature "smears out" the Fermi ball. Instead we define the following:

Definition 7.2.2. Define the projections P and $Q = 1-P$ onto low and high momenta by

$$\hat{P}(k) = \chi_{(|k|<k_F^\kappa)}, \qquad \hat{Q}(k) = 1-\hat{P}(k), \qquad k_F^\kappa := \left[\mu+\beta^{-1}\kappa\right]_+^{1/2}, \tag{7.2.2}$$

where $[x]_+ = \max\{0,x\}$ denotes the positive part. The parameter $\kappa>0$ will be chosen large so that $k_F^\kappa>0$. In fact, we shall choose

$$\kappa = \zeta(a^3\rho_0)^{-\alpha}, \qquad \zeta := 1+|\log z|, \tag{7.2.3}$$

for some (small) $\alpha>0$; for small $a^3\rho_0$ then $k_F^\kappa \gg \rho_0^{1/3}$, see Eq. (7.3.3) below. (Recall that $z=e^{\beta\mu}$ denotes the fugacity.) The temperature dependence of the error terms are naturally given in terms of ζ. Here and in the following, we use the notation

Notation 7.2.3. We denote by ρ_0 the particle density of the free gas in finite volume.

The integral kernels of P and Q are, with a slight abuse of notation,

$$\begin{aligned} P(x-y) &= \frac{1}{L^3}\sum_k \hat{P}(k)e^{ik(x-y)}, \\ Q(x-y) &= \frac{1}{L^3}\sum_k \hat{Q}(k)e^{ik(x-y)} = \delta(x-y) - P(x-y). \end{aligned}$$

The momentum k_F^κ serves as an enlarged Fermi momentum. The operators P and Q are chosen so that the approximations

$$P\gamma_0 \approx \gamma_0, \qquad Q \approx \mathbb{1}$$

are both good in appropriate senses. Here γ_0 is the one-particle density matrix of the free Gibbs state Γ_0.

As in the zero-temperature setting studied in Chapter 4 and [FGHP21; Gia23a] we introduce creation and annihilation operators for small and large momentum. They are defined as follows.

Definition 7.2.4. Define the operators

$$c_k = \hat{P}(k)a_k, \qquad b_k = \hat{Q}(k)a_k,$$

Define further the operator-valued distributions

$$c_x = \frac{1}{L^{3/2}}\sum_k e^{ikx}c_k = \frac{1}{L^{3/2}}\sum_k e^{ikx}\hat{P}(k)a_k, \qquad b_x = \frac{1}{L^{3/2}}\sum_k e^{ikx}b_k = \frac{1}{L^{3/2}}\sum_k e^{ikx}\hat{Q}(k)a_k.$$

We will further need a regularized version of b. We define

$$b_k^r = \hat{Q}^r(k)a_k, \qquad b_x^r = \frac{1}{L^{3/2}}\sum_k e^{ikx}b_k^r,$$

with $\hat{Q}^r : \mathbb{R}^3 \to [0,1]$ a smooth function with

$$\hat{Q}^r(k) = \begin{cases} 0 & |k| \leq k_F^\kappa, \\ 1 & |k| \geq 2k_F^\kappa, \end{cases} \qquad |\nabla Q^r(k)| \leq C(k_F^\kappa)^{-1}\chi_{(k_F^\kappa \leq |k| \leq 2k_F^\kappa)}.$$

Remark 7.2.5. Contrary to Chapter 4 we do not define c_x with the opposite sign in the exponent. Since we do not conjugate by the particle hole transform (which is not readily available at positive temperature), it is more convenient to define c_x as done here.

The function $\hat{Q}^r$ naturally defines an operator Q^r on $\mathfrak{h} = L^2(\Lambda;\mathbb{C})$ with integral kernel (with a slight abuse of notation)

$$Q^r(x-y) = \frac{1}{L^3}\sum_k \hat{Q}^r(k)e^{ik(x-y)}.$$

As in [FGHP21, Proposition 4.2] we have

Lemma 7.2.6. *Let $P^r = \delta - Q^r$. Then $\|P^r\|_{L^1(\Lambda)} \leq C$ for sufficiently large L.*

7.2.3 The scattering function

We define the scattering function φ as in Chapter 4 (see also [Gia23a]) only with k_F replaced by k_F^κ. For completeness we recall the details here.

Let $\chi_\varphi : [0, \infty) \to [0, 1]$ be a smooth function with

$$\chi_\varphi(t) = \begin{cases} 1 & t \leq 1, \\ 0 & t \geq 2. \end{cases}$$

Define then

$$\varphi(x) = \varphi_0(x)\chi_\varphi(k_F^\kappa|x|) \tag{7.2.4}$$

with φ_0 the p-wave scattering function defined in Definition 7.1.2. More precisely φ is the periodization of the right-hand-side.

Remark 7.2.7. We will in general abuse notation slightly and refer to any (compactly supported) function and its periodization by the same name. For L larger than the range of the function, at most one summand in the periodization is non-zero and so no issue will arise.

The function φ does not satisfy the p-wave scattering equation (7.1.4) exactly. We define the discrepancy

$$\begin{aligned} \mathcal{E}_\varphi(x) &= x\Delta\varphi(x) + 2\nabla\varphi(x) + \frac{1}{2}xV(x)(1 - \varphi(x)) \\ &= 2k_F^\kappa x\nabla^\mu\varphi_0(x)\nabla^\mu\chi_\varphi(k_F^\kappa|x|) + (k_F^\kappa)^2 x\varphi_0(x)\Delta\chi_\varphi(k_F^\kappa|x|) + 2k_F^\kappa\varphi_0(x)\nabla\chi_\varphi(k_F^\kappa|x|). \end{aligned} \tag{7.2.5}$$

Again, more precisely, $\mathcal{E}_\varphi$ is the periodization of the right-hand-side. Here we have used the notation:

Notation 7.2.8. We adopt the Einstein summation convention of summing over repeated indices denoting components of a vector, i.e., $x^\mu y^\mu = \sum_{\mu=1}^3 x^\mu y^\mu = x \cdot y$ for vectors $x, y \in \mathbb{R}^3$.

7.2.4 The operator $\mathcal{B}$

With the definitions above we can define the operator $\mathcal{B}$ implementing the correlations. It is defined as

$$\begin{aligned} \mathcal{B} &= -\frac{1}{2}\iint \varphi(z - z')(b_z^r)^*(b_{z'}^r)^* c_{z'}c_z \,\mathrm{d}z\,\mathrm{d}z' - \text{h.c.} \\ &= -\frac{1}{2L^3}\sum_{p,k,k'} \hat{\varphi}(p)(b_{k+p}^r)^*(b_{k'-p}^r)^* c_{k'}c_k - \text{h.c.}. \end{aligned} \tag{7.2.6}$$

We expect that the Gibbs state of the interacting gas is then approximately given by $e^{\mathcal{B}}\Gamma_0 e^{-\mathcal{B}}$. This is analogous to the zero-temperature setting in Chapter 4, where one expects that the interacting ground state is approximately given by $e^{\mathcal{B}}\Psi_0$, with Ψ_0 the ground state of the free gas.

Remark 7.2.9 (Comparison to Chapter 4 and [FGHP21; Gia23a])**.** In Chapter 4 and [FGHP21; Gia23a] an analogous operator B is constructed. There, however, also a particle-hole transformation is used and so the operator B is not particle number preserving. Conjugating the operator B by the particle-hole transformation, however, we recover the operator $\mathcal{B}$ (up to the precise momentum cut-offs in the operators c_k, b_k, and the inclusion of spin considered in [FGHP21; Gia23a], in which case a different function φ needs to be used).

With the operator $\mathcal{B}$ above we define for any state Γ

$$\Gamma^{\lambda} := e^{-\lambda \mathcal{B}} \Gamma e^{\lambda \mathcal{B}}, \qquad 0 \leq \lambda \leq 1. \tag{7.2.7}$$

Any state Γ thus satisfies $\Gamma = e^{\mathcal{B}} \Gamma^1 e^{-\mathcal{B}}$.

7.2.5 Implementation

To prove Theorem 7.1.3 we shall consider the pressure functional evaluated on appropriate states. Let $\mathcal{N} = \mathrm{d}\Gamma(1)$ denote the particle number operator. We shall consider the following states:

Definition 7.2.10. A state Γ is said to be an *approximate Gibbs state* if it is translation invariant and satisfies

$$\langle \mathcal{N} \rangle_{\Gamma} \leq C L^3 \rho_0 \quad , \quad \langle \mathcal{H} \rangle_{\Gamma} - \frac{1}{\beta} S(\Gamma) \leq -\frac{1}{\beta} \log Z_0 + C L^3 a^3 \rho_0^{8/3} \tag{7.2.8}$$

for some $C > 0$ (independent of L, $a^3 \rho_0$ and z).

Remark 7.2.11. We note that the Gibbs state of the interacting gas is indeed an approximate Gibbs state (for L large enough, $a^3\rho_0$ small enough and $1/z$ bounded). Indeed, this follows from Theorem 6.1.2 and Corollary 6.1.4.

An immediate consequence of Definition 7.2.10 is that in an approximate Gibbs state Γ we have

$$\langle \mathcal{V} \rangle_{\Gamma} \leq C L^3 a^3 \rho_0^{8/3} . \tag{7.2.9}$$

We shall now sketch the proof of Theorem 7.1.3. Using (7.2.7) above, any state Γ can be written as $\Gamma = e^{\mathcal{B}} \Gamma^1 e^{-\mathcal{B}}$. As discussed above, we expect that if Γ is the (interacting) Gibbs state, then Γ^1 is approximately given by the free Gibbs state Γ_0. Hence, it is natural to write $\langle \mathcal{H} \rangle_{\Gamma} = \left\langle e^{-\mathcal{B}} \mathcal{H} e^{\mathcal{B}} \right\rangle_{\Gamma^1}$. Heuristically to compute $e^{-\mathcal{B}} \mathcal{H} e^{\mathcal{B}}$ we would expand to second order in a Baker–Campbell–Hausdorff expansion. To do this rigorously, we instead do a Duhamel expansion as follows.

Note that for any operator $\mathcal{A}$ we have (for any $0 \leq \lambda, \lambda' \leq 1$, recall (7.2.7))

$$\langle \mathcal{A} \rangle_{\Gamma^{\lambda}} = \langle \mathcal{A} \rangle_{\Gamma^{\lambda'}} - \int_{\lambda}^{\lambda'} \mathrm{d}\lambda'' \, \partial_{\lambda''} \langle \mathcal{A} \rangle_{\Gamma^{\lambda''}} = \langle \mathcal{A} \rangle_{\Gamma^{\lambda'}} + \int_{\lambda}^{\lambda'} \mathrm{d}\lambda'' \, \langle [\mathcal{A}, \mathcal{B}] \rangle_{\Gamma^{\lambda''}} . \tag{7.2.10}$$

We decompose the interaction $\mathcal{V}$ as

$$\mathcal{V} = \mathrm{d}\Gamma(V) = \mathcal{V}_P + \mathcal{V}_Q + \mathcal{V}_{\mathsf{OD}} + \mathcal{Q}_V, \tag{7.2.11}$$

with (denoting the two-body projection $P \otimes P$ by PP and similar)

$$\mathcal{V}_P = \mathrm{d}\Gamma(PPVPP), \qquad \mathcal{V}_Q = \mathrm{d}\Gamma(QQVQQ), \qquad \mathcal{V}_{\mathsf{OD}} = \mathrm{d}\Gamma(PPVQQ + QQVPP). \tag{7.2.12}$$

The operator $\mathcal{Q}_V$ containing all the remaining terms will not contribute to the pressure to the desired accuracy, i.e., it is an error term.

Decomposing as in (7.2.11) and employing (7.2.10) we find for any state Γ the formula

$$\begin{aligned}\langle\mathcal{H}\rangle_\Gamma &= \langle\mathcal{V}_P\rangle_\Gamma + \langle\mathcal{H}_0+\mathcal{V}_Q+\mathcal{V}_{\mathsf{OD}}\rangle_\Gamma + \langle\mathcal{Q}_V\rangle_\Gamma \\ &= \langle\mathcal{V}_P\rangle_\Gamma + \langle\mathcal{H}_0+\mathcal{V}_Q\rangle_{\Gamma^1} + \langle\mathcal{Q}_V\rangle_\Gamma + \int_0^1 \mathsf{d}\lambda\,\langle[\mathcal{H}_0+\mathcal{V}_Q,\mathcal{B}]+\mathcal{V}_{\mathsf{OD}}\rangle_{\Gamma^\lambda} \\ &\quad + \int_0^1 \mathsf{d}\lambda\,\langle[\mathcal{V}_{\mathsf{OD}},\mathcal{B}]\rangle_{\Gamma^\lambda} - \int_0^1 \mathsf{d}\lambda \int_\lambda^1 \mathsf{d}\lambda'\,\langle[\mathcal{V}_{\mathsf{OD}},\mathcal{B}]\rangle_{\Gamma^{\lambda'}} \\ &= \langle\mathcal{V}_P\rangle_\Gamma + \langle\mathcal{H}_0+\mathcal{V}_Q\rangle_{\Gamma^1} + \langle\mathcal{Q}_V\rangle_\Gamma + \int_0^1 \mathsf{d}\lambda\,\langle[\mathcal{H}_0+\mathcal{V}_Q,\mathcal{B}]+\mathcal{V}_{\mathsf{OD}}\rangle_{\Gamma^\lambda} \\ &\quad + \int_0^1 \mathsf{d}\lambda\,(1-\lambda)\,\langle[\mathcal{V}_{\mathsf{OD}},\mathcal{B}]\rangle_{\Gamma^\lambda}\,.\end{aligned}$$

We shall write $[\mathcal{V}_{\mathsf{OD}},\mathcal{B}] = 2(\mathcal{W}_P-\mathcal{V}_P)+\mathcal{Q}_{\mathsf{OD}}$, with $W = V(1-\varphi)$ and $\mathcal{W}_P = \mathsf{d}\Gamma(PPWPP)$. The term $\mathcal{Q}_{\mathsf{OD}}$ is then an error term. Again using (7.2.10),

$$\langle[\mathcal{V}_{\mathsf{OD}},\mathcal{B}]\rangle_{\Gamma^\lambda} = 2\,\langle\mathcal{W}_P-\mathcal{V}_P\rangle_\Gamma - 2\int_0^\lambda \mathsf{d}\lambda'\,\langle[\mathcal{W}_P-\mathcal{V}_P,\mathcal{B}]\rangle_{\Gamma^{\lambda'}} + \langle\mathcal{Q}_{\mathsf{OD}}\rangle_{\Gamma^\lambda}\,.$$

Defining $\mathcal{Q}_{V\varphi} = [\mathcal{V}_P-\mathcal{W}_P,\mathcal{B}]$ and the error terms

$$\mathcal{E}_V(\Gamma) = \langle\mathcal{Q}_V\rangle_\Gamma\,, \tag{7.2.13}$$

$$\mathcal{E}_{\mathsf{scat}}(\Gamma) = \int_0^1 \mathsf{d}\lambda\,\langle[\mathcal{H}_0+\mathcal{V}_Q,\mathcal{B}]+\mathcal{V}_{\mathsf{OD}}\rangle_{\Gamma^\lambda}\,, \tag{7.2.14}$$

$$\mathcal{E}_{\mathsf{OD}}(\Gamma) = \int_0^1 \mathsf{d}\lambda\,(1-\lambda)\,\langle\mathcal{Q}_{\mathsf{OD}}\rangle_{\Gamma^\lambda}\,, \tag{7.2.15}$$

$$\mathcal{E}_{V\varphi}(\Gamma) = \int_0^1 \mathsf{d}\lambda\,(1-\lambda)^2\,\langle\mathcal{Q}_{V\varphi}\rangle_{\Gamma^\lambda}\,, \tag{7.2.16}$$

we find for any state Γ

$$\langle\mathcal{H}\rangle_\Gamma = \langle\mathcal{H}_0\rangle_{\Gamma^1} + \langle\mathcal{W}_P\rangle_\Gamma + \langle\mathcal{V}_Q\rangle_{\Gamma^1} + \mathcal{E}_V(\Gamma) + \mathcal{E}_{\mathsf{scat}}(\Gamma) + \mathcal{E}_{\mathsf{OD}}(\Gamma) + \mathcal{E}_{V\varphi}(\Gamma).$$

This is analogous to the similar formula (4.2.11) in the zero-temperature setting.

The desired leading contribution from the interaction is the term $\langle\mathcal{W}_P\rangle_\Gamma$. In fact, we expect that to leading order we can replace Γ by Γ_0 in this expression, and drop the projection P (i.e., replace it by 1). With $\mathcal{W} = \mathsf{d}\Gamma(W)$, let us consequently define the difference between $\langle\mathcal{W}_P\rangle_\Gamma$ and $\langle\mathcal{W}\rangle_{\Gamma_0}$ by $\mathcal{E}_{\mathsf{pt}}$; i.e.,

$$\langle\mathcal{W}_P\rangle_\Gamma = \langle\mathcal{W}\rangle_{\Gamma_0} + \mathcal{E}_{\mathsf{pt}}(\Gamma)\,. \tag{7.2.17}$$

The term $\mathcal{E}_{\mathsf{pt}}(\Gamma)$ is another error term. It quantifies, to some extent, the validity of *first order perturbation theory*, as we shall explain in more detail Section 7.7. Furthermore, by the Gibbs variational principle (applied to the free system) we have

$$\langle\mathcal{H}_0\rangle_{\Gamma^1} - \frac{1}{\beta}S(\Gamma^1) \geq \langle\mathcal{H}_0\rangle_{\Gamma_0} - \frac{1}{\beta}S(\Gamma_0) = -\frac{1}{\beta}\log Z_0.$$

Finally, $\mathcal{V}_Q \geq 0$ and $S(\Gamma^1) = S(\Gamma)$ since $e^{\mathcal{B}}$ is unitary. Thus we find for any state Γ the lower bound

$$\boxed{\langle\mathcal{H}\rangle_\Gamma - \frac{1}{\beta}S(\Gamma) \geq -\frac{1}{\beta}\log Z_0 + \langle\mathcal{W}\rangle_{\Gamma_0} + \mathcal{E}_{\mathsf{pt}}(\Gamma) + \mathcal{E}_V(\Gamma) + \mathcal{E}_{\mathsf{scat}}(\Gamma) + \mathcal{E}_{\mathsf{OD}}(\Gamma) + \mathcal{E}_{V\varphi}(\Gamma).} \tag{7.2.18}$$

To evaluate $\langle \mathcal{W} \rangle_{\Gamma_0}$ we use Lemma 7.3.1 below. Note that $\int |x|^2 W = 24\pi a^3$. Indeed, by the compact support of V we have for small enough $a^3\rho_0$

$$\int_{\mathbb{R}^3} |x|^2 W(x)\, \mathrm{d}x = \int_{|x|<(k_F^\kappa)^{-1}} |x|^2 V(x)(1-\varphi_0(x))\, \mathrm{d}x = 24\pi a^3.$$

The first '=' follows from the fact that $\varphi(x) = \varphi_0(x)$ for $|x| \leq (k_F^\kappa)^{-1}$, noting the asymptotics for k_F^κ in (7.3.3). The last '=' follows from a simple integration by parts using the scattering equation (7.1.4). Bounding also $\int |x|^4 W \leq Ca^5$ (the integral $\int |x|^4 W$ is some constant of dimension (length)^5 and hence we write it as Ca^5, cf. Remark 7.1.4) we have

$$\langle \mathcal{W} \rangle_{\Gamma_0} = 24\pi^2 \frac{-\operatorname{Li}_{5/2}(-z)}{(-\operatorname{Li}_{3/2}(-z))^{5/3}} L^3 a^3 \rho_0^{8/3} \left[1 + O(a^2\rho_0^{2/3}) + \mathfrak{e}_L\right]. \tag{7.2.19}$$

Here we have used the notation

Notation 7.2.12. We denote by $\mathfrak{e}_L$ any term vanishing as L^{-1} in the limit $L \to \infty$.

The main part of this paper concerns bounding the error terms $\mathcal{E}_{\mathrm{pt}}(\Gamma)$, $\mathcal{E}_V(\Gamma)$, $\mathcal{E}_{\mathrm{scat}}(\Gamma)$, $\mathcal{E}_{\mathrm{OD}}(\Gamma)$ and $\mathcal{E}_{V\varphi}(\Gamma)$. They are bounded as follows. Recall our choice $\kappa = \zeta(a^3\rho_0)^{-\alpha}$ for some (small) $\alpha > 0$ in (7.2.3).

Proposition 7.2.13. *Let Γ be an approximate Gibbs state. Then, for any $\alpha > 0$ sufficiently small,*

$$\mathcal{E}_{\mathrm{pt}}(\Gamma) \geq -C(z) L^3 a^3 \rho_0^{8/3} (a^3\rho_0)^{1/16 - 21\alpha/32} - L^3 \mathfrak{e}_L,$$

with the function $C(z)$ uniformly bounded on compact subsets of $(0,\infty)$.

Proposition 7.2.14. *Let Γ be an approximate Gibbs state. Then, for any $\alpha > 0$,*

$$\mathcal{E}_V(\Gamma) \geq -C L^3 a^3 \rho_0^{8/3} (a^3\rho_0)^{1/2 - 5\alpha/2} - L^3 \mathfrak{e}_L.$$

Proposition 7.2.15. *Let Γ be an approximate Gibbs state. Then, for any $\alpha > 0$ sufficiently small,*

$$|\mathcal{E}_{\mathrm{scat}}(\Gamma)| \leq C L^3 a^3 \rho_0^{8/3} (a^3\rho_0)^{1/5 - 2\alpha} \left|\log a^3\rho_0\right|^{2/5} + L^3 \mathfrak{e}_L.$$

Proposition 7.2.16. *Let Γ be an approximate Gibbs state. Then, for any $\alpha > 0$ sufficiently small,*

$$|\mathcal{E}_{\mathrm{OD}}(\Gamma)| \leq C L^3 a^3 \rho_0^{8/3} (a^3\rho_0)^{1/2 - 13\alpha/4} + L^3 \mathfrak{e}_L.$$

Proposition 7.2.17. *Let Γ be an approximate Gibbs state. Then, for any $\alpha > 0$,*

$$|\mathcal{E}_{V\varphi}(\Gamma)| \leq C L^3 a^3 \rho_0^{8/3} (a^3\rho_0)^{2/3 - 4\alpha} + L^3 \mathfrak{e}_L.$$

With these we may give the

Proof of Theorem 7.1.3. We evaluate the first two terms in (7.2.18) using (7.2.1) and (7.2.19) and bound the error terms by Propositions 7.2.13–7.2.17. Taking an infinite volume limit, we obtain the desired bound (7.1.5). □

Remark 7.2.18. We note that the error bounds in Propositions 7.2.14–7.2.17 are uniform in the temperature, while the bound in Proposition 7.2.13 is not.

Remark 7.2.19. Propositions 7.2.14–7.2.17 are analogous to Propositions 4.2.8, 4.2.9 and 4.2.10. The main novelty of the present paper is Proposition 7.2.13.

The remainder of the paper deals with the proofs of Propositions 7.2.13–7.2.17.

Structure of the paper:

First, in Section 7.3, we recall some useful results from Chapters 4 and 6, give some a priori bounds for approximate Gibbs states and conclude with the proof of Proposition 7.2.14. Next, in Section 7.4, we calculate the commutators $[\mathcal{H}_0, \mathcal{B}]$, $[\mathcal{V}_Q, \mathcal{B}]$, $[\mathcal{V}_P - \mathcal{W}_P, \mathcal{B}]$, and $[\mathcal{V}_{\mathrm{OD}}, \mathcal{B}]$ and extract the claimed leading terms. The error terms arising from the commutators are estimated in Section 7.5. In Section 7.6, we propagate the a priori bounds to the states Γ^λ and conclude the proof of Propositions 7.2.15, 7.2.16 and 7.2.17. Finally, in Section 7.7, we employ the method of [Sei06a] in order to estimate the validity of first order perturbation theory at positive temperature, and conclude the proof of Proposition 7.2.13 and thereby of Theorem 7.1.3.

In Section 7.A we estimate certain Riemann sums needed in the proof, and in Section 7.B we sketch how to adapt the proof to the two-dimensional setting, and hence to prove Theorem 7.1.7.

7.3 Preliminaries

7.3.1 Reduced densities

We recall from Chapter 6 the following properties for the reduced k-particle densities $\rho_0^{(k)}$ of the free gas.

Lemma 7.3.1 (Lemma 6.3.6)**.** *The reduced densities of the free Fermi gas satisfy*

$$\rho_0^{(1)}(x_1) = \rho_0 = \frac{1}{(4\pi)^{3/2}}\beta^{-3/2}(-\operatorname{Li}_{3/2}(-z))\left[1 + O(L^{-1}\zeta\rho_0^{-1/3})\right], \tag{7.3.1}$$

$$\rho_0^{(2)}(x_1,x_2) = 2\pi\frac{-\operatorname{Li}_{5/2}(-z)}{(-\operatorname{Li}_{3/2}(-z))^{5/3}}\rho_0^{8/3}|x_1-x_2|^2\left[1 + O(\rho_0^{2/3}|x_1-x_2|^2) + O(L^{-1}\zeta\rho_0^{-1/3})\right]. \tag{7.3.2}$$

For bounded $1/z = e^{-\beta\mu}$, we have the asymptotic behavior

$$\beta \sim \zeta\rho_0^{-2/3}, \qquad |\mu| \le C\rho_0^{2/3}, \qquad k_F^\kappa \sim \kappa^{1/2}\zeta^{-1/2}\rho_0^{1/3} \sim \rho_0^{1/3}(a^3\rho_0)^{-\alpha/2}. \tag{7.3.3}$$

Indeed, the asymptotics for β and for positive μ follows from Remark 6.3.7. For $1/z$ bounded we have $\mu \ge -C\beta^{-1} \ge -C\zeta^{-1}\rho_0^{2/3}$ and the bound for μ follows for negative μ. The asymptotics for k_F^κ follows from the first two by recalling (7.2.3) noting that for $a^3\rho_0$ small we have $\beta^{-1}\kappa \gg -\mu$.

7.3.2 The scattering function

We recall from Chapter 6 that the scattering function φ and the function $\mathcal{E}_\varphi$, defined in (7.2.4) and (7.2.5), satisfy

Lemma 7.3.2 (Lemma 4.3.6 and Remark 4.3.7)**.** *The scattering function φ satisfies*

$$\begin{aligned}
&\||\cdot|^n\varphi\|_{L^1} \le Ca^3(k_F^\kappa)^{-n}, \quad n=1,2, && \||\cdot|^n\nabla^n\varphi\|_{L^1} \le Ca^3\left|\log ak_F^\kappa\right|, \quad n=0,1,2\\
&\||\cdot|\varphi\|_{L^2} \le Ca^{3/2+1}, && \||\cdot|^n\nabla^n\varphi\|_{L^2} \le Ca^{3/2}, \qquad n=0,1.
\end{aligned}$$

Here ∇^n represents any combination of n derivatives and $|\cdot|$ denotes the metric on the torus in the sense that $|x|$ is the distance between x and the point 0.

Moreover, $\mathcal{E}_\varphi$ satisfies the same bounds as φ only with an additional power k_F^κ.

7.3.3 Relative entropy

The relative entropy of a state Γ with respect to the free Gibbs state Γ_0 is given by

$$\frac{1}{\beta}S(\Gamma,\Gamma_0) = \langle \mathcal{H}_0\rangle_\Gamma - \frac{1}{\beta}S(\Gamma) + \frac{1}{\beta}\log Z_0.$$

For a translation invariant state Γ with one-particle density matrix γ, we have $S(\Gamma) \le \mathcal{S}(\gamma)$, where the 'one-particle-density' entropy is given in terms of the Fourier coefficients $\hat\gamma(k)$ of γ as $\mathcal{S}(\gamma) = -\sum_k [\hat\gamma(k)\log\hat\gamma(k) + (1-\hat\gamma(k))\log(1-\hat\gamma(k))]$. Moreover, $S(\Gamma_0) = \mathcal{S}(\gamma_0)$ with γ_0 the one-particle-density matrix of Γ_0, since Γ_0 is a quasi-free state. In particular, using that $\hat\gamma_0(k) = (1+e^{\beta(|k|^2-\mu)})^{-1}$,

$$\begin{aligned}\frac{1}{\beta}\mathcal{S}(\gamma,\gamma_0) &:= \frac{1}{\beta}\sum_k\left[\hat\gamma(k)\log\frac{\hat\gamma(k)}{\hat\gamma_0(k)} + (1-\hat\gamma(k))\log\frac{1-\hat\gamma(k)}{1-\hat\gamma_0(k)}\right] \\ &= \langle\mathcal{H}_0\rangle_\Gamma - \langle\mathcal{H}_0\rangle_{\Gamma_0} - \frac{1}{\beta}\mathcal{S}(\gamma) + \frac{1}{\beta}\mathcal{S}(\gamma_0) \le \frac{1}{\beta}S(\Gamma,\Gamma_0).\end{aligned}$$

Recalling (7.2.8), we thus have for an approximate Gibbs state Γ

$$\mathcal{S}(\gamma,\gamma_0) \le S(\Gamma,\Gamma_0) \le CL^3a^3\rho_0^{8/3}\beta \le CL^3\zeta a^3\rho_0^2, \tag{7.3.4}$$

where we used the asymptotics of β from (7.3.3) in the last bound.

7.3.4 Highly excited particles

To state many of the intermediary bounds in the proof of Propositions 7.2.14–7.2.17 it is convenient to define

$$\mathcal{N}_Q = \sum_k b_k^*b_k = \int b_x^*b_x\,\mathrm{d}x, \qquad \mathcal{K}_Q = \sum_k |k|^2 b_k^*b_k = \int \nabla b_x^*\nabla b_x\,\mathrm{d}x, \tag{7.3.5}$$

being the number and kinetic energy of highly excited particles. We shall prove the following lemma.

Lemma 7.3.3. *For any translation invariant state Γ with one-particle density matrix γ, we have*

$$\begin{aligned}\langle\mathcal{N}_Q\rangle_\Gamma &\lesssim \kappa^{-1}\left(\mathcal{S}(\gamma,\gamma_0) + L^3\beta^{-1}k_F^\kappa e^{-\kappa/3} + L^3\mathfrak{e}_L\right)\\ \langle\mathcal{K}_Q\rangle_\Gamma &\lesssim \left(\beta^{-1} + \rho_0^{2/3}\kappa^{-1}\right)\left(\mathcal{S}(\gamma,\gamma_0) + L^3\beta^{-1}k_F^\kappa e^{-\kappa/3} + L^3\mathfrak{e}_L\right)\end{aligned}$$

Applying this Lemma for the choice $\kappa = \zeta(a^3\rho_0)^{-\alpha}$ in (7.2.3) and recalling (7.3.3) and (7.3.4) we find for any approximate Gibbs state Γ

$$\langle\mathcal{N}_Q\rangle_\Gamma \le CL^3\zeta\kappa^{-1}a^3\rho_0^2 + L^3\mathfrak{e}_L, \qquad \langle\mathcal{K}_Q\rangle_\Gamma \le CL^3a^3\rho_0^{8/3} + L^3\mathfrak{e}_L \tag{7.3.6}$$

with the constants $C>0$ depending only on $\alpha>0$.

Proof. Define the functions

$$s(t) = -t\log t - (1-t)\log(1-t), \qquad s(t,t') = t\log\frac{t}{t'} + (1-t)\log\frac{1-t}{1-t'}.$$

Then for any translation-invariant density matrices γ,γ' we have $\mathcal{S}(\gamma) = \sum_k s(\hat\gamma(k))$ and $\mathcal{S}(\gamma,\gamma') = \sum_k s(\hat\gamma(k),\hat\gamma'(k))$.

Let $h > 0$. We claim that for all $t \in [0, 1]$

$$ht \leq 2s(t, t_0) + \frac{h}{1 + e^{h/2}}, \qquad t_0 = \frac{1}{1 + e^h} \tag{7.3.7}$$

To prove this we define $F(h) := -\log(1 + e^{-h}) = ht_0 - s(t_0)$ the 'free energy' of the 'Hamiltonian' h and note that $s(t, t_0) = ht - s(t) - F(h)$. Then, by the Gibbs variational principle applied to the 'Hamiltonian' $h/2$ we have

$$2s(t, t_0) - ht = 2\left[\frac{1}{2}ht - s(t) - F(h)\right] \geq 2\left[F(h/2) - F(h)\right] = -2h \int_{1/2}^{1} F'(uh)\,\mathrm{d}u.$$

Clearly $|F'(uh)| \leq (1 + e^{h/2})^{-1}$ for any $u \in [1/2, 1]$, yielding (7.3.7).

In order to prove the lemma we apply (7.3.7) for $h = \beta(|k|^2 - \mu)\hat{Q}(k)$ and $t = \hat{\gamma}(k)$ and sum in k. Noting that $t_0 = (1 + e^h)^{-1} = \hat{\gamma}_0(k)\hat{Q}(k)$ on the support of $\hat{Q}$, and $s(\hat{\gamma}(k), \hat{\gamma}_0(k)) \geq 0$, we have

$$\sum_{|k| > k_F^\kappa} \beta(|k|^2 - \mu)\hat{\gamma}(k) \leq 2\mathcal{S}(\gamma, \gamma_0) + \sum_{|k| > k_F^\kappa} \frac{\beta(|k|^2 - \mu)}{1 + e^{\frac{\beta}{2}(|k|^2 - \mu)}}.$$

The sum on the right hand side can be bounded as

$$\sum_{|k| > k_F^\kappa} \frac{\beta(|k|^2 - \mu)}{1 + e^{\frac{\beta}{2}(|k|^2 - \mu)}} \leq CL^3\beta^{-3/2}(1 + k_F^\kappa \beta^{1/2})e^{-\kappa/3} + L^3\mathfrak{e}_L \leq CL^3\beta^{-1}k_F^\kappa e^{-\kappa/3} + L^3\mathfrak{e}_L. \tag{7.3.8}$$

This follows by viewing the sum as a Riemann sum and computing the corresponding integral; we shall give the details in Section 7.A. The bounds in the lemma then follow by noting that $\beta((k_F^\kappa)^2 - \mu) = \kappa$ according to (7.2.2) and

$$\begin{aligned}
\langle \mathcal{N}_Q \rangle_\Gamma &= \sum_k \hat{Q}(k)\hat{\gamma}(k) \leq [\beta((k_F^\kappa)^2 - \mu)]^{-1} \sum_{|k| > k_F^\kappa} \beta(|k|^2 - \mu)\gamma(k), \\
\langle \mathcal{K}_Q \rangle_\Gamma &= \sum_k \hat{Q}(k)|k|^2\hat{\gamma}(k) = \beta^{-1} \sum_{|k| > k_F^\kappa} \beta(|k|^2 - \mu)\gamma(k) + \mu \langle \mathcal{N}_Q \rangle_\Gamma.
\end{aligned}$$

Using (7.3.3) to bound μ yields the statement of the Lemma. □

7.3.5 The interaction V

We shall now give a priori bounds for the interaction V and prove Proposition 7.2.14. This is analogous to what is done in Section 4.3.2.

Recall the definition of $\mathcal{E}_V$ in (7.2.13)) and (7.2.11).

Lemma 7.3.4. *For any state Γ and any $\varepsilon > 0$ we have the lower bound*

$$\mathcal{E}_V(\Gamma) \geq -\varepsilon \langle \mathcal{V}_P \rangle_\Gamma - \varepsilon \langle \mathcal{V}_Q \rangle_\Gamma - C\varepsilon^{-1}a^3(k_F^\kappa)^3 \left[\langle \mathcal{K}_Q \rangle_\Gamma + (k_F^\kappa)^2 \langle \mathcal{N}_Q \rangle_\Gamma\right]$$

Proof. Again denoting by PP the two-body operator $P \otimes P$, we can write

$$V = [PP + PQ + QP + QQ]V[PP + PQ + QP + QQ].$$

Expanding out the product we may bound the cross-terms as

$$\begin{aligned}
(QQV(PQ + QP) + \text{h.c.}) &\geq -\varepsilon QQVQQ - \frac{1}{\varepsilon}(PQ + QP)V(PQ + QP) \\
(PPV(PQ + QP) + \text{h.c.}) &\geq -\varepsilon PPVPP - \frac{1}{\varepsilon}(PQ + QP)V(PQ + QP).
\end{aligned}$$

With the definitions in (7.2.12) we thus obtain the bound

$$\mathcal{V} \geq (1-\varepsilon)\mathcal{V}_P + (1-\varepsilon)\mathcal{V}_Q + \mathcal{V}_{\mathsf{OD}} + \left(1 - \frac{2}{\varepsilon}\right)\mathcal{V}_{\mathsf{X}}$$

with

$$\mathcal{V}_{\mathsf{X}} = \mathrm{d}\Gamma((PQ+QP)V(PQ+QP)) = \frac{1}{2}\iint V(x-y)(b_x^* c_y^* + c_x^* b_y^*)(b_y c_x + c_y b_x)\,\mathrm{d}x\,\mathrm{d}y.$$

For any state Γ define the function $\phi(x,y) = \left\langle (b_x^* c_y^* + c_x^* b_y^*)(b_y c_x + c_y b_x)\right\rangle_\Gamma$. We note that $\phi(x,x) = 0$ and $\phi(x,y) = \phi(y,x)$. Hence, Taylor expanding in y around $y = x$, the zeroth and first orders vanish. (The path from x to y used in the Taylor expansion should be interpreted as the shortest path on the torus Λ.) Then

$$\phi(x,y) = (y-x)^\mu (y-x)^\nu \int_0^1 \mathrm{d}t\,(1-t)[\nabla_2^\mu \nabla_2^\nu \phi](x, x+t(y-x))$$

where ∇_2^μ denotes the derivative in the second variable. Changing variables to $z = y - x$, we have

$$\langle \mathcal{V}_{\mathsf{X}}\rangle_\Gamma = \frac{1}{2}\int_0^1 \mathrm{d}t\,(1-t)\int \mathrm{d}z\, z^\mu z^\nu V(z)\int \mathrm{d}x\,[\nabla_2^\mu \nabla_2^\nu \phi](x, x+tz).$$

The x-integral is given by (with derivatives now being with respect to x and the brackets indicating that the derivatives are of the product of operators in the brackets)

$$\begin{aligned}\int \mathrm{d}x \Big\langle & b_x^* \nabla^\mu \nabla^\nu [c_{x+tz}^* b_{x+tz}] c_x + c_x^* \nabla^\mu \nabla^\nu [b_{x+tz}^* b_{x+tz}] c_x \\ & + b_x^* \nabla^\mu \nabla^\nu [c_{x+tz}^* c_{x+tz}] b_x + c_x^* \nabla^\mu \nabla^\nu [b_{x+tz}^* c_{x+tz}] b_x \Big\rangle.\end{aligned}$$

Integrating by parts once, so that no factor b or b^* carry two derivatives we may bound this using Cauchy–Schwarz by

$$\begin{aligned}\left|\int \mathrm{d}x\,[\nabla_2^\mu \nabla_2^\nu \phi](x,x+tz)\right| &\leq C(k_F^\kappa)^3 \int \mathrm{d}x\,\langle \nabla b_x^* \nabla b_x\rangle_\Gamma + C(k_F^\kappa)^5 \int \mathrm{d}x\,\langle b_x^* b_x\rangle_\Gamma \\ &= C(k_F^\kappa)^3 \langle \mathcal{K}_Q\rangle_\Gamma + C(k_F^\kappa)^5 \langle \mathcal{N}_Q\rangle_\Gamma\end{aligned}$$

using that $\|\nabla^n c\| \leq C(k_F^\kappa)^{3/2+n}$. We conclude that

$$|\langle \mathcal{V}_{\mathsf{X}}\rangle_\Gamma| \leq C \left\| |\cdot|^2 V\right\|_{L^1} (k_F^\kappa)^3 \left[\langle \mathcal{K}_Q\rangle_\Gamma + (k_F^\kappa)^2 \langle \mathcal{N}_Q\rangle_\Gamma\right].$$

Noting finally that $\int |x|^2 V \leq Ca^3$ (it is some constant of dimension (length)^3, cf. Remark 7.1.4) we conclude the proof of the lemma. □

Lemma 7.3.5 (A priori bound for $\mathcal{V}_P$)**.** *For any state* Γ *we have*

$$\langle \mathcal{V}_P\rangle_\Gamma \leq Ca^3 (k_F^\kappa)^5 \langle \mathcal{N}\rangle_\Gamma.$$

Proof. We have

$$\langle \mathcal{V}_P\rangle_\Gamma = \frac{1}{2}\iint \mathrm{d}x\,\mathrm{d}y V(x-y)\left\langle c_x^* c_y^* c_y c_x\right\rangle_\Gamma.$$

We Taylor expand the factors c_y and c_y^* as

$$c_y = c_x + (y-x)^\mu \int_0^1 \mathrm{d}t\, \nabla^\mu c_{x+t(y-x)}, \tag{7.3.9}$$

where again the path from x to y should be understood as the shortest on the torus Λ. Since c_x is a bounded fermionic operator $c_x^2 = 0$. Doing this Taylor expansion for both c_y and c_y^* and changing variables to $z = y - x$ we have

$$\langle \mathcal{V}_P \rangle_\Gamma = \frac{1}{2} \iint \mathrm{d}x\, \mathrm{d}z\, V(z) z^\mu z^\nu \int_0^1 \mathrm{d}t \int_0^1 \mathrm{d}s \left\langle c_x^* \nabla^\mu c_{x+tz}^* \nabla^\nu c_{x+sz} c_x \right\rangle_\Gamma$$

To bound this we can use that $\|\nabla c\| \leq C(k_F^\kappa)^{3/2+1}$. Thus, with $\|\cdot\|_{\mathfrak{S}_2}$ denoting the Hilbert–Schmidt norm, the Cauchy–Schwarz inequality implies that

$$\langle \mathcal{V}_P \rangle_\Gamma \leq C \iint \mathrm{d}x\, \mathrm{d}z\, V(z) |z|^2 (k_F^\kappa)^5 \left\| \Gamma^{1/2} c_x^* \right\|_{\mathfrak{S}_2} \left\| c_x \Gamma^{1/2} \right\|_{\mathfrak{S}_2}.$$

Noting that $\left\|\Gamma^{1/2} c_x^*\right\|_{\mathfrak{S}_2} = (\mathrm{Tr}[\Gamma^{1/2} c_x^* c_x \Gamma^{1/2}])^{1/2} = \langle c_x^* c_x \rangle_\Gamma^{1/2}$, that $\int \langle c_x^* c_x \rangle_\Gamma \,\mathrm{d}x \leq \langle \mathcal{N} \rangle_\Gamma$ and that $\int |x|^2 V \leq C a^3$ we obtain the desired bound. ☐

Lemma 7.3.6 (A priori bound for $\mathcal{V}_{\mathrm{OD}}$)**.** *For any state Γ and any $\delta > 0$ we have*

$$|\langle \mathcal{V}_{\mathrm{OD}} \rangle_\Gamma| \leq \delta \langle \mathcal{V}_Q \rangle_\Gamma + \delta^{-1} \langle \mathcal{V}_P \rangle_\Gamma \leq \delta \langle \mathcal{V}_Q \rangle_\Gamma + C \delta^{-1} a^3 (k_F^\kappa)^5 \langle \mathcal{N} \rangle_\Gamma.$$

Proof. By Cauchy–Schwarz we have for any $\delta > 0$

$$|\langle \mathcal{V}_{\mathrm{OD}} \rangle_\Gamma| \leq \frac{1}{2} \iint V(x-y) \left| \left\langle b_x^* b_y^* c_y c_x + \mathrm{h.c.} \right\rangle_\Gamma \right| \mathrm{d}x\, \mathrm{d}y \leq \delta \langle \mathcal{V}_Q \rangle_\Gamma + \delta^{-1} \langle \mathcal{V}_P \rangle_\Gamma.$$

Using the bound of $\langle \mathcal{V}_P \rangle_\Gamma$ in Lemma 7.3.5 we conclude the desired bound. ☐

Lemma 7.3.7 (A priori bound for $\mathcal{V}_Q$)**.** *For any approximate Gibbs state Γ we have*

$$\langle \mathcal{V}_Q \rangle_\Gamma \leq C L^3 a^3 \rho_0 (k_F^\kappa)^5 + L^3 \mathfrak{e}_L$$

Proof. Recalling (7.2.11) and applying Lemma 7.3.4 and Lemma 7.3.6 with $\delta = 1/2$ we have the lower bound

$$\langle \mathcal{V} \rangle_\Gamma \geq -(1+\varepsilon) \langle \mathcal{V}_P \rangle_\Gamma + \left(\frac{1}{2} - \varepsilon\right) \langle \mathcal{V}_Q \rangle_\Gamma - \varepsilon^{-1} C a^3 (k_F^\kappa)^3 \left[\langle \mathcal{K}_Q \rangle_\Gamma + (k_F^\kappa)^2 \langle \mathcal{N}_Q \rangle_\Gamma \right].$$

Moreover, $\langle \mathcal{V} \rangle_\Gamma$ is bounded above as in (7.2.9). Bounding $\langle \mathcal{V}_P \rangle_\Gamma$ using Lemma 7.3.5, choosing $\varepsilon = 1/4$, and using the bounds of $\mathcal{N}_Q$ and $\mathcal{K}_Q$ in (7.3.6) we conclude the proof of the lemma. ☐

Finally we can the give the

Proof of Proposition 7.2.14. We start with Lemma 7.3.4 and apply the bounds of Lemmas 7.3.5 and 7.3.7 as well as (7.3.6). We conclude for any $\varepsilon > 0$ the bound

$$\mathcal{E}_V(\Gamma) \geq -C\varepsilon L^3 a^3 \rho_0 (k_F^\kappa)^5 - C \varepsilon^{-1} L^3 a^6 \rho_0^2 (k_F^\kappa)^5 - L^3 \mathfrak{e}_L$$

Choosing the optimal $\varepsilon = a^{3/2} \rho_0^{1/2}$ and recalling the asymptotic behavior of k_F^κ in (7.3.3) we arrive at the claimed bound. ☐

7.4 Calculation of commutators

As detailed in Section 7.2.5, our method of proof requires the calculation of the commutator of the operator $\mathcal{B}$ defined in (7.2.6) with various other operators. These commutators are analogous to the corresponding ones in the zero-temperature setting in Chapter 4 and [FGHP21; Gia23a]. The calculations are essentially the same as those of Section 4.4, only the particle-hole transformation used there is now absent. For completeness we give the details here.

7.4.1 $[\mathcal{H}_0, \mathcal{B}]$:

Recall the formulas for $\mathcal{H}_0$ and $\mathcal{B}$ from (7.1.3) and (7.2.6). We have

$$[\mathcal{H}_0, \mathcal{B}] = -\frac{1}{2L^3}\sum_{k,k',p,q}(|q|^2-\mu)\hat{\varphi}(p)[a_q^*a_q, (b_{k+p}^r)^*(b_{k'-p}^r)^*c_{k'}c_k] + \text{h.c.}.$$

To calculate the commutator we note that $[a_q^*a_q, a_k] = -\delta_{q,k}a_k$. Thus,

$$[a_q^*a_q, (b_{k+p}^r)^*(b_{k'-p}^r)^*c_{k'}c_k] = (\delta_{q,k+p}+\delta_{q,k'-p}-\delta_{q,k'}-\delta_{q,k})(b_{k+p}^r)^*(b_{k'-p}^r)^*c_{k'}c_k$$

Noting further that

$$(|k+p|^2-\mu)+(|k-'p|^2-\mu)-(|k'|^2-\mu)-(|k|^2-\mu) = 2|p|^2+2p\cdot(k-k')$$

we have

$$[\mathcal{H}_0, \mathcal{B}] = -\frac{1}{L^3}\sum_{k,k',p}(|p|^2+p\cdot(k-k'))\hat{\varphi}(p)(b_{k+p}^r)^*(b_{k'-p}^r)^*c_{k'}c_k + \text{h.c.}.$$

Using the symmetry of interchanging $k \leftrightarrow k'$ and $p \to -p$ and writing in configuration space we have

$$[\mathcal{H}_0, \mathcal{B}] = \iint \mathrm{d}x\,\mathrm{d}y\left(\Delta\varphi(x-y)(b_x^r)^*(b_y^r)^*c_yc_x + 2\nabla^\mu\varphi(x-y)(b_x^r)^*(b_y^r)^*c_y\nabla^\mu c_x\right) + \text{h.c.}$$

As a first step we replace the b^r's by b's and write

$$[\mathcal{H}_0, \mathcal{B}] = \iint \mathrm{d}x\,\mathrm{d}y\left(\Delta\varphi(x-y)b_x^*b_y^*c_yc_x + 2\nabla^\mu\varphi(x-y)b_x^*b_y^*c_y\nabla^\mu c_x\right) + \text{h.c.} + \mathcal{H}_{0;\mathcal{B}}^{\div r}, \quad (7.4.1)$$

with $\mathcal{H}_{0;\mathcal{B}}^{\div r}$ defined so that this holds. In the first term in this expression we Taylor expand c_x around $x=y$. More precisely we have (as in Equation (4.4.2))

$$c_x = c_y + (x-y)^\mu\nabla^\mu c_x - (x-y)^\mu(x-y)^\nu\int_0^1 \mathrm{d}t\,(1-t)\nabla^\mu\nabla^\nu c_{x+t(y-x)}. \quad (7.4.2)$$

Note here that the first order term is evaluated at x and not at y. With this we have

$$[\mathcal{H}_0, \mathcal{B}] = \iint \mathrm{d}x\,\mathrm{d}y\left([(\cdot)^\mu\Delta\varphi + 2\nabla^\mu\varphi](x-y)b_x^*b_y^*c_y\nabla^\mu c_x\right) + \text{h.c.} + \mathcal{H}_{0;\mathcal{B}}^{\text{Taylor}} + \mathcal{H}_{0;\mathcal{B}}^{\div r}, \quad (7.4.3)$$

with $\mathcal{H}_{0;\mathcal{B}}^{\text{Taylor}}$ defined such that this holds, i.e. as the first term in (7.4.1) only with c_x replaced by the last term in (7.4.2).

7.4.2 $[\mathcal{V}_Q, \mathcal{B}]$:

The operator $\mathcal{V}_Q$ defined in (7.2.12) is given by

$$\mathcal{V}_Q = \frac{1}{2} \iint \mathrm{d}x\, \mathrm{d}y\, V(x-y) b_x^* b_y^* b_y b_x.$$

Thus, recalling again the formula for $\mathcal{B}$ in (7.2.6),

$$[\mathcal{V}_Q, \mathcal{B}] = -\frac{1}{4} \iiiint \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z\, \mathrm{d}z'\, V(x-y)\varphi(z-z')[b_x^* b_y^* b_y b_x, (b_z^r)^*(b_{z'}^r)^* c_{z'} c_z] + \text{h.c.}. \tag{7.4.4}$$

Since b's and c's anti-commute, the commutator is given by

$$[b_x^* b_y^* b_y b_x, (b_z^r)^*(b_{z'}^r)^* c_{z'} c_z] = b_x^* b_y^* [b_y b_x, (b_z^r)^*(b_{z'}^r)^*] c_{z'} c_z.$$

Using that

$$\{b_x, (b_z^r)^*\} = \frac{1}{L^3} \sum_k \hat{Q}^r(k) e^{ik(x-z)} = Q^r(x-z),$$

one computes

$$\begin{aligned}
[b_y b_x, (b_z^r)^*(b_{z'}^r)^*] = {} & Q^r(x-z)Q^r(y-z') - Q^r(y-z)Q^r(x-z') \\
& - Q^r(x-z)(b_{z'}^r)^* b_y + Q^r(y-z)(b_{z'}^r)^* b_x \\
& + Q^r(x-z')(b_z^r)^* b_y - Q^r(y-z')(b_z^r)^* b_x.
\end{aligned} \tag{7.4.5}$$

The first two and the last four terms give the same contribution to $[\mathcal{V}_Q, \mathcal{B}]$ when the integrations in (7.4.4) are computed, by the symmetries of interchanging $x \leftrightarrow y$ or $z \leftrightarrow z'$. By writing $Q^r = \delta - P^r$ we thus obtain

$$[\mathcal{V}_Q, \mathcal{B}] = -\frac{1}{2} \iint \mathrm{d}x\, \mathrm{d}y\, V(x-y)\varphi(x-y) b_x^* b_y^* c_y c_x + \text{h.c.} + \mathcal{Q}_{[\mathcal{V}_Q, \mathcal{B}]} \tag{7.4.6}$$

with

$$\begin{aligned}
\mathcal{Q}_{[\mathcal{V}_Q, \mathcal{B}]} = \frac{1}{2} \iiiint V(x-y)\varphi(z-z') \Big[& (\delta(x-z) - P^r(x-z)) b_x^* b_y^* (b_{z'}^r)^* b_y c_{z'} c_z \\
& + (2\delta(x-z)P^r(y-z') - P^r(x-z)P^r(y-z'))\, b_x^* b_y^* c_{z'} c_z \Big] \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z\, \mathrm{d}z' + \text{h.c.}.
\end{aligned} \tag{7.4.7}$$

In the first term in (7.4.6) we again Taylor expand the factor c_x using (7.4.2). Then,

$$[\mathcal{V}_Q, \mathcal{B}] = -\frac{1}{2} \iint \mathrm{d}x\, \mathrm{d}y\, (x-y)^\mu V(x-y)\varphi(x-y) b_x^* b_y^* c_y \nabla^\mu c_x + \text{h.c.} + \mathcal{V}_{Q;\mathcal{B}}^{\text{Taylor}} + \mathcal{Q}_{[\mathcal{V}_Q, \mathcal{B}]} \tag{7.4.8}$$

with $\mathcal{V}_{Q;\mathcal{B}}^{\text{Taylor}}$ as in the first term of (7.4.6) only with c_x replaced by the last term in (7.4.2).

7.4.3 $[\mathcal{V}_P - \mathcal{W}_P, \mathcal{B}]$:

We start by noting that

$$\mathcal{V}_P - \mathcal{W}_P = \frac{1}{2} \iint \mathrm{d}x\, \mathrm{d}y\, V(x-y)\varphi(x-y) c_x^* c_y^* c_y c_x.$$

Thus, recalling again the formula for $\mathcal{B}$ in (7.2.6),

$$\begin{aligned}\mathcal{Q}_{V\varphi} &= [\mathcal{V}_P - \mathcal{W}_P, \mathcal{B}] \\ &= -\frac{1}{4}\iiiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\, V(x-y)\varphi(x-y)\varphi(z-z')[c_x^* c_y^* c_y c_x, (b_z^r)^*(b_{z'}^r)^* c_{z'} c_z] + \text{h.c.}.\end{aligned}$$

The commutator is given by

$$[c_x^* c_y^* c_y c_x, (b_z^r)^*(b_{z'}^r)^* c_{z'} c_z] = (b_z^r)^*(b_{z'}^r)^*[c_x^* c_y^*, c_{z'} c_z] c_y c_x$$

To bound this term it is convenient to order the c's and b's not in normal order, but instead according to their indices x, y and z, z' such that factors c and b with indices z, z' are first. This corresponds to anti-normal ordering the c-commutator. Using that

$$\{c_x^*, c_z\} = \frac{1}{L^3}\sum_k \hat{P}(k) e^{ik(z-x)} = P(z-x) = P(x-z)$$

we calculate

$$\begin{aligned}[c_x^* c_y^*, c_{z'} c_z] &= P(x-z)P(y-z') - P(x-z')P(y-z) \\ &\quad - P(x-z)c_{z'}c_y^* + P(y-z)c_{z'}c_x^* + P(x-z')c_z c_y^* - P(y-z')c_z c_x^*.\end{aligned} \tag{7.4.9}$$

From the symmetries of interchanging $x \leftrightarrow y$ or $z \leftrightarrow z'$ the first two as well as the last four terms give the same contribution to $[\mathcal{V}_P - \mathcal{W}_P, \mathcal{B}]$ when the integrations are performed. Thus we find

$$\begin{aligned}\mathcal{Q}_{V\varphi} = -\frac{1}{2}\iiiint & \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\, V(x-y)\varphi(x-y)\varphi(z-z') \\ \times & \Big[P(x-z)P(y-z')(b_z^r)^*(b_{z'}^r)^* c_y c_x - 2P(x-z)(b_z^r)^*(b_{z'}^r)^* c_{z'} c_y^* c_y c_x\Big] + \text{h.c.}.\end{aligned} \tag{7.4.10}$$

7.4.4 $[\mathcal{V}_{\mathsf{OD}}, \mathcal{B}]$:

The operator $\mathcal{V}_{\mathsf{OD}}$ defined in (7.2.12) takes the form

$$\mathcal{V}_{\mathsf{OD}} = \frac{1}{2}\iint \mathrm{d}x\,\mathrm{d}y\, V(x-y) c_x^* c_y^* b_y b_x + \text{h.c.}.$$

Recalling again the formula for $\mathcal{B}$ in (7.2.6), we have

$$[\mathcal{V}_{\mathsf{OD}}, \mathcal{B}] = -\frac{1}{4}\iiiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\, V(x-y)\varphi(z-z')[c_x^* c_y^* b_y b_x, (b_z^r)^*(b_{z'}^r)^* c_{z'} c_z] + \text{h.c.}.$$

The commutator is given by

$$[c_x^* c_y^* b_y b_x, (b_z^r)^*(b_{z'}^r)^* c_{z'} c_z] = c_x^* c_y^*[b_y b_x, (b_z^r)^*(b_{z'}^r)^*] c_{z'} c_z - (b_z^r)^*(b_{z'}^r)^*[c_{z'} c_z, c_x^* c_y^*] b_y b_x.$$

The first term is the leading one. Using the formula in (7.4.5) and writing $Q^r = \delta - P^r$ the main term is the term with two δ's. The rest are error terms. Thus we have

$$[\mathcal{V}_{\mathsf{OD}}, \mathcal{B}] = 2(\mathcal{W}_P - \mathcal{V}_P) + \mathcal{Q}_{\mathsf{OD}}$$

with

$$\begin{aligned}\mathcal{Q}_{\mathsf{OD}} = \frac{-1}{4}\iiiint & V(x-y)\varphi(z-z')\Big[-4(\delta(x-z) - P^r(x-z))c_x^* c_y^* (b_{z'}^r)^* b_y c_{z'} c_z \\ & + (-4\delta(x-z)P^r(y-z') + 2P^r(x-z)P^r(y-z'))\, c_x^* c_y^* c_{z'} c_z \\ & + (b_z^r)^*(b_{z'}^r)^*[c_x^* c_y^*, c_{z'} c_z] b_y b_x\Big]\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z' + \text{h.c.}.\end{aligned} \tag{7.4.11}$$

7.5 Bounding commutators

To bound the error terms $\mathcal{E}_{\text{scat}}$, $\mathcal{E}_{\text{OD}}$ and $\mathcal{E}_{V\varphi}$ defined in (7.2.14)–(7.2.16), in this section we first derive useful bounds on the expectation values of the operators $[\mathcal{H}_0 + \mathcal{V}_Q, \mathcal{B}] + \mathcal{V}_{\text{OD}}$, $\mathcal{Q}_{\text{OD}}$, and $\mathcal{Q}_{V\varphi}$ in general states. In the subsequent Section 7.6 we shall use these bound for the particular states Γ^λ with Γ an approximate Gibbs state to conclude the proof of Propositions 7.2.15, 7.2.16 and 7.2.17.

To show that $[\mathcal{H}_0 + \mathcal{V}_Q, \mathcal{B}] + \mathcal{V}_{\text{OD}}$ is appropriately small, we write

$$\begin{aligned} \mathcal{V}_{\text{OD}} &= \frac{1}{2} \iint \mathrm{d}x \, \mathrm{d}y \, V(x-y) b_x^* b_y^* c_y c_x + \text{h.c.} \\ &= \frac{1}{2} \iint \mathrm{d}x \, \mathrm{d}y \, (x-y)^\mu V(x-y) b_x^* b_y^* c_y \nabla^\mu c_x + \text{h.c.} + \mathcal{V}_{\text{OD}}^{\text{Taylor}} \end{aligned} \tag{7.5.1}$$

by Taylor expanding c_x as in (7.4.2) and with $\mathcal{V}_{\text{OD}}^{\text{Taylor}}$ appropriately defined. Recalling (7.4.3) and (7.4.8) as well as (7.2.5), we obtain

$$[\mathcal{H}_0 + \mathcal{V}_Q, \mathcal{B}] + \mathcal{V}_{\text{OD}} = \mathcal{Q}_{\text{scat}} + \mathcal{H}_{0;\mathcal{B}}^{\div r} + \mathcal{H}_{0;\mathcal{B}}^{\text{Taylor}} + \mathcal{Q}_{[\mathcal{V}_Q,\mathcal{B}]} + \mathcal{V}_{Q;\mathcal{B}}^{\text{Taylor}} + \mathcal{V}_{\text{OD}}^{\text{Taylor}}, \tag{7.5.2}$$

with

$$\mathcal{Q}_{\text{scat}} = \iint \mathrm{d}x \, \mathrm{d}y \, \mathcal{E}_\varphi^\mu(x-y) b_x^* b_y^* c_y \nabla^\mu c_x + \text{h.c.}.$$

The main result of this section are bounds on the operators

$$\mathcal{H}_{0;\mathcal{B}}^{\div r}, \quad \mathcal{Q}_{\text{Taylor}} := \mathcal{H}_{0;\mathcal{B}}^{\text{Taylor}} + \mathcal{V}_{Q;\mathcal{B}}^{\text{Taylor}} + \mathcal{V}_{\text{OD}}^{\text{Taylor}}, \quad \mathcal{Q}_{\text{scat}}, \quad \mathcal{Q}_{[\mathcal{V}_Q,\mathcal{B}]}, \quad \mathcal{Q}_{V\varphi}, \quad \mathcal{Q}_{\text{OD}}.$$

To state the bounds it will be convenient to define for any (small) $\delta > 0$

$$k_F^{\delta^{-1}\kappa} = [\beta^{-1} + \mu\delta^{-1}\kappa]_+^{1/2}, \qquad \mathcal{N}_{Q^>} = \sum_{|k| > k_F^{\delta^{-1}\kappa}} a_k^* a_k. \tag{7.5.3}$$

That is, $k_F^{\delta^{-1}\kappa}$ is defined as k_F^κ in (7.2.2) only with κ replaced by $\delta^{-1}\kappa$. Recall that κ is chosen in (7.2.3) as $\kappa = \zeta(a^3\rho_0)^{-\alpha}$ for some (small) $\alpha > 0$. Recall also the definition of the operators $\mathcal{N}_Q$ and $\mathcal{K}_Q$ in (7.3.5).

Remark 7.5.1 (Bound on $\mathcal{N}_{Q^>}$)**.** Noting that $\mathcal{N}_{Q^>}$ is defined as $\mathcal{N}_Q$ only with κ replaced by $\delta^{-1}\kappa$ we can apply Lemma 7.3.3 and conclude that $\mathcal{N}_{Q^>}$ satisfies the same bound as $\mathcal{N}_Q$ only with κ replaced by $\delta^{-1}\kappa$. In particular, recalling (7.3.3) and (7.3.4) we conclude as in (7.3.6) that for an approximate Gibbs state Γ we have

$$\langle \mathcal{N}_{Q^>} \rangle_\Gamma \le C L^3 \zeta \delta \kappa^{-1} a^3 \rho_0^2 + L^3 \mathfrak{e}_L.$$

We shall prove (analogously to Lemma 4.5.1)

Lemma 7.5.2. *Let Γ be any state. Then, for $\alpha > 0$ sufficiently small and any $0 < \delta < 1$,*

$$\left| \left\langle \mathcal{H}_{0;\mathcal{B}}^{\div r} \right\rangle_\Gamma \right| \le C a^3 (k_F^\kappa)^4 \left| \log a k_F^\kappa \right| \left[k_F^\kappa \langle \mathcal{N}_Q \rangle_\Gamma^{1/2} + \langle \mathcal{K}_Q \rangle_\Gamma^{1/2} \right] \langle \mathcal{N} \rangle_\Gamma^{1/2}, \tag{7.5.4}$$

$$\begin{aligned} \left| \langle \mathcal{Q}_{\text{Taylor}} \rangle_\Gamma \right| + \left| \langle \mathcal{Q}_{\text{scat}} \rangle_\Gamma \right| &\le C a^3 \left| \log a k_F^\kappa \right| (k_F^{\delta^{-1}\kappa})^{3/2} (k_F^\kappa)^{3/2+2} \langle \mathcal{N}_Q \rangle_\Gamma^{1/2} \langle \mathcal{N} \rangle_\Gamma^{1/2} \\ &\quad + C L^{3/2} a^{3/2} (k_F^\kappa)^5 \langle \mathcal{N}_{Q^>} \rangle_\Gamma^{1/2}, \end{aligned} \tag{7.5.5}$$

$$\left| \left\langle \mathcal{Q}_{[\mathcal{V}_Q,\mathcal{B}]} \right\rangle_\Gamma \right| \le C a^3 (k_F^\kappa)^4 \left[\langle \mathcal{N}_Q \rangle_\Gamma^{1/2} + (a k_F^\kappa)^{1/2} \langle \mathcal{N} \rangle_\Gamma^{1/2} \right] \langle \mathcal{V}_Q \rangle_\Gamma^{1/2}, \tag{7.5.6}$$

$$\left| \langle \mathcal{Q}_{V\varphi} \rangle_\Gamma \right| \le C a^{2+3/2} (k_F^\kappa)^{4+3/2} \langle \mathcal{N}_Q \rangle_\Gamma^{1/2} \langle \mathcal{N} \rangle_\Gamma^{1/2}, \tag{7.5.7}$$

$$\left| \langle \mathcal{Q}_{\text{OD}} \rangle_\Gamma \right| \le C a^{4+1/2} (k_F^\kappa)^{6+1/2} \langle \mathcal{N} \rangle_\Gamma + C a^2 (k_F^\kappa)^3 \langle \mathcal{V}_Q \rangle_\Gamma^{1/2} \langle \mathcal{N}_Q \rangle_\Gamma^{1/2}. \tag{7.5.8}$$

For the proof the following lemma from Chapter 4 will be very useful.

Lemma 7.5.3 (Lemma 4.5.2). *Let F be a compactly supported function with $F(x) = 0$ for $|x| \geq C(k_F^\kappa)^{-1}$. Then, uniformly in $x \in \Lambda$ and $t \in [0,1]$, (with ∇^n denoting any n'th derivative)*

$$\left\| \int F(x-y) a_y^* c_y \, \mathrm{d}y \right\| \leq C(k_F^\kappa)^{3/2} \|F\|_{L^2} ,$$

$$\left\| \int F(x-y) a_y^* c_y \nabla^n c_{ty+(1-t)x} \, \mathrm{d}y \right\| \leq C(k_F^\kappa)^{3+n} \|F\|_{L^2} .$$

As straightforward consequences we obtain as in (4.5.5), (4.5.6)

$$\left\| \int \varphi(z-z')(b_{z'}^r)^* c_{z'} \, \mathrm{d}z' \right\| \leq C(k_F^\kappa)^3 \|\varphi\|_{L^1} + C(k_F^\kappa)^{3/2} \|\varphi\|_{L^2} \leq C(ak_F^\kappa)^{3/2} \tag{7.5.9}$$

$$\left\| \int \varphi(z-z')(b_{z'}^r)^* c_{z'} c_z \, \mathrm{d}z' \right\| \leq C(k_F^\kappa)^{4+3/2} \| |\cdot| \varphi\|_{L^1} + C(k_F^\kappa)^4 \| |\cdot| \varphi\|_{L^2} \leq C(k_F^\kappa)^{3/2}(ak_F^\kappa)^{5/2} \tag{7.5.10}$$

where we used Lemma 7.3.2 in the last step.

The remainder of this section is devoted to the proof of Lemma 7.5.2.

Remark 7.5.4. Many of the bounds and computations in the following are similar to the analogous bounds and computations in Chapter 4. There, however, the operators are conjugated by a particle-hole transformation. At positive temperature there is no such natural 'particle-hole transformation' — there is no filled Fermi ball in the free system. Hence the bounds given here appear somewhat different than in the zero-temperature case studied in Chapter 4.

7.5.1 (Non-)regularization of $[\mathcal{H}_0, \mathcal{B}]$

According to (7.4.1), $\mathcal{H}_{0;\mathcal{B}}^{\div r}$ is given by

$$\mathcal{H}_{0;\mathcal{B}}^{\div r} = \iint \mathrm{d}x \, \mathrm{d}y \, \Big((b_x^r)^* (b_y^r)^* - b_x^* b_y^* \Big) \Big(\Delta\varphi(x-y) c_y c_x + 2\nabla^\mu \varphi(x-y) c_y \nabla^\mu c_x \Big) + \text{h.c.}. \tag{7.5.11}$$

To bound this write $b_x^r = b_x + b_x^{\div r}$ with $b_x^{\div r} = L^{-3/2} \sum_k e^{ikx} b_k^{\div r}$ and $b_k^{\div r} = (\hat{Q}^r(k) - \hat{Q}(k)) a_k$. We note that $\hat{Q}^r - \hat{Q}$ is supported on the set $k_F^\kappa \leq |k| \leq 2k_F^\kappa$. In particular $\|b_x^{\div r}\| \leq C(k_F^\kappa)^{3/2}$. We further Taylor expand the factor c_x in the first term in the integrand in (7.5.11) around $x = y$ as in (7.3.9) (with x and y interchanged) and change variables to $z = x - y$. Then for any state Γ we obtain the identity

$$\begin{aligned}
&\left\langle \mathcal{H}_{0;\mathcal{B}}^{\div r} \right\rangle_\Gamma \\
&= 2\,\mathrm{Re} \iint \mathrm{d}z \, \mathrm{d}y \, z^\mu \Delta\varphi(z) \int_0^1 \mathrm{d}t \, \left\langle \Big(b_{y+z}^* (b_y^{\div r})^* + (b_{y+z}^{\div r})^* b_y^* + (b_{y+z}^{\div r})^* (b_y^{\div r})^* \Big) c_y \nabla^\mu c_{y+tz} \right\rangle_\Gamma \\
&\quad + 2\,\mathrm{Re} \iint \mathrm{d}z \, \mathrm{d}y \, \nabla^\mu \varphi(z) \left\langle \Big(b_{y+z}^* (b_y^{\div r})^* + (b_{y+z}^{\div r})^* b_y^* + (b_{y+z}^{\div r})^* (b_y^{\div r})^* \Big) c_y \nabla^\mu c_{y+z} \right\rangle_\Gamma .
\end{aligned} \tag{7.5.12}$$

The two terms are treated similarly. We start with the first. Define the function $\phi_y(z) = \left\langle \Big(b_{y+z}^* (b_y^{\div r})^* + (b_{y+z}^{\div r})^* b_y^* + (b_{y+z}^{\div r})^* (b_y^{\div r})^* \Big) c_y \nabla^\mu c_{y+tz} \right\rangle_\Gamma$. Note that it vanishes at $z = 0$, and hence

$$\phi_y(z) = z^\nu \int_0^1 \mathrm{d}s\, \nabla^\nu \phi_y(sz).$$

The derivative hits either a factor ∇c, $(b^{\div r})^*$ or b^*. In the case where the derivative hits either ∇c or a factor $(b^{\div r})^*$ we bound the factor ∇c and a factor $(b^{\div r})^*$ in norm (in the term with two $(b^{\div r})^*$'s we keep one factor $(b^{\div r})^*$ without a derivative). These terms are then bounded by

$$\begin{aligned}&(k_F^\kappa)^5 \iint \mathrm{d}z\,\mathrm{d}y\,|z|^2|\Delta\varphi(z)| \left(\left\|\Gamma^{1/2}b_y^*\right\|_{\mathfrak{S}_2} + \left\|\Gamma^{1/2}(b_y^{\div r})^*\right\|_{\mathfrak{S}_2}\right)\left\|c_y\Gamma^{1/2}\right\|_{\mathfrak{S}_2}\\ &\quad\le C\left\||\cdot|^2\Delta\varphi\right\|_{L^1}(k_F^\kappa)^5 \left\langle \mathcal{N}_Q\right\rangle_\Gamma^{1/2}\left\langle\mathcal{N}\right\rangle_\Gamma^{1/2}.\end{aligned}$$

For the terms where the derivative hits a factor b^* we again bound the factors ∇c and $(b^{\div r})^*$ in norm. These terms are then bounded by

$$(k_F^\kappa)^4 \iint \mathrm{d}z\,\mathrm{d}y\,|z|^2|\Delta\varphi(z)|\left\|\Gamma^{1/2}\nabla b_y^*\right\|_{\mathfrak{S}_2}\left\|c_y\Gamma^{1/2}\right\|_{\mathfrak{S}_2} \le C\left\||\cdot|^2\Delta\varphi\right\|_{L^1}(k_F^\kappa)^4\left\langle\mathcal{K}_Q\right\rangle_\Gamma^{1/2}\left\langle\mathcal{N}\right\rangle_\Gamma^{1/2}.$$

The second term in (7.5.12) is treated analogously, only the bound has a factor $\||\cdot|\nabla\varphi\|_{L^1}$ instead of $\||\cdot|^2\Delta\varphi\|_{L^1}$. Together with the bounds of Lemma 7.3.2 this completes the proof of (7.5.4).

7.5.2 Taylor expansion errors

According to (7.4.3), (7.4.8) and (7.5.1) the term $\mathcal{Q}_{\mathsf{Taylor}}$ is given by

$$\mathcal{Q}_{\mathsf{Taylor}} = \iint \mathrm{d}x\,\mathrm{d}y\,F^{\mu\nu}(x-y)b_x^*b_y^*c_y\int_0^1 \mathrm{d}t\,(1-t)\nabla^\mu\nabla^\nu c_{x+t(y-x)} + \text{h.c.}, \tag{7.5.13}$$

where

$$F^{\mu\nu}(x) = -\left[x^\mu x^\nu\Delta\varphi(x) + \frac{1}{2}x^\mu x^\nu V(x)(1-\varphi(x))\right] = 2x^\mu\nabla^\nu\varphi(x) - x^\mu\mathcal{E}_\varphi^\nu(x),$$

using (7.2.5). To bound this we write

$$b_x^* = (b_x^<)^* + (b_x^>)^*, \qquad b_x^> = L^{-3/2}\sum_k \hat{Q}^>(k)e^{ikx}a_k, \qquad \hat{Q}^>(k) = \chi_{(|k|>k_F^{\delta^{-1}\kappa})}$$

for some $0<\delta<1$, with $k_F^{\delta^{-1}\kappa}$ defined in (7.5.3), i.e. as k_F^κ only with κ replaced by $\delta^{-1}\kappa$. In the term with $(b_x^>)^*$ we shall use Lemma 7.5.3. To do this we first write $b_y^* = a_y^* - c_y^*$, and rewrite $\mathcal{Q}_{\mathsf{Taylor}}$ as

$$\begin{aligned}&\mathcal{Q}_{\mathsf{Taylor}}\\ &= \iint \mathrm{d}x\,\mathrm{d}y\,F^{\mu\nu}(x-y)\left[(b_x^<)^*b_y^* + (b_x^>)^*a_y^* - (b_x^>)^*c_y^*\right]c_y\int_0^1 \mathrm{d}t\,(1-t)\nabla^\mu\nabla^\nu c_{x+t(y-x)} + \text{h.c.}\\ &=: \mathcal{Q}_{\mathsf{Taylor}}^< + \mathcal{Q}_{\mathsf{Taylor}}^> + \mathcal{Q}_{\mathsf{Taylor}}^c.\end{aligned}$$

First, for the term $\mathcal{Q}_{\mathsf{Taylor}}^<$ containing $(b_x^<)^*$, we note that $\|(b_x^<)^*\| \le C(k_F^{\delta^{-1}\kappa})^{3/2}$. Thus, bounding also $\nabla^2 c$ in norm we have

$$\begin{aligned}\left|\left\langle\mathcal{Q}_{\mathsf{Taylor}}^<\right\rangle_\Gamma\right| &\le C\iint \mathrm{d}x\,\mathrm{d}y\,|F(x-y)|\left\|\Gamma^{1/2}b_y^*\right\|_{\mathfrak{S}_2}(k_F^{\delta^{-1}\kappa})^{3/2}(k_F^\kappa)^{3/2+2}\left\|c_y\Gamma^{1/2}\right\|_{\mathfrak{S}_2}\\ &\le C\|F\|_{L^1}(k_F^{\delta^{-1}\kappa})^{3/2}(k_F^\kappa)^{3/2+2}\left\langle\mathcal{N}_Q\right\rangle_\Gamma^{1/2}\left\langle\mathcal{N}\right\rangle_\Gamma^{1/2}.\end{aligned}$$

Next, for the term $\mathcal{Q}^{c}_{\mathsf{Taylor}}$ containing c^*_y, we bound c^*_y and $\nabla^2 c$ in norm. Then this term is bounded by

$$\begin{aligned}\left|\left\langle \mathcal{Q}^{c}_{\mathsf{Taylor}}\right\rangle_\Gamma\right| &\leq C \iint \mathrm{d}x\,\mathrm{d}y\ |F(x-y)| \left\|\Gamma^{1/2}(b^>_x)^*\right\|_{\mathfrak{S}_2} (k_F^\kappa)^5 \left\|c_y\Gamma^{1/2}\right\|_{\mathfrak{S}_2} \\ &\leq C\,\|F\|_{L^1} (k_F^\kappa)^5 \left\langle \mathcal{N}_{Q^>}\right\rangle_\Gamma^{1/2} \left\langle \mathcal{N}\right\rangle_\Gamma^{1/2}.\end{aligned}$$

Finally, for the term $\mathcal{Q}^{>}_{\mathsf{Taylor}}$ we use Lemma 7.5.3 to bound the y-integral. This term is then bounded by

$$\begin{aligned}\left|\left\langle \mathcal{Q}^{>}_{\mathsf{Taylor}}\right\rangle_\Gamma\right| &\leq 2\int \mathrm{d}x \int_0^1 \mathrm{d}t \left\|\Gamma^{1/2}(b^>_x)^*\right\|_{\mathfrak{S}_2} \left\|\int \mathrm{d}y\, F^{\mu\nu}(x-y) a^*_y c_y \nabla^\mu\nabla^\nu c_{x+t(y-x)}\right\| \\ &\leq CL^{3/2}\,\|F\|_{L^2} (k_F^\kappa)^5 \left\langle \mathcal{N}_{Q^>}\right\rangle_\Gamma^{1/2}.\end{aligned}$$

Combining the bounds for $\mathcal{Q}^{\leq}_{\mathsf{Taylor}}$, $\mathcal{Q}^{>}_{\mathsf{Taylor}}$ and $\mathcal{Q}^{c}_{\mathsf{Taylor}}$, using Lemma 7.3.2 and noting that $\mathcal{N}_{Q^>} \leq \mathcal{N}_Q$ and $k_F^\kappa \leq k_F^{\delta^{-1}\kappa}$ we thus obtain the bound (7.5.5) for the expectation value of $\mathcal{Q}_{\mathsf{Taylor}}$.

7.5.3 Scattering equation cancellation

We can bound $\mathcal{Q}_{\mathsf{scat}}$ analogously to $\mathcal{Q}_{\mathsf{Taylor}}$. The only difference is that $\nabla^2 c$ is replaced by ∇c, hence the bounds have one fewer power of k_F^κ, and F is replaced by $\mathcal{E}_\varphi$, leading to an additional factor k_F^κ. Hence we arrive at the same bound.

7.5.4 Error terms from $[\mathcal{V}_Q, \mathcal{B}]$

Recall the definition of $\mathcal{Q}_{[\mathcal{V}_Q,\mathcal{B}]}$ in (7.4.7). We split the operator into 4 terms and bound each separately:

1. The quartic term with one δ and one P^r,
2. The quartic term with two P^r's,
3. The sextic term with δ, and
4. The sextic term with P^r.

7.5.4.1 Quartic term with one δ and one P^r

This term is of the form

$$\mathcal{A}_{4,\delta} = \iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z'\,V(x-y)\varphi(x-z')P^r(y-z')b^*_x b^*_y c_{z'} c_x + \text{h.c.}.$$

Taylor expanding $c_{z'}$ around $z'=x$ as in (7.3.9) and bounding in norm $\|\nabla c\| \leq C(k_F^\kappa)^{3/2+1}$ and $\|P^r\|_{L^\infty} \leq C(k_F^\kappa)^3$ we obtain the bound

$$\begin{aligned}\left|\left\langle \mathcal{A}_{4,\delta}\right\rangle_\Gamma\right| &\leq C(k_F^\kappa)^{3/2+4}\, \||\cdot|\varphi\|_{L^1} \iint V(x-y) \left\|\Gamma^{1/2} b^*_x b^*_y\right\|_{\mathfrak{S}_2} \left\|c_x\Gamma^{1/2}\right\|_{\mathfrak{S}_2} \mathrm{d}x\,\mathrm{d}y \\ &\leq C(k_F^\kappa)^{3/2+4}\, \||\cdot|\varphi\|_{L^1} \|V\|_{L^1}^{1/2} \left\langle \mathcal{V}_Q\right\rangle_\Gamma^{1/2} \left\langle \mathcal{N}\right\rangle_\Gamma^{1/2} \leq Ca^{3+1/2}(k_F^\kappa)^{3/2+3} \left\langle \mathcal{V}_Q\right\rangle_\Gamma^{1/2} \left\langle \mathcal{N}\right\rangle_\Gamma^{1/2}\end{aligned} \tag{7.5.14}$$

using Lemma 7.3.2 in the last step.

7.5.4.2 Quartic term with two P^r's

This term is of the form

$$\mathcal{A}_{4,P} = -\frac{1}{2} \iiiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\, V(x-y)\varphi(z-z')P^r(x-z)P^r(y-z')b_x^* b_y^* c_{z'} c_z + \text{h.c.}.$$

As above we Taylor expand $c_{z'}$ and bound ∇c in norm. By Cauchy–Schwarz

$$\begin{aligned}
&\left|\langle \mathcal{A}_{4,P}\rangle_\Gamma\right| \\
&\quad \leq C(k_F^\kappa)^{3/2+1} \iiiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\, V(x-y)|z-z'||\varphi(z-z')||P^r(x-z)||P^r(y-z')| \\
&\qquad \times \left\|\Gamma^{1/2} b_x^* b_y^*\right\|_{\mathfrak{S}_2} \left\|c_z \Gamma^{1/2}\right\|_{\mathfrak{S}_2} \\
&\quad \leq C(k_F^\kappa)^{3/2+1} \left[\iiiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\, V(x-y) \left\|\Gamma^{1/2} b_x^* b_y^*\right\|_{\mathfrak{S}_2}^2 |z-z'||\varphi(z-z')||P^r(x-z)|^2\right]^{1/2} \\
&\qquad \times \left[\iiiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\, V(x-y)|z-z'||\varphi(z-z')||P^r(y-z')|^2 \left\|c_z \Gamma^{1/2}\right\|_{\mathfrak{S}_2}^2\right]^{1/2} \\
&\quad \leq C(k_F^\kappa)^{3/2+1} \left\||\cdot||\varphi|\right\|_{L^1} \|V\|_{L^1}^{1/2} \|P^r\|_{L^2}^2 \langle \mathcal{V}_Q\rangle_\Gamma^{1/2} \langle \mathcal{N}\rangle_\Gamma^{1/2} \\
&\quad \leq C a^{3+1/2}(k_F^\kappa)^{3/2+3} \langle \mathcal{V}_Q\rangle_\Gamma^{1/2} \langle \mathcal{N}\rangle_\Gamma^{1/2}
\end{aligned} \tag{7.5.15}$$

using again Lemma 7.3.2.

7.5.4.3 Sextic term with δ

This term is of the form

$$\mathcal{A}_{6,\delta} = \frac{1}{2} \iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z'\, V(x-y)\varphi(x-z')b_x^* b_y^* (b_{z'}^r)^* b_y c_{z'} c_x + \text{h.c.}.$$

We use (7.5.10) to bound the z'-integral. Thus, by Cauchy–Schwarz,

$$\begin{aligned}
\left|\langle \mathcal{A}_{6,\delta}\rangle_\Gamma\right| &\leq \iint \mathrm{d}x\,\mathrm{d}y\, V(x-y) \left\|\Gamma^{1/2} b_x^* b_y^*\right\|_{\mathfrak{S}_2} \left\|\int \mathrm{d}z'\, \varphi(x-z')(b_{z'}^r)^* c_{z'} c_x\right\| \left\|b_y \Gamma^{1/2}\right\|_{\mathfrak{S}_2} \\
&\leq C(k_F^\kappa)^{3/2}(a k_F^\kappa)^{5/2} \|V\|_{L^1}^{1/2} \langle \mathcal{V}_Q\rangle_\Gamma^{1/2} \langle \mathcal{N}_Q\rangle_\Gamma^{1/2} \leq C a^3 (k_F^\kappa)^4 \langle \mathcal{V}_Q\rangle_\Gamma^{1/2} \langle \mathcal{N}_Q\rangle_\Gamma^{1/2}.
\end{aligned} \tag{7.5.16}$$

7.5.4.4 Sextic term with P^r

This term is of the form

$$\mathcal{A}_{6,P} = -\frac{1}{2} \iiiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\, V(x-y)\varphi(z-z')P^r(x-z)b_x^* b_y^* (b_{z'}^r)^* b_y c_{z'} c_z + \text{h.c.}.$$

As above we use (7.5.10) to bound the z'-integral. The z-integral afterwards is then bounded by $\|P^r\|_{L^1} \leq C$. As above then

$$\left|\langle \mathcal{A}_{6,P}\rangle_\Gamma\right| \leq C a^3 (k_F^\kappa)^4 \langle \mathcal{V}_Q\rangle_\Gamma^{1/2} \langle \mathcal{N}_Q\rangle_\Gamma^{1/2}. \tag{7.5.17}$$

Combining (7.5.14)–(7.5.17) we conclude the proof of (7.5.6).

7.5.5 Error terms from $[\mathcal{V}_P - \mathcal{W}_P, \mathcal{B}]$

Recall the definition of $\mathcal{Q}_{V\varphi}$ in (7.4.10). We consider the two terms separately:

1. The quartic term,
2. The sextic term.

7.5.5.1 Quartic term

This term is of the form

$$\mathcal{A}_4 = -\frac{1}{2} \iiiint \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z\, \mathrm{d}z'\, V(x-y)\varphi(x-y)\varphi(z-z')P(x-z)P(y-z')(b_z^r)^*(b_{z'}^r)^* c_y c_x + \text{h.c.}.$$

We bound its expectation value in an arbitrary state Γ as

$$\begin{aligned} |\langle \mathcal{A}_4 \rangle_\Gamma| \le \iiint \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z\, V(x-y)\varphi(x-y)|P(x-z)| \left\| \Gamma^{1/2}(b_z^r)^* \right\|_{\mathfrak{S}_2} \\ \times \left\| \int \mathrm{d}z'\, P(y-z')\varphi(z-z')(b_{z'}^r)^* \right\| \left\| c_y c_x \Gamma^{1/2} \right\|_{\mathfrak{S}_2}. \end{aligned}$$

To bound this we note that since $\hat{Q}^r \le 1$ we have

$$\left\| \int \mathrm{d}z'\, P(y-z')\varphi(z-z')(b_{z'}^r)^* \right\| \le \left\| \int \mathrm{d}z'\, P(y-z')\varphi(z-z')a_{z'}^* \right\| = (P^2 * \varphi^2(y-z))^{1/2}$$

with $*$ denoting convolution. Then, noting that $\varphi \le 1$, we have by Cauchy–Schwarz

$$\begin{aligned} |\langle \mathcal{A}_4 \rangle_\Gamma| &\le \left[\iiint \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z\, V(x-y)\, |P(x-z)|^2 \left\| c_y c_x \Gamma^{1/2} \right\|_{\mathfrak{S}_2}^2 \right]^{1/2} \\ &\quad \times \left[\iiint \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z\, V(x-y) P^2 * \varphi^2(y-z) \left\| \Gamma^{1/2}(b_z^r)^* \right\|_{\mathfrak{S}_2}^2 \right]^{1/2} \\ &\le C(k_F^\kappa)^3 \|V\|_{L^1}^{1/2} \|\varphi\|_{L^2} \langle \mathcal{V}_P \rangle_\Gamma^{1/2} \langle \mathcal{N}_Q \rangle_\Gamma^{1/2} \\ &\le C a^{2+3/2} (k_F^\kappa)^{4+3/2} \langle \mathcal{N}_Q \rangle_\Gamma^{1/2} \langle \mathcal{N} \rangle_\Gamma^{1/2}, \end{aligned} \tag{7.5.18}$$

where we used Lemmas 7.3.2 and 7.3.5.

7.5.5.2 Sextic term

This term is of the form

$$\begin{aligned} \mathcal{A}_6 &= \iiiint \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z\, \mathrm{d}z'\, V(x-y)\varphi(x-y)\varphi(z-z')P(x-z)(b_z^r)^*(b_{z'}^r)^* c_{z'} c_y^* c_y c_x + \text{h.c.} \\ &= \iint \mathrm{d}y\, \mathrm{d}z\, P(y-z) \left[\int \mathrm{d}z'\, \varphi(z-z')(b_z^r)^*(b_{z'}^r)^* c_{z'} \right] \left[\int \mathrm{d}x\, V(x-y)\varphi(x-y) c_y^* c_y c_x \right] \\ &\quad + \text{h.c.}. \end{aligned}$$

Noting that as operators $P \le \mathbb{1}$ we thus have by Cauchy–Schwarz for any $\lambda > 0$

$$\begin{aligned} \pm \mathcal{A}_6 &\le \lambda \int \mathrm{d}z \left[\int \mathrm{d}z'\, \varphi(z-z')(b_z^r)^*(b_{z'}^r)^* c_{z'} \right] \left[\int \mathrm{d}x\, \varphi(z-x) c_x^* b_x^r b_z^r \right] \\ &\qquad + \lambda^{-1} \int \mathrm{d}y \left[\int \mathrm{d}z\, V(z-y)\varphi(z-y) c_z^* c_y^* c_y \right] \left[\int \mathrm{d}x\, V(x-y)\varphi(x-y) c_y^* c_y c_x \right] \\ &=: \lambda \mathcal{A}_6^\varphi + \lambda^{-1} \mathcal{A}_6^V. \end{aligned}$$

We bound $\mathcal{A}_6^\varphi$ using the bound in (7.5.9). This yields

$$\begin{aligned}\langle \mathcal{A}_6^\varphi\rangle_\Gamma &\leq \int \mathrm{d}z \left\|\Gamma^{1/2}(b_z^r)^*\right\|_{\mathfrak{S}_2} \left\|\int \mathrm{d}z'\,\varphi(z-z')(b_{z'}^r)^* c_{z'}\right\| \left\|\int \mathrm{d}x\,\varphi(z-x)c_x^* b_x^r\right\| \left\|b_z^r\Gamma^{1/2}\right\|_{\mathfrak{S}_2} \\ &\leq C(ak_F^\kappa)^3 \langle \mathcal{N}_Q\rangle_\Gamma .\end{aligned} \tag{7.5.19}$$

To bound $\mathcal{A}_6^V$ we again note that $\varphi \leq 1$. Then, by Lemma 7.3.5,

$$\begin{aligned}\left\langle \mathcal{A}_6^V\right\rangle_\Gamma &\leq \iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z V(z-y)V(x-y)\left\|\Gamma^{1/2}c_z^*c_y^*\right\|_{\mathfrak{S}_2}\left\|c_yc_y^*\right\|\left\|c_yc_z\Gamma^{1/2}\right\|_{\mathfrak{S}_2} \\ &\leq C(k_F^\kappa)^3\|V\|_{L^1}\langle \mathcal{V}_P\rangle_\Gamma \leq Ca^4(k_F^\kappa)^8\langle\mathcal{N}\rangle_\Gamma .\end{aligned}$$

Choosing the optimal λ we thus find

$$|\langle \mathcal{A}_6\rangle_\Gamma| \leq Ca^{2+3/2}(k_F^\kappa)^{4+3/2}\langle\mathcal{N}\rangle_\Gamma^{1/2}\langle\mathcal{N}_Q\rangle_\Gamma^{1/2}. \tag{7.5.20}$$

Combining (7.5.18) and (7.5.20) we conclude the proof of (7.5.7).

7.5.6 Error terms from $[\mathcal{V}_{\mathrm{OD}}, \mathcal{B}]$

Recall the definition of $\mathcal{Q}_{\mathrm{OD}}$ in (7.4.11). Writing the c-commutator using (7.4.9) we have four types of terms, which we treat separately.

1. The quartic term with only c's,
2. The sextic term with four c's and two b's,
3. The quartic term with only b's, and
4. The sextic term with four b's and two c's.

7.5.6.1 Quartic term with only c's

We have two terms,

a. The term with one factor δ and one factor P^r, and

b. The term with two factors P^r.

They are of the form

$$\begin{aligned}\mathcal{A}_{4,c,\delta} &= \iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z'\,V(x-y)\varphi(x-z')P^r(y-z')c_x^*c_y^*c_{z'}c_x + \text{h.c.}, \\ \mathcal{A}_{4,c,P} &= -\frac{1}{2}\iiiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\,V(x-y)\varphi(z-z')P^r(x-z)P^r(y-z')c_x^*c_y^*c_{z'}c_z + \text{h.c.}.\end{aligned}$$

To bound the first term we Taylor expand $c_{z'}$ around $z'=x$. Then by Cauchy–Schwarz

$$\begin{aligned}\left|\langle \mathcal{A}_{4,c,\delta}\rangle_\Gamma\right| &\leq C(k_F^\kappa)^{3/2+1}\iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z'\,V(x-y)|x-z'|\varphi(x-z')|P^r(y-z')| \\ &\quad\times\left\|\Gamma^{1/2}c_x^*c_y^*\right\|_{\mathfrak{S}_2}\left\|c_x\Gamma^{1/2}\right\|_{\mathfrak{S}_2} \\ &\leq C(k_F^\kappa)^{3/2+1}\|V\|_{L^1}^{1/2}\||\cdot|\varphi\|_{L^2}\|P^r\|_{L^2}\langle\mathcal{V}_P\rangle_\Gamma^{1/2}\langle\mathcal{N}\rangle_\Gamma^{1/2} \leq Ca^{4+1/2}(k_F^\kappa)^{6+1/2}\langle\mathcal{N}\rangle_\Gamma\end{aligned} \tag{7.5.21}$$

by Lemmas 7.3.2 and 7.3.5. Similarly we have for the second term, again using Lemmas 7.3.2 and 7.3.5,

$$
\begin{aligned}
&|\langle \mathcal{A}_{4,c,P}\rangle| \\
&\leq C(k_F^\kappa)^{3/2+1}\left[\iiiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\,V(x-y)|z-z'|\varphi(z-z')|P^r(x-z)|^2\left\|\Gamma^{1/2}c_x^*c_y^*\right\|_{\mathfrak{S}_2}^2\right]^{1/2} \\
&\quad\times\left[\iiiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\,V(x-y)|z-z'|\varphi(z-z')|P^r(y-z')|^2\left\|c_z\Gamma^{1/2}\right\|_{\mathfrak{S}_2}^2\right]^{1/2} \\
&\leq C(k_F^\kappa)^{3/2+1}\,\||\cdot|\varphi\|_{L^1}\,\|P^r\|_{L^2}^2\,\|V\|_{L^1}^{1/2}\,\langle\mathcal{V}_P\rangle_\Gamma^{1/2}\,\langle\mathcal{N}\rangle_\Gamma^{1/2}\leq Ca^5(k_F^\kappa)^7\,\langle\mathcal{N}\rangle_\Gamma\,. \qquad (7.5.22)
\end{aligned}
$$

7.5.6.2 Sextic term with four c's and two b's

We have two terms,

a. The term with a factor δ, and

b. The term with a factor P^r.

They are of the form

$$
\begin{aligned}
\mathcal{A}_{6,c,\delta} &= \iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z'\,V(x-y)\varphi(x-z')c_x^*c_y^*(b_{z'}^r)^*b_yc_{z'}c_x+\text{h.c.}, \\
\mathcal{A}_{6,c,P} &= -\iiiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\,V(x-y)\varphi(z-z')P^r(x-z)c_x^*c_y^*(b_{z'}^r)^*b_yc_{z'}c_z+\text{h.c.}.
\end{aligned}
$$

To bound the first term we use (7.5.10) to bound the z'-integral. We have

$$
\begin{aligned}
\left|\langle\mathcal{A}_{6,c,\delta}\rangle_\Gamma\right| &\leq 2\iint \mathrm{d}x\,\mathrm{d}y\,V(x-y)\left\|\Gamma^{1/2}c_x^*c_y^*\right\|_{\mathfrak{S}_2}\left\|\int \mathrm{d}z'\,\varphi(x-z')(b_{z'}^r)^*c_{z'}c_x\right\|\left\|b_y\Gamma^{1/2}\right\|_{\mathfrak{S}_2} \\
&\leq C(k_F^\kappa)^{3/2}(ak_F^\kappa)^{5/2}\|V\|_{L^1}^{1/2}\langle\mathcal{V}_P\rangle_\Gamma^{1/2}\langle\mathcal{N}_Q\rangle_\Gamma^{1/2}\leq Ca^{4+1/2}(k_F^\kappa)^{6+1/2}\langle\mathcal{N}_Q\rangle_\Gamma^{1/2}\langle\mathcal{N}\rangle_\Gamma^{1/2}, \qquad (7.5.23)
\end{aligned}
$$

where we used Lemma 7.3.5. The second term is bounded similarly, only the z-integral is bounded by $\|P^r\|_{L^1}\leq C$. We conclude that

$$
\left|\langle\mathcal{A}_{6,c,P}\rangle_\Gamma\right|\leq Ca^{4+1/2}(k_F^\kappa)^{6+1/2}\langle\mathcal{N}_Q\rangle_\Gamma^{1/2}\langle\mathcal{N}\rangle_\Gamma^{1/2}. \qquad (7.5.24)
$$

7.5.6.3 Quartic term with only b's

This term is of the form

$$
\mathcal{A}_{4,b} = -\frac{1}{2}\iiiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'\,V(x-y)\varphi(z-z')P(x-z)P(y-z')(b_z^r)^*(b_{z'}^r)^*b_yb_x+\text{h.c.}.
$$

We bound its expectation value as

$$
\begin{aligned}
\left|\langle\mathcal{A}_{4,b}\rangle_\Gamma\right| &\leq \iiint \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,V(x-y)|P(x-z)| \\
&\qquad\times\left\|\Gamma^{1/2}(b_z^r)^*\right\|_{\mathfrak{S}_2}\left\|\int \mathrm{d}z'\,\varphi(z-z')P(y-z')(b_{z'}^r)^*\right\|\left\|b_yb_x\Gamma^{1/2}\right\|_{\mathfrak{S}_2}
\end{aligned}
$$

Then, since $0 \leq \hat{Q}^r(k) \leq 1$ we have

$$\left\| \int \mathrm{d}z' \, \varphi(z-z') P(y-z') (b_{z'}^r)^* \right\| \leq \left\| \int \mathrm{d}z' \, \varphi(z-z') P(y-z') a_{z'}^* \right\| = (\varphi^2 * P^2(y-z))^{1/2}$$

with $*$ denoting convolution. Hence, by Cauchy–Schwarz, using Lemma 7.3.2,

$$\begin{aligned}
\left| \langle \mathcal{A}_{4,b} \rangle_\Gamma \right| &\leq \left[\iiint \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z \, V(x-y) |P(x-z)|^2 \left\| b_y b_x \Gamma^{1/2} \right\|_{\mathfrak{S}_2}^2 \right]^{1/2} \\
&\quad \times \left[\iiint \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z \, V(x-y) \varphi^2 * P^2(y-z) \left\| \Gamma^{1/2} (b_z^r)^* \right\|_{\mathfrak{S}_2}^2 \right]^{1/2} \\
&\leq C \|V\|_{L^1}^{1/2} \|P\|_{L^2}^2 \|\varphi\|_{L^2} \langle \mathcal{V}_Q \rangle_\Gamma^{1/2} \langle \mathcal{N}_Q \rangle_\Gamma^{1/2} \leq C a^2 (k_F^\kappa)^3 \langle \mathcal{V}_Q \rangle_\Gamma^{1/2} \langle \mathcal{N}_Q \rangle_\Gamma^{1/2}. \quad (7.5.25)
\end{aligned}$$

7.5.6.4 Sextic term with four b's and two c's

This term is of the form

$$\begin{aligned}
\mathcal{A}_{6,b} &= \iiiint \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z \, \mathrm{d}z' \, V(x-y) \varphi(z-z') P(x-z) (b_z^r)^* (b_{z'}^r)^* c_{z'} c_y^* b_y b_x + \text{h.c.} \\
&= \iint \mathrm{d}x \, \mathrm{d}z \, P(x-z) \left[\int \mathrm{d}z' \, \varphi(z-z') (b_z^r)^* (b_{z'}^r)^* c_{z'} \right] \left[\int \mathrm{d}y \, V(x-y) c_y^* b_y b_x \right] + \text{h.c.}.
\end{aligned}$$

To bound it we note that as operators $0 \leq P \leq \mathbb{1}$. Thus by Cauchy–Schwarz we have for any $\lambda > 0$ the bound

$$\begin{aligned}
\pm \mathcal{A}_{6,b} &\leq \lambda \int \mathrm{d}z \left[\int \mathrm{d}z' \, \varphi(z-z') (b_z^r)^* (b_{z'}^r)^* c_{z'} \right] \left[\int \mathrm{d}x \, \varphi(z-x) c_x^* b_x^r b_z^r \right] \\
&\quad + \lambda^{-1} \int \mathrm{d}y \left[\int \mathrm{d}z \, V(z-y) b_z^* b_y^* c_y \right] \left[\int \mathrm{d}x \, V(x-y) c_y^* b_y b_x \right] \\
&=: \lambda \mathcal{A}_{6,b}^\varphi + \lambda^{-1} \mathcal{A}_{6,b}^V.
\end{aligned}$$

Note that $\mathcal{A}_{6,b}^\varphi = \mathcal{A}_6^\varphi$ from the bound of $\mathcal{Q}_{V\varphi}$, see (7.5.19). In particular,

$$\langle \mathcal{A}_6^\varphi \rangle_\Gamma \leq C (a k_F^\kappa)^3 \langle \mathcal{N}_Q \rangle_\Gamma .$$

With Cauchy–Schwarz we bound $\mathcal{A}_{6,b}^V$ as

$$\begin{aligned}
\left\langle \mathcal{A}_{6,b}^V \right\rangle_\Gamma &\leq C (k_F^\kappa)^3 \iiint \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z \, V(z-y) V(x-y) \left\| \Gamma^{1/2} b_z^* b_y^* \right\|_{\mathfrak{S}_2} \left\| b_y b_x \Gamma^{1/2} \right\|_{\mathfrak{S}_2} \\
&\leq C \|V\|_{L^1} (k_F^\kappa)^3 \langle \mathcal{V}_Q \rangle_\Gamma \leq C a (k_F^\kappa)^3 \langle \mathcal{V}_Q \rangle_\Gamma .
\end{aligned}$$

Choosing the optimal λ we find

$$\left| \langle \mathcal{A}_{6,b} \rangle_\Gamma \right| \leq C a^2 (k_F^\kappa)^3 \langle \mathcal{V}_Q \rangle_\Gamma^{1/2} \langle \mathcal{N}_Q \rangle_\Gamma^{1/2} . \tag{7.5.26}$$

Combining (7.5.21)–(7.5.26) we conclude the proof of (7.5.8). Hence the proof of Lemma 7.5.2 is complete.

7.6 Propagating a priori bounds — Bounding $\mathcal{E}_{\mathsf{scat}}, \mathcal{E}_{\mathsf{OD}}, \mathcal{E}_{V\varphi}$

To bound the error terms $\mathcal{E}_{\mathsf{scat}}, \mathcal{E}_{\mathsf{OD}}$ and $\mathcal{E}_{V\varphi}$ in (7.2.14)–(7.2.16), we use Lemma 7.5.2. Thus, we need bounds on

$$\langle \mathcal{N} \rangle_{\Gamma^\lambda}, \qquad \langle \mathcal{N}_Q \rangle_{\Gamma^\lambda}, \qquad \langle \mathcal{K}_Q \rangle_{\Gamma^\lambda}, \qquad \langle \mathcal{V}_Q \rangle_{\Gamma^\lambda}$$

for $0 \le \lambda \le 1$ (recall the definition of Γ^λ in (7.2.7)). For an approximate Gibbs state Γ the states Γ^λ are not necessarily approximate Gibbs states, so we cannot directly apply the bounds of (7.3.6) and Lemma 7.3.7. Instead, we obtain the desired bounds by propagating the corresponding bounds for the state Γ. This is similar to what is done in Chapter 4 and [FGHP21; Gia23a].

7.6.1 General propagation estimates

To start, we consider propagation estimates for a general state Γ. First, since $\mathcal{B}$ is particle number preserving we have

$$\langle \mathcal{N} \rangle_{\Gamma^\lambda} = \langle \mathcal{N} \rangle_{\Gamma}$$

for any state Γ. Next, we have

Lemma 7.6.1 (Propagation of $\mathcal{N}_Q$)**.** *Let Γ be any state and let Γ^λ be defined as in* (7.2.7)*. Then,*

$$\langle \mathcal{N}_Q \rangle_{\Gamma^\lambda} \le C \langle \mathcal{N}_Q \rangle_{\Gamma^{\lambda'}} + C L^3 (k_F^\kappa)^3 (a k_F^\kappa)^5$$

for any $0 \le \lambda, \lambda' \le 1$.

Proof. This is an application of Grönwall's lemma. We calculate

$$\frac{\mathsf{d}}{\mathsf{d}\lambda} \langle \mathcal{N}_Q \rangle_{\Gamma^\lambda} = - \langle [\mathcal{N}_Q, \mathcal{B}] \rangle_{\Gamma^\lambda} = 2 \operatorname{Re} \iint \mathsf{d}z \, \mathsf{d}z' \, \varphi(z - z') \left\langle (b_z^r)^* (b_{z'}^r)^* c_{z'} c_z \right\rangle_{\Gamma^\lambda}.$$

Using (7.5.10) to bound the z'-integral we find

$$\left| \frac{\mathsf{d}}{\mathsf{d}\lambda} \langle \mathcal{N}_Q \rangle_{\Gamma^\lambda} \right| \le C L^{3/2} (k_F^\kappa)^{3/2} (a k_F^\kappa)^{5/2} \langle \mathcal{N}_Q \rangle_{\Gamma^\lambda}^{1/2}.$$

By Grönwall's lemma we easily obtain the desired bound. □

Lemma 7.6.2 (Propagation of $\mathcal{K}_Q$)**.** *Let Γ be any state and let Γ^λ be defined as in* (7.2.7)*. Then,*

$$\langle \mathcal{K}_Q \rangle_{\Gamma^\lambda} \le C \langle \mathcal{K}_Q \rangle_{\Gamma^{\lambda'}} + C a^3 (k_F^\kappa)^8 \left[L^3 + a^3 \left| \log a k_F^\kappa \right|^2 \langle \mathcal{N} \rangle_\Gamma \right]$$

for any $0 \le \lambda, \lambda' \le 1$.

Proof. This is again an application of Grönwall's lemma. We calculate

$$\frac{\mathsf{d}}{\mathsf{d}\lambda} \langle \mathcal{K}_Q \rangle_{\Gamma^\lambda} = - \langle [\mathcal{K}_Q, \mathcal{B}] \rangle_{\Gamma^\lambda} = \operatorname{Re} \frac{1}{L^3} \sum_{k,k',p} (|k+p|^2 + |k'-p|^2) \hat{\varphi}(p) \left\langle (b_{k+p}^r)^* (b_{k'-p}^r)^* c_{k'} c_k \right\rangle_{\Gamma^\lambda}.$$

Noting the symmetry of interchanging k with k' and p with $-p$ we write this in configuration space as

$$\frac{\mathsf{d}}{\mathsf{d}\lambda} \langle \mathcal{K}_Q \rangle_{\Gamma^\lambda} = -2 \operatorname{Re} \iint \varphi(x - y) \left\langle (\Delta b_x^r)^* (b_y^r)^* c_y c_x \right\rangle_{\Gamma^\lambda} \mathsf{d}x \, \mathsf{d}y.$$

Taylor expanding c_x around $x = y$ and integrating by parts once in the x-integral we have (with the derivatives being with respect to x)

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle \mathcal{K}_Q\rangle_{\Gamma^\lambda} = 2\,\mathrm{Re}\iint \left\langle (\nabla^\nu b_x^r)^*(b_y^r)^* c_y \int_0^1 \mathrm{d}t\, \nabla^\nu \left[(x-y)^\mu \varphi(x-y)\nabla^\mu c_{y+t(x-y)}\right]\right\rangle_{\Gamma^\lambda} \mathrm{d}x\,\mathrm{d}y$$

We bound the y-integral using Lemma 7.5.3. Write first $(b_y^r)^* = a_y^* - (c_y^r)^*$. We bound the term with $(c_y^r)^*$ by, using Lemma 7.3.2,

$$\begin{aligned}&C(k_F^\kappa)^4 \iint \mathrm{d}x\,\mathrm{d}y \left\|(\Gamma^\lambda)^{1/2}(\nabla^\nu b_x^r)^*\right\|_{\mathfrak{S}_2} [(\varphi + |\cdot||\nabla\varphi|)(x-y)] \left\|c_y(\Gamma^\lambda)^{1/2}\right\|_{\mathfrak{S}_2}\\ &\quad\leq C(k_F^\kappa)^4 \left[\|\varphi\|_{L^1} + \||\cdot|\nabla\varphi\|_{L^1}\right] \langle\mathcal{K}_Q\rangle_{\Gamma^\lambda}^{1/2}\langle\mathcal{N}\rangle_{\Gamma^\lambda}^{1/2} \leq a^3(k_F^\kappa)^4 \left|\log ak_F^\kappa\right| \langle\mathcal{K}_Q\rangle_{\Gamma^\lambda}^{1/2}\langle\mathcal{N}\rangle_{\Gamma^\lambda}^{1/2}.\end{aligned}$$

Using Lemmas 7.3.2 and 7.5.3 the term with a_y^* is bounded by

$$\begin{aligned}&\int_0^1 \mathrm{d}t \int \mathrm{d}x \left\|(\Gamma^\lambda)^{1/2}(\nabla^\nu b_x^r)^*\right\|_{\mathfrak{S}_2}\\ &\qquad\times \left\| \int \mathrm{d}y \Big[\left(\delta^{\mu\nu}\varphi(x-y) + (x-y)^\mu\nabla^\nu\varphi(x-y)\right) a_y^* c_y \nabla^\mu c_{y+t(x-y)}\\ &\qquad\qquad + t(x-y)^\mu\varphi(x-y) a_y^* c_y \nabla^\mu\nabla^\nu c_{y+t(x-y)}\Big]\right\|\\ &\quad\leq CL^{3/2}(k_F^\kappa)^4\left(\|\varphi\|_{L^2} + \||\cdot|\nabla\varphi\|_{L^2} + k_F^\kappa\||\cdot|\varphi\|_{L^2}\right)\langle\mathcal{K}_Q\rangle_{\Gamma^\lambda}^{1/2}\\ &\quad\leq CL^{3/2}a^{3/2}(k_F^\kappa)^4\langle\mathcal{K}_Q\rangle_{\Gamma^\lambda}^{1/2}.\end{aligned}$$

Using that $\langle\mathcal{N}\rangle_{\Gamma^\lambda} = \langle\mathcal{N}\rangle_\Gamma$ we obtain the bound

$$\left|\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle\mathcal{K}_Q\rangle_{\Gamma^\lambda}\right| \leq Ca^{3/2}(k_F^\kappa)^4\left[L^{3/2} + a^{3/2}\left|\log ak_F^\kappa\right|\langle\mathcal{N}\rangle_\Gamma^{1/2}\right]\langle\mathcal{K}_Q\rangle_{\Gamma^\lambda}^{1/2}.$$

By Grönwall's lemma this proves the lemma. □

Lemma 7.6.3 (Propagation of $\mathcal{V}_Q$)**.** *Let Γ be any state and let Γ^λ be defined as in* (7.2.7)*. Then,*

$$\langle\mathcal{V}_Q\rangle_{\Gamma^\lambda} \leq C\langle\mathcal{V}_Q\rangle_{\Gamma^{\lambda'}} + Ca^3(k_F^\kappa)^5\langle\mathcal{N}\rangle_\Gamma$$

for any $0 \leq \lambda, \lambda' \leq 1$.

Proof. We again employ Grönwall's lemma. Recalling (7.4.6) we have

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle\mathcal{V}_Q\rangle_{\Gamma^\lambda} = -\langle[\mathcal{V}_Q,\mathcal{B}]\rangle_{\Gamma^\lambda} = \mathrm{Re}\iint \mathrm{d}x\,\mathrm{d}y\, V(x-y)\varphi(x-y)\left\langle b_x^* b_y^* c_y c_x\right\rangle_{\Gamma^\lambda} - \left\langle \mathcal{Q}_{[\mathcal{V}_Q,\mathcal{B}]}\right\rangle_{\Gamma^\lambda}.$$

The second term is bounded in Lemma 7.5.2. Using that $\varphi \leq 1$ we bound the first term with the aid of Cauchy–Schwarz by

$$\begin{aligned}&\left[\iint V(x-y)\varphi(x-y)\left\langle b_x^* b_y^* b_y b_x\right\rangle_{\Gamma^\lambda}\right]^{1/2}\left[\iint V(x-y)\varphi(x-y)\left\langle c_x^* c_y^* c_y c_x\right\rangle_{\Gamma^\lambda}\right]^{1/2}\\ &\quad\leq \langle\mathcal{V}_Q\rangle_{\Gamma^\lambda}^{1/2}\langle\mathcal{V}_P\rangle_{\Gamma^\lambda}^{1/2}.\end{aligned}$$

Using Lemmas 7.3.5 and 7.5.2 and recalling that $\langle\mathcal{N}\rangle_{\Gamma^\lambda} = \langle\mathcal{N}\rangle_\Gamma$ we obtain the bound

$$\begin{aligned}\left|\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle\mathcal{V}_Q\rangle_{\Gamma^\lambda}\right| &\le Ca^3(k_F^\kappa)^4\left[\langle\mathcal{N}_Q\rangle_{\Gamma^\lambda}^{1/2} + (ak_F^\kappa)^{1/2}\langle\mathcal{N}\rangle_\Gamma^{1/2}\right]\langle\mathcal{V}_Q\rangle_{\Gamma^\lambda}^{1/2} \\ &\quad + Ca^{3/2}(k_F^\kappa)^{5/2}\langle\mathcal{N}\rangle_\Gamma^{1/2}\langle\mathcal{V}_Q\rangle_{\Gamma^\lambda}^{1/2} \\ &\le Ca^{3/2}(k_F^\kappa)^{5/2}\langle\mathcal{N}\rangle_\Gamma^{1/2}\langle\mathcal{V}_Q\rangle_{\Gamma^\lambda}^{1/2}.\end{aligned}$$

By Grönwall's lemma this yields the desired bound. □

7.6.2 Bounding $\mathcal{E}_{\mathsf{scat}}, \mathcal{E}_{\mathsf{OD}}, \mathcal{E}_{V\varphi}$

We now apply the propagation estimates above to approximate Gibbs states Γ.

Lemma 7.6.4. *Let Γ be an approximate Gibbs state. Then, (for any $0 \le \lambda \le 1$)*

$$\langle\mathcal{N}_Q\rangle_{\Gamma^\lambda} \le CL^3\zeta\kappa^{-1}a^3\rho_0^2 + L^3\mathfrak{e}_L, \tag{7.6.1}$$

$$\langle\mathcal{K}_Q\rangle_{\Gamma^\lambda} \le CL^3\zeta^{-4}\kappa^4a^3\rho_0^{8/3} + L^3\mathfrak{e}_L, \tag{7.6.2}$$

$$\langle\mathcal{V}_Q\rangle_{\Gamma^\lambda} \le CL^3\zeta^{-5/2}\kappa^{5/2}a^3\rho_0^{8/3} + L^3\mathfrak{e}_L. \tag{7.6.3}$$

Proof. Apply Lemmas 7.6.1, 7.6.2 and 7.6.3 for $\lambda' = 0$, use the bounds in (7.3.6) and Lemma 7.3.7 and recall the bound in (7.3.3) for k_F^κ. The statement of the lemma follows. □

The bounds of Lemma 7.6.4 can be used to prove Propositions 7.2.15, 7.2.16 and 7.2.17.

Proof of Proposition 7.2.15. Recall the definition of $\mathcal{E}_{\mathsf{scat}}$ in (7.2.14) and the formula (7.5.2). Combining Lemma 7.5.2 and the bounds in (7.3.3), (7.6.1), (7.6.2) and (7.6.3) we have for any $0 < \delta \ll 1$ (using that $\mathcal{N}_{Q^>}$ satisfies the same bounds as $\mathcal{N}_Q$ only with κ replaced by $\delta^{-1}\kappa$, recall Remark 7.5.1)

$$\begin{aligned}\left|\left\langle\mathcal{H}_{0;\mathcal{B}}^{\div r}\right\rangle_{\Gamma^\lambda}\right| &\le CL^3a^3\rho_0^{8/3}\zeta^{-4}\kappa^4(a^3\rho_0)^{1/2}\left|\log a^3\rho_0\right| + L^3\mathfrak{e}_L, \\ \left|\langle\mathcal{Q}_{\mathsf{Taylor}}\rangle_{\Gamma^\lambda}\right| + |\langle\mathcal{Q}_{\mathsf{scat}}\rangle_{\Gamma^\lambda}| &\le CL^3a^3\rho_0^{8/3}\left[\zeta^{-2}\kappa^2\delta^{-3/4}(a^3\rho_0)^{1/2}\left|\log a^3\rho_0\right| + \zeta^{-2}\kappa^2\delta^{1/2}\right] + L^3\mathfrak{e}_L, \\ \left|\left\langle\mathcal{Q}_{[\mathcal{V}_Q,\mathcal{B}]}\right\rangle_{\Gamma^\lambda}\right| &\le CL^3a^3\rho_0^{8/3}\left[\zeta^{-11/4}\kappa^{11/4}a^3\rho_0 + \zeta^{-4}\kappa^4(a^3\rho_0)^{2/3}\right] + L^3\mathfrak{e}_L.\end{aligned}$$

Choosing the optimal $\delta = (a^3\rho_0)^{2/5}\left|\log a^3\rho_0\right|^{4/5}$ we conclude the desired statement for $\alpha > 0$ small enough. (Recall that $\kappa = \zeta(a^3\rho_0)^{-\alpha}$ as per (7.2.3).) □

Proof of Proposition 7.2.16. Recall the definition of $\mathcal{E}_{\mathsf{OD}}$ in (7.2.15). Combining Lemma 7.5.2 and the bounds in (7.3.3), (7.6.1) and (7.6.3) we have

$$|\langle\mathcal{Q}_{\mathsf{OD}}\rangle_{\Gamma^\lambda}| \le CL^3a^3\rho_0^{8/3}\left[\zeta^{-13/4}\kappa^{13/4}(a^3\rho_0)^{1/2} + \zeta^{-4}\kappa^4(a^3\rho_0)^{2/3}\right] + L^3\mathfrak{e}_L.$$

We conclude the desired bound by taking $\alpha > 0$ small enough. □

Proof of Proposition 7.2.17. Recall the definition of $\mathcal{E}_{V\varphi}$ in (7.2.16). Combining Lemma 7.5.2 and the bounds in (7.3.3) and (7.6.1) we have

$$\left|\langle\mathcal{Q}_{V\varphi}\rangle_\Gamma\right| \le CL^3a^3\rho_0^{8/3}\zeta^{-4}\kappa^4(a^3\rho_0)^{2/3} + L^3\mathfrak{e}_L\,,$$

from which the statement follows. □

7.7 Validity of perturbation theory — Bounding $\mathcal{E}_{\mathrm{pt}}$

In this section we give the proof of Proposition 7.2.13. In broad strokes this amounts to showing the validity of first order perturbation theory in an appropriate regime. The main idea is to use the a priori bound (7.3.4) on the relative entropy to show that the expectation value of $\mathcal{W}_P = \mathrm{d}\Gamma(PPWPP)$ in an approximate Gibbs state Γ is to leading order the same as in the non-interacting state Γ_0, which in turn can be replaced by the $\langle \mathcal{W} \rangle_{\Gamma_0}$ (i.e., the projection P can be dropped).

The main result of this section is the following proposition. A key ingredient in its proof is the method of [Sei06a] for obtaining correlation estimates at positive temperature (see also [Sei08], and [GS94] for earlier work at zero temperature.)

Recall the definition of $\mathcal{E}_{\mathrm{pt}}(\Gamma)$ in (7.2.17).

Proposition 7.7.1. *For any state Γ, any $a \leq R < L$, any $\rho_0^{-1/3} \lesssim d \leq L$, any $0 < q_F < k_F^\kappa$ with $\beta(k_F^\kappa - q_F)^2 \gtrsim 1$ any $n \in \mathbb{N}$ and any $z \gtrsim 1$*

$$\begin{aligned}
\mathcal{E}_{\mathrm{pt}}(\Gamma) \gtrsim & -L^3 a^3 R^2 \rho_0^{2+4/3} - (k_F^\kappa)^7 a^3 R^2 \langle \mathcal{N} \rangle_\Gamma - L^3 a^3 \rho_0^{8/3} R d^{-1} \\
& - L^{9/4} \left[a^6 R^{-5} \rho_0^{2+2/3} d^{-3} + a^6 \rho_0^{3+4/3} (d^{-3} + \rho_0) \right]^{1/2} \Big[d^3 S(\Gamma, \Gamma_0) + L^3 \beta^4 (k_F^\kappa)^7 d^{-1} \\
& \quad + L^3 d^3 \beta^{-1} (k_F^\kappa - q_F) e^{-\kappa + \beta(2k_F^\kappa q_F - q_F^2)} + C_n d^3 (d q_F)^{-2n} \log Z_0 \Big]^{1/4} - L^3 \mathfrak{e}_L.
\end{aligned} \tag{7.7.1}$$

The constant $C_n > 0$ depends only on n.

Remark 7.7.2 (Interpretation of parameters)**.** In Proposition 7.7.1 appear many free parameters. They may be understood heuristically as follows: The length R is the range of a new interaction. To prove Proposition 7.7.1 we use in particular an argument that can be viewed as an analogue of the "Dyson lemma" (see Section 7.7.1) where the interaction W gets replaced by a weaker and longer ranged interaction U of range R. The length d is a localization length. To prove Proposition 7.7.1 we split the box Λ into many smaller regions of size of order d and separated by a distance of order d, see Section 7.7.2. The momentum cut-off q_F and the integer n are technical parameters introduced to estimate non-leading error terms.

Remark 7.7.3 (Non-uniformity in the temperature)**.** We do now know how to prove the result of Theorem 7.1.3 uniformly in temperatures $T \lesssim T_F$. This is due to the temperature dependence of the error bounds in Proposition 7.7.1. We illustrate this here.

As in Chapter 6 we can, for sufficiently small temperatures, i.e. large ζ, simply compare to the zero-temperature result in Chapter 4. For $\zeta \gg (a^3\rho_0)^{-1/2}$ the contribution of the main term $\psi_0(\beta, \mu)$ resulting from the temperature is negligible compared to the leading interaction term of order $a^3 \overline{\rho}_0^{8/3}$; see Section 6.1.2 for the details. Thus, to get a bound uniformly in temperatures $T \lesssim T_F$ it suffices to consider $\zeta \lesssim (a^3\rho_0)^{-1/2}$.

Further, one might consider changing the choice of κ in (7.2.3) to $\kappa = \zeta^{1-\varepsilon}(a^3\rho)^{-\alpha}$ for some $\varepsilon \geq 0$. As in (7.3.3) we then have $k_F^\kappa \sim (1 + \zeta^{-1/2}\kappa^{1/2})\rho_0^{1/3}$.

Using the bounds from (7.3.3) and (7.3.4) and this new choice of κ, two of the error terms in Proposition 7.7.1 are bounded as

$$\begin{aligned}
& L^{9/4} a^3 \rho_0^{8/3} \left[d^3 S(\Gamma, \Gamma_0) + L^3 \beta^4 (k_F^\kappa)^7 d^{-1} \right]^{1/4} \\
& \quad \leq C L^3 a^3 \rho_0^{8/3} \left[\zeta^{1/4} (a^3\rho_0)^{1/4} (d^3\rho_0)^{1/4} + \zeta \left[1 + \zeta^{-7/8}\kappa^{7/8} \right] (d^3\rho_0)^{-1/12} \right].
\end{aligned}$$

For $\zeta \sim (a^3\rho_0)^{-1/2}$ these terms are of order

$$L^3 a^3 \rho_0^{8/3} \left[(a^3\rho_0)^{1/8}(d^3\rho_0)^{1/4} + (a^3\rho_0)^{-1/2}\left[1+(a^3\rho_0)^{7\varepsilon/16-7\alpha/8}\right](d^3\rho_0)^{-1/12}\right].$$

It is impossible to choose d such that both of these terms are negligible compared to the leading term of order $L^3a^3\rho_0^{8/3}$.

With Proposition 7.7.1 at hand we can give the

Proof of Proposition 7.2.13. We shall apply Proposition 7.7.1 with $q_F = \zeta^{-1/2}\rho_0^{1/3}$. Recalling (7.3.3) then

$$\beta k_F^\kappa q_F \sim \kappa^{1/2} \ll \kappa, \qquad \beta q_F^2 \sim 1 \ll \kappa, \qquad \beta(k_F^\kappa - q_F)^2 \sim \kappa \gg 1.$$

We shall choose $d \gg \zeta^{1/2}\rho_0^{-1/3}$. Then, by taking n large enough, we can ensure that the last two summands in $[\ldots]^{1/4}$ in (7.7.1) are negligible.

We can use (7.2.8) to bound $\langle \mathcal{N}\rangle_\Gamma$, and (7.3.4) to bound $S(\Gamma,\Gamma_0)$. Thus, using (7.3.3), the leading terms in the lower bound on $\mathcal{E}_{\text{pt}}(\Gamma)$ are

$$\begin{aligned} &- L^3a^3\rho_0^{8/3}\left[\kappa^{7/2}\zeta^{-7/2}R^2\rho_0^{2/3} + Rd^{-1}\right] \\ &- L^3\left[a^3R^{-5/2}\rho_0^{4/3}d^{-3/2} + a^3\rho_0^{8/3}\right]\left[\zeta d^3a^3\rho_0^2 + \zeta^{1/2}\kappa^{7/2}\rho_0^{-1/3}d^{-1}\right]^{1/4}\end{aligned}$$

We shall restrict our attention to a compact set of z's, i.e., we can assume that $\zeta \sim 1$ and hence $\kappa \sim (a^3\rho_0)^{-\alpha}$. We shall choose

$$d = \rho_0^{-1/3}(a^3\rho_0)^{-s}, \qquad R = \rho_0^{-1/3}(a^3\rho_0)^t$$

for some $s,t>0$ to be determined. Then, $\mathcal{E}_{\text{pt}}(\Gamma) \geq -C(z)L^3a^3\rho_0^{8/3}\left[(a^3\rho_0)^\sigma + \mathfrak{e}_L\right]$ with $C(z)$ bounded uniformly on compact sets of z's and

$$\sigma = \frac{1}{8}\min\Big\{16t-28\alpha,\, 2+6s-20t,\, 2-6s,\, 14s-20t-7\alpha,\, 2s-7\alpha\Big\}.$$

The choice

$$s = \frac{1}{4}+\frac{7}{8}\alpha, \qquad t = \frac{1}{32}+\frac{91}{64}\alpha$$

yields $\sigma = 1/16 - 21\alpha/32$, and hence the desired bound. □

The rest of this section is devoted to the proof of Proposition 7.7.1. It is divided into three parts. We first introduce some convenient notation.

Notation 7.7.4. We write

$$\mathrm{Tr} = \mathrm{Tr}_{\mathcal{F}(\mathfrak{h})}, \qquad \mathrm{tr} = \mathrm{Tr}_{\mathfrak{h}}.$$

That is, tr for the trace of the one-particle space $\mathfrak{h} = L^2(\Lambda;\mathbb{C})$ and Tr for the trace over the Fock space $\mathcal{F}(\mathfrak{h})$.

Definition 7.7.5 (See also [LNR21, Definition 5.5] and [HLS09, Appendix A])**.** For any projection X on $\mathfrak{h}$ and state Γ we define the operator Γ_X as the state Γ restricted to the space $\mathcal{F}(X\mathfrak{h})$ as follows: Any operator $\mathcal{A}$ on $\mathcal{F}(X\mathfrak{h})$ may naturally be extended as $\mathcal{A}\otimes \mathbb{1}_{\mathcal{F}(X^\perp\mathfrak{h})}$ on $\mathcal{F}(X\mathfrak{h})\otimes\mathcal{F}(X^\perp\mathfrak{h}) \simeq \mathcal{F}(\mathfrak{h})$. With this extension and unitary equivalence hidden in the notation, the state Γ_X is defined by duality satisfying $\mathrm{Tr}\,\mathcal{A}\Gamma_X = \mathrm{Tr}\,\mathcal{A}\Gamma$ for all $\mathcal{A}$ on $\mathcal{F}(X\mathfrak{h})$.

7.7.1 Regularizing the interaction

As a first step we shall replace the effective interaction $W = V(1-\varphi)$ by a much weaker interaction U of longer range. This step is, at least in spirit, analogous to the "Dyson lemma" [Dys57, Lemma 1] (see also [LY98, Lemma 1]) applied first for dilute Bose gases. In our case, the presence of the projection P effectively smears out the particle coordinates on a length scale $(k_F^\kappa)^{-1} \gg a$, allowing us to replace $W = V(1-\varphi)$ by U as long as the range of U is $\ll (k_F^\kappa)^{-1}$ and $\int |x|^2 U = \int |x|^2 W = 24\pi a^3$. For any interaction U we define

$$\mathcal{U} = \mathrm{d}\Gamma(U), \qquad \mathcal{U}_P = \mathrm{d}\Gamma(PPUPP).$$

More concretely we show

Lemma 7.7.6. *Let U be a radial function with $\int |x|^2 U = \int |x|^2 W$. Then for any state Γ,*

$$\langle \mathcal{W}_P \rangle_\Gamma = \langle \mathcal{U}_P \rangle_\Gamma + O\left((k_F^\kappa)^7 \left\| |\cdot|^4 (U-W) \right\|_{L^1} \langle \mathcal{N} \rangle_\Gamma \right).$$

Proof. We start by writing

$$\mathcal{W}_P - \mathcal{U}_P = \mathrm{d}\Gamma(PP(W-U)PP) = \frac{1}{2} \iint (W-U)(x-y) c_x^* c_y^* c_y c_x \, \mathrm{d}x \, \mathrm{d}y.$$

We Taylor expand c_y and c_y^* around $y = x$ as in (7.3.9). Changing variables to $z = y - x$ we have

$$\mathcal{W}_P - \mathcal{U}_P = \frac{1}{2} \iint (W-U)(z) z^\mu z^\nu \int_0^1 \mathrm{d}t \int_0^1 \mathrm{d}s \, c_x^* \nabla^\mu c_{x+tz}^* \nabla^\nu c_{x+sz} c_x \, \mathrm{d}x \, \mathrm{d}z$$

Evaluating in the state Γ we define the function(s) $\phi_x^{\mu\nu}(z) = \left\langle c_x^* \nabla^\mu c_{x+tz}^* \nabla^\nu c_{x+sz} c_x \right\rangle_\Gamma$. We shall Taylor expand $\phi_x^{\mu\nu}$ around $z = 0$. Noting that $\|\nabla^n c\| \leq C (k_F^\kappa)^{3/2+n}$ we can bound

$$|\nabla^2 \phi_x^{\mu\nu}(z)| \leq C \left\| \Gamma^{1/2} c_x^* \right\|_{\mathfrak{S}_2} (k_F^\kappa)^7 \left\| c_x \Gamma^{1/2} \right\|_{\mathfrak{S}_2} = C (k_F^\kappa)^7 \langle c_x^* c_x \rangle_\Gamma .$$

Consequently

$$\left| \phi_x^{\mu\nu}(z) - \phi_x^{\mu\nu}(0) - z^\lambda \nabla^\lambda \phi_x^{\mu\nu}(0) \right| \lesssim |z|^2 (k_F^\kappa)^7 \langle c_x^* c_x \rangle_\Gamma .$$

Noting further that $\int z^\mu z^\nu U = \int z^\mu z^\nu W$ and $\int z^\mu z^\nu z^\lambda U = 0 = \int z^\mu z^\nu z^\lambda W$ we find

$$|\langle \mathcal{W}_P - \mathcal{U}_P \rangle_\Gamma| \leq C (k_F^\kappa)^7 \int |z|^4 |U - W| \, \mathrm{d}z \int \langle c_x^* c_x \rangle_\Gamma \, \mathrm{d}x.$$

Since $\int c_x^* c_x \, \mathrm{d}x \leq \mathcal{N}$ this proves the lemma. $\square$

7.7.2 Localizing the relative entropy

Because of Lemma 7.7.6, our task is now to evaluate $\langle \mathcal{U}_P \rangle_\Gamma$ for an appropriate choice of U in an approximate Gibbs state Γ. Our goal is to show that we can replace Γ by Γ_0 to leading order, which amounts to showing the validity of first order perturbation theory. To be able to utilize the a priori bound (7.3.4) on the relative entropy $S(\Gamma, \Gamma_0)$, we shall localize the latter in a suitable way, following the method in [Sei06a, Proof of Theorem 3.1]. Due to the presence of the projection P, the case considered here is slightly different from the one considered in [Sei06a], hence we cannot just quote the result but give the complete argument here.

A first step is localizing the relative entropy $S(\Gamma_P, \Gamma_d)$ for a state Γ_d closely related to the free Gibbs state Γ_0, but with a cut-off the removes all correlations between well separated regions. The state Γ_d is defined as follows.

Let $\eta : \mathbb{R}^3 \to \mathbb{R}$ be a smooth function with

- $\eta(0) = 1$ and $\eta(x) = 0$ for $|x| \geq 1$,
- $\hat{\eta}(p) = \int \mathrm{d}x\, \eta(x) e^{-ipx} \geq 0$ for all $p \in \mathbb{R}^3$.

(To construct such a function η simply take any smooth compactly supported function and convolve it with itself.) Define then for $0 < d \leq L/2$ the function $\eta_d(x) = \eta(x/d)$ (more precisely its periodization $\eta_d(x) = \sum_{n\in\mathbb{Z}^3} \eta\left(\frac{x+nL}{d}\right)$). Let Γ_d be the quasi-free state on $\mathcal{F}(\mathfrak{h})$ with one-particle density matrix

$$\gamma_d(x;y) = \gamma_0(x;y)\eta_d(x-y),$$

with γ_0 the one-particle density matrix of the free Gibbs state. Define then $\overline{d} \geq d$ by $L/2\overline{d} = \lfloor L/2d \rfloor$ (here $\lfloor\cdot\rfloor$ denotes the integer part) and define for $r \leq d/2$

$$X_r(x) = \sum_{\xi \in 2\overline{d}\mathbb{Z}^3 \cap [0,L)^3} \chi_{r,\xi}(x).$$

Noting that η_d vanishes outside a ball of radius $d \leq 2\overline{d} - 2r$ we have

$$X_r \gamma_d X_r = \sum_{\xi \in 2\overline{d}\mathbb{Z}^3 \cap [0,L)^3} \chi_{r,\xi}\gamma_d\chi_{r,\xi}.$$

Thus,

$$(\Gamma_d)_{X_r} \simeq \bigotimes_{\xi \in 2\overline{d}\mathbb{Z}^3 \cap [0,L)^3} (\Gamma_d)_{\chi_{r,\xi}}$$

Next, we note that the relative entropy is monotone decreasing under restriction [OP04, Theorem 1.5] and further that it is superadditive for its right argument being a product state (which follows easily from the subadditivity of the von Neumann entropy). Concretely this means that

$$S(\Gamma_P, \Gamma_d) \geq S\left((\Gamma_P)_{X_r}, (\Gamma_d)_{X_r}\right) \geq \sum_{\xi \in 2\overline{d}\mathbb{Z}^3 \cap [0,L)^3} S\left((\Gamma_P)_{\chi_{r,\xi}}, (\Gamma_d)_{\chi_{r,\xi}}\right).$$

Replacing X_r by $X_r(\cdot + a)$ for $a \in [0, 2\overline{d}]^3$ and averaging over a we find for any $r \leq d/2$ (this is [Sei06a, (5.10)])

$$S(\Gamma_P, \Gamma_d) \geq \frac{1}{(2\overline{d})^3} \int_\Lambda \mathrm{d}\xi\, S\left((\Gamma_P)_{\chi_{r,\xi}}, (\Gamma_d)_{\chi_{r,\xi}}\right). \tag{7.7.2}$$

The next step is relating the relative entropy $S(\Gamma_P, \Gamma_d)$ to the relative entropy $S(\Gamma, \Gamma_0)$ for which we have a priori bounds. In the absence of the projection P, this is done in [Sei06a, Section 5.2]. We claim that (compare to [Sei06a, Eq. (5.31)])

Lemma 7.7.7. *Let Γ be any state and let $0 < q_F < k_F^\kappa$ with $\beta(k_F^\kappa - q_F)^2 \gtrsim 1$. Then, for any $n \in \mathbb{N}$*

$$\begin{aligned} S(\Gamma_P, \Gamma_d) \lesssim{} & S(\Gamma, \Gamma_0) + L^3\beta^4(k_F^\kappa)^7 d^{-4} \\ & + L^3\beta^{-1}(k_F^\kappa - q_F)e^{-\kappa+\beta(2k_F^\kappa q_F - q_F^2)} + C_n(dq_F)^{-2n}\log Z_0 + L^3\mathfrak{e}_L. \end{aligned}$$

The constant C_n depends only on n.

Combining Lemma 7.7.7 and Equation (7.7.2) we thus find that

$$\begin{aligned}\int_\Lambda \mathrm{d}\xi\, S\left((\Gamma_P)_{\chi_{r,\xi}}, (\Gamma_d)_{\chi_{r,\xi}}\right) &\lesssim d^3 S(\Gamma,\Gamma_0) + L^3\beta^4 (k_F^\kappa)^7 d^{-1} + C_n d^3 (dq_F)^{-2n}\log Z_0 \\ &\quad + L^3 d^3 \beta^{-1}(k_F^\kappa - q_F) e^{-\kappa+\beta(2k_F^\kappa q_F - q_F^2)} + L^3 \mathfrak{e}_L.\end{aligned} \tag{7.7.3}$$

for any $0 < r \le d/2 \le L/4$.

Proof of Lemma 7.7.7. Following [Sei06a, Section 5.2], we first make the following observation. Denote by Γ_ω the quasi-free state with one-particle-density matrix ω. Then for any state Γ (whose one-particle-density matrix we denote by γ) we have that

$$S(\Gamma,\Gamma_\omega) = \operatorname{Tr}\Gamma\log\Gamma - \operatorname{tr}\gamma\log\omega - \operatorname{tr}(1-\gamma)\log(1-\omega) \tag{7.7.4}$$

is convex in ω. We may write γ_d as a convex combination

$$\gamma_d = \frac{1}{|\Lambda|}\sum_{q\in\frac{2\pi}{L}\mathbb{Z}^3} \hat\eta_d(q)\gamma_q, \qquad \hat\gamma_q(p) = \frac{1}{2}\left(\hat\gamma_0(p+q) + \hat\gamma_0(p-q)\right).$$

(Note that for $q=0$ we indeed have $\gamma_q = \gamma_0$.) Recalling that $\hat\eta_d \ge 0$ and $\frac{1}{|\Lambda|}\sum\hat\eta_d = \eta(0) = 1$ by construction, we thus have

$$S(\Gamma_P,\Gamma_d) \le \frac{1}{|\Lambda|}\sum_{q\in\frac{2\pi}{L}\mathbb{Z}^3}\hat\eta_d(q) S(\Gamma_P,\Gamma_{\gamma_q}). \tag{7.7.5}$$

We claim that for any $t>0$ (compare to [Sei06a, (5.14)])

$$\begin{aligned} S(\Gamma_P,\Gamma_{\gamma_q}) &\le (1+t^{-1})S(\Gamma_P,(\Gamma_0)_P) - \operatorname{tr} Q\log(1-\gamma_q) \\ &\quad + \operatorname{tr} P(h_q - h_0)\left(\frac{1}{1+e^{(1+t)h_0 - th_q}} - \frac{1}{1+e^{h_q}}\right)\end{aligned} \tag{7.7.6}$$

where $h_q = \log\frac{1-\gamma_q}{\gamma_q}$, i.e., $\gamma_q = (1+e^{h_q})^{-1}$. We will later choose $t=1$ but for now it is convenient to leave it as a variable.

To prove Equation (7.7.6) we first note that $(\Gamma_0)_P$ is a quasi-free state with one-particle density matrix $P\gamma_0$. Using the formula in Equation (7.7.4) we have

$$\begin{aligned}&(1+t^{-1})S(\Gamma_P,(\Gamma_0)_P) - S(\Gamma_P,\Gamma_{\gamma_q}) \\ &\ = t^{-1}\operatorname{Tr}\Gamma_P\log\Gamma_P + \operatorname{tr} Q\log(1-\gamma_q) \\ &\quad\ + \operatorname{tr} P\left[\gamma\log\gamma_q + (1-\gamma)\log(1-\gamma_q) - (1+t^{-1})\gamma\log\gamma_0 - (1+t^{-1})(1-\gamma)\log(1-\gamma_0)\right] \\ &\ = t^{-1}\left[\operatorname{Tr}\Gamma_P\log\Gamma_P + \operatorname{tr} P\gamma((1+t)h_0 - th_q)\right] + \operatorname{tr} Q\log(1-\gamma_q) \\ &\quad\ - \operatorname{tr} P\log(1+e^{-h_q}) + (1+t^{-1})\operatorname{tr} P\log(1+e^{-h_0}).\end{aligned}$$

By the Gibbs variational principle applied to the one-body Hamiltonian $P((1+t)h_0 - th_q)$ and Taylor expanding we have

$$\begin{aligned}&\operatorname{Tr}\Gamma_P\log\Gamma_P + \operatorname{tr} P\gamma((1+t)h_0 - th_q) \\ &\quad\ge -\operatorname{tr} P\log\left(1+e^{-(1+t)h_0 + th_q}\right) \\ &\quad= -\operatorname{tr} P\log\left(1+e^{-h_0}\right) + t\int_0^1 \mathrm{d}s\ \operatorname{tr} P(h_0 - h_q)\frac{1}{1+e^{(1+st)h_0 - sth_q}}\end{aligned}$$

Similarly we have

$$-\operatorname{tr} P \log(1+e^{-h_q}) = -\operatorname{tr} P \log(1+e^{-h_0}) + \int_0^1 \mathrm{d}s \ \operatorname{tr} P(h_q - h_0)\frac{1}{1+e^{(1-s)h_0+sh_q}}$$

Combining these equations and noting the the integrands in the s-integrals are monotone in s we conclude the proof of Equation (7.7.6).

To bound the first term on the right-hand-side of (7.7.6) we note that $S(\Gamma_P, (\Gamma_0)_P) \le S(\Gamma, \Gamma_0)$, since the relative entropy is decreasing in restrictions [OP04, Theorem 1.5]. Next, we bound the last term on the right-hand-side of (7.7.6) similarly to [Sei06a, (5.27)]. Taylor expanding to first order in t we find that

$$\left|\operatorname{tr} P(h_q - h_0)\left(\frac{1}{1+e^{(1+t)h_0 - th_q}} - \frac{1}{1+e^{h_q}}\right)\right| \le (1+t)\operatorname{tr} P(h_q-h_0)^2.$$

To estimate the latter trace we recall the bound [Sei06a, Lemma 5.1]

$$|h_q(p) - h_0(p)| \le C\beta q^2(\zeta + \beta p^2).$$

Then clearly (recalling $\zeta \sim \beta\rho_0^{2/3}$ from (7.3.3))

$$\operatorname{tr} P(h_q - h_0)^2 \le C \sum_{|p|\le k_F^\kappa} \beta^2 q^4 (\zeta+\beta p^2)^2 \le CL^3\beta^4 (k_F^\kappa)^7 q^4.$$

To bound the second term on the right-hand-side of (7.7.6) we can use convexity of $\gamma \mapsto -\log(1-\gamma)$ and the symmetry $p \to -p$ to conclude that

$$-\operatorname{tr} Q \log(1-\gamma_q) \le \sum_{|p|>k_F^\kappa} \log\left(1+e^{-\beta((p+q)^2-\mu)}\right).$$

We treat this sum separately for large and small q's. Let $0 < q_F < k_F^\kappa$ and assume that $|q| < q_F$. In this case

$$\begin{aligned} -\operatorname{tr} Q \log(1-\gamma_q) &\le \sum_{|p|>k_F^\kappa - q_F} \log\left(1+e^{-\beta(p^2-\mu)}\right) \\ &\le CL^3\beta^{-3/2}[\beta^{1/2}(k_F^\kappa - q_F)+1]e^{-\beta((k_F^\kappa-q_F)^2-\mu)} + L^3\mathfrak{e}_L, \end{aligned} \tag{7.7.7}$$

To prove this we view the sum as a Riemann sum for the corresponding integral and compute the integral explicitly. We give the details in Section 7.A. For $|q| \ge q_F$ we shall simply bound

$$-\operatorname{tr} Q\log(1-\gamma_q) \le \sum_{p\in\frac{2\pi}{L}\mathbb{Z}^3} \log\left(1+e^{-\beta(p^2-\mu)}\right) = \log Z_0,$$

where Z_0 is the partition function of the free gas. Combining these bounds and choosing $t=1$ we conclude that (for $\beta(k_F^\kappa - q_F)^2 \gtrsim 1$)

$$\begin{aligned} S(\Gamma_P, \Gamma_{\gamma_q}) &\lesssim S(\Gamma,\Gamma_0) + L^3\beta^4(k_F^\kappa)^7 q^4 \\ &\quad + L^3\beta^{-1}(k_F^\kappa - q_F)e^{-\beta((k_F^\kappa-q_F)^2-\mu)}\chi_{(|q|<q_F)} + \log Z_0 \chi_{(|q|\ge q_F)} + L^3\mathfrak{e}_L. \end{aligned}$$

We insert this bound in (7.7.5). To evaluate the q-summation we note that

$$\frac{1}{|\Lambda|}\sum_{q\in\frac{2\pi}{L}\mathbb{Z}^3} \hat{\eta}_d(q) q^{2n} = (-\Delta)^n \eta(0) d^{-2n} = C_n d^{-2n}$$

for any integer $n \geq 0$. (Recall also that $\eta(0) = 1$.) In particular for any $n \in \mathbb{N}$

$$\frac{1}{L^3}\sum_q \hat{\eta}_d(q) \log Z_0 \chi_{(|q|>q_F)} \leq q_F^{-2n} \log Z_0 \frac{1}{L^3} \sum_{|q|>q_F} \hat{\eta}_d(q) q^{2n} \leq C_n (q_F d)^{-2n} \log Z_0.$$

Noting that $-\beta((k_F^\kappa - q_F)^2 - \mu) = -\kappa + \beta(2k_F^\kappa q_F - q_F^2)$ we conclude the proof of the lemma. $\square$

7.7.3 Localizing the interaction

The bound (7.7.3) allows us to conclude that the states Γ_P and Γ_d are suitably close when viewed on a ball of some radius r. As long as r is large compared to R (the range of U) this will thus allow us to obtain the desired estimate on the expectation value $\langle \mathcal{U}_P \rangle_\Gamma$, and to bound the difference $\langle \mathcal{U}_P\rangle_\Gamma - \langle \mathcal{U}\rangle_{\Gamma_0}$ by the localized relative entropy.

To do this precisely, we need to also localize the interaction into balls. The subsequent analysis follows closely the corresponding analysis in [Sei06a, Section 5.3]. We recall that, for a state Γ, the state Γ_X denotes its localization using the projection X, see Definition 7.7.5. The state Γ_0 is the free Gibbs state and the state Γ_d is defined in Section 7.7.2. We shall prove

Lemma 7.7.8. *Let Γ be any state and let $U \geq 0$ be compactly supported with range R. Then, for any $0 < r \leq d/2 \leq L/4$ with $d \gtrsim \rho_0^{-1/3}$ and $1/z$ bounded, we have*

$$\begin{aligned}\langle \mathcal{U}_P\rangle_\Gamma \geq \langle \mathcal{U}\rangle_{\Gamma_0} &- CL^3 \left\| |\cdot|^2 U\right\|_{L^1} \rho_0^{8/3} \frac{R}{r} \\ &- CL^{9/4}\left[\||\cdot| U\|_{L^2}^2 \rho_0^{2+2/3} + C\left\| |\cdot|^2 U\right\|_{L^1}^2 \rho_0^{3+4/3}(1+r^3\rho_0)\right]^{1/2} \\ &\times r^{-3/2}\left[\int_\Lambda \mathrm{d}\xi\, S((\Gamma_P)_{\chi_{r,\xi}}, (\Gamma_d)_{\chi_{r,\xi}})\right]^{1/4} - L^3 \mathfrak{e}_L.\end{aligned}$$

Proof. Write for any $r > 0$

$$\begin{aligned}U(x-y) &= \frac{3}{4\pi r^3}\int_\Lambda \mathrm{d}\xi\, U(x-y)\chi_{r,\xi}(y) \\ &= \frac{3}{4\pi r^3}\int_\Lambda \mathrm{d}\xi\, \chi_{r,\xi}(x) U(x-y)\chi_{r,\xi}(y) + \frac{3}{4\pi r^3}\int_\Lambda \mathrm{d}\xi\, (1-\chi_{r,\xi}(x))U(x-y)\chi_{r,\xi}(y)\end{aligned}$$

with $\chi_{r,\xi}$ the characteristic function of a ball of radius r centered at ξ. As a lower bound we may keep only the first term since $U \geq 0$. Define $U_{r,\xi}(x,y) = \chi_{r,\xi}(x)U(x-y)\chi_{r,\xi}(y)$ and $\mathcal{U}_{r,\xi} = \mathrm{d}\Gamma(U_{r,\xi})$. Then

$$\langle \mathcal{U}_P\rangle_\Gamma = \langle \mathcal{U}\rangle_{\Gamma_P} \geq \frac{3}{4\pi r^3}\int_\Lambda \mathrm{d}\xi\, \operatorname{Tr}\left[\mathcal{U}_{r,\xi}\Gamma_P\right] = \frac{3}{4\pi r^3}\int_\Lambda \mathrm{d}\xi\, \operatorname{Tr}\left[\mathcal{U}_{r,\xi}(\Gamma_P)_{\chi_{r,\xi}}\right]$$

since we may replace Γ_P by $(\Gamma_P)_{\chi_{r,\xi}}$ since $U_{r,\xi}$ is localized to this domain.

For any K we introduce

$$f_K(t) = \min\{t, K\} = t - [t-K]_+, \qquad [\cdot]_+ = \min\{\cdot, 0\}.$$

Then $t \geq f_K(t)$ for any t. Using this on $t = \mathcal{U}_{r,\xi}$ we thus have (with Γ_d as above)

$$\begin{aligned}
\langle \mathcal{U}_P \rangle_\Gamma &\geq \frac{3}{4\pi r^3} \int_\Lambda \mathsf{d}\xi \ \mathrm{Tr}\left[f_K\left(\mathcal{U}_{r,\xi}\right) (\Gamma_P)_{\chi_{r,\xi}} \right] \\
&= \frac{3}{4\pi r^3} \int_\Lambda \mathsf{d}\xi \ \mathrm{Tr}\left[f_K\left(\mathcal{U}_{r,\xi}\right) (\Gamma_d)_{\chi_{r,\xi}} \right] \\
&\quad + \frac{3}{4\pi r^3} \int_\Lambda \mathsf{d}\xi \ \mathrm{Tr}\left[f_K\left(\mathcal{U}_{r,\xi}\right) \left((\Gamma_P)_{\chi_{r,\xi}} - (\Gamma_d)_{\chi_{r,\xi}} \right) \right] \\
&=: \mathcal{I} + \mathcal{E}_{\mathsf{state}}
\end{aligned} \tag{7.7.8}$$

The first term $\mathcal{I}$ is the main term. To evaluate it, we use $f_K(t) = t - [t-K]_+$ and bound $[t-K]_+ \leq t^2/4K$. Thus

$$\mathrm{Tr}\left[f_K\left(\mathcal{U}_{r,\xi}\right) (\Gamma_d)_{\chi_{r,\xi}} \right] \geq \mathrm{Tr}\left[\mathcal{U}_{r,\xi} (\Gamma_d)_{\chi_{r,\xi}} \right] - \frac{1}{4K} \mathrm{Tr}\left[\left(\mathcal{U}_{r,\xi}\right)^2 (\Gamma_d)_{\chi_{r,\xi}} \right].$$

For the first term we note that $(\Gamma_d)_{\chi_{r,\xi}}$ is quasi-free and has two-particle density

$$\begin{aligned}
\rho_d^{(2)}(x,y)\chi_{r,\xi}(x)\chi_{r,\xi}(y) &= (\rho_0^2 - |\gamma_d(x-y)|^2)\chi_{r,\xi}(x)\chi_{r,\xi}(y) \\
&\geq \rho_0^{(2)}(x,y)\chi_{r,\xi}(x)\chi_{r,\xi}(y)
\end{aligned}$$

since $|\gamma_d| \leq |\gamma_0|$ by construction. In particular,

$$\begin{aligned}
&\mathrm{Tr}\left[\mathcal{U}_{r,\xi} (\Gamma_d)_{\chi_{r,\xi}} \right] \\
&\geq \frac{1}{2} \iint_{(B_{r,\xi})^2} U(x-y)\rho_0^{(2)}(x,y) \,\mathsf{d}x\,\mathsf{d}y \\
&= \frac{1}{2} \iint_{\Lambda \times B_{r,\xi}} U(x-y)\rho_0^{(2)}(x,y) \,\mathsf{d}x\,\mathsf{d}y - \frac{1}{2} \iint_{(\Lambda \setminus B_{r,\xi}) \times B_{r,\xi}} U(x-y)\rho_0^{(2)}(x,y) \,\mathsf{d}x\,\mathsf{d}y.
\end{aligned}$$

Integrating this over ξ we get

$$\begin{aligned}
\frac{3}{4\pi r^3} \int_\Lambda \mathsf{d}\xi \ \mathrm{Tr}\left[\mathcal{U}_{r,\xi} (\Gamma_d)_{\chi_{r,\xi}} \right] &\geq \mathrm{Tr}\left[\mathcal{U}\Gamma_0 \right] \\
&\quad - \frac{3}{8\pi r^3} \int_\Lambda \mathsf{d}\xi \iint_{(\Lambda \setminus B_{r,\xi}) \times B_{r,\xi}} \mathsf{d}x\,\mathsf{d}y \, U(x-y)\rho_0^{(2)}(x,y).
\end{aligned}$$

We conclude that

$$\begin{aligned}
\mathcal{I} \geq \langle \mathcal{U} \rangle_{\Gamma_0} &- \underbrace{\frac{3}{16\pi K r^3} \int_\Lambda \mathsf{d}\xi \ \mathrm{Tr}\left[\mathcal{U}_{r,\xi}^2 (\Gamma_d)_{\chi_{r,\xi}} \right]}_{\mathcal{E}_d :=} \\
&- \underbrace{\frac{3}{8\pi r^3} \int_\Lambda \mathsf{d}\xi \iint_{(\Lambda \setminus B_{r,\xi}) \times B_{r,\xi}} \mathsf{d}x\,\mathsf{d}y \, U(x-y)\rho_0^{(2)}(x,y)}_{\mathcal{E}_{\mathsf{local}} :=}.
\end{aligned} \tag{7.7.9}$$

We are left with bounding the three error terms $\mathcal{E}_{\mathsf{local}}$, $\mathcal{E}_d$ and $\mathcal{E}_{\mathsf{state}}$.

First, we bound the error term $\mathcal{E}_{\mathsf{local}}$ from (7.7.9). Using that U has compact support of range R and recalling the formula in (7.3.2) for $\rho_0^{(2)}$ we have for $1/z$ bounded

$$\begin{aligned}
|\mathcal{E}_{\mathsf{local}}| &\leq \frac{C}{r^3} \int_\Lambda \mathsf{d}\xi \int_{B_{r+R,\xi} \setminus B_{r,\xi}} \mathsf{d}x \int_\Lambda \mathsf{d}z \, |z|^2 U(z) \rho_0^{8/3} \left[1 + L^{-1}\zeta\rho_0^{-1/3} \right] \\
&\leq C L^3 \rho_0^{8/3} \left\| |\cdot|^2 U \right\|_{L^1} \frac{R}{r} + L^3 \mathfrak{e}_L.
\end{aligned}$$

The error term $\mathcal{E}_d$ in (7.7.9) can be evaluated explicitly since Γ_d is a quasi-free state. We have

$$\operatorname{Tr}\left[(\mathcal{U}_{r,\xi})^2 (\Gamma_d)_{\chi_{r,\xi}}\right] = \iiiint_{(B_{r,\xi})^4} U(x-y)U(z-z') \operatorname{Tr}\left[a_x^* a_y^* a_y a_x a_z^* a_{z'}^* a_{z'} a_z \Gamma_d\right] \,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'. \tag{7.7.10}$$

Normal ordering and using $\operatorname{Tr}\left[a_{x_1}^* \cdots a_{x_n}^* a_{x_n} \cdots a_{x_1}\Gamma_d\right] = \rho_d^{(n)}(x_1,\ldots,x_n)$ we find

$$\begin{aligned}
(7.7.10) = 2 &\iint_{(B_{r,\xi})^2} U(x-y)^2 \rho_d^{(2)}(x,y)\,\mathrm{d}x\,\mathrm{d}y \\
&+ 4 \iiint_{(B_{r,\xi})^3} U(x-y)U(x-z')\rho_d^{(3)}(x,y,z')\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z' \\
&+ \iiiint_{(B_{r,\xi})^4} U(x-y)U(z-z')\rho_d^{(4)}(x,y,z,z')\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}z'.
\end{aligned}$$

We may Taylor expand the reduced densities as in Lemma 6.3.6, to conclude that as long as $d \gtrsim \rho_0^{-1/3}$ and $1/z$ is bounded

$$\begin{aligned}
\rho_d^{(2)}(x,y) &\leq C\rho_0^{2+2/3}|x-y|^2\left[1 + L^{-1}\zeta\rho_0^{-1/3}\right], \\
\rho_d^{(3)}(x,y,z') &\leq C\rho_0^{3+4/3}|x-y|^2|x-z'|^2\left[1 + L^{-1}\zeta\rho_0^{-1/3}\right], \\
\rho_d^{(4)}(x,y,z,z') &\leq C\rho_0^{4+4/3}|x-y|^2|z-z'|^2\left[1 + L^{-1}\zeta\rho_0^{-1/3}\right].
\end{aligned}$$

This gives the bound

$$\begin{aligned}
(7.7.10) \leq Cr^3\rho_0^{2+2/3} &\left[\int |x|^2U^2\,\mathrm{d}x + \rho_0^{1+2/3}\left(\int |x|^2U\,\mathrm{d}x\right)^2 + r^3\rho_0^{2+2/3}\left(\int |x|^2U\,\mathrm{d}x\right)^2\right] \\
&\times\left[1 + L^{-1}\zeta\rho_0^{-1/3}\right].
\end{aligned}$$

Thus

$$|\mathcal{E}_d| \leq CK^{-1}L^3\left[\||\cdot|U\|_{L^2}^2\,\rho_0^{2+2/3} + \left\||\cdot|^2U\right\|_{L^1}^2\rho_0^{3+4/3}(1+r^3\rho_0) + \mathfrak{e}_L\right]. \tag{7.7.11}$$

Finally we bound the error term $\mathcal{E}_{\text{state}}$ from (7.7.8). Since $f_K(t) \leq K$ for any t we have

$$|\mathcal{E}_{\text{state}}| \leq \frac{3K}{4\pi r^3}\int_\Lambda \mathrm{d}\xi\,\left\|(\Gamma_P)_{\chi_{r,\xi}} - (\Gamma_d)_{\chi_{r,\xi}}\right\|_{\mathfrak{S}_1} \leq \frac{3\sqrt{2}K}{4\pi r^3}L^{3/2}\left(\int_\Lambda \mathrm{d}\xi\,S((\Gamma_P)_{\chi_{r,\xi}},(\Gamma_d)_{\chi_{r,\xi}})\right)^{1/2}$$

using the Cauchy–Schwarz inequality and that $\left\|(\Gamma_P)_{\chi_{r,\xi}} - (\Gamma_d)_{\chi_{r,\xi}}\right\|_{\mathfrak{S}_1}^2 \leq 2S((\Gamma_P)_{\chi_{r,\xi}},(\Gamma_d)_{\chi_{r,\xi}})$ [OP04, Theorem 1.15]. Combining this with the bound for $\mathcal{E}_d$ and choosing the optimal K we have

$$\begin{aligned}
|\mathcal{E}_d| + |\mathcal{E}_{\text{state}}| \leq CL^{9/4} &\left[\||\cdot|U\|_{L^2}^2\,\rho_0^{2+2/3} + \left\||\cdot|^2U\right\|_{L^1}^2\rho_0^{3+4/3}(1+r^3\rho_0) + \mathfrak{e}_L\right]^{1/2} \\
&\times r^{-3/2}\left(\int_\Lambda \mathrm{d}\xi\,S((\Gamma_P)_{\chi_{r,\xi}},(\Gamma_d)_{\chi_{r,\xi}})\right)^{1/4}.
\end{aligned}$$

Together with the bound of $\mathcal{E}_{\text{local}}$ above we conclude the proof of the lemma. □

7.7.4 Combining the parts

Finally, we combine the three parts above and give the

Proof of Proposition 7.7.1. Consider the function U given by

$$U(x) = 30a^3 R^{-5} \chi_{|x|\le R}.$$

This has

$$\left\| |\cdot|^2 U \right\|_{L^1} = 24\pi a^3, \qquad \left\| |\cdot|^4 U \right\|_{L^1} = Ca^3R^2, \qquad \| |\cdot| U\|_{L^2}^2 = Ca^6R^{-5}.$$

Note also that $\| |\cdot|^4 W\|_{L^1} \le Ca^5$ and $a \lesssim R$. Combining Lemmas 7.7.6 and 7.7.8 and Equation (7.7.3) we have

$$\begin{aligned}\langle \mathcal{W}_P\rangle_\Gamma \ge \langle \mathcal{U}\rangle_{\Gamma_0} &- C(k_F^\kappa)^7 a^3 R^2 \langle \mathcal{N}\rangle_\Gamma - CL^3a^3\rho_0^{8/3} R r^{-1} \\ &- CL^{9/4}\left[a^6R^{-5}r^{-3}\rho_0^{2+2/3} + a^6\rho_0^{3+4/3}(r^{-3}+\rho_0)\right]^{1/2}\Big[d^3 S(\Gamma,\Gamma_0) + L^3\beta^4(k_F^\kappa)^7 d^{-1} \\ &\quad + L^3 d^3 \beta^{-1}(k_F^\kappa - q_F)e^{-\kappa+\beta(2k_F^\kappa q_F - q_F^2)} + C_n d^3 (dq_F)^{-2n}\log Z_0 + L^3\mathfrak{e}_L\Big]^{1/4} - L^3\mathfrak{e}_L.\end{aligned}$$

Recalling the formula from $\rho_0^{(2)}$ from (7.3.2), we have

$$\begin{aligned}\langle \mathcal{U}\rangle_{\Gamma_0} &= \frac{1}{2}\iint U(x-y)\rho_0^{(2)}(x,y)\,\mathrm{d}x\,\mathrm{d}y \\ &= 2\pi\frac{-\operatorname{Li}_{5/2}(-z)}{(-\operatorname{Li}_{3/2}(-z))^{5/3}} L^3\rho_0^{2+2/3}\int |x|^2 U(x)\left[1 + O(|x|^2\rho_0^{2/3}) + O(L^{-1}\zeta\rho_0^{-1/3})\right]\mathrm{d}x \\ &= \langle \mathcal{W}\rangle_{\Gamma_0} + O(L^3a^3R^2\rho_0^{10/3}) + L^3\mathfrak{e}_L\,,\end{aligned}$$

where we have used that $\int |x|^2 U(x)\,\mathrm{d}x = \int |x|^2 W(x)\,\mathrm{d}x$ and that $a \lesssim R$ in the last step. Choosing finally $r = d/2$ (as this is clearly the optimal choice) and recalling that $\mathcal{E}_{\mathrm{pt}}(\Gamma) = \langle \mathcal{W}_P\rangle_\Gamma - \langle \mathcal{W}\rangle_{\Gamma_0}$ this concludes the proof of Proposition 7.7.1. $\square$

7.A Bounding Riemann sums

In this section we prove (7.3.8) and (7.7.7). We do this by viewing the sums as Riemann sums for the corresponding integrals. To estimate their difference, note that for any function F and any $k \in \frac{2\pi}{L}\mathbb{Z}^3$ we have

$$\frac{1}{L^3}F(k) = \frac{1}{(2\pi)^3}\int_{[-\frac{\pi}{L},\frac{\pi}{L}]^3} \mathrm{d}\xi\,\left[F(k+\xi) - \int_0^1 \mathrm{d}t\,\partial_t F(k+t\xi)\right]. \qquad (7.A.1)$$

When summed over k, the first term gives the integral $\int F$ and the second term will in general be of order L^{-1} for large L.

Proof of (7.3.8). We shall apply the bound $h(1+e^{h/2})^{-1} \le Ce^{-h/3}$ to $h = \beta(|k|^2-\mu)$, obtaining

$$\sum_{|k|>k_F^\kappa} \frac{\beta(|k|^2-\mu)}{1+e^{\frac{\beta}{2}(|k|^2-\mu)}} \le C\sum_{|k|>k_F^\kappa} z^{1/3}e^{-\beta|k|^2/3}$$

Let $F(k) = z^{1/3}e^{-\beta|k|^2/3}$ and note that

$$\partial_t F(k+t\xi) = -\frac{2}{3}z^{1/3}\beta(k+t\xi)\xi e^{-\beta(k+t\xi)^2/3}.$$

Using that $|\xi| \leq CL^{-1}$ for $\xi \in [-\frac{\pi}{L}, \frac{\pi}{L}]^3$, we may bound this by

$$|\partial_t F(k+t\xi)| \leq Cz^{1/3}\beta\left[L^{-1}|k+\xi| + L^{-2}\right] e^{-\beta(k+\xi)^2/3}e^{C\beta(|k+\xi|L^{-1}+L^{-2})}.$$

This is clearly integrable in $k+\xi$ and subleading in L. (More precisely it is of the order L^{-1}.) Thus, using (7.A.1),

$$\sum_{|k|>k_F^\kappa} z^{1/3}e^{-\beta k^2/3} = \frac{L^3}{(2\pi)^3}\int_{|k|\geq k_F^\kappa} z^{1/3}e^{-\beta k^2/3}\,\mathrm{d}k + L^3\mathfrak{e}_L.$$

The integral is explicitly given by

$$\int_{|k|\geq k_F^\kappa} z^{1/3}e^{-\beta|k|^2/3}\,\mathrm{d}k = \pi z^{1/3}(\beta/3)^{-3/2}\left(\sqrt{\pi}\,\mathrm{erfc}((\beta/3)^{1/2}k_F^\kappa) + 2(\beta/3)^{1/2}k_F^\kappa e^{-\beta(k_F^\kappa)^2/3}\right),$$

with erfc the complementary error function [NIS, (7.2.2)]. Bounding $\mathrm{erfc}(z) \leq \frac{1}{z+1}e^{-z^2}$ [NIS, (7.8.3)] we thus have

$$\int_{|k|\geq k_F^\kappa - q_F} z^{1/3}e^{-\beta k^2}\,\mathrm{d}k \leq C\beta^{-3/2}\left(\beta^{1/2}k_F^\kappa + 1\right)e^{-\beta((k_F^\kappa)^2-\mu)/3} = C\beta^{-3/2}\left(\beta^{1/2}k_F^\kappa + 1\right)e^{-\kappa/3}$$

proving (7.3.8). □

Proof of (7.7.7). For any $t > -1$ we have $\log(1+t) \leq t$. Thus, in order to prove (7.7.7) we need to bound $\sum_{|k|>k_F^\kappa - q_F} ze^{-\beta|k|^2}$. Define $F(k) = ze^{-\beta|k|^2}$ and note that

$$\partial_t F(k+t\xi) = -2z\beta(k+t\xi)\xi e^{-\beta(k+t\xi)^2}.$$

Using that $|\xi| \leq CL^{-1}$ for $\xi \in [-\frac{\pi}{L}, \frac{\pi}{L}]^3$, we may bound this by,

$$|\partial_t F(k+t\xi)| \leq Cz\beta\left[L^{-1}|k+\xi| + L^{-2}\right] e^{-\beta(k+\xi)^2}e^{C\beta(|k+\xi|L^{-1}+L^{-2})}.$$

As in the proof of (7.3.8) above, this is clearly integrable in $k+\xi$ and of the order L^{-1}. Thus, using (7.A.1),

$$\sum_{|k|>k_F^\kappa - q_F} ze^{-\beta k^2} = \frac{L^3}{(2\pi)^3}\int_{|k|\geq k_F^\kappa - q_F} ze^{-\beta k^2}\,\mathrm{d}k + L^3\mathfrak{e}_L.$$

The integral is explicitly given by

$$\int_{|k|\geq k_F^\kappa - q_F} ze^{-\beta|k|^2}\,\mathrm{d}k = \pi\beta^{-3/2}z\left(\sqrt{\pi}\,\mathrm{erfc}(\beta^{1/2}(k_F^\kappa - q_F)) + 2\beta^{1/2}(k_F^\kappa - q_F)e^{-\beta(k_F^\kappa - q_F)^2}\right),$$

with erfc the complementary error function [NIS, (7.2.2)]. Bounding $\mathrm{erfc}(z) \leq \frac{1}{z+1}e^{-z^2}$ [NIS, (7.8.3)] as in the proof of (7.3.8) above we thus have

$$\int_{|k|\geq k_F^\kappa - q_F} ze^{-\beta k^2}\,\mathrm{d}k \leq C\beta^{-3/2}z\left(\beta^{1/2}(k_F^\kappa - q_F) + 1\right)e^{-\beta(k_F^\kappa - q_F)^2}.$$

This concludes the proof of (7.7.7). □

7.B Two dimensions

In this appendix we shall sketch the (straightforward) changes to the argument to get the bounds also in dimension $D = 2$, i.e., to prove Theorem 7.1.7. To illustrate the dimensional dependence and make clear which parts of the argument fails in dimension $D = 1$ we consider here general dimension $D = 1, 2$. The main steps in the proof are Lemma 7.5.2 and Proposition 7.7.1 together with the a priori bounds of Lemma 7.6.4. In general dimension D they read

Lemma 7.B.1 (Lemma 7.5.2 in D dimensions)**.** *Let $D = 1, 2$ and let Γ be any state. Then, for $\alpha > 0$ sufficiently small and any $0 < \delta < 1$,*

$$\begin{aligned}
\left|\left\langle \mathcal{H}_{0;\mathcal{B}}^{\div r}\right\rangle_\Gamma\right| &\leq Ca^D (k_F^\kappa)^{D+1} \left|\log ak_F^\kappa\right| \left[k_F^\kappa \left\langle \mathcal{N}_Q\right\rangle_\Gamma^{1/2} + \left\langle \mathcal{K}_Q\right\rangle_\Gamma^{1/2}\right] \left\langle \mathcal{N}\right\rangle_\Gamma^{1/2}, \\
\left|\left\langle \mathcal{Q}_{\mathsf{Taylor}}\right\rangle_\Gamma\right| + \left|\left\langle \mathcal{Q}_{\mathsf{scat}}\right\rangle_\Gamma\right| &\leq Ca^D \left|\log ak_F^\kappa\right| (k_F^{\delta^{-1}\kappa})^{D/2} (k_F^\kappa)^{D/2+2} \left\langle \mathcal{N}_Q\right\rangle_\Gamma^{1/2} \left\langle \mathcal{N}\right\rangle_\Gamma^{1/2} \\
&\quad + CL^{D/2} a^{D/2} (k_F^\kappa)^{D+2} \left\langle \mathcal{N}_{Q^>}\right\rangle_\Gamma^{1/2} \\
\left|\left\langle \mathcal{Q}_{[\mathcal{V}_Q,\mathcal{B}]}\right\rangle_\Gamma\right| &\leq \begin{cases} Ca^{1/2} (k_F^\kappa)^{3/2} \left\langle \mathcal{V}_Q\right\rangle_\Gamma^{1/2} \left\langle \mathcal{N}\right\rangle_\Gamma^{1/2} & D = 1, \\ Ca^2 (k_F^\kappa)^3 \left|\log ak_F^\kappa\right|^{1/2} \left\langle \mathcal{V}_Q\right\rangle_\Gamma^{1/2} \left\langle \mathcal{N}\right\rangle_\Gamma^{1/2} & D = 2, \end{cases} \\
\left|\left\langle \mathcal{Q}_{V\varphi}\right\rangle_\Gamma\right| &\leq Ca^{3D/2-1} (k_F^\kappa)^{3D/2+1} \left\langle \mathcal{N}_Q\right\rangle_\Gamma^{1/2} \left\langle \mathcal{N}\right\rangle_\Gamma^{1/2}, \\
\left|\left\langle \mathcal{Q}_{\mathsf{OD}}\right\rangle_\Gamma\right| &\leq \begin{cases} Ca (k_F^\kappa)^3 \left\langle \mathcal{N}\right\rangle_\Gamma + Ck_F^\kappa \left\langle \mathcal{V}_Q\right\rangle_\Gamma^{1/2} \left\langle \mathcal{N}_Q\right\rangle_\Gamma^{1/2} & D = 1, \\ Ca^3 (k_F^\kappa)^5 \left|\log ak_F^\kappa\right|^{1/2} \left\langle \mathcal{N}\right\rangle_\Gamma + Ca (k_F^\kappa)^2 \left\langle \mathcal{V}_Q\right\rangle_\Gamma^{1/2} \left\langle \mathcal{N}_Q\right\rangle_\Gamma^{1/2} & D = 2. \end{cases}
\end{aligned}$$

Lemma 7.B.2 (Proposition 7.7.1 in D dimensions)**.** *Let $D = 1, 2$ and let Γ be any state. Then, for any $0 < d, R < L$, any $0 < q_F < k_F^\kappa$ with $\beta(k_F^\kappa - q_F)^2 \gtrsim 1$ any $n \in \mathbb{N}$ and any $z \gtrsim 1$*

$$\begin{aligned}
\mathcal{E}_{\mathsf{pt}}(\Gamma) \gtrsim{} & -L^D a^D R^2 \rho_0^{2+4/D} - (k_F^\kappa)^{D+4} a^D R^4 \left\langle \mathcal{N}\right\rangle_\Gamma - L^D a^D \rho_0^{2+2/D} R d^{-1} \\
& - L^{3D/4} \left[a^{2D} R^{-D-2} \rho_0^{2+2/D} d^{-D} + a^{2D} \rho_0^{3+4/D} (d^{-D} + \rho_0)\right]^{1/2} \Big[d^D S(\Gamma, \Gamma_0) \\
& \quad + L^D \beta^4 (k_F^\kappa)^{D+4} d^{D-4} + L^D \beta^{-D/2} e^{-\kappa + \beta(2k_F^\kappa q_F - q_F^2)} + C_n (dq_F)^{-2n} \log Z_0\Big]^{1/4} \\
& - L^D \mathfrak{e}_L.
\end{aligned}$$

Lemma 7.B.3 (Lemma 7.6.4 in D dimensions)**.** *Let $D = 1, 2$ and let Γ be an approximate Gibbs state. Then, for any $0 \leq \lambda \leq 1$,*

$$\begin{aligned}
\left\langle \mathcal{N}_Q\right\rangle_{\Gamma^\lambda} &\leq CL^D \zeta \kappa^{-1} a^D \rho_0^2 + L^D \mathfrak{e}_L, \\
\left\langle \mathcal{K}_Q\right\rangle_{\Gamma^\lambda} &\leq CL^D \zeta^{-D-1} \kappa^{D+1} a^D \rho_0^{2+2/D} + L^D \mathfrak{e}_L, \\
\left\langle \mathcal{V}_Q\right\rangle_{\Gamma^\lambda} &\leq CL^D \zeta^{-D/2-1} \kappa^{D/2+1} a^D \rho_0^{2+2/D} + L^D \mathfrak{e}_L.
\end{aligned}$$

With Lemma 7.B.2 at hand we may prove the analogue of Proposition 7.2.13:

Lemma 7.B.4 (Proposition 7.2.13 in D dimensions)**.** *Let Γ be an approximate Gibbs state. Then, for $\alpha > 0$ sufficiently small,*

$$\mathcal{E}_{\mathsf{pt}}(\Gamma) \geq -C(z) L^D a^D \rho_0^{2+2/D} (a^D \rho_0)^\sigma - L^D \mathfrak{e}_L, \qquad \sigma = \begin{cases} \frac{2}{11} - \frac{30}{44}\alpha & D = 1, \\ \frac{1}{8} - \frac{3}{8}\alpha & D = 2, \end{cases}$$

with the function $C(z)$ uniformly bounded on compact subsets of $(0, \infty)$.

With these we may then give the

Proof of Theorem 7.1.7. Recall (7.2.18). Similarly as in (7.2.19) we evaluate (see also Lemma 6.3.6)

$$\langle \mathcal{W}\rangle_{\Gamma_0} = 8\pi^2 \frac{-\operatorname{Li}_2(-z)}{(-\operatorname{Li}_1(-z))^2} a^2\rho_0^3 \left[1 + O(a^2\rho_0) + \mathfrak{e}_L\right].$$

We bound $\mathcal{E}_V(\Gamma)$ similarly as in Proposition 7.2.14, $\mathcal{E}_{V\varphi}(\Gamma)$, $\mathcal{E}_{\mathsf{scat}}(\Gamma)$ and $\mathcal{E}_{\mathsf{OD}}(\Gamma)$ using Lemmas 7.B.1 and 7.B.3 and choosing the optimal $\delta = (a^2\rho_0)^{1/2}\left|\log a^2\rho_0\right|$, and $\mathcal{E}_{\mathsf{pt}}(\Gamma)$ using Lemma 7.B.4. □

Remark 7.B.5 (The case of $D = 1$ dimensions)**.** The method presented here does not allow proving the one-dimensional analogue of Theorems 7.1.3 and 7.1.7. Indeed, combining the propagated a priori bounds of Lemma 7.B.3 with the bounds in Lemma 7.B.1, the bounds on the error terms $\mathcal{Q}_{[\mathcal{V}_Q,\mathcal{B}]}$, $\mathcal{Q}_{V\varphi}$ and $\mathcal{Q}_{\mathsf{OD}}$ are too large. A similar issue occurs in the zero-temperature setting, see Remark 4.A.4.

The proofs of Lemmas 7.B.1–7.B.4 are as those of Lemmas 7.5.2 and 7.6.4 and Propositions 7.2.13 and 7.7.1 only with straightforward changes, which we shall sketch here. Recall first the bounds on the scattering function:

Lemma 7.B.6 (Lemma 4.A.2 and Remark 4.A.4)**.** *The scattering function φ satisfies*

$$\left\| |\cdot|^n \varphi\right\|_{L^1} \le C a^D (k_F^\kappa)^{-n}, \qquad n = 1,2, \quad \left\| |\cdot|^n \nabla^n \varphi\right\|_{L^1} \le C a^D \left|\log a k_F^\kappa\right|, \quad n = 0,1,2$$

$$\left\| |\cdot| \varphi\right\|_{L^2} \le \begin{cases} C a (k_F^\kappa)^{-1/2} & D = 1, \\ C a^2 \left|\log a k_F\right|^{1/2} & D = 2, \end{cases} \qquad \left\| |\cdot|^n \nabla^n \varphi\right\|_{L^2} \le C a^{D/2}, \qquad n = 0,1.$$

Furthermore, we have the analogues of (7.5.9) and (7.5.10):

$$\begin{aligned}
\left\| \int \varphi(z - z')(b_{z'}^r)^* c_{z'} \,\mathrm{d}z' \right\| &\le C\left[(k_F^\kappa)^D \left\|\varphi\right\|_{L^1} + (k_F^\kappa)^{D/2} \left\|\varphi\right\|_{L^2}\right] \\
\left\| \int \varphi(z - z')(b_{z'}^r)^* c_{z'} c_z \,\mathrm{d}z' \right\| &\le C\left[(k_F^\kappa)^{3D/2+1} \left\| |\cdot|\varphi\right\|_{L^1} + (k_F^\kappa)^{D+1} \left\| |\cdot|\varphi\right\|_{L^2}\right].
\end{aligned}$$

Proof of Lemma 7.B.1. The proof of Lemma 7.B.1 is exactly as that of Lemma 7.5.2 given in Section 7.5. We simply state here all the intermediary bounds.

We may bound $\mathcal{H}_{0;B}^{\div r}$, $\mathcal{Q}_{\mathsf{Taylor}}$ and $\mathcal{Q}_{\mathsf{scat}}$ as

$$\begin{aligned}
\left|\left\langle \mathcal{H}_{0;B}^{\div r}\right\rangle_\Gamma\right| &\le C(k_F^\kappa)^D \left[\left\| |\cdot| \nabla\varphi\right\|_{L^1} + \left\| |\cdot|^2 \Delta\varphi\right\|_{L^1}\right] \\
&\quad \times \left[k_F^\kappa \left\langle \mathcal{N}_Q\right\rangle_\Gamma^{1/2} + \left\langle \mathcal{K}_Q\right\rangle_\Gamma^{1/2}\right] \left\langle \mathcal{N}\right\rangle_\Gamma^{1/2}, \\
\left|\left\langle \mathcal{Q}_{\mathsf{Taylor}}\right\rangle_\Gamma\right| + \left|\left\langle \mathcal{Q}_{\mathsf{scat}}\right\rangle_\Gamma\right| &\le C(k_F^{\delta^{-1}\kappa})^{D/2} (k_F^\kappa)^{D/2+} \left[k_F^\kappa \left\|F\right\|_{L^1} + \left\|\mathcal{E}_\varphi\right\|_{L^1}\right] \left\langle \mathcal{N}_Q\right\rangle_\Gamma^{1/2} \left\langle \mathcal{N}\right\rangle_\Gamma^{1/2} \\
&\quad + C L^{D/2} (k_F^\kappa)^{D+1} \left[k_F^\kappa \left\|F\right\|_{L^2} + \left\|\mathcal{E}_\varphi\right\|_{L^2}\right] \left\langle \mathcal{N}_{Q^>}\right\rangle_\Gamma^{1/2}.
\end{aligned}$$

To bound $\mathcal{Q}_{[\mathcal{V}_Q,\mathcal{B}]}$ we have the bounds

$$\begin{aligned}
\left|\left\langle \mathcal{A}_{4,\delta}\right\rangle_\Gamma\right| + \left|\left\langle \mathcal{A}_{4,P}\right\rangle_\Gamma\right| &\le C(\kappa_F^\kappa)^{3D/2+1} \left\| |\cdot|\varphi\right\|_{L^1} \left\|V\right\|_{L^1}^{1/2} \left\langle \mathcal{V}_Q\right\rangle_\Gamma^{1/2} \left\langle \mathcal{N}\right\rangle_\Gamma^{1/2}, \\
\left|\left\langle \mathcal{A}_{6,\delta}\right\rangle_\Gamma\right| + \left|\left\langle \mathcal{A}_{6,P}\right\rangle_\Gamma\right| &\le C\left[(k_F^\kappa)^{3D/2+1} \left\| |\cdot|\varphi\right\|_{L^1} + (k_F^\kappa)^{D+1} \left\| |\cdot|\varphi\right\|_{L^2}\right] \\
&\quad \times \left\|V\right\|_{L^1}^{1/2} \left\langle \mathcal{V}_Q\right\rangle_\Gamma^{1/2} \left\langle \mathcal{N}\right\rangle_\Gamma^{1/2}.
\end{aligned}$$

To bound $\mathcal{Q}_{V\varphi}$ we have the bounds

$$|\langle \mathcal{A}_4 \rangle_\Gamma| \leq C a^{D/2} (k_F^\kappa)^{3D/2+1} \|V\|_{L^1}^{1/2} \|\varphi\|_{L^2} \langle \mathcal{N}_Q \rangle_\Gamma^{1/2} \langle \mathcal{N} \rangle_\Gamma^{1/2},$$
$$|\langle \mathcal{A}_6 \rangle_\Gamma| \leq C a^{D/2} (k_F^\kappa)^{D+1} \Big[(k_F^\kappa)^D \|\varphi\|_{L^1} + (k_F^\kappa)^{D/2} \|\varphi\|_{L^2} \Big] \|V\|_{L^1}^{1/2} \langle \mathcal{N}_Q \rangle_\Gamma^{1/2} \langle \mathcal{N} \rangle_\Gamma^{1/2}.$$

To bound $\mathcal{Q}_{\mathsf{OD}}$ we have the bounds

$$\begin{aligned}
\left| \langle \mathcal{A}_{4,c,\delta} \rangle_\Gamma \right| &\leq C a^{D/2} (k_F^\kappa)^{3D/2+2} \|V\|_{L^1}^{1/2} \||\cdot|\varphi\|_{L^2} \langle \mathcal{N} \rangle_\Gamma, \\
\left| \langle \mathcal{A}_{4,c,P} \rangle_\Gamma \right| &\leq C a^{D/2} (k_F^\kappa)^{2D+2} \||\cdot|\varphi\|_{L^1} \|V\|_{L^1}^{1/2} \langle \mathcal{N} \rangle_\Gamma, \\
\left| \langle \mathcal{A}_{6,c,\delta} \rangle_\Gamma \right| + \left| \langle \mathcal{A}_{6,c,P} \rangle_\Gamma \right| &\leq C a^{D/2} (k_F^\kappa)^{D/2+1} \Big[(k_F^\kappa)^{3D/2+1} \||\cdot|\varphi\|_{L^1} + (k_F^\kappa)^{D+1} \||\cdot|\varphi\|_{L^2} \Big] \\
&\qquad \times \|V\|_{L^1}^{1/2} \langle \mathcal{N}_Q \rangle_\Gamma^{1/2} \langle \mathcal{N} \rangle_\Gamma^{1/2}, \\
\left| \langle \mathcal{A}_{4,b} \rangle_\Gamma \right| &\leq C (k_F^\kappa)^D \|V\|_{L^1}^{1/2} \|\varphi\|_{L^2} \langle \mathcal{V}_Q \rangle_\Gamma^{1/2} \langle \mathcal{N}_Q \rangle_\Gamma^{1/2}, \\
\left| \langle \mathcal{A}_{6,b} \rangle_\Gamma \right| &\leq C (k_F^\kappa)^{D/2} \Big[(k_F^\kappa)^D \|\varphi\|_{L^1} + (k_F^\kappa)^{D/2} \|\varphi\|_{L^2} \Big] \\
&\qquad \times \|V\|_{L^1}^{1/2} \langle \mathcal{V}_Q \rangle_\Gamma^{1/2} \langle \mathcal{N}_Q \rangle_\Gamma^{1/2}.
\end{aligned}$$

Combining with the bounds in Lemma 7.B.6 we conclude of the lemma. □

Proof of Lemma 7.B.2. The proof is (almost) the same as that for Proposition 7.7.1 given in Section 7.7. The only non-immediate change is the bound for the sum $\sum_{|k|>k_F^\kappa - q_F} z e^{-\beta|k|^2}$. Similarly as in Section 7.A we have

$$\sum_{|k|>k_F^\kappa - q_F} z e^{-\beta|k|^2} \leq \begin{cases} CL\beta^{-1/2} z \frac{1}{1+\beta^{1/2}(k_F^\kappa - q_F)} e^{-\beta(k_F^\kappa - q_F)^2} + L\mathfrak{e}_L & D=1, \\ CL^2 \beta^{-1} z e^{-\beta(k_F^\kappa - q_F)^2} + L^2 \mathfrak{e}_L & D=2, \end{cases}$$

This way we obtain the proof of the lemma. □

Proof of Lemma 7.B.3. Same as that for Lemma 7.6.4. □

Proof of Lemma 7.B.4. We use Lemma 7.B.2 with $q_F = \zeta^{-1/2} \rho_0^{1/D}$. Choosing in addition $d \gg \zeta^{1/2} \rho_0^{-1/D}$ then, as in the proof of Proposition 7.2.13 above, by taking n large enough, we can ensure that the last two summands in $[\ldots]^{1/4}$ are negligible. Then,

$$\begin{aligned}
\mathcal{E}_{\mathsf{pt}}(\Gamma) \gtrsim & -L^D a^D \rho_0^{2+2/D} \Big[\kappa^{D/2+2} \zeta^{-D/2+2} R^2 \rho_0^{2/D} + R d^{-1} \Big] \\
& - L^D \Big[a^D R^{-D/2-1} \rho_0^{4/D} d^{-D/2} + a^D \rho_0^{2+2/D} \Big] \\
& \quad \times \Big[\zeta d^D a^D \rho_0^2 + \zeta^{-D/2+2} \kappa^{D/2+2} \rho_0^{1-4/D} d^{D-4} \Big]^{1/4} - L^D \mathfrak{e}_L.
\end{aligned}$$

Restricting to a compact set of z's we take

$$d = \rho_0^{-1/D} (a^D \rho_0)^{-s}, \qquad R = \rho_0^{-1/D} (a^D \rho_0)^t$$

for some $s, t > 0$ to be determined. Then, $\mathcal{E}_{\mathsf{pt}}(\Gamma) \geq -C(z) L^D a^D \rho_0^{2+2/D} \Big[(a^D \rho_0)^\sigma - \mathfrak{e}_L \Big]$ with $C(z)$ bounded uniformly on compact sets of z's and

$$\begin{aligned}
\sigma = \frac{1}{8} \min \Big\{ & 16t - (4D+16)\alpha, \, 2 - (4D+8)t + 2Ds, \\
& - (4D+8)t + (2D+8)s - (D+4)\alpha, \, 2 - 2Ds, \, (8-2D)s - (D+4)\alpha \Big\}
\end{aligned}$$

Choosing

$$s = \begin{cases} \frac{3}{11} + \frac{30}{11}\alpha & D = 1, \\ \frac{1}{4} + \frac{3}{4}\alpha & D = 2, \end{cases} \qquad t = \begin{cases} \frac{1}{11} + \frac{10}{11}\alpha & D = 1, \\ \frac{1}{16} + \frac{21}{16}\alpha & D = 2, \end{cases}$$

we find

$$\sigma = \begin{cases} \frac{2}{11} - \frac{30}{44}\alpha & D = 1, \\ \frac{1}{8} - \frac{3}{8}\alpha & D = 2. \end{cases}$$

This concludes the proof of Lemma 7.B.4 $\square$

Part II

Universalities in BCS Theory

CHAPTER 8

Brief introduction to the BCS theory of superconductivity

Superconductivity is an important physical phenomenon with many applications ranging from quantum computers to high-speed levitating trains. It was first observed experimentally by Kamerlingh Onnes in 1911, see [DK10] for the history, with the first microscopic theory thereof being BCS theory, developed by Bardeen, Cooper and Schrieffer in 1957 [BCS57]. We give here only a brief introduction to BCS theory. For a more detailed introduction we refer the reader to the PhD theses of Deuchert [Deu16], Maier [Mai22] and Roos [Roo23], the review [HS16], or my master's thesis [Lau20].

An important aspect of BCS theory is that the effective interaction between the electrons in some superconductor is sufficiently attractive. Physically this arises from the (attractive) interactions between electrons and the ions in the crystal lattice. "Integrating out" the degrees of freedom from the vibrations of the lattice ions, this then yields an effective attractive interaction between the electrons.

An important feature of a superconductor is its critical temperature T_c. The superconductor is only superconducting for temperatures smaller than this critical temperature. For larger temperatures it is a normal metal. A second important feature of BCS theory is its associated energy gap Ξ. This is the energy required to excite the superconductor out of the superconducting state.

Both the energy gap and critical temperature measure the 'stability' of the superconducting phase. While they both depend heavily on the microscopic details of any specific superconductor, what is perhaps surprising is that they exhibit a certain universal behaviour, however. Namely, in multiple limiting regimes, their ratio Ξ/T_c is *universal* meaning that it is *independent of the microscopic details of the material*. In general this is expected to appear as soon as "superconductivity is weak", meaning that both Ξ and T_c are small. The ratio Ξ/T_c is then given by a universal function depending only on the reduced temperature T/T_c [LT23; Leg06].

Mathematically, BCS theory is described by the non-linear BCS gap equation, an equation in the *gap function* Δ depending on the temperature of the superconductor. For temperatures larger than the critical, no non-zero solution Δ exists, while for temperatures below the critical there exists some non-zero function Δ solving the gap equation. The BCS gap equation arises as the Euler–Lagrange equations of the *BCS functional* [HHSS08; HS16; Leg80]. Using this functional formulation, many aspects of BCS theory have been put on rigorous grounds. In particular, asymptotic formulas for the critical temperature [FHNS07; HS08a; HS08b; Hen22] and energy gap [HS08b; Lau21] have been proven.

Further, BCS theory has been studied for temperatures close to the critical. For these temperatures superconductivity is also well-described by the phenomenological Ginzburg–Landau (GL) theory [GL50]. For temperatures close to the critical, BCS theory in fact recovers GL theory [Gor59]. This was recently proved, even including external electric and magnetic fields, [DHM23a; DHM23b; FHSS12a; FHSS16; FL16]. For further discussion on the link between BCS and GL theory and the effect of external fields we refer the reader to the PhD thesis of Maier [Mai22].

We consider here BCS theory in the translation invariant setting and in infinite volume. In particular, there are no boundary effects included and this describes the bulk properties of a superconductor. For a discussion of the non-translation invariant setting and including boundary effects we refer the reader to the PhD thesis of Roos [Roo23], see also [DGHL18; HRS23; Roo24; RS23; RS24].

8.1 Universalities in BCS theory

We give next a precise definition of the critical temperature and energy gap in the translation invariant setting. Further, we discuss their universal behaviour studied in Part II of the thesis. Again, we refer the reader to [Deu16; HS16; Lau20; Mai22; Roo23] for a more detailed introduction and extensions to more general settings.

The BCS theory of superconductivity is described by the non-linear gap equation (being an equation in the function Δ)

$$\Delta(p) = -\frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \hat{V}(p-q) \frac{\Delta(q)}{K_T^\Delta(q)} \, \mathrm{d}q, \tag{8.1.1}$$

where

$$K_T^\Delta(p) = \frac{E_\Delta(p)}{\tanh \frac{E_\Delta(p)}{2T}}, \qquad E_\Delta(p) = \sqrt{|p^2-\mu|^2 + |\Delta(p)|^2}.$$

The central statement of BCS theory is that, if the effective interaction V is sufficiently attractive, then there exists some critical temperature $T_c > 0$ such that for $T \geq T_c$ Equation (8.1.1) has only the trivial solution, being the solution $\Delta(p) \equiv 0$, whereas for $T < T_c$ there exists some non-trivial solution Δ. A sufficient assumption on V is that it is of negative type $\hat{V} \leq 0$ (and non-zero $\hat{V} \neq 0$), in which case also the gap function Δ is unique up to a constant global complex phase.

The function $E_\Delta(p)$ has the interpretation as the dispersion relation of associated quasi-particles, see [HHSS08, Appendix A]. In particular the value $\Xi = \inf_p E_\Delta(p)$ is naturally interpreted as an energy gap. For negative type interactions, where Δ is unique up to a constant global phase, the energy gap is even uniquely defined.

The universal features of BCS theory studied in the thesis relate to the ratio Ξ/T_c. As discussed above, this ratio is universal in appropriate limiting regimes, where “superconductivity is weak”, meaning that T_c is small. Proving various notions of this is the contents of Part II of the thesis.

We consider two such universal properties, the first being the formula

$$\frac{\Xi(T=0)}{T_c} \approx \pi e^{-\gamma} \approx 1.76, \tag{8.1.2}$$

with $\gamma \approx 0.577$ the Euler–Mascheroni constant, for the ratio of the zero-temperature energy gap and the critical temperature. This formula is well-known in the physics literature [BCS57; NS85]. In the mathematical physics literature this was first proven in the weak coupling limit [FHNS07; HS08b], where one replaces the interaction V by λV and considers the limit $\lambda \to 0$. This was later extended to also cover the low-density limit $\mu \to 0$ [HS08a; Lau21]. In Chapter 9 we prove this formula in the weak coupling limit in $d = 1, 2$ dimensions and in Chapter 10 we prove this formula in the high-density limit $\mu \to \infty$ by establishing an asymptotic formula for the zero-temperature energy gap and using a similar formula for the critical temperature of Henheik [Hen22]. Further, we give in Chapter 9 an exemplary proof and compare it to the other proofs of this universality in the literature and Chapter 10 in various limits.

The second universality we consider is the positive temperature extension of (8.1.2). More precisely one has the formula [LT23; Leg06]

$$\frac{\Xi(T)}{T_c} \approx \mathsf{f}_{\mathsf{BCS}}\left(\sqrt{1 - T/T_c}\right), \tag{8.1.3}$$

for some universal function $\mathsf{f}_{\mathsf{BCS}}$ described in detail in Chapter 11. In particular, for temperatures close to the critical, we have the formula

$$\frac{\Xi(T)}{T_c} \approx \sqrt{\frac{8\pi^2}{7\zeta(3)}}\sqrt{1 - T/T_c} \approx 3.06\sqrt{1 - T/T_c},$$

with $\zeta(s) = \sum_{n=1}^{\infty} n^{-s}$ the Riemann zeta function. Both universalities (8.1.2) and (8.1.3) are illustrated in Figure 8.1.1.

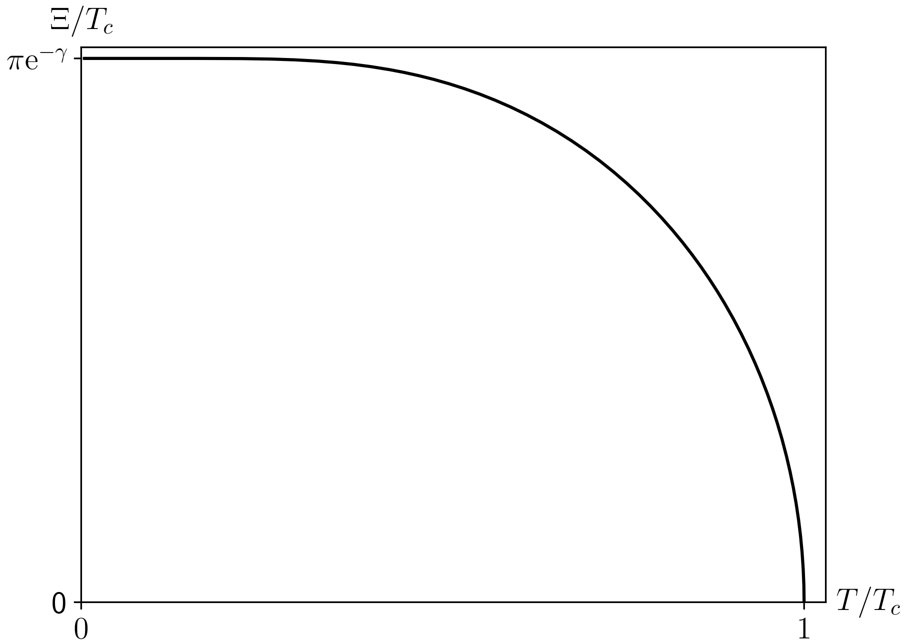


Figure 8.1.1: (Copied from Chapter 11.) The ratio of the BCS energy gap and the critical temperature, Ξ/T_c, is well approximated by a *universal function* of the relative temperature T/T_c. At $T = 0$, it approaches the well-known constant $\pi e^{-\gamma} \approx 1.76$.

We prove in Chapter 11 the validity of the formula in (8.1.3) in the weak coupling limit. This partially builds on and extends recent work of Langmann and Triola [LT23] showing the validity of (8.1.3) for temperatures $T \in [0, (1-\varepsilon)T_c]$.

For the precise statement of the universalities discussed here and proved in Chapters 9, 10 and 11, we refer the reader to the corresponding chapters.

8.2 Birman–Schwinger principle

The proofs of the universal formulas in Chapters 9, 10 and 11 follow mostly the same structure. A central ingredient is the Birman–Schwinger principle. We sketch the main ideas here.

First, we note that the BCS gap equation (8.1.1) is equivalent to the operator $K_T^\Delta + V$ having 0 as its lowest eigenvalue and the associated eigenvector is given by the minimizer α of the BCS functional. We use this in particular for the temperatures $T = 0$ (in which case $K_T^\Delta = E_\Delta$) and $T = T_c$ (in which case $\Delta = 0$). The Birman–Schwinger principle then says that the Birman–Schwinger operator

$$B_{T,\Delta} = \operatorname{sgn} V |V|^{1/2} (K_T^\Delta)^{-1} |V|^{1/2}$$

has -1 as its lowest eigenvalue with associated eigenvector $\operatorname{sgn} V|V|^{1/2}\alpha$. To study the Birman–Schwinger operator we define the integral

$$m(T,\Delta) = \frac{1}{|\mathbb{S}^{d-1}|} \int_{|p| \leq \sqrt{2\mu}} \frac{1}{K_T^\Delta(p)} \, \mathrm{d}p.$$

In the limit of weak superconductivity, where T_c and Δ are both small, this integral can be computed directly. At $T = 0$ and $T = T_c$ one finds

$$\begin{aligned} m(T=0,\Delta) &\approx \mu^{d/2-1} \left[\log \frac{\mu}{\Xi(T=0)} + \log(2c_d) \right], \\ m(T_c, \Delta = 0) &\approx \mu^{d/2-1} \left[\log \frac{\mu}{T_c} + \log \frac{e^\gamma}{\pi} + \log(2c_d) \right], \end{aligned} \tag{8.2.1}$$

for an explicit dimension-dependent constant c_d.

Using the integral $m(T,\Delta)$ we decompose the Birman–Schwinger operator into a dominant term and an error term as

$$B_{T,\Delta} = m(T,\Delta) \operatorname{sgn} V |V|^{1/2} \mathfrak{F}_\mu^\dagger \mathfrak{F}_\mu |V|^{1/2} + \operatorname{sgn} V |V|^{1/2} M_{T,\Delta} |V|^{1/2},$$

with $\mathfrak{F}_\mu : L^1(\mathbb{R}^d) \to L^2(\mathbb{S}^{d-1})$ a rescaled Fourier transform and $M_{T,\Delta}$ defined such that this holds. It is an error term. Using that $B_{T,\Delta}$ has -1 as its lowest eigenvalue and the decomposition above we find

$$m(T,\Delta) = -\left[\inf \operatorname{spec} \left(\mathfrak{F}_\mu |V|^{1/2} \frac{1}{1 + \operatorname{sgn} V |V|^{1/2} M_{T,\Delta} |V|^{1/2}} \operatorname{sgn} V |V|^{1/2} \mathfrak{F}_\mu^\dagger \right) \right]^{-1}. \tag{8.2.2}$$

Neglecting the error term and considering the temperatures $T = 0$ and $T = T_c$ we thus find that

$$m(T=0,\Delta) \approx m(T_c, \Delta = 0) \approx \frac{-1}{e_\mu}, \qquad e_\mu = \inf \operatorname{spec} \left(\mathfrak{F}_\mu V \mathfrak{F}_\mu^\dagger \right) < 0.$$

Combining with the direct evaluation of the integral $m(T, \Delta)$ in (8.2.1) we find the asymptotic formulas

$$T_c \approx 2c_d \frac{e^\gamma}{\pi} \exp\left(\frac{1}{\mu^{d/2-1} e_\mu}\right), \qquad \Xi(T=0) \approx 2c_d \exp\left(\frac{1}{\mu^{d/2-1} e_\mu}\right),$$

from which the universal ratio $\Xi(T=0)/T_c \approx \pi e^{-\gamma}$ follows.

For the proof that $\Xi/T_c \approx \mathsf{f}_{\mathsf{BCS}}(\sqrt{1-T/T_c})$ in Chapter 11 a more refined analysis is required. In particular one needs to treat the '$\log$-divergence' of the BCS gap equation (8.1.1). This '$\log$-divergence' can be understood as the logarithmic divergence of the integral $m(T, \Delta)$ in the limit $T, \Delta \to 0$, recall (8.2.1).

For temperatures not too close to the critical the analysis is comparable to the analysis sketched above with one key difference: In Chapter 11 we use the fact that $B_{T,\Delta}$ has lowest eigenvalue -1 simultaneously for two different temperatures. More precisely, using (8.2.2) for any temperature T together with the temperature T_c we find a formula for the difference $m(T, \Delta) - m(T_c, \Delta = 0)$. We bound this as being exponentially small in the coupling, see the details in Chapter 11. Further, the formula $m(T, \Delta) - m(T_c, \Delta = 0) \approx 0$ is essentially the defining equation for the function $\mathsf{f}_{\mathsf{BCS}}$, and so we find that $\Xi/T_c \approx \mathsf{f}_{\mathsf{BCS}}(\sqrt{1-T/T_c})$ as desired.

For temperatures close to the critical we instead use the relation of BCS theory to GL theory: Defining the (rather simple in our case) GL 'functional' $\mathcal{E}_{\mathsf{GL}} : \mathbb{C} \to \mathbb{R}$, the BCS gap function is given by $\Delta \approx \sqrt{1-T/T_c}|\psi_{\mathsf{GL}}|\Delta_0$, with ψ_{GL} the minimizer of the GL functional and Δ_0 a specific function used to define the GL functional, see Chapter 11. A precise analysis of the GL minimizer ψ_{GL} yields $|\psi_{\mathsf{GL}}| \approx \sqrt{\frac{8\pi^2}{7\zeta(3)} \frac{T_c}{\Delta_0(\sqrt{\mu})}}$ and thus

$$\frac{\Xi}{T_c} \approx \frac{\Delta(\sqrt{\mu})}{T_c} \approx \sqrt{\frac{8\pi^2}{7\zeta(3)}} \sqrt{1-T/T_c}.$$

This is exactly the value of the function $\mathsf{f}_{\mathsf{BCS}}$ for temperatures close to the critical, and so we find the universal ratio $\Xi/T_c \approx \mathsf{f}_{\mathsf{BCS}}(\sqrt{1-T/T_c})$ for temperatures close to the critical as claimed.

Chapter 9

Universality in low-dimensional BCS theory

This chapter contains the paper

[LowDim] J. Henheik, A. B. Lauritsen, and B. Roos. "Universality in low-dimensional BCS theory", *Rev. Math. Phys.* (2023), p. 2360005. DOI: 10.1142/S0129055X2360005X.

Abstract. It is a remarkable property of BCS theory that the ratio of the energy gap at zero temperature Ξ and the critical temperature T_c is (approximately) given by a universal constant, independent of the microscopic details of the fermionic interaction. This universality has rigorously been proven quite recently in three spatial dimensions and three different limiting regimes: weak coupling, low density, and high density. The goal of this short note is to extend the universal behavior to lower dimensions $d = 1, 2$ and give an exemplary proof in the weak coupling limit.

Contents

9.1 Introduction

The Bardeen–Cooper–Schrieffer (BCS) theory of superconductivity [BCS57] is governed by the *BCS gap equation*. For translation invariant systems without external fields the BCS gap equation is

$$\Delta(p) = -\frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \hat{V}(p-q) \frac{\Delta(q)}{E_\Delta(p)} \tanh\left(\frac{E_\Delta(p)}{2T}\right) \mathrm{d}q \tag{9.1.1}$$

with dispersion relation $E_\Delta(p) = \sqrt{(p^2-\mu)^2 + |\Delta(p)|^2}$. Here, $T \geq 0$ denotes the temperature and $\mu > 0$ the chemical potential. We consider dimensions $d \in \{1,2,3\}$. The Fourier transform of the potential $V \in L^1(\mathbb{R}^d) \cap L^{p_V}(\mathbb{R}^d)$ (with a d-dependent $p_V \geq 1$ to be specified below), modeling their effective interaction, is denoted by $\hat{V}(p) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} V(x) e^{-ip\cdot x}\, \mathrm{d}x$.

According to BCS theory, a system is in a superconducting state, if there exists a non-zero solution Δ to the gap equation (9.1.1). The question of existence of such a non-trivial solution Δ hinges, in particular, on the temperature T. It turns out, there exists a critical temperature $T_c \geq 0$ such that for $T < T_c$ there exists a non-trivial solution, and for $T \geq T_c$ it does not [HHSS08, Theorem 9.1.3 and Definition 9.1.4]. This critical temperature is one of the key (physically measurable) quantities of the theory and its asymptotic behavior, in three spatial dimensions, has been studied in three physically rather different limiting regimes: In a weak-coupling limit (i.e. replacing $V \to \lambda V$ and taking $\lambda \to 0$) [FHNS07; HS08b], in a low-density limit (i.e. $\mu \to 0$) [HS08a], and in a high-density limit (i.e. $\mu \to \infty$) [Hen22].

As already indicated above, at zero temperature, the function E_Δ may be interpreted as the dispersion relation of a certain 'approximate' Hamiltonian of the quantum many-body system, see [HHSS08, Appendix A]. In particular

$$\Xi := \inf_{p\in\mathbb{R}^d} E_\Delta(p) \tag{9.1.2}$$

has the interpretation of an energy gap associated with the approximate BCS Hamiltonian and as such represents a second key quantity of the theory. Analogously to the critical temperature, the asymptotic behavior of this energy gap, again in three spatial dimensions, has been studied in the same three different limiting regimes: In a weak coupling limit [HS08b], in a low density limit [Lau21], and in a high density limit [Chapter 10].

In this paper, we focus on a remarkable feature of BCS theory, which is well known in the physics literature [BCS57; LTB19; NS85]: The ratio of the energy gap Ξ and critical temperature T_c tends to a *universal constant, independent of the microscopic details* of the interaction between the fermions, i.e. the potential V. More precisely, in three spatial dimension, it holds that

$$\frac{\Xi}{T_c} \approx \frac{\pi}{e^\gamma} \approx 1.76\,, \tag{9.1.3}$$

where $\gamma \approx 0.577$ is the Euler-Mascheroni constant, in each of the three physically very different limits mentioned above. This result follows as a limiting equality by combining asymptotic formulas for the critical temperature T_c (see [FHNS07; HS08a; HS08b; Hen22]) and the energy gap Ξ (see [HS08b; Lau21] and Chapter 10) in the three different regimes. Although these scenarios (weak coupling, low density, and high density) are physically rather different, they all have in common that 'superconductivity is weak' and one can hence derive an asymptotic formula for T_c and Ξ as they depart from being zero (in the extreme cases $\lambda = 0$, $\mu = 0$, $\mu = \infty$, respectively). However, all the asymptotic expressions are *not perturbative*, as they depend exponentially on the natural dimensionless small parameter in the respective limit. We refer to the above mentioned original works for details.

The goal of this note is to prove the *same* universal behavior (9.1.3), which has already been established in three spatial dimension, also in dimensions $d = 1,2$ in the weak coupling limit (i.e. replacing $V \to \lambda V$ and taking $\lambda \to 0$). This situation serves as a showcase for the methods involved in the proofs of the various limits in three dimensions (see Remark 9.3.6 and Remark 9.3.9 below). Apart from the mathematical curiosity in $d = 1,2$, there have been recent studies in lower-dimensional superconductors in the physics literature, out of which we mention one-dimensional superconducting nanowires [NTH12] and two-dimensional 'magic angle' graphene [Cao+18].

In the remainder of this introduction, we briefly recall the mathematical formulation of BCS theory, which has been developed mostly by Hainzl and Seiringer, but also other co-authors [FHNS07; HHSS08; HS16]. Apart from the universality discussed here, also many other properties of BCS theory have been shown using this formulation: Most prominently, Ginzburg-Landau theory, as an effective theory describing superconductors close to the critical temperature, has been derived from BCS theory [DHM23a; DHM23b; FHSS12b; FL16]. More recently, it has been shown that the effect of boundary superconductivity occurs in the BCS model [HRS23]. We refer to [HS16] for a more comprehensive review of developments in the mathematical formulation of BCS theory. The universal behavior in the weak coupling limit for lower dimensions $d = 1, 2$ is presented in Section 9.2. Finally, in Section 9.3, we provide the proofs of the statements from Section 9.2.

9.1.1 Mathematical formulation of BCS theory

We will now briefly recall the mathematical formulation [HHSS08; HS16] of BCS theory [BCS57], which is an effective theory developed for describing superconductivity of a fermionic gas. In the following, we consider these fermions in $\mathbb{R}^d$, $d = 1, 2$, at temperature $T \geq 0$ and chemical potential $\mu \in \mathbb{R}$, interacting via a two-body potential V, for which we assume the following.

Assumption 9.1.1. We have that V is real-valued, reflection symmetric, i.e. $V(x) = V(-x)$ for all $x \in \mathbb{R}^d$, and it satisfies $V \in L^{p_V}(\mathbb{R}^d)$, where $p_V = 1$ if $d = 1$, $p_V \in (1, \infty)$ if $d = 2$.

Moreover, we neglect external fields, in which case the system is translation invariant.

The central object in the mathematical formulation of the theory is the BCS functional, which can naturally be viewed as a function of BCS states Γ. These states are given by a pair of functions (γ, α) and can be conveniently represented as a 2×2 matrix valued Fourier multiplier on $L^2(\mathbb{R}^d) \oplus L^2(\mathbb{R}^d)$ of the form

$$\hat{\Gamma}(p) = \begin{pmatrix} \hat{\gamma}(p) & \hat{\alpha}(p) \\ \overline{\hat{\alpha}(p)} & 1 - \hat{\gamma}(p) \end{pmatrix} \tag{9.1.4}$$

for all $p \in \mathbb{R}^d$. In (9.1.4), $\hat{\gamma}(p)$ denotes the Fourier transform of the one particle density matrix and $\hat{\alpha}(p)$ is the Fourier transform of the Cooper pair wave function. We require reflection symmetry of $\hat{\alpha}$, i.e. $\hat{\alpha}(-p) = \hat{\alpha}(p)$, as well as $0 \leq \hat{\Gamma}(p) \leq 1$ as a matrix.

The *BCS free energy functional* takes the form

$$\mathcal{F}_T[\Gamma] := \int_{\mathbb{R}^d} (p^2 - \mu)\hat{\gamma}(p)\, \mathrm{d}p - TS[\Gamma] + \int_{\mathbb{R}^d} V(x)|\alpha(x)|^2\, \mathrm{d}x\,, \qquad \Gamma \in \mathcal{D}, \tag{9.1.5}$$

$$\mathcal{D} := \left\{ \hat{\Gamma}(p) = \begin{pmatrix} \hat{\gamma}(p) & \hat{\alpha}(p) \\ \overline{\hat{\alpha}(p)} & 1 - \hat{\gamma}(p) \end{pmatrix} : 0 \leq \hat{\Gamma} \leq 1\,,\ \hat{\gamma} \in L^1(\mathbb{R}^d, (1+p^2)\, \mathrm{d}p)\,,\ \alpha \in H^1_{\mathrm{sym}}(\mathbb{R}^d) \right\},$$

where the *entropy density* is defined as

$$S[\Gamma] = -\int_{\mathbb{R}^d} \mathrm{Tr}_{\mathbb{C}^2}\left[\hat{\Gamma}(p) \log \hat{\Gamma}(p)\right] \mathrm{d}p\,.$$

The minimization problem associated with (9.1.5) is well defined. In fact, the following result has only been proven for $d = 3$ and $V \in L^{3/2}(\mathbb{R}^3)$, but its extension to $d = 1, 2$ is straightforward.

Proposition 9.1.2 ([HHSS08], see also [HS16])**.** *Under Assumption 9.1.1 on V, the BCS free energy is bounded below on $\mathcal{D}$ and attains its minimum.*

The BCS gap equation (9.1.1) arises as the Euler–Lagrange equations of this functional [HHSS08]. Namely by defining $\Delta = -2\widehat{V\alpha}$, the Euler–Lagrange equation for α takes the form of the BCS gap equation (9.1.1). Additionally, one has the following linear criterion for the BCS gap equation to have non-trivial solutions. Again, so far, a proof has only been given in spatial dimension $d = 3$ and for $V \in L^{3/2}(\mathbb{R}^3)$, but its extension to $d = 1, 2$ is straightforward.

Theorem 9.1.3 ([HHSS08, Thm. 1])**.** *Let V satisfy Assumption 9.1.1 and let $\mu \in \mathbb{R}$ as well as $T \geq 0$. Then, writing $\mathcal{F}_T[\Gamma] \equiv \mathcal{F}_T(\gamma, \alpha)$, the following are equivalent.*

1. *The minimizer of $\mathcal{F}_T$ is not attained with $\alpha = 0$, i.e.*

$$\inf_{(\gamma,\alpha)\in\mathcal{D}} \mathcal{F}_T(\gamma, \alpha) < \inf_{(\gamma,0)\in\mathcal{D}} \mathcal{F}_T(\gamma, 0),$$

2. *There exists a pair $(\gamma, \alpha) \in \mathcal{D}$ with $\alpha \neq 0$ such that $\Delta = -2\widehat{V\alpha}$ satisfies the BCS gap equation* (9.1.1)*,*

3. *The linear operator $K_T + V$, where $K_T(p) = \frac{p^2-\mu}{\tanh((p^2-\mu)/(2T))}$ has at least one negative eigenvalue.*

The third item immediately leads to the following definition of the *critical temperature* T_c for the existence of non-trivial solutions of the BCS gap equation (9.1.1).

Definition 9.1.4 (Critical temperature, see [FHNS07, Def. 1])**.** For V satisfying Assumption 9.1.1, we define the critical temperature $T_c \geq 0$ as

$$T_c := \inf\{T > 0 : K_T + V \geq 0\}\,. \tag{9.1.6}$$

By $K_T(p) \geq 2T$ and the asymptotic behavior $K_T(p) \sim p^2$ for $|p| \to \infty$, Sobolev's inequality [LL01, Thm. 8.3] implies that the critical temperature is well defined.

The other object we study is the energy gap Ξ defined in (9.1.2). The energy gap depends on the solution Δ of the gap equation (9.1.1) at $T = 0$. A priori, Δ may not be unique. However, for potentials with non-positive Fourier transform, this possibility can be ruled out.

Proposition 9.1.5 (see [HS08b, (21)-(22) and Lemma 2])**.** *Let V satisfy Assumption 9.1.1 (and additionally $V \in L^1(\mathbb{R}^2)$ in case that $d = 2$). Moreover, we assume that $\hat{V} \leq 0$ and $\hat{V}(0) < 0$. Then, there exists a unique minimizer Γ of $\mathcal{F}_0$ (up to a constant phase in α). One can choose the phase such that α has strictly positive Fourier transform $\hat{\alpha} > 0$.*

In particular, we conclude that Δ is strictly positive. Moreover, by means of the gap equation (9.1.1), Δ is continuous and thus $\Xi > 0$.

9.2 Main Results

As explained in the introduction, our main result in this short note is the extension of the universality (9.1.3) from $d = 3$ to lower spatial dimensions $d = 1, 2$ in the limit of weak coupling (i.e., replacing $V \to \lambda V$ and taking $\lambda \to 0$). We assume the following properties for the interaction potential V.

Assumption 9.2.1. Let $d \in \{1, 2\}$ and assume that V satisfies Assumption 9.1.1 as well as $\hat{V} \leq 0$, $\hat{V}(0) < 0$. Moreover, for $d = 1$ we assume that $(1 + |\cdot|^{\varepsilon})V \in L^1(\mathbb{R}^1)$ for some $\varepsilon > 0$. Finally, in case that $d = 2$, we suppose that $V \in L^1(\mathbb{R}^2)$ is radial.

By Proposition 9.1.5, this means that, in particular, the minimizer of $\mathcal{F}_0$ is unique (up to a phase) and the associated energy gap at zero temperature (9.1.2) is strictly positive, $\Xi > 0$. We are now ready to state our main result.

Theorem 9.2.2 (BCS Universality in one and two dimensions)**.** *Let V be as in Assumption 9.2.1. Then the critical temperature $T_c(\lambda)$ (defined in* (9.1.6)*) and the energy gap $\Xi(\lambda)$ (defined in* (9.1.2)*) are strictly positive for all $\lambda > 0$ and it holds that*

$$\lim_{\lambda \to 0} \frac{\Xi(\lambda)}{T_c(\lambda)} = \frac{\pi}{e^{\gamma}} \,,$$

where $\gamma \approx 0.577$ is the Euler-Mascheroni constant.

To prove the universality, we separately establish asymptotic formulas for T_c (see Theorem 9.2.5) and Ξ (see Theorem 9.2.7), valid to second order, and compare them by taking their ratio. The asymptotic formula for T_c is valid under weaker conditions on V than Assumption 9.2.1, because we do not need uniqueness of Δ. To obtain the asymptotic formulas, we first introduce two self-adjoint operators $\mathcal{V}_{\mu}^{(d)}$ and $\mathcal{W}_{\mu}^{(d)}$ mapping $L^2(\mathbb{S}^{d-1}) \to L^2(\mathbb{S}^{d-1})$ and as such measuring the strength of the interaction $\hat{V}$ on the (rescaled) Fermi surface (see [HS08b; Hen22] and Chapter 10). To assure that $\mathcal{V}_{\mu}^{(d)}$ and $\mathcal{W}_{\mu}^{(d)}$ will be well-defined and compact, we assume the following.

Assumption 9.2.3. Let V satisfy Assumption 9.1.1. Additionally, assume that for $d = 1$, $\Big(1 + (\ln(1 + |\cdot|))^2\Big)V \in L^1(\mathbb{R}^1)$ and for $d = 2$, $V \in L^1(\mathbb{R}^2)$.

First, in order to capture the strength to leading order, we define $\mathcal{V}_{\mu}^{(d)}$ via

$$(\mathcal{V}_{\mu}^{(d)} u)(p) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{S}^{d-1}} \hat{V}(\sqrt{\mu}(p - q))u(q) \, \mathrm{d}\omega(q) \,,$$

where $\mathrm{d}\omega$ is the Lebesgue measure on $\mathbb{S}^{d-1}$. Since $V \in L^1(\mathbb{R}^d)$, we have that $\hat{V}$ is a bounded continuous function and hence $\mathcal{V}_{\mu}^{(d)}$ is a Hilbert-Schmidt operator (in fact, trace class with trace being equal to $(2\pi)^{-d}|\mathbb{S}^{d-1}| \int_{\mathbb{R}^d} V(x) \, \mathrm{d}x$). Therefore, its lowest eigenvalue $e_{\mu}^{(d)} := \inf \operatorname{spec} \mathcal{V}_{\mu}^{(d)}$ satisfies $e_{\mu}^{(d)} \leq 0$ and it is strictly negative if e.g. $\int V < 0$ as in Assumption 9.2.1.

Second, in order to capture the strength of $\hat{V}$ to next to leading order, we define the operator $\mathcal{W}_\mu^{(d)}$ via its quadratic form

$$\begin{aligned}&\left\langle u\middle|\mathcal{W}_\mu^{(d)}\middle|u\right\rangle\\&=\mu^{d/2-1}\left[\int_{|p|<\sqrt{2}}\frac{1}{|p^2-1|}\left(|\psi(\sqrt{\mu}p)|^2-|\psi(\sqrt{\mu}p/|p|)|^2\right)\mathrm{d}p\right.\\&\quad\left.+\int_{|p|>\sqrt{2}}\frac{1}{|p^2-1|}|\psi(\sqrt{\mu}p)|^2\,\mathrm{d}p\right],\end{aligned}$$

where $\psi(p)=\frac{1}{(2\pi)^{d/2}}\int_{\mathbb{S}^{d-1}}\hat{V}(p-\sqrt{\mu}q)u(q)\,\mathrm{d}\omega(q)$ and $u\in L^2(\mathbb{S}^{d-1})$. The proof of the following proposition shall be given in Section 9.3.3.

Proposition 9.2.4. *Let $d\in\{1,2\}$ and let V satisfy Assumption 9.2.3. The operator $\mathcal{W}_\mu^{(d)}$ is well-defined and Hilbert-Schmidt.*

Next, we define the self-adjoint Hilbert-Schmidt operator

$$\mathcal{B}_\mu^{(d)}(\lambda):=\frac{\pi}{2}\left(\lambda\mathcal{V}_\mu^{(d)}-\lambda^2\mathcal{W}_\mu^{(d)}\right)$$

on $L^2(\mathbb{S}^{d-1})$ and its ground state energy

$$b_\mu^{(d)}(\lambda):=\inf\operatorname{spec}\left(\mathcal{B}_\mu^{(d)}(\lambda)\right). \tag{9.2.1}$$

Note that if $e_\mu^{(d)}<0$, then also $b_\mu^{(d)}(\lambda)<0$ for small enough λ. After these preparatory definitions, we are ready to state the separate asymptotic formulas for the critical temperature and the energy gap in one and two dimensions, which immediately imply Theorem 9.2.2.

Theorem 9.2.5 (Critical Temperature for $d=1,2$)**.** *Let $\mu>0$. Let V satisfy Assumption 9.2.3 and additionally $e_\mu^{(d)}<0$. Then the critical temperature T_c, given in Definition 9.1.4, is strictly positive and satisfies*

$$\lim_{\lambda\to0}\left(\ln\left(\frac{\mu}{T_c(\lambda)}\right)+\frac{\pi}{2\,\mu^{d/2-1}\,b_\mu^{(d)}(\lambda)}\right)=-\gamma-\ln\left(\frac{2c_d}{\pi}\right),$$

where γ denotes the Euler-Mascheroni constant and $c_1=\frac{4}{1+\sqrt{2}}$ and $c_2=1$.

Here, the Assumptions on V are weaker than Assumption 9.2.1, since $\hat{V}(0)<0$ implies that $e_\mu^{(d)}<0$. We thus have the asymptotic behavior

$$T_c(\lambda)=2c_d\,\frac{e^\gamma}{\pi}\left(1+o(1)\right)\mu\,e^{\pi/(2\mu^{d/2-1}b_\mu^{(d)}(\lambda))}$$

in the limit of small λ.

Remark 9.2.6. Theorem 9.2.5 is essentially a special case of [HS10, Theorem 2]. We give the proof here for two main reasons.

(i) There is still some work required to translate the statement of [HS10, Theorem 2] into a form in which it is comparable to that of Theorem 9.2.7 (in order to prove Theorem 9.2.2). The main difficulty is that the operator $\mathcal{W}_\mu^{(d)}$ in [HS10] is only defined via a limit, [HS10, Equation (2.10)].

(ii) The goal of this paper is to give an exemplary proof of Theorem 9.2.5 in order to compare it to the proofs of the similar statements in the literature concerning the asymptotic behavior of the critical temperature in various limits [HS08a; HS08b; Hen22].

Theorem 9.2.5 is complemented by the following asymptotics for the energy gap.

Theorem 9.2.7 (Energy Gap for $d = 1, 2$)**.** *Let V satisfy Assumption 9.2.1 and let $\mu > 0$. Then there exists a unique radially symmetric minimizer (up to a constant phase) of the BCS functional* (9.1.5) *at temperature $T = 0$. The associated energy gap Ξ, given in* (9.1.2)*, is strictly positive and satisfies*

$$\lim_{\lambda \to 0} \left(\ln\left(\frac{\mu}{\Xi}\right) + \frac{\pi}{2\,\mu^{d/2-1}\, b_\mu^{(d)}(\lambda)} \right) = -\ln(2c_d)\,,$$

where $b_\mu^{(d)}$ is defined in (9.2.1) *and $c_1 = \frac{4}{1+\sqrt{2}}$ and $c_2 = 1$.*

In other words, we have the asymptotic behavior

$$\Xi(\lambda) = 2c_d \Big(1 + o(1)\Big) \mu\, e^{\pi/(2\mu^{d/2-1} b_\mu^{(d)}(\lambda))}$$

in the limit of small λ. Now, Theorem 9.2.2 follows immediately from Theorems 9.2.5 and 9.2.7.

Remark 9.2.8 (Other limits in dimensions $d = 1, 2$)**.** Similarly to the presented results, one could also consider the limits of low and high density. We expect that also here the universality $\frac{\Xi}{T_c} \approx \frac{\pi}{e^{\gamma}}$ holds. As mentioned in the introduction, this has already been shown in three spatial dimensions [HS08a; Hen22; Lau21], [Chapter 10]. We expect that one could generalize the arguments of [HS08a; Hen22; Lau21], [Chapter 10] to lower dimensions, but that there will be some non-trivial technical difficulties in doing so. Also for the weak coupling limit presented here, the overall structure and ideas of the proof are the same in lower dimensions as in three dimensions [HS08b], but with non-trivial technical differences, see Remark 9.3.3.

The following is an example of such a non-trivial difference in the low-density limit. In three spatial dimensions [HS08a; Lau21] the asymptotic formulas for T_c and Ξ were obtained for attractive potentials V not creating bound states of $-\nabla^2 + V$. This latter condition ensures that the low-density limit is given by $\mu \to 0$. However, in spatial dimensions one and two, attractive potentials, no matter how weak, always give rise to bound states of $-\nabla^2 + V$, see [Sim76]. This means that one should not take the limit $\mu \to 0$, but rather the limit $\mu \to -E_b$, with $-E_b < 0$ the energy of the (lowest energy) bound state, see [HS12]. We will not deal with the low- and high-density limits here.

The rest of the paper is devoted to proving Theorem 9.2.5 and Theorem 9.2.7.

9.3 Proofs

The overall structure of our proofs is as follows: First, we argue that the Schrödinger type operators $K_{T_c} + \lambda V$ and $E_\Delta + \lambda V$ have lowest eigenvalue zero. The second step is to study the corresponding Birman-Schwinger operators

$$B_T^{(d)} := \lambda V^{1/2} K_T^{-1} |V|^{1/2} \quad \text{and} \quad B_\Delta^{(d)} := \lambda V^{1/2} E_\Delta^{-1} |V|^{1/2}\,,$$

where $V(x)^{1/2} = \operatorname{sgn}(V(x))|V(x)|^{1/2}$. According to the Birman-Schwinger principle, the lowest eigenvalue of $B_{T_c}^{(d)}$ and $B_{\Delta}^{(d)}$ is -1. It turns out, that for $X \in \{T, \Delta\}$ one can decompose

$$B_X^{(d)} = \lambda m_\mu^{(d)}(X) V^{1/2} (\mathfrak{F}_\mu^{(d)})^\dagger \mathfrak{F}_\mu^{(d)} |V|^{1/2} + \lambda V^{1/2} M_X^{(d)} |V|^{1/2}, \tag{9.3.1}$$

where $V^{1/2} M_X^{(d)} |V|^{1/2}$ are bounded operators,

$$m_\mu^{(d)}(T) = \frac{1}{|\mathbb{S}^{d-1}|} \int_{|p|<\sqrt{2\mu}} \frac{1}{K_T(p)} \mathrm{d}p, \tag{9.3.2}$$

$$m_\mu^{(d)}(\Delta) = \frac{1}{|\mathbb{S}^{d-1}|} \int_{|p|<\sqrt{2\mu}} \frac{1}{E_\Delta(p)} \mathrm{d}p, \tag{9.3.3}$$

and $\mathfrak{F}_\mu^{(d)} : L^1(\mathbb{R}^d) \to L^2(\mathbb{S}^{d-1})$ is the (scaled) Fourier transform restricted to the (rescaled) Fermi sphere,

$$\left(\mathfrak{F}_\mu^{(d)} \psi\right)(p) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \psi(x) e^{-i\sqrt{\mu} p \cdot x} \, \mathrm{d}x \, .$$

Note that for an L^1-function, pointwise values of its Fourier transform are well-defined by the Riemann–Lebesgue lemma. (In particular the restriction to a co–dimension 1 manifold of a sphere is well-defined.)

To satisfy the constraint that the lowest eigenvalue of the Birman-Schwinger operators is -1, the functions $m_\mu^{(d)}$ must diverge as $\lambda \to 0$. It turns out that this is only possible if T and Δ go to zero. For each $m_\mu^{(d)}$ one then derives the asymptotics up to second order in two ways, once from the constraint that $B_X^{(d)}$ has lowest eigenvalue -1 and once by directly computing the asymptotics of $m_\mu^{(d)}$ for T and Δ going to zero.

Indeed, for the critical temperature we obtain the following asymptotics, which, by combining them, immediately prove Theorem 9.2.5.

Proposition 9.3.1. *Let $\mu > 0$. Let V satisfy Assumption 9.2.3 and additionally $e_\mu^{(d)} < 0$. Then, the critical temperature T_c is positive and, as $\lambda \to 0$, we have that*

$$m_\mu^{(d)}(T_c) = -\frac{\pi}{2 b_\mu^{(d)}(\lambda)} + o(1) \, ,$$

$$m_\mu^{(d)}(T_c) = \mu^{d/2-1} \left(\ln\left(\frac{\mu}{T_c}\right) + \gamma + \ln\left(\frac{2c_d}{\pi}\right) + o(1) \right) .$$

For the energy gap we obtain the following asymptotics, which, again by combining them, immediately prove Theorem 9.2.7.

Proposition 9.3.2. *Let V satisfy Assumption 9.2.1 and let $\mu > 0$. Then (by Proposition 9.1.5) we have a strictly positive radially symmetric gap function Δ and associated energy gap Ξ, which, as $\lambda \to 0$, satisfy the asymptotics*

$$\Xi = \Delta(\sqrt{\mu})\Big(1 + o(1)\Big)$$

$$m_\mu^{(d)}(\Delta) = -\frac{\pi}{2 b_\mu^{(d)}(\lambda)} + o(1)$$

$$m_\mu^{(d)}(\Delta) = \mu^{d/2-1} \left(\ln\left(\frac{\mu}{\Delta(\sqrt{\mu})}\right) + \ln(2c_d) + o(1) \right)$$

With a slight abuse of notation, using radiality of Δ, we wrote $\Delta(\sqrt{\mu})$ instead of $\Delta(\sqrt{\mu}\hat{p})$ for some $\hat{p} \in \mathbb{S}^{d-1}$.

Remark 9.3.3. The main technical differences between $d \in \{1,2\}$ considered here and the proof for $d=3$ in [HS08b] arise when bounding $V^{1/2} M_X^{(d)} |V|^{1/2}$. The underlying reason is that the Fourier transform of the constant function on the sphere $j_d(x) = (2\pi)^{-d/2} \int_{\mathbb{S}^{d-1}} e^{ip\cdot x}\, \mathrm{d}\omega(p)$ decays like $1/|x|$ for large $|x|$ in three dimensions, but only like $|x|^{-1/2}$ in two dimensions and does not decay for $d=1$.

Remark 9.3.4. In [CM21], Cuenin and Merz use the Tomas-Stein theorem to define $\mathfrak{F}_\mu^{(d)}$ on a larger space than $L^1(\mathbb{R}^d)$. With this they are able to prove a general version of Theorem 9.2.5 under slightly weaker conditions on V. However, we do not pursue this here, see Remark 9.2.6.

9.3.1 Proof of Proposition 9.3.1

Proof of Proposition 9.3.1. The argument is divided into several steps.

1. A priori spectral information on $K_{T_c} + \lambda V$. First note that, due to Theorem 9.1.3 and Definition 9.1.4, the critical temperature T_c is determined by the lowest eigenvalue of $K_T + \lambda V$ being 0 exactly for $T = T_c$.

2. Birman-Schwinger principle. Next, we employ the Birman-Schwinger principle, which says that the compact Birman-Schwinger operator $B_T^{(d)} = \lambda V^{1/2} K_T^{-1} |V|^{1/2}$ has -1 as its lowest eigenvalue exactly for $T = T_c$, see [FHNS07; HS08b].

Using the notation for the Fourier transform restricted to the rescaled Fermi sphere introduced above, we now decompose the Birman-Schwinger operator as in (9.3.1), where $M_T^{(d)}$ is defined through the integral kernel

$$\begin{aligned} M_T^{(d)}(x,y) = \frac{1}{(2\pi)^d} \Bigg[&\int_{|p|<\sqrt{2\mu}} \frac{1}{K_T(p)} \left(e^{ip\cdot(x-y)} - e^{i\sqrt{\mu}p/|p|\cdot(x-y)} \right) \mathrm{d}p \\ &+ \int_{|p|>\sqrt{2\mu}} \frac{1}{K_T} e^{ip\cdot(x-y)}\, \mathrm{d}p \Bigg] . \end{aligned} \tag{9.3.4}$$

We claim that $V^{1/2} M_T^{(d)} |V|^{1/2}$ is uniformly bounded.

Lemma 9.3.5. *Let $\mu > 0$. Let V satisfy Assumption 9.2.3. Then we have for all $T \geq 0$*

$$\left\| V^{1/2} M_T^{(d)} |V|^{1/2} \right\|_{\mathsf{HS}} \leq C \,,$$

where $C > 0$ denotes some positive constant and $\|\cdot\|_{\mathsf{HS}}$ is the Hilbert-Schmidt norm.

Armed with this bound, we have that for sufficiently small λ that $1 + \lambda V^{1/2} M_T^{(d)} |V|^{1/2}$ is invertible, and hence

$$1 + B_T^{(d)} = (1 + \lambda V^{1/2} M_T^{(d)} |V|^{1/2}) \left(1 + \frac{\lambda m_\mu^{(d)}(T)}{1 + \lambda V^{1/2} M_T^{(d)} |V|^{1/2}} V^{1/2} (\mathfrak{F}_\mu^{(d)})^\dagger \mathfrak{F}_\mu^{(d)} |V|^{1/2} \right) .$$

Thus, the fact that $B_T^{(d)}$ has lowest eigenvalue -1 at $T = T_c$ is equivalent to

$$\lambda m_\mu^{(d)}(T) \mathfrak{F}_\mu^{(d)} |V|^{1/2} \frac{1}{1 + \lambda V^{1/2} M_T^{(d)} |V|^{1/2}} V^{1/2} (\mathfrak{F}_\mu^{(d)})^\dagger \tag{9.3.5}$$

having lowest eigenvalue -1, again at $T = T_c$, as it is isospectral to the rightmost operator on the right-hand-side above. (Recall that for bounded operators A, B, the operators AB and

BA have the same spectrum apart from possibly at 0. However, in our case, both operators are compact on an infinite dimensional space and hence 0 is in both spectra.)

We now prove Lemma 9.3.5.

Proof of Lemma 9.3.5. We want to bound the integral kernel (9.3.4) of $M_T^{(d)}$ uniformly in T. Hence, we will bound $K_T \geq |p^2-\mu|$. The computation is slightly different in $d=1$ and $d=2$, so we do them separately.

$\underline{d=1.}$ The second integral in (9.3.4) is bounded by

$$2\int_{|p|>\sqrt{2\mu}} \frac{1}{|p^2-\mu|}\,\mathrm{d}p = \frac{2\operatorname{arcoth}\sqrt{2}}{\sqrt{\mu}}.$$

For the first integral, we use that $|e^{ix}-e^{iy}| \leq \min\{|x-y|,2\}$, $|p^2-\mu| \geq \sqrt{\mu}||p|-\sqrt{\mu}|$, and increase the domain of integration to obtain the bound

$$\begin{aligned}\frac{2}{\sqrt{\mu}}\int_0^{2\sqrt{\mu}} \frac{\min\left\{||p-\sqrt{\mu}||x-y|,2\right\}}{|p-\sqrt{\mu}|}\,\mathrm{d}p &= \frac{8}{\sqrt{\mu}}\left[1+\ln\left(\max\left\{\frac{|x-y|\sqrt{\mu}}{2},1\right\}\right)\right]\\ &\leq \frac{8}{\sqrt{\mu}}(1+\ln(1+\sqrt{\mu}\max\{|x|,|y|\}).\end{aligned}$$

We conclude that $|M_T^{(1)}(x,y)| \lesssim \frac{1}{\sqrt{\mu}}(1+\ln(1+\sqrt{\mu}\max\{|x|,|y|\}))$. Hence,

$$\left\|V^{1/2}M_T^{(1)}|V|^{1/2}\right\|_{\mathsf{HS}}^2 \lesssim \frac{1}{\mu}\left(\|V\|_{L^1(\mathbb{R})}^2 + \|V\|_{L^1(\mathbb{R})}\int_{\mathbb{R}}|V(x)|(1+\ln(1+\sqrt{\mu}|x|))^2\,\mathrm{d}x\right).$$

$\underline{d=2}$. We first compute the angular integral. Note that $\int_{\mathbb{S}^1} e^{ipx}\,\mathrm{d}\omega(p) = 2\pi J_0(|x|)$, where J_0 is the zeroth order Bessel function. For the second integral in (9.3.4) we may bound $|p^2-\mu| \geq cp^2$. Up to some finite factor, the second integral is hence bounded by

$$\int_{\sqrt{2\mu}}^{\infty} \frac{1}{p}|J_0(p|x-y|)|\,\mathrm{d}p \leq C\int_{\sqrt{2\mu}}^{\infty}\frac{1}{p^{1+\lambda}}|x-y|^{-\lambda}\,\mathrm{d}p \leq C_\lambda|x-y|^{-\lambda},$$

for any $0<\lambda\leq 1/2$ since $|J_0(x)|\leq C$ and $\sqrt{x}J_0(x)\leq C$, see e.g. [BSMM12, (9.55f), (9.57a)]. For the first integral we get the bound

$$\int_0^{\sqrt{2\mu}} \frac{p}{|p^2-\mu|}\,|J_0(p|x-y|)-J_0(\sqrt{\mu}|x-y|)|\,\mathrm{d}p.$$

Here we use that J_0 is Lipschitz, since its derivative J_{-1} is bounded (see e.g. [BSMM12, (9.55a), (9.55f)]), so that

$$|J_0(x)-J_0(y)| \leq C|x-y|^{1/3}(|J_0(x)|+|J_0(y)|)^{2/3} \leq C|x-y|^{1/3}\left(x^{-1/3}+y^{-1/3}\right).$$

That is

$$|J_0(p|x-y|)-J_0(\sqrt{\mu}|x-y|)| \leq C\frac{|p-\sqrt{\mu}|^{1/3}}{p^{1/3}+\sqrt{\mu}^{1/3}}.$$

This shows that the first integral is bounded. We conclude that $|M_T^{(2)}(x,y)| \lesssim 1 + \frac{1}{|x-y|^\lambda}$ for any $0 < \lambda \leq 1/2$. Then, by the Hardy–Littlewood–Sobolev inequality [LL01, Theorem 4.3] we have that

$$\left\| V^{1/2} M_T^{(2)} |V|^{1/2} \right\|_{\mathsf{HS}}^2 = \iint |V(x)||M_T^{(2)}(x,y)||V(y)| \,\mathsf{d}x\,\mathsf{d}y \lesssim \|V\|_{L^1(\mathbb{R}^2)}^2 + \|V\|_{L^p(\mathbb{R}^2)}^2$$

for any $1 < p \leq 4/3$. □

3. First order. Evaluating (9.3.5) at $T = T_c$ and expanding the geometric series to first order we get

$$\begin{aligned} -1 &= \lambda m_\mu^{(d)}(T_c) \inf \operatorname{spec} \left(\mathfrak{F}_\mu^{(d)} |V|^{1/2} \frac{1}{1 + \lambda V^{1/2} M_{T_c}^{(d)} |V|^{1/2}} V^{1/2} (\mathfrak{F}_\mu^{(d)})^\dagger \right) \\ &= \lambda\, m_\mu^{(d)}(T_c) \, \inf \operatorname{spec} \mathcal{V}_\mu^{(d)} (1 + O(\lambda)) = \lambda\, m_\mu^{(d)}(T_c)\, e_\mu^{(d)} (1 + O(\lambda)) \end{aligned}$$

where we used $\mathcal{V}_\mu^{(d)} = \mathfrak{F}_\mu^{(d)} V (\mathfrak{F}_\mu^{(d)})^\dagger$. Since by assumption $e_\mu^{(d)} < 0$, this shows that $m_\mu^{(d)}(T_c) \to \infty$ as $\lambda \to 0$.

4. A priori bounds on T_c. By (9.3.2), the divergence of $m_\mu^{(d)}$ as $\lambda \to 0$ in particular shows that $T_c/\mu \to 0$ in the limit $\lambda \to 0$.

5. Calculation of the integral $m_\mu^{(d)}(T_c)$. This step is very similar to [HS08b, Lemma 1] and [HRS23, Lemma 3.5], where the asymptotics have been computed for slightly different definitions of $m_\mu^{(d)}$ in three and one spatial dimension, respectively. Integrating over the angular variable and substituting $s = \left| \frac{|p|^2}{\mu} - 1 \right|$, we get

$$m_\mu^{(d)}(T_c) = \mu^{d/2-1} \int_0^1 \tanh\left(\frac{s}{2(T_c/\mu)} \right) \frac{(1+s)^{d/2-1} + (1-s)^{d/2-1}}{2s} \,\mathsf{d}s.$$

According to [HS08b, Lemma 1],

$$\lim_{T_c \downarrow 0} \left(\int_0^1 \frac{\tanh\left(\frac{s}{2(T_c/\mu)}\right)}{s} \,\mathsf{d}s - \ln \frac{\mu}{T_c} \right) = \gamma - \ln \frac{\pi}{2}.$$

By monotone convergence, it follows that

$$m_\mu^{(d)}(T_c) = \mu^{d/2-1} \left[\ln \frac{\mu}{T_c} + \gamma - \ln \frac{\pi}{2} + \int_0^1 \frac{(1-s)^{d/2-1} + (1+s)^{d/2-1} - 2}{2s} \,\mathsf{d}s + o(1) \right].$$

The remaining integral equals $\ln c_d$ and we have thus proven the second item in Proposition 9.3.1.

Combining this with the third step, one immediately sees that the critical temperature vanishes exponentially fast, $T_c \sim e^{1/\lambda e_\mu}$, as $\lambda \to 0$, recalling that $e_\mu^{(d)} < 0$ by assumption.

6. Second order. Now, to show the universality, we need to compute the next order correction. To do so, we expand the geometric series in (9.3.5) and employ first order perturbation theory, yielding that

$$m_\mu^{(d)}(T_c) = \frac{-1}{\lambda \left\langle u \middle| \mathfrak{F}_\mu^{(d)} V (\mathfrak{F}_\mu^{(d)})^\dagger \middle| u \right\rangle - \lambda^2 \left\langle u \middle| \mathfrak{F}_\mu^{(d)} V M_{T_c}^{(d)} V (\mathfrak{F}_\mu^{(d)})^\dagger \middle| u \right\rangle + O(\lambda^3)}, \tag{9.3.6}$$

where u is the (normalized) ground state (eigenstate of lowest eigenvalue) of $\mathfrak{F}_\mu^{(d)} V (\mathfrak{F}_\mu^{(d)})^\dagger$. (In case of a degenerate ground state, u is the ground state minimizing the second order term.)

This second order term in the denominator of (9.3.6) is close to $\mathcal{W}_\mu^{(d)}$. More precisely, it holds that

$$\lim_{\lambda\to 0} \left\langle u \middle| \mathfrak{F}_\mu^{(d)} V M_{T_c}^{(d)} V (\mathfrak{F}_\mu^{(d)})^\dagger \middle| u \right\rangle = \left\langle u \middle| \mathcal{W}_\mu^{(d)} \middle| u \right\rangle , \tag{9.3.7}$$

which easily follows from dominated convergence, noting that $\frac{1}{K_T}$ increases to $\frac{1}{|p^2-\mu|}$ as $T \to 0$. We then conclude that

$$\lim_{\lambda\to 0} \left(m_\mu^{(d)}(T_c) + \frac{\pi}{2 b_\mu^{(d)}(\lambda)} \right) = 0 ,$$

since $\left\langle u \middle| \lambda \mathcal{V}_\mu^{(d)} - \lambda^2 \mathcal{W}_\mu^{(d)} \middle| u \right\rangle = \inf \operatorname{spec}(\lambda \mathcal{V}_\mu^{(d)} - \lambda^2 \mathcal{W}_\mu^{(d)}) + O(\lambda^3) = \frac{\pi}{2} b_\mu^{(d)}(\lambda) + O(\lambda^3)$, again by first-order perturbation theory. This concludes the proof of Proposition 9.3.1. □

We conclude this subsection with several remarks, comparing our proof with those of similar results from the literature.

Remark 9.3.6 (Structure here vs. in earlier papers on T_c)**.** We compare the structure of our proof to that of the different limits in three dimensions [HS08a; HS08b; Hen22]:

- **Weak coupling:** The structure of the proof we gave here is quite similar to that of [HS08b], only they do Steps 5 and 6 in the opposite order. Also the leading term for T_c was shown already in [FHNS07], where a computation somewhat similar to Steps 1–4 is given.
- **High density:** For $\mu \to \infty$, the structure of the proof in [Hen22] is slightly different compared to the one given here. This is basically due to the facts that (i) the necessary a priori bound $T_c = o(\mu)$ already requires the Birman-Schwinger decomposition and (ii) the second order requires strengthened assumptions compared to the first order. To conclude, the order of steps in [Hen22] can be thought of as: 1, 5, 4 (establishing $T_c = O(\mu)$), 2, 3, 4 (establishing $T_c = o(\mu)$), 2 (again), 6. Here the final step is much more involved than in the other limits considered.
- **Low density:** As above, for the proof of the low density limit in [HS08a] the structure is slightly different. One first needs the a priori bound $T_c = o(\mu)$ on the critical temperature before one uses the Birman-Schwinger principle and decomposes the Birman-Schwinger operator.[1] Also, the decomposition of the Birman-Schwinger operator is again different. For the full decomposition and analysis of the Birman-Schwinger operator one needs also the first-order analysis, that is Step 2, which is done in two parts. The order of the steps in [HS08a] can then mostly be though of as: 1, 4, 5, 2, 3, 2 (again), 6.

9.3.2 Proof of Proposition 9.3.2

Proof of Proposition 9.3.2. The structure of the proof is parallel to that of Proposition 9.3.1 for the critical temperature.

1. A priori spectral information on $E_\Delta + \lambda V$**.** First, it is proven in [HS08b, Lemma 2] that

[1]Strictly speaking, in [HS08a], it is only proven that $T_c = O(\mu)$ (which is sufficient for applying the Birman-Schwinger principle), while the full $T_c = o(\mu)$ itself requires the Birman-Schwinger decomposition (see [Lau20, Remark 4.12] for details).

$\mathcal{F}_0$ has a unique minimizer α which has strictly positive Fourier transform. Using radiality of V, it immediately follows that this minimizer is rotationally symmetric (since otherwise rotating α would give a different minimizer) and hence also $\Delta = -2\lambda\hat{V} \star \hat{\alpha}$ is rotation invariant. It directly follows from [HS08b, (43) and Lemma 3] that that $E_\Delta + \lambda V$ has lowest eigenvalue 0, and that the minimizer α is the corresponding eigenfunction.

2. Birman-Schwinger principle. This implies, by means of the Birman-Schwinger principle, that the Birman-Schwinger operator $B_\Delta^{(d)} = \lambda V^{1/2} E_\Delta^{-1} |V|^{1/2}$ has -1 as its lowest eigenvalue. As in the proof of Proposition 9.3.1, we decompose it as described in (9.3.1) and prove the second summand to be uniformly bounded.

Lemma 9.3.7. *Let $\mu > 0$. Let V satisfy Assumption 9.2.3. Then, uniformly in small λ, we have*

$$\left\| V^{1/2} M_\Delta^{(d)} |V|^{1/2} \right\|_{\mathsf{HS}} \leq C\,.$$

With this one may similarly factor

$$1+B_\Delta^{(d)} = (1+\lambda V^{1/2} M_\Delta^{(d)} |V|^{1/2}) \left(1 + \frac{\lambda m_\mu^{(d)}(\Delta)}{1+\lambda V^{1/2} M_\Delta^{(d)} |V|^{1/2}} V^{1/2} (\mathfrak{F}_\mu^{(d)})^\dagger \mathfrak{F}_\mu^{(d)} |V|^{1/2} \right) \tag{9.3.8}$$

and conclude that

$$T_\Delta^{(d)} := \lambda m_\mu^{(d)}(\Delta) \mathfrak{F}_\mu^{(d)} |V|^{1/2} \frac{1}{1+\lambda V^{1/2} M_\Delta^{(d)} |V|^{1/2}} V^{1/2} (\mathfrak{F}_\mu^{(d)})^\dagger \tag{9.3.9}$$

has lowest eigenvalue -1.

Proof of Lemma 9.3.7. Note that M_Δ has kernel

$$\begin{aligned} M_\Delta(x,y) = \frac{1}{(2\pi)^d} \Bigg[&\int_{|p|<\sqrt{2\mu}} \frac{1}{E_\Delta(p)} \left(e^{ip\cdot(x-y)} - e^{i\sqrt{\mu}p/|p|\cdot(x-y)} \right) \mathsf{d}p \\ &+ \int_{|p|>\sqrt{2\mu}} \frac{1}{E_\Delta(p)} e^{ip\cdot(x-y)} \,\mathsf{d}p \Bigg] . \end{aligned}$$

We may bound this exactly as in the proof of Lemma 9.3.5 using that $E_\Delta(p) \geq |p^2 - \mu|$. □

3. First order. Expanding the geometric series in (9.3.9) to first order, we see that

$$\begin{aligned} -1 &= \lambda m_\mu^{(d)}(\Delta) \inf \operatorname{spec} \left(\mathfrak{F}_\mu^{(d)} |V|^{1/2} \frac{1}{1+\lambda V^{1/2} M_\Delta^{(d)} |V|^{1/2}} V^{1/2} (\mathfrak{F}_\mu^{(d)})^\dagger \right) \\ &= \lambda m_\mu^{(d)}(\Delta) \inf \operatorname{spec} \mathcal{V}_\mu^{(d)} (1+O(\lambda)) = \lambda e_\mu^{(d)} m_\mu^{(d)}(\Delta)(1+O(\lambda)). \end{aligned}$$

Hence, in particular, $m_\mu^{(d)}(\Delta) \sim -\frac{1}{\lambda e_\mu^{(d)}} \to \infty$ as $\lambda \to 0$.

4. A priori bounds on Δ. We now prepare for the computation of the integral $m_\mu^{(d)}(\Delta)$ in terms of $\Delta(\sqrt{\mu})$. This requires two types of bounds on Δ: One bound estimating the gap function $\Delta(p)$ at general momentum $p \in \mathbb{R}^d$ in terms of $\Delta(\sqrt{\mu})$ (see (9.3.10)), and one bound controlling the difference $|\Delta(p) - \Delta(q)|$ in some kind of Hölder-continuity estimate (see (9.3.11)).

Lemma 9.3.8. *Suppose that V is as in Assumption 9.2.1. Then for λ small enough*

$$\Delta(p) = f(\lambda)\left(\int_{\mathbb{S}^{d-1}} \hat{V}(p-\sqrt{\mu}q)\,\mathrm{d}\omega(q) + \lambda\eta_\lambda(p)\right),$$

where f is some function of λ and $\|\eta_\lambda\|_{L^\infty(\mathbb{R}^d)}$ is bounded uniformly in λ.

Proof. Recall that α is the eigenfunction of $E_\Delta + \lambda V$ with lowest eigenvalue 0. Then, by the Birman-Schwinger principle, $\phi = V^{1/2}\alpha$ satisfies

$$B_\Delta\phi = \lambda V^{1/2}\frac{1}{E_\Delta}|V|^{1/2}V^{1/2}\alpha = -\phi.$$

With the decomposition Equation (9.3.8) then ϕ is an eigenfunction of

$$\frac{\lambda m_\mu^{(d)}(\Delta)}{1+\lambda V^{1/2}M_\Delta^{(d)}|V|^{1/2}}V^{1/2}(\mathfrak{F}_\mu^{(d)})^\dagger\mathfrak{F}_\mu^{(d)}|V|^{1/2}$$

of eigenvalue -1. Thus, $\mathfrak{F}_\mu^{(d)}|V|^{1/2}\phi$ is an eigenfunction of $T_\Delta^{(d)}$ of (lowest) eigenvalue -1. Now $u = |\mathbb{S}^{d-1}|^{-1/2}$ is the unique eigenfunction corresponding to the lowest eigenvalue of $\mathcal{V}_\mu^{(d)}$ by radiality of V and the assumption $\hat{V}\le 0$ (see e.g. [FHNS07]). Hence, for λ small enough, u is the unique eigenfunction of $T_\Delta^{(d)}$ of smallest eigenvalue. Thus,

$$\phi = f(\lambda)\frac{1}{1+\lambda V^{1/2}M_\Delta^{(d)}|V|^{1/2}}V^{1/2}(\mathfrak{F}_\mu^{(d)})^\dagger u = f(\lambda)\left(V^{1/2}(\mathfrak{F}_\mu^{(d)})^\dagger u + \lambda\xi_\lambda\right)$$

for some number $f(\lambda)$. The function ξ_λ satisfies $\|\xi_\lambda\|_{L^2(\mathbb{R}^d)}\le C$ by Lemma 9.3.7. Noting that $\Delta = -2\widehat{|V|^{1/2}\phi}$ and bounding $\left\|\widehat{|V|^{1/2}\xi_\lambda}\right\|_{L^\infty} \le \|V\|_{L^1}^{1/2}\|\xi_\lambda\|_{L^2}$ we get the desired. □

Evaluating the formula in Lemma 9.3.8 at $p=\sqrt{\mu}$ we get $|f(\lambda)|\le C\Delta(\sqrt{\mu})$ for λ small enough. This in turn implies that

$$\Delta(p)\le C\Delta(\sqrt{\mu}). \tag{9.3.10}$$

For the Hölder-continuity, we have by rotation invariance

$$\begin{aligned}
&\left|\int \hat{V}(p-\sqrt{\mu}r)-\hat{V}(q-\sqrt{\mu}r)\,\mathrm{d}\omega(r)\right| = \left|\int \hat{V}(|p|e_1-\sqrt{\mu}r)-\hat{V}(|q|e_1-\sqrt{\mu}r)\,\mathrm{d}\omega(r)\right| \\
&\quad= \left|\frac{1}{(2\pi)^{d/2}}\int_{\mathbb{R}^d}\mathrm{d}x\left(V(x)\left(e^{i|p|x_1}-e^{i|q|x_1}\right)\int_{\mathbb{S}^{d-1}}e^{-i\sqrt{\mu}x\cdot r}\,\mathrm{d}\omega(r)\right)\right| \\
&\quad\le C_\varepsilon\mu^{-\varepsilon/2}||p|-|q||^\varepsilon\int\mathrm{d}x\left(|V(x)|(\sqrt{\mu}|x|)^\varepsilon\left|\int_{\mathbb{S}^{d-1}}e^{-i\sqrt{\mu}x\cdot r}\,\mathrm{d}\omega(r)\right|\right),
\end{aligned}$$

for any $0<\varepsilon\le 1$. For $d=2$ we have $V\in L^1(\mathbb{R}^2)$ and

$$\left|\int_{\mathbb{S}^{d-1}}e^{-i\sqrt{\mu}xr}\,\mathrm{d}\omega(r)\right| = |J_0(\sqrt{\mu}|x|)|\le(\sqrt{\mu}|x|)^{-1/2}.$$

For $d=1$ we have $|x|^\varepsilon V\in L^1(\mathbb{R})$ for some $\varepsilon>0$ and

$$\left|\int_{\mathbb{S}^{d-1}}e^{-i\sqrt{\mu}x\cdot r}\,\mathrm{d}\omega(r)\right| = 2|\cos(\sqrt{\mu}|x|)|\le 2.$$

We conclude that with $\varepsilon = 1/2$ for $d=2$ and small enough $\varepsilon > 0$ for $d=1$

$$|\Delta(p) - \Delta(q)| \leq C|f(\lambda)| \left(\mu^{-\varepsilon/2}||p|-|q||^{\varepsilon} + \lambda\right) \leq C|\Delta(\sqrt{\mu})| \left(\mu^{-\varepsilon/2}||p|-|q||^{\varepsilon} + \lambda\right). \tag{9.3.11}$$

Additionally, since $m_\mu^{(d)}(\Delta) \to \infty$ we have that $\Delta(p) \to 0$ at least for some $p \in \mathbb{R}^d$ by (9.3.3). Then it follows from Lemma 9.3.8 that $f(\lambda) \to 0$, i.e. that $\Delta(p) \to 0$ for all p.

5. Calculation of the integral $m_\mu^{(d)}(\Delta)$. Armed with the a priori bounds (9.3.10) and (9.3.11), we can now compute the integral $m_\mu^{(d)}(\Delta)$. Carrying out the angular integration and substituting $s = \left|\frac{|p|^2-\mu}{\mu}\right|$ we have

$$\begin{aligned} m_\mu^{(d)}(\Delta) = \frac{\mu^{d/2-1}}{2} \Bigg[&\int_0^1 \left(\frac{(1-s)^{d/2-1} - 1}{\sqrt{s^2 + x_-(s)^2}} + \frac{(1+s)^{d/2-1} - 1}{\sqrt{s^2 + x_+(s)^2}} \right) \mathrm{d}s \\ &+ \int_0^1 \left(\frac{1}{\sqrt{s^2 + x_-(s)^2}} + \frac{1}{\sqrt{s^2 + x_+(s)^2}} \right) \mathrm{d}s \Bigg], \end{aligned}$$

where $x_\pm(s) = \frac{\Delta(\sqrt{\mu}\sqrt{1\pm s})}{\mu}$. By dominated convergence, using that $x_\pm(s) \to 0$, the first integral is easily seen to converge to

$$\int_0^1 \left(\frac{(1-s)^{d/2-1} - 1}{s} + \frac{(1+s)^{d/2-1} - 1}{s} \right) \mathrm{d}s = 2 \ln c_d$$

for $\lambda \to 0$. For the second integral, we will now show that

$$\int_0^1 \left(\frac{1}{\sqrt{s^2 + x_\pm(s)^2}} - \frac{1}{\sqrt{s^2 + x_\pm(0)^2}} \right) \mathrm{d}s \to 0\,.$$

In fact, the integrand is bounded by

$$\begin{aligned} &\left| \frac{1}{\sqrt{s^2 + x_\pm(s)^2}} - \frac{1}{\sqrt{s^2 + x_\pm(0)^2}} \right| \\ &\quad = \frac{|x_\pm(0)^2 - x_\pm(s)^2|}{\sqrt{s^2 + x_\pm(s)^2}\sqrt{s^2 + x_\pm(0)^2}(\sqrt{s^2 + x_\pm(s)^2} + \sqrt{s^2 + x_\pm(0)^2})} \\ &\quad \leq \frac{C x_\pm(0)(s^\varepsilon + \lambda)}{\sqrt{s^2 + x_\pm(s)^2}\sqrt{s^2 + x_\pm(0)^2}}, \end{aligned}$$

using the Hölder continuity from (9.3.11). By continuity of $\hat{V}$ there exists some s_0 (independent of λ) such that for $s < s_0$ we have $x_\pm(s) \geq c x_\pm(0)$. We now split the integration into $\int_0^{s_0}$ and $\int_{s_0}^1$. For the first we have

$$\begin{aligned} \int_0^{s_0} \left| \frac{1}{\sqrt{s^2 + x_\pm(s)^2}} - \frac{1}{\sqrt{s^2 + x_\pm(0)^2}} \right| \mathrm{d}s &\leq C \int_0^{s_0} \frac{x_\pm(0)}{s^2 + x_\pm(0)^2} (s^\varepsilon + \lambda)\, \mathrm{d}s \\ &= O(x_\pm(0)^\varepsilon + \lambda)\,. \end{aligned}$$

For the second we have

$$\int_{s_0}^1 \left| \frac{1}{\sqrt{s^2 + x_\pm(s)^2}} - \frac{1}{\sqrt{s^2 + x_\pm(0)^2}} \right| \mathrm{d}s \leq C \int_{s_0}^1 x_\pm(0) \frac{s^\varepsilon + \lambda}{s^2}\, \mathrm{d}s = O(x_\pm(0))\,.$$

Collecting all the estimates, we have thus shown that $m_\mu^{(d)}(\Delta)$ equals

$$\mu^{d/2-1}\left(\ln c_d+\int_0^1 \frac{1}{\sqrt{s^2+\Delta(\sqrt{\mu})^2/\mu^2}}\,\mathrm{d}s+o(1)\right)$$
$$=\mu^{d/2-1}\left(\ln c_d+\ln\left(\frac{\mu+\sqrt{\mu^2+\Delta(\sqrt{\mu})^2}}{|\Delta(\sqrt{\mu})|}\right)+o(1)\right)=\mu^{d/2-1}\ln\left(\frac{2\mu c_d}{|\Delta(\sqrt{\mu})|}+o(1)\right).$$

This proves the third inequality in Proposition 9.3.2.

Combining this with the third step, one immediately sees that the gap function evaluated on the Fermi sphere vanishes exponentially fast, $\Delta(\sqrt{\mu})\sim e^{1/\lambda e_\mu}$, as $\lambda\to 0$, recalling that $e_\mu^{(d)}<0$ by assumption.

6. Second order. To obtain the next order, we recall that $T_\Delta^{(d)}$ has lowest eigenvalue -1 (see (9.3.9)), and hence, by first-order perturbation theory,

$$m_\mu^{(d)}(\Delta)=\frac{-1}{\lambda\left\langle u\middle|\mathfrak{F}_\mu^{(d)}V(\mathfrak{F}_\mu^{(d)})^\dagger\middle|u\right\rangle-\lambda^2\left\langle u\middle|\mathfrak{F}_\mu^{(d)}VM_\Delta^{(d)}V(\mathfrak{F}_\mu^{(d)})^\dagger\middle|u\right\rangle+O(\lambda^3)},\tag{9.3.12}$$

where $u(p)=|\mathbb{S}^{d-1}|^{-1/2}$ is the constant function on the sphere. Recall that u is the unique ground state of $\mathcal{V}_\mu^{(d)}$.

In the second order term we have that

$$\lim_{\lambda\to 0}\left\langle u\middle|\mathfrak{F}_\mu^{(d)}VM_\Delta^{(d)}V(\mathfrak{F}_\mu^{(d)})^\dagger\middle|u\right\rangle=\left\langle u\middle|\mathcal{W}_\mu^{(d)}\middle|u\right\rangle,$$

which follows from a simple dominated convergence argument as for T_c, noting that $\Delta(p)\to 0$ pointwise.

By again employing first–order perturbation theory, similarly to the last step in the proof of Proposition 9.3.1, we conclude the second equality in Proposition 9.3.2.

7. Comparing $\Delta(\sqrt{\mu})$ to Ξ. To prove the first equality in Proposition 9.3.2 we separately prove upper and lower bounds. The upper bound is immediate from

$$\Xi=\inf_{p\in\mathbb{R}^d}E_\Delta(p)=\inf_{p\in\mathbb{R}^d}\sqrt{|p^2-\mu|+\Delta(p)^2}\le\Delta(\sqrt{\mu}).$$

Hence, for the lower bound, take $p\in\mathbb{R}^d$ with $\sqrt{|p^2-\mu|}\le\Xi\le\Delta(\sqrt{\mu})$. Then by (9.3.11)

$$\begin{aligned}\Delta(p)\ge\Delta(\sqrt{\mu})-|\Delta(p)-\Delta(\sqrt{\mu})|\ge\Delta(\sqrt{\mu})-C\Delta(\sqrt{\mu})\left(||p|-\sqrt{\mu}|^\varepsilon+\lambda\right)&\\ \ge\Delta(\sqrt{\mu})(1+o(1)).&\end{aligned}$$

In combination with the upper bound, we have thus shown that $\Xi=\Delta(\sqrt{\mu})(1+o(1))$ as desired. This concludes the proof of Proposition 9.3.2. □

We conclude this subsection with several remarks, comparing our proof with those of similar results from the literature.

Remark 9.3.9 (Structure here vs. in earlier papers on Ξ)**.** We now compare the proof above to the proofs of the three different limits in 3 dimensions [HS08b; Lau21], [Chapter 10]:

- **Weak coupling:** The structure of our proof here is very similar to that of [HS08b]. Essentially, only the technical details in Lemma 9.3.7 and the calculation of $m_\mu^{(d)}(\Delta)$ in Step 5 are different.

- **High density:** For the high-density limit in Chapter 10, we needed some additional a priori bounds on Δ before we could employ the Birman-Schwinger argument. Apart from that, in Chapter 10 the comparison of $\Delta(\sqrt{\mu})$ and Ξ are done right after these a priori bounds. Additionally, since one starts with finding a priori bounds on Δ, one does not need the first-order analysis in Step 3. One may think of the structure in Chapter 10 as being ordered in the above steps as follows: 4, 7, 1, 2, 4 (again), 5, 6.

- **Low density:** For the low-density limit in [Lau21] the structure is quite different. Again, one first needs some a priori bounds on Δ before one can use the Birman-Schwinger argument. One then improves these bounds on Δ using the Birman-Schwinger argument, which in turn can be used to get better bounds on the error term in the decomposition of the Birman–Schwinger operator. In this sense, the Steps 2–4 are too interwoven to be meaningfully separated. Also, Step 5 is done in two parts.

9.3.3 Proof of Proposition 9.2.4

Note that $\mathcal{W}_\mu^{(d)} = \mathfrak{F}_\mu^{(d)} V M_0^{(d)} V (\mathfrak{F}_\mu^{(d)})^\dagger$, where $M_0^{(d)}$ is defined in (9.3.4). By Lemma 9.3.5, $V^{1/2} M_0^{(d)} V^{1/2}$ is Hilbert-Schmidt. The integral kernel of $\mathcal{W}_\mu^{(d)}$ is bounded by

$$|\mathcal{W}_\mu^{(d)}(p,q)| \leq \frac{1}{(2\pi)^d} \int_{\mathbb{R}^{2d}} |V(x)||M_0^{(d)}(x,y)||V(y)| \,\mathrm{d}x \,\mathrm{d}y \leq \frac{1}{(2\pi)^d} \|V\|_1 \|V^{1/2} M_0^{(d)} V^{1/2}\|_{\mathsf{HS}}. \tag{9.3.13}$$

It follows that $\|\mathcal{W}_\mu^{(d)}\|_{\mathsf{HS}} \leq \frac{|\mathbb{S}^{d-1}|}{(2\pi)^d} \|V\|_1 \|V^{1/2} M_0^{(d)} V^{1/2}\|_{\mathsf{HS}}$. □

Chapter 10

The BCS energy gap at high density

This chapter contains the paper

[HighDen] J. Henheik and A. B. Lauritsen. "The BCS Energy Gap at High Density", *J Stat Phys* **189**.5 (2022). DOI: 10.1007/s10955-022-02965-9.

Abstract. We study the BCS energy gap Ξ in the high–density limit and derive an asymptotic formula, which strongly depends on the strength of the interaction potential V on the Fermi surface. In combination with the recent result by one of us (Math. Phys. Anal. Geom. 25, 2022) on the critical temperature T_c at high densities, we prove the universality of the ratio of the energy gap and the critical temperature.

Contents

10.1 Introduction and Main Results

The Bardeen–Cooper–Schrieffer (BCS) theory [BCS57] (see [HS16] for a review of recent rigorous mathematical work) has been an important theory of superconductivity since its conception. More recently, it has also gained attraction for describing the phenomenon of superfluidity in ultra cold fermionic gases, see [BDZ08; CSTL05] for reviews. In either context, BCS theory is often formulated in terms of the BCS gap equation (at zero temperature)

$$\Delta(p) = -\frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \hat{V}(p-q) \frac{\Delta(q)}{E_{\Delta,\mu}(q)} \, \mathrm{d}q \,, \tag{10.1.1}$$

where $E_{\Delta,\mu}(p) = \sqrt{(p^2-\mu)^2 + |\Delta(p)|^2}$. At finite temperature $T > 0$ one replaces $E_{\Delta,\mu}$ by $E_{\Delta,\mu}/\tanh(E_{\Delta,\mu}/2T)$. The function Δ is interpreted as the order parameter describing the Cooper pairs (paired fermions). The interaction is local and given by the potential V, which we will assume satisfies $V \in L^1(\mathbb{R}^3)$, in which case it has a Fourier transform given by $(\mathfrak{F}V)(p) = \hat{V}(p) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} V(x) e^{-ip\cdot x} \,\mathrm{d}x$.

The chemical potential μ controls the density of the fermions, and we investigate the high–density limit, i.e. $\mu \to \infty$, here. Recently this limit was studied by one of us [Hen22], where an asymptotic formula for the critical temperature T_c was found. For temperatures T below the critical temperature, $T < T_c$, the gap equation at temperature T (Equation (10.1.1) with $E_{\Delta,\mu}$ replaced as prescribed) admits a non–trivial solution, for $T \geq T_c$ it does not. The critical temperature may equivalently be characterized by the existence of a negative eigenvalue of a certain linear operator, see [HHSS08]. Physically, a system at temperature T is superconducting/–fluid if $T < T_c$, if $T \geq T_c$ it is not.

In this paper we study the energy gap (at zero temperature)

$$\Xi = \inf_p E_{\Delta,\mu}(p) = \inf_p \sqrt{(p^2-\mu)^2 + |\Delta(p)|^2}\,. \tag{10.1.2}$$

The function $E_{\Delta,\mu}$ has the interpretation of the dispersion relation for the corresponding BCS Hamiltonian, and so Ξ is indeed an energy gap (see Appendix A in [HHSS08]). We show that, in the high–density limit, $\mu \to \infty$, the ratio of the energy gap and the critical temperature tends to a universal constant independent of the interaction potential,

$$\frac{\Xi}{T_c} \approx \frac{\pi}{e^\gamma}\,, \tag{10.1.3}$$

where $\gamma \approx 0.577$ denotes the Euler–Mascheroni constant. This universality is well–known in the physics literature, see, e.g., [GM61], and was rigorously verified in the weak–coupling limit by Hainzl and Seiringer [HS08b] and in the low–density limit, $\mu \to 0$, by one of us [Lau21] building on a work by Hainzl and Seiringer [HS08a]. The general strategy for proving the universality in these limits has been to establish sufficiently good asymptotic formulas for both, T_c and Ξ, and compare them afterwards.

The weak–coupling limit is studied in [FHNS07; HS08b], where one considers a potential λV for V fixed and a small coupling constant $\lambda \to 0$. In this limit, Hainzl and Seiringer [HS08b] have shown that the critical temperature and energy gap satisfies $T_c \sim A\exp(-B/\lambda)$ and $\Xi \sim C\exp(-B/\lambda)$ respectively for explicit constants $A, B, C > 0$ depending on the interaction potential V and the chemical potential μ. This limit exhibits the same universality and the ratio $C/A = \pi e^{-\gamma}$ is independent of the interaction potential V and the chemical potential μ.

The low–density limit $\mu \to 0$ is studied in [HS08a; Lau21]. In this limit Hainzl and Seiringer [HS08a] have shown that the critical temperature satisfies $T_c \sim \mu A \exp(-B/\sqrt{\mu})$ and one of us [Lau21] has shown that the energy gap satisfies $\Xi \sim \mu C \exp(-B/\sqrt{\mu})$, for some (different) explicit constants $A, B, C > 0$ depending on the interaction potential V. Also in this limit we have the same universality and the ratio $C/A = \pi e^{-\gamma}$ is independent of the interaction potential V. These results together with the present paper thus show that the universality (10.1.3) holds in both, the low– and high–density limit, as well as in the weak–coupling limit.

To show the universality, we prove in Theorem 10.1.3 an asymptotic formula for the energy gap Ξ in the high–density limit, similar to the corresponding formula for the critical temperature given in Theorem 7 in [Hen22]. This formula, as well as the one given in Theorem 10.1.3, depends strongly on the strength of the interaction potential V on the Fermi sphere $\{p^2 = \mu\}$, which becomes weak due to the decay of $\hat{V}$ in momentum space. Together with the formula for the critical temperature [Hen22] we prove the universality (10.1.3) in Corollary 10.1.5. All proofs are given in Section 10.2. We now introduce some technical constructions and give the precise statements of our results.

10.1.1 Preliminaries

We will work with the formulation of BCS theory of [FHNS07; HHSS08; HS08a; HS16; HS08b; Hen22; Lau21]. There one considers minimizers of the BCS functional (at zero temperature)

$$\mathcal{F}(\alpha) = \frac{1}{2}\int_{\mathbb{R}^3} |p^2-\mu|\left(1-\sqrt{1-4|\hat{\alpha}(p)|^2}\right) \mathrm{d}p + \int_{\mathbb{R}^3} V(x)|\alpha(x)|^2 \,\mathrm{d}x\,. \tag{10.1.4}$$

If α is a minimizer of this, then $\Delta = -2\widehat{V\alpha}$ satisfies the BCS gap equation (10.1.1). As discussed in [HS08b] the minimizer α is in general not necessarily unique, hence also Δ and Ξ are not necessarily unique. However, since we will assume that the interaction V has non–positive Fourier transform, α and thus Ξ is unique (see Lemma 2 in [HS08b]).

A crucial role for the investigation of the energy gap (10.1.2) in the high–density limit is played by the (rescaled) operator $\mathcal{V}_\mu : L^2(\mathbb{S}^2) \to L^2(\mathbb{S}^2)$ measuring the strength of the interaction potential $\hat{V}$ on the Fermi surface. It is defined as

$$\left(\mathcal{V}_\mu u\right)(p) = \frac{1}{(2\pi)^{3/2}}\int_{\mathbb{S}^2} \hat{V}(\sqrt{\mu}(p-q))u(q)\,\mathbb{D}\omega(q)\,, \tag{10.1.5}$$

where $\mathrm{d}\omega$ denotes the uniform (Lebesgue) measure on the unit sphere $\mathbb{S}^2$. The pointwise evaluation of $\hat{V}$ (and in particular on a $\mathrm{codim}-1$ submanifold) is well defined since $V \in L^1(\mathbb{R}^3)$. The condition that $V \in L^1(\mathbb{R}^3)$ could potentially be relaxed, see [CM21] and Remark 9 in [Hen22]. The lowest eigenvalue of $\mathcal{V}_\mu$, which we denote by

$$e_\mu = \inf \operatorname{spec} \mathcal{V}_\mu$$

will be of particular importance. Note, that $\mathcal{V}_\mu$ is a trace–class operator (see the argument above Equation (3.2) in [FHNS07]) with

$$\operatorname{tr}(\mathcal{V}_\mu) = \frac{1}{2\pi^2}\int_{\mathbb{R}^3} V(x)\,\mathrm{d}x = \sqrt{\frac{2}{\pi}}\,\hat{V}(0)\,.$$

We will assume that $\hat{V}(0) < 0$ in which case $e_\mu < 0$. This corresponds to an attractive interaction between (some) electrons on the Fermi sphere.

In this work, we restrict ourselves to the special case of radial potentials V, where the spectrum of $\mathcal{V}_\mu$ can be determined more explicitly (see, e.g., Section 2.1 in [FHNS07]). Indeed, for radial V, the eigenfunctions of $\mathcal{V}_\mu$ are spherical harmonics and the corresponding eigenvalues are

$$\frac{1}{2\pi^2}\int_{\mathbb{R}^3} V(x)\left(j_\ell(\sqrt{\mu}|x|)\right)^2 \,\mathrm{d}x\,. \tag{10.1.6}$$

The lowest eigenvalue e_μ is thus given by

$$e_\mu = \frac{1}{2\pi^2}\inf_{\ell\in\mathbb{N}_0}\int_{\mathbb{R}^3} V(x)\left(j_\ell(\sqrt{\mu}|x|)\right)^2 \,\mathrm{d}x\,.$$

Here, j_ℓ denotes the spherical Bessel function of order $\ell \in \mathbb{N}_0$. Additionally, in case that $\hat{V} \leq 0$, we have, by the Perron–Frobenius theorem, that the minimal eigenvalue is attained for the constant eigenfunction (i.e. with $\ell = 0$). Thus

$$e_\mu = \frac{1}{2\pi^2} \int_{\mathbb{R}^3} V(x) \left(\frac{\sin(\sqrt{\mu}|x|)}{\sqrt{\mu}|x|} \right)^2 \mathrm{d}x \,. \tag{10.1.7}$$

For further discussions of the radiality assumption on V, see Remark 8 in [Hen22].

In order to obtain an asymptotic formula for the energy gap that is valid up to second order (see [HS08b; Hen22]), we define the operator $\mathcal{W}_\mu^{(\kappa)}$ on $u \in L^2(\mathbb{S}^2)$ via its quadratic form

$$\begin{aligned} \left\langle u \middle| \mathcal{W}_\mu^{(\kappa)} \middle| u \right\rangle = \sqrt{\mu} \int_0^\infty \mathrm{d}|p| \Bigg(\frac{|p|^2}{||p|^2 - 1|} \left[\int_{\mathbb{S}^2} \mathrm{d}\omega(p) \left(|\hat{\varphi}(\sqrt{\mu}p)|^2 - |\hat{\varphi}(\sqrt{\mu}p/|p|)|^2 \right) \right] \\ + \frac{|p|^2}{|p|^2 + \kappa^2} \int_{\mathbb{S}^2} \mathrm{d}\omega(p) |\hat{\varphi}(\sqrt{\mu}p/|p|)|^2 \Bigg) \end{aligned} \tag{10.1.8}$$

for any fixed $\kappa \geq 0$ (cf. Equation (10) in [Hen22] resp. Equation (13) in [HS08b] for an analogous definition with $\kappa = 0$). Here $\hat{\varphi}(p) = (2\pi)^{-3/2} \int_{\mathbb{S}^2} \hat{V}(p - \sqrt{\mu}q) u(q) \, \mathrm{d}\omega(q)$, and $(|p|, \omega(p)) \in (0, \infty) \times \mathbb{S}^2$ denote spherical coordinates for $p \in \mathbb{R}^3$. To see that this operator is well–defined note that the map $|p| \mapsto \int_{\mathbb{S}^2} \mathrm{d}\omega(p) |\hat{\varphi}(p)|^2$ is Lipschitz continuous for any $u \in L^2(\mathbb{S}^2)$ since $V \in L^1(\mathbb{R}^3)$. Hence the radial integral in Equation (10.1.8) is well defined for $|p| \sim 1$. We will further assume that $V \in L^{3/2}(\mathbb{R}^3)$, in which case the integral is well–defined for large $|p|$ as well. We formulate our result in Theorem 10.1.3 only for $\kappa = 0$, but the case of a positive parameter $\kappa > 0$ is crucial in the proof of this statement. For example, $\kappa > 0$ ensures that the second term in the decomposition of the Birman–Schwinger operator associated with $E_{\Delta,\mu} + V$ is small (cf. Equation (10.2.2)). Whenever it does not lead to confusion, we will refer to some κ–dependent quantity at $\kappa = 0$ by simply dropping the (κ)–superscript.

We now define the operator

$$\mathcal{B}_\mu^{(\kappa)} = \frac{\pi}{2} \left(\mathcal{V}_\mu - \mathcal{W}_\mu^{(\kappa)} \right) , \tag{10.1.9}$$

which captures the strength of the interaction potential near the Fermi surface to second order and denote its lowest eigenvalue by

$$b_\mu^{(\kappa)} = \inf \operatorname{spec} \mathcal{B}_\mu^{(\kappa)} \,. \tag{10.1.10}$$

The factor $\pi/2$ is introduced in Equation (10.1.9) since for this scaling, the eigenvalue $b_\mu^{(\kappa)}$ has the interpretation of an effective scattering length in the case of small μ (see Proposition 1 in [HS08b]). Moreover, it was shown during the proof of Theorem 7 in [Hen22] that if $e_\mu < 0$ then also $b_\mu^{(\kappa)} < 0$ for μ large enough. This will also follow from Equation (10.2.17) in the proof below.

10.1.2 Results

The following definition characterizes the class of interaction potentials for which our asymptotic formula will hold.

Definition 10.1.1 (Admissible potentials)**.** Let $V \in L^1(\mathbb{R}^3) \cap L^{3/2}(\mathbb{R}^3)$ be a radial real–valued function with non–positive Fourier transform $\hat{V} \leq 0$ and $\hat{V}(0) < 0$. Denote

$$s_\pm^* := \sup \left\{ s \geq 0 : |\cdot|^{-s} V_\pm \in L^1(\mathbb{R}^3) \right\} , \qquad s^* := \min\{s_+^*, s_-^*\} \,, \tag{10.1.11}$$

where $V_\pm = \max\{\pm V, 0\}$ are the positive and negative parts of V. We say that V is *admissible* if the following is satisfied:

(a) There exists $a > 0$ such that

$$\sup\left\{r \geq 0 : \lim_{\varepsilon \to 0} \frac{1}{\varepsilon^r} \int_{B_\varepsilon} V_\pm(x)\,\mathrm{d}x = 0\right\} = \sup\left\{r \geq 0 : \lim_{\varepsilon \to 0} \frac{1}{\varepsilon^r} \int_{B_\varepsilon} V_\pm|_{B_a}^*(x)\,\mathrm{d}x = 0\right\},$$

where $V_\pm|_{B_a}^*$ denotes the symmetric decreasing rearrangement of $V_\pm|_{B_a}$, the restriction of $V_\pm$ to the ball of radius a around 0,

(b) if $|\cdot|^{-2}V \notin L^1(\mathbb{R}^3)$, we have $s^* = s_-^* < s_+^*$, and

(c) $|\cdot|V \in L^2(\mathbb{R}^3)$ and $s^* > 7/5$.

As discussed around Equation (10.1.4), the definiteness of the Fourier transform is needed for ensuring uniqueness of the energy gap Ξ. Intuitively, the other criteria may be though as follows: Assumption (a) captures that the strongest singularity of V near the origin is in fact at the origin, assumption (b) captures that V is predominantly attractive, and assumption (c) captures that V is slightly less divergent at the origin, than allowed by the $L^{3/2}(\mathbb{R}^3)$-assumption. In view of assumption (a), we remark that it is natural that the system is sensitive to the short range behavior of the interaction potential, since the interparticle distance as the physically relevant length scale that depends on the particle density tends to zero in the high–density limit. Furthermore, note that for $V \in L^1(\mathbb{R}^3) \cap L^{3/2}(\mathbb{R}^3)$, the condition $|\cdot|V \in L^2(\mathbb{R}^3)$ is mainly about regularity away from 0 and infinity.

The most important examples of allowed interaction potentials include the cases of attractive Gaussian, Lorentzian and Yukawa potentials, also discussed in [LTB19]. That is

$$V_{\mathsf{Gauss}}(x) = -(2\pi)^{-3/2} e^{-x^2/2}, \quad V_{\mathsf{Lorentz}}(x) = -\frac{1}{\pi^2(1+x^2)^2}, \quad V_{\mathsf{Yukawa}}(x) = -\frac{1}{4\pi|x|} e^{-|x|}.$$

Remark 10.1.2. The proof of our main result formulated in Theorem 10.1.3 works without change if we assume $|\cdot|V \in L^r(\mathbb{R}^3)$ for some $2 \geq r > f(s^*)$ instead of $|\cdot|V \in L^2(\mathbb{R}^3)$, where f is some complicated (explicit) expression, see the proof of Proposition 10.2.9. We do not state the theorem with this slight generalization for simplicity. We will however give the proof under this more general assumption for the purpose of illuminating where the assumption on $r = 2$ comes from. Additionally, to further illuminate where the conditions are used, all propositions and lemmas are stated with only the conditions needed on V for that specific statement. (Beyond the conditions that $V \in L^1(\mathbb{R}^3) \cap L^{3/2}(\mathbb{R}^3)$ is real–valued, radial and has $\hat{V} \leq 0, \hat{V}(0) < 0$, which is always assumed.)

We can now state our main result for admissible interaction potentials.

Theorem 10.1.3. *Let V be an admissible potential. Then the energy gap Ξ is positive and satisfies*

$$\lim_{\mu \to \infty} \left(\log \frac{\mu}{\Xi} + \frac{\pi}{2\sqrt{\mu} b_\mu}\right) = 2 - \log(8). \tag{10.1.12}$$

In other words,

$$\Xi = \mu\left(8\,e^{-2} + o(1)\right)\exp\left(\frac{\pi}{2\sqrt{\mu}b_\mu}\right)$$

in the limit $\mu \to \infty$. Similarly as for the critical temperature [Hen22], this asymptotic formula is completely analogous to the weak–coupling case [HS08b] (replace $V \to \lambda V$ and take the limit $\lambda \to 0$) but we have coupling parameter $\lambda = 1$ here. This similarity is not entirely surprising. From a physical perspective, only those fermions with momenta close to the Fermi surface $\{p^2 = \mu\}$ contribute to the superconductivity/–fluidity. Thus, by the decay of the interaction $\hat{V}$ in Fourier space, the high–density limit, $\mu \to \infty$, is effectively a weak–coupling limit.

In order to deduce universality as in Equation (10.1.3) in the high–density limit, we show that every admissible potential in the sense of Definition 10.1.1 satisfies the imposed conditions for the proof of an analogous formula for the critical temperature. These conditions were formulated in Definition 5 in [Hen22].

Proposition 10.1.4. *Every admissible potential satisfies the conditions of Definition 5 in [Hen22].*

Proof. By comparing the two definitions, the statement is trivial apart from the following two points. First, the additional requirement $\int_{\mathbb{R}^3} \frac{V(x)}{|x|^2}\,\mathrm{d}x < 0$ from Definition 5 in [Hen22] in the case $|\cdot|^{-2}V \in L^1(\mathbb{R}^3)$ is automatically fulfilled, since

$$-\Delta_p \widehat{\frac{V}{|\cdot|^2}}(p) = \hat{V}(p) \le 0\,.$$

That is, the radial function $\widehat{\frac{V}{|\cdot|^2}}$ is subharmonic and approaches 0 as $|p| \to \infty$ (by the Riemann–Lebesgue Lemma), and thus by the maximum principle assumes a strictly negative value at 0. Second, since $\hat{V} \le 0$ and by application of the Perron–Frobenius Theorem, the constant spherical harmonic is the unique normalized ground state of $\mathcal{V}_\mu$ and thus condition (d) from Definition 5 in [Hen22] can be dropped. □

Therefore, by means of Theorem 7 in [Hen22], the critical temperature T_c satisfies

$$T_c = \mu\left(\frac{8}{\pi}e^{\gamma-2} + o(1)\right)\exp\left(\frac{\pi}{2\sqrt{\mu}b_\mu}\right)$$

for any admissible potential. Here $\gamma \approx 0.577$ is the Euler–Mascheroni constant. Together with Theorem 10.1.3, this immediately proves the following.

Corollary 10.1.5. *Let V be an admissible potential. Then*

$$\lim_{\mu\to\infty}\frac{\Xi}{T_c} = \frac{\pi}{e^\gamma} \approx 1.764\,.$$

This universality of the ratio between the energy gap and the critical temperature is well known in the physics literature (see, e.g., [GM61]) and has been previously established rigorously in the weak–coupling and low–density limits (see [HS08b] resp. [Lau21]).

10.2 Proofs

As in the analysis of the critical temperature [Hen22] we introduce the parameter $\kappa > 0$. We have the following comparison of $b_\mu^{(\kappa)}$ with the $\kappa = 0$ quantity.

Lemma 10.2.1 ([Hen22, Lemma 15])**.** *Let V be admissible and $\kappa > 0$. In the limit of high density, $\mu \to \infty$, we have*

$$\frac{\pi}{2\sqrt{\mu}b_\mu} = \frac{\pi}{2\sqrt{\mu}b_\mu^{(\kappa)}} + \kappa\frac{\pi}{2} + o(1)\,.$$

Proof. This is immediate from Lemma 15 in [Hen22] by invoking Proposition 10.1.4. □

Now, one important ingredient in our proof is the asymptotic behavior of

$$m_\mu^{(\kappa)}(\Delta) = \frac{1}{4\pi}\int_{\mathbb{R}^3}\left(\frac{1}{E_{\Delta,\mu}(p)} - \frac{1}{p^2+\kappa^2\mu}\right)\mathrm{d}p$$

for fixed $\kappa > 0$ (recall that $E_{\Delta,\mu}(p) = \sqrt{(p^2-\mu)^2 + |\Delta(p)|^2}$). This is similar to the strategy for the weak–coupling, low–density, and high–density limits of the critical temperature (see [HS08a; HS08b; Hen22]), and for the weak–coupling and low–density limits of the energy gap (see [HS08b; Lau21]).

Lemma 10.2.2. *Let V be admissible and $\kappa > 0$. In the limit of high density, $\mu \to \infty$, we have*

$$\begin{aligned}
\Xi &= \Delta(\sqrt{\mu})(1+o(1))\,,\\
m_\mu^{(\kappa)}(\Delta) &= \sqrt{\mu}\left(\log\frac{\mu}{\Delta(\sqrt{\mu})} - 2 + \kappa\frac{\pi}{2} + \log(8) + o(1)\right)\,,\\
\frac{m_\mu^{(\kappa)}(\Delta)}{\sqrt{\mu}} &= -\frac{\pi}{2\sqrt{\mu}b_\mu^{(\kappa)}} + o(1)\,.
\end{aligned}$$

These three asymptotic equalities are proven in Propositions 10.2.5, 10.2.9, and 10.2.10 respectively.

Proof of Theorem 10.1.3. By Lemma 10.2.2 and Lemma 10.2.1 we get

$$\begin{aligned}
&\lim_{\mu\to\infty}\left(\log\frac{\mu}{\Xi} + \frac{\pi}{2\sqrt{\mu}b_\mu}\right) = \lim_{\mu\to\infty}\left(\log\frac{\mu}{\Delta(\sqrt{\mu})} + \frac{\pi}{2\sqrt{\mu}b_\mu}\right)\\
&= \lim_{\mu\to\infty}\left(\log\frac{\mu}{\Delta(\sqrt{\mu})} + \frac{\pi}{2\sqrt{\mu}b_\mu^{(\kappa)}}\right) + \kappa\frac{\pi}{2} = \lim_{\mu\to\infty}\left(\log\frac{\mu}{\Delta(\sqrt{\mu})} - \frac{m_\mu^{(\kappa)}(\Delta)}{\sqrt{\mu}}\right) + \kappa\frac{\pi}{2}\\
&= \ 2 - \kappa\frac{\pi}{2} + \log(8) + \kappa\frac{\pi}{2} = 2 - \log(8)\,,
\end{aligned}$$

which yields (10.1.12) and we have proven Theorem 10.1.3. □

The rest of this paper is devoted to the proof of Lemma 10.2.2.

10.2.1 Proof of Lemma 10.2.2

As remarked, a key idea is to study the integral $m_\mu^{(\kappa)}(\Delta)$. As in [HS08b; Lau21] we first need some control of Δ in the form of a Lipschitz–like bound (given in Lemma 10.2.4) and a bound controlling $\Delta(p)$ in terms of $\Delta(\sqrt{\mu}q)$ for $q \in \mathbb{S}^2$ (given in Equation (10.2.10)). First, we recall some properties (from [HS08b]) of the minimizer α of the BCS functional at zero temperature

$$\mathcal{F}(\alpha) = \frac{1}{2}\int_{\mathbb{R}^3} |p^2-\mu| \left(1-\sqrt{1-4|\hat{\alpha}(p)|^2}\right) \mathrm{d}p + \int_{\mathbb{R}^3} V(x)|\alpha(x)|^2 \,\mathrm{d}x\,. \tag{10.2.1}$$

In [HS08b, Lemma 2] it is shown that for potentials V with non-positive Fourier transform there exists a unique minimizer α with (strictly) positive Fourier transform. Moreover, for radial V the BCS functional is invariant under rotations. Hence α and thus also $\Delta = -2\widehat{V\alpha}$ are radial functions. Therefore, with a slight abuse of notation, we will write $\Delta(|p|)$ and mean $\Delta(p)$ for some (any) vector p. (In general for any radial function f, we will write $f(|p|)$ for the value of $f(p)$.) Additionally, since $\hat{V} \le 0$ we have that $\Delta \ge 0$. In fact, by the BCS gap equation (10.1.1), we even have $\Delta > 0$, see Lemma 2 in [HS08b]. Now, we give some *a priori* bounds on the minimizer α. The proofs of Lemma 10.2.3 and Lemma 10.2.4 are given in Section 10.2.2.

Lemma 10.2.3. *Let α be the minimizer of the BCS functional* (10.2.1). *Then for large μ*

$$\|\alpha\|_{L^2} \le C\mu^{7/20} \quad \text{and} \quad \|\alpha\|_{H^1} \le C\mu^{3/4}.$$

These estimates on the minimizer α now translate to bounds on $\Delta = -2\widehat{V\alpha}$.

Lemma 10.2.4. *Suppose $V \in L^r(\mathbb{R}^3)$ for some $6/5 \le r \le 2$. Define $\delta_r = \frac{3}{4} - \frac{6}{5r}$. Then for sufficiently large μ we have*

$$\|\Delta\|_{L^\infty} \le C\mu^{\frac{24-5r}{20r}} = C\mu^{\frac{1}{2}-\delta_r}.$$

Similarly, if $|\cdot|V \in L^r(\mathbb{R}^3)$ then

$$|\Delta(p)-\Delta(q)| \le C\mu^{\frac{24-5r}{20r}}||p|-|q|| = C\mu^{\frac{1}{2}-\delta_r}||p|-|q||$$

for all p,q. In particular, if $r > 8/5$ then $\delta_r > 0$ and thus $1/2-\delta_r < 1/2$.

We will use the first bound as $\|\Delta\|_{L^\infty} \le C\mu^{11/20} = o(\mu)$ for $r = 3/2$, and the second bound as $|\Delta(p)-\Delta(q)| \le C\mu^{7/20}||p|-|q||$ for $r = 2$.

Armed with these *a* priori bounds on Δ, we can now prove the asymptotic formulas in Lemma 10.2.2 and start with the first one.

Proposition 10.2.5. *Suppose $|\cdot|V \in L^r(\mathbb{R}^3)$ for $r > 8/5$. Then $\Xi = \Delta(\sqrt{\mu})(1+o(1))$.*

Proof. Clearly $\Xi = \inf\sqrt{|p^2-\mu|^2+|\Delta(p)|^2} \le \Delta(\sqrt{\mu})$. Take now p with $|p^2-\mu| \le \Xi \le \Delta(\sqrt{\mu})$. Then

$$|\Delta(p)-\Delta(\sqrt{\mu})| \le C\mu^{1/2-\delta_r}||p|-\sqrt{\mu}| \le C\mu^{1/2-\delta_r}\frac{\Delta(\sqrt{\mu})}{|p|+\sqrt{\mu}} \le C\mu^{-\delta_r}\Delta(\sqrt{\mu})$$

where $\delta_r > 0$ by assumption. Hence, $\Delta(p) = \Delta(\sqrt{\mu})(1+o(1))$ for any such p and we conclude the desired. □

The proofs of the second and third equality (Proposition 10.2.9 and Proposition 10.2.10, respectively) heavily use Lemma 10.2.6 and Lemma 10.2.7, which we import from [Hen22]. Lemma 10.2.6 provides an upper bound for integrals of the potential against spherical Bessel functions j_ℓ, uniformly in $\ell \in \mathbb{N}_0$. These naturally arise by the spherical symmetry of V (cf. Equation (10.1.6)).

Lemma 10.2.6 ([Hen22, Lemma 12]). *Let $V \in L^1(\mathbb{R}^3) \cap L^{3/2}(\mathbb{R}^3)$ and assume that $s^* > 1$, with s^* as in Definition 10.1.1. Set*

$$\beta^* = \begin{cases} \frac{s^*}{2} & \text{for} \quad s^* \in (1, 5/3] \\ \min\left(\frac{4s^*-4}{9s^*-7} + \frac{1}{2}, \frac{19}{22}\right) & \text{for} \quad s^* > 5/3\,. \end{cases}$$

Note that β^* depends continuously on s^* and is (strictly) monotonically increasing (between 1 and 2), and $\beta^* \leq \min(s^*, 2)/2$ for any $s^* > 1$. Then for any $\delta > 0$ there exists an $\varepsilon_0 > 0$ such that for all $\varepsilon \in [0, \varepsilon_0]$ we have

$$\limsup_{\mu \to \infty} \mu^{\beta^* - \delta} \sup_{\ell \in \mathbb{N}_0} \int_{\mathbb{R}^3} \mathrm{d}x |V(x)| |j_\ell(\sqrt{\mu}|x|)|^{2-\epsilon} = 0\,.$$

Lemma 10.2.7 gives a lower bound on the quantity e_μ that measures the strength of the interaction potential on the Fermi surface (see Equation (10.1.7)).

Lemma 10.2.7 ([Hen22, Lemma 13]). *Let V be an admissible potential (cf. Definition 10.1.1). Then for any $\delta > 0$ there exists $c_\delta > 0$ such that*

$$\liminf_{\mu \to \infty} |\mu^{\min(s^*+\delta, 2)/2}\, e_\mu| \geq c_\delta\,.$$

Proof. This is immediate from Lemma 13 in [Hen22] by invoking Proposition 10.1.4. □

An upper bound is trivially obtained as $|e_\mu| \leq C_\delta \mu^{-\min(s^*-\delta,2)/2}$ for any $\delta > 0$ by definition of s^* in Equation (10.1.11) (see also Equation (10.2.9)). Note that both, upper and lower bound, remain true if we replace the exponent with $\min(s^*, 2)/2 \pm \delta$, i.e. $c_\delta \mu^{-\min(s^*,2)/2-\delta} \leq |e_\mu| \leq C_\delta \mu^{-\min(s^*,2)/2+\delta}$. This is the formulation we will use.

Beside these two Lemmas, we will use the following observation: It can easily be checked (see Lemma 3 in [HS08b]) that the operator $E_{\Delta,\mu}(p) + V(x)$ has 0 as its lowest eigenvalue, and that α is the (unique) eigenvector with this eigenvalue. By employing the Birman–Schwinger principle (see [FHNS07; HHSS08; HS16]), this is equivalent to the fact that the Birman–Schwinger operator

$$B_{\Delta,\mu} = V^{1/2} \frac{1}{E_{\Delta,\mu}} |V|^{1/2}$$

has -1 as its lowest eigenvalue with $V^{1/2}\alpha$ being the corresponding (unique) eigenvector. Here we used the notation $V(x)^{1/2} = \operatorname{sgn}(V(x))|V(x)|^{1/2}$. In the following we need a convenient decomposition of $B_{\Delta,\mu}$ in a dominant singular term and other error terms. For this purpose we let $\mathfrak{F}_\mu : L^1(\mathbb{R}^3) \to L^2(\mathbb{S}^2)$ denote the (rescaled) Fourier transform restricted to $\mathbb{S}^2$ with

$$\left(\mathfrak{F}_\mu \psi\right)(p) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{-\mathrm{i}\sqrt{\mu} p \cdot x} \psi(x)\, \mathrm{d}x\,,$$

which is well–defined by the Riemann–Lebesgue Lemma. Now, we decompose the Birman–Schwinger operator as

$$B_{\Delta,\mu} = m_\mu^{(\kappa)}(\Delta)\, V^{1/2} \mathfrak{F}_\mu{}^\dagger \mathfrak{F}_\mu |V|^{1/2} + V^{1/2} M_{\Delta,\mu}^{(\kappa)} |V|^{1/2}\,, \tag{10.2.2}$$

where $M^{(\kappa)}_{\Delta,\mu}$ is such that this holds. For the first term, note that $V^{1/2}\mathfrak{F}_\mu{}^\dagger\mathfrak{F}_\mu|V|^{1/2}$ is isospectral to $\mathcal{V}_\mu = \mathfrak{F}_\mu V \mathfrak{F}_\mu{}^\dagger$. In fact, the spectra agree at first except possibly at 0, but 0 is in both spectra as the operators are compact on an infinite dimensional space. This first term in the decomposition (10.2.2) will be the dominant term, which is how the third equality in Lemma 10.2.2 will arise.

Analogously to the proof of Lemma 14 in [Hen22] and the proof of Theorem 1 in [HS08b], we further decompose

$$V^{1/2}M^{(\kappa)}_{\Delta,\mu}|V|^{1/2} = V^{1/2}\frac{1}{p^2+\kappa^2\mu}|V|^{1/2} + A^{(\kappa)}_{\Delta,\mu} =: L^{(\kappa)}_\mu + A^{(\kappa)}_{\Delta,\mu}\,, \tag{10.2.3}$$

where now $A^{(\kappa)}_{\Delta,\mu}$ is such that this holds. During the proof of Lemma 14 in [Hen22] (see the Equation in the middle of page 15) it was shown that

$$\left\|L^{(\kappa)}_\mu\right\|_{\mathrm{op}} \leq C\,\mu^{1/2}\int_0^\infty \mathrm{d}p\frac{p^2}{p^2+\kappa^2}\sup_{\ell\in\mathbb{N}_0}\int_{\mathbb{R}^3}\mathrm{d}x|V(x)|\,|j_\ell(\sqrt{\mu}p|x|)|^2\,,$$

which may be bounded by $\mu^{-\beta^*+1/2+\delta}$ for any $\delta>0$ by means of Lemma 10.2.6. We continue with a bound on the operator norm of $A^{(\kappa)}_{\Delta,\mu}$ by estimating the matrix elements $\langle f|A^{(\kappa)}_{\Delta,\mu}|g\rangle$ for functions $f,g\in L^2(\mathbb{R}^3)$. This computation is analogous to the computation in the proof of Theorem 2 in [Hen22]. We give it here for completeness.

Note that, since V is radial, it is enough to restrict to functions of definite angular momentum. That is, with a slight abuse of notation, functions of the form $f(x)=Y_\ell^m(\hat{x})f(|x|)$, where Y_ℓ^m denotes the spherical harmonics and we write $\hat{x}=x/|x|$. The operator $A^{(\kappa)}_{\Delta,\mu}$ is indeed block–diagonal in the angular momentum as will follow from the computations below. Since functions of definite angular momentum span $L^2(\mathbb{R}^3)$ [Hal13, Sections 17.6-17.7] it is thus enough to bound $\langle f|A^{(\kappa)}_{\Delta,\mu}|g\rangle$ for f,g of the form $f(x)=Y_\ell^m(\hat{x})f(|x|)$, $g(x)=Y_{\ell'}^{m'}(\hat{x})g(|x|)$.

Now, $A^{(\kappa)}_{\Delta,\mu}$ has integral kernel

$$A^{(\kappa)}_{\Delta,\mu}(x,y) = CV^{1/2}(x)|V(y)|^{1/2}\int_{\mathbb{R}^3}\left(\frac{1}{E_{\Delta,\mu}(p)}-\frac{1}{p^2+\kappa^2\mu}\right)\left(e^{ip\cdot(x-y)}-e^{i\sqrt{\mu}\hat{p}\cdot(x-y)}\right)\mathrm{d}p\,.$$

Thus, by the radiality of V we get

$$\begin{aligned}\left\langle f\middle|A^{(\kappa)}_{\Delta,\mu}\middle|g\right\rangle = C&\int_0^\infty \mathrm{d}|x|\,|x|^2V^{1/2}(|x|)\overline{f(|x|)}\int_0^\infty \mathrm{d}|y|\,|y|^2|V(|y|)|^{1/2}g(|y|)\\ &\times\int_0^\infty \mathrm{d}|p|\,|p|^2\left(\frac{1}{E_{\Delta,\mu}(|p|)}-\frac{1}{|p|^2+\kappa^2\mu}\right)\int_{\mathbb{S}^2}\mathrm{d}\omega(\hat{p})\\ &\times\int_{\mathbb{S}^2}\mathrm{d}\omega(\hat{x})\int_{\mathbb{S}^2}\mathrm{d}\omega(\hat{y})\,\overline{Y_\ell^m(\hat{x})}Y_{\ell'}^{m'}(\hat{y})\left(e^{-ip\cdot(x-y)}-e^{-i\sqrt{\mu}\hat{p}\cdot(x-y)}\right)\,.\end{aligned} \tag{10.2.4}$$

Now, using the plane–wave expansion $e^{ip\cdot x}=4\pi\sum_{\ell=0}^\infty\sum_{m=-\ell}^{\ell} i^\ell j_\ell(|p||x|)Y_\ell^m(\hat{p})\overline{Y_\ell^m(\hat{x})}$, the spherical integrations in x and y may be evaluated as

$$16\pi^2(-i)^{\ell+\ell'}\left(j_\ell(|p||x|)j_{\ell'}(|p||y|)-j_\ell(\sqrt{\mu}|x|)j_{\ell'}(\sqrt{\mu}|y|)\right)\overline{Y_\ell^m(\hat{p})}Y_{\ell'}^{m'}(\hat{p})$$

using the orthogonality of the spherical harmonics. The spherical p–integral of this gives a factor $\delta_{\ell\ell'}\delta_{mm'}$ again by orthogonality of the spherical harmonics. (This shows that $A^{(\kappa)}_{\Delta,\mu}$ is block–diagonal in the angular momentum as claimed.) We may thus restrict to the case of $\ell = \ell'$ and $m = m'$. Hereinafter, we will write x, y, and p instead of $|x|$, $|y|$, and $|p|$.

Recall the following bounds on spherical Bessel functions

$$\sup_{\ell\in\mathbb{N}_0}\sup_{x\geq 0}|j_\ell(x)| \leq 1\,, \qquad \sup_{\ell\in\mathbb{N}_0}\sup_{x\geq 0}|j_\ell'(x)| \leq 1\,, \qquad \sup_{\ell\in\mathbb{N}_0}\sup_{x\geq 0}x^{5/6}|j_\ell(x)| \leq C\,,$$

where the first one is elementary, the second one follows from [AS14, Eq. 10.1.20], and the third one may be found in [Lan00, Eq. 1] (see also Proposition 16 in [Hen22]). Adding $\pm j_\ell(px)j_\ell(\sqrt{\mu}y)$ and using these bounds we may estimate for any $0 < \varepsilon < 5/11$

$$\begin{aligned}
&|j_\ell(px)j_\ell(py) - j_\ell(\sqrt{\mu}x)j_\ell(\sqrt{\mu}y)| \\
&\quad\leq C|p-\sqrt{\mu}|^\varepsilon\left(p^{-\varepsilon} + (\sqrt{\mu})^{-\varepsilon}\right)\left(|j_\ell(px)|^{1-11\varepsilon/5} + |j_\ell(\sqrt{\mu}x)|^{1-11\varepsilon/5}\right) \\
&\qquad\times\left(|j_\ell(py)|^{1-11\varepsilon/5} + |j_\ell(\sqrt{\mu}y)|^{1-11\varepsilon/5}\right).
\end{aligned} \tag{10.2.5}$$

The radial p–integral in Equation (10.2.4) is then (a constant times)

$$\int_0^\infty \mathrm{d}p\left(\frac{1}{E_{\Delta,\mu}(p)} - \frac{1}{p^2+\kappa^2\mu}\right)\left(j_\ell(px)j_\ell(py) - j_\ell(\sqrt{\mu}x)j_\ell(\sqrt{\mu}y)\right) \tag{10.2.6}$$

Using Equation (10.2.5) and changing integration variable $p \to \sqrt{\mu}p$ we get

$$\begin{aligned}
|(10.2.6)| \leq C\mu^{1/2}&\int_0^\infty \mathrm{d}p\, p^2\left|\frac{1}{\sqrt{(p^2-1)^2 + |\Delta(\sqrt{\mu}p)/\mu|^2}} - \frac{1}{p^2+\kappa^2}\right||p-1|^\varepsilon\left(\frac{1}{p^\varepsilon}+1\right) \\
&\times\left(|j_\ell(\sqrt{\mu}px)|^{1-11\varepsilon/5} + |j_\ell(\sqrt{\mu}x)|^{1-11\varepsilon/5}\right) \\
&\times\left(|j_\ell(\sqrt{\mu}py)|^{1-11\varepsilon/5} + |j_\ell(\sqrt{\mu}y)|^{1-11\varepsilon/5}\right).
\end{aligned}$$

Plugging this into Equation (10.2.4) and using Hölder for the x– and y–integrations we thus get

$$\begin{aligned}
&\left|\left\langle f\middle|A_{\Delta,\mu}^{(\kappa)}\middle|g\right\rangle\right| \\
&\quad\leq C\mu^{1/2}\int_0^\infty \mathrm{d}p\, p^2\left|\frac{1}{\sqrt{(p^2-1)^2+|\Delta(\sqrt{\mu}p)/\mu|^2}} - \frac{1}{p^2+\kappa^2}\right||p-1|^\varepsilon\left(\frac{1}{p^\varepsilon}+1\right) \\
&\qquad\times\int_{\mathbb{R}^3}\mathrm{d}x\,|V(x)|\left(|j_\ell(\sqrt{\mu}p|x|)|^{2-22\varepsilon/5} + |j_\ell(\sqrt{\mu}|x|)|^{2-22\varepsilon/5}\right),
\end{aligned}$$

where we changed back to x denoting a vector in $\mathbb{R}^3$. By Lemma 10.2.6 we may bound the x–integral by $\mu^{-\beta^*+\delta}(1+p^{-\beta^*+\delta})$ for any $\delta > 0$. Also, $\|\Delta\|_{L^\infty} = o(\mu)$ by Lemma 10.2.4. Hence the p–integral will be finite uniformly in μ for μ large enough. We conclude that

$$\left\|A_{\Delta,\mu}^{(\kappa)}\right\|_{\mathrm{op}} \leq C\mu^{-\beta^*+1/2+\delta}$$

for any $\delta > 0$ and for μ large enough. Combining this with the bound on $\|L_\mu^{(\kappa)}\|_{\mathrm{op}}$ from above, we get

$$\limsup_{\mu\to\infty}\mu^{\beta^*-1/2-\delta}\left\|V^{1/2}M_{\Delta,\mu}^{(\kappa)}|V|^{1/2}\right\|_{\mathrm{op}} = 0 \tag{10.2.7}$$

for any $\delta > 0$. Also, since $V^{1/2}\mathfrak{F}_\mu^\dagger \mathfrak{F}_\mu |V|^{1/2}$ is isospectral to $\mathcal{V}_\mu$, so its eigenvalues are given by Equation (10.1.6), one can easily see, using Lemma 10.2.6 again, that

$$\limsup_{\mu\to\infty} \mu^{\beta^*-\delta} \left\| V^{1/2}\mathfrak{F}_\mu^\dagger \mathfrak{F}_\mu |V|^{1/2} \right\|_{\mathrm{op}} = 0\,, \tag{10.2.8}$$

for any $\delta > 0$. Finally, by definition of s^* (see Equation (10.1.11)), we get for any $\delta > 0$ that

$$\limsup_{\mu\to\infty} \mu^{\min(s^*,2)/2-\delta} \int_{\mathbb{R}^3} |V(x)| \left(\frac{\sin(\sqrt{\mu}|x|)}{\sqrt{\mu}|x|} \right)^2 \mathrm{d}x = 0\,. \tag{10.2.9}$$

As the last ingredient we need the following Lemma, which provides a bound controlling $\Delta(p)$ in terms of $\Delta(\sqrt{\mu})$. Its proof is given in Section 10.2.2.

Lemma 10.2.8. *Suppose $s^* > 1$ and let $u(p) = (4\pi)^{-1/2}$ be the constant function on the sphere $\mathbb{S}^2$ and let*

$$\hat{\varphi}(p) = \sqrt{4\pi}\mathfrak{F}V\mathfrak{F}_\mu^\dagger u(p) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{S}^2} \hat{V}(p - \sqrt{\mu}q)\, \mathrm{d}\omega(q)\,,$$

where $\mathfrak{F}$ denotes the usual Fourier transform. Then

$$\Delta(p) = f(\mu)\left[\hat{\varphi}(p) + \eta_\mu(p)\right],$$

for some function $f(\mu)$. The function η_μ satisfies

$$\limsup_{\mu\to\infty} \mu^{\beta^*+\min(s^*,2)/4-1/2-\delta} \|\eta_\mu\|_{L^\infty} = 0 \;\; \textit{and} \;\; \limsup_{\mu\to\infty} \mu^{\beta^*+\min(s^*,2)/2-1/2-\delta} |\eta_\mu(\sqrt{\mu})| = 0$$

for any $\delta > 0$.

Note that $\hat{\varphi}(\sqrt{\mu}) = \sqrt{4\pi}\mathfrak{F}_\mu V \mathfrak{F}_\mu^\dagger u(1) = e_\mu$. Now, combining this with Lemmas 10.2.6 and 10.2.7, we see that $\Delta(\sqrt{\mu}) = f(\mu)e_\mu(1 + o(1))$, from which we conclude that

$$\Delta(p) = \frac{\hat{\varphi}(p) + \eta_\mu(p)}{e_\mu + \eta_\mu(\sqrt{\mu})}\Delta(\sqrt{\mu}) = \left[1 + \frac{\hat{\varphi}(p) - \hat{\varphi}(\sqrt{\mu})}{e_\mu} + \frac{\eta_\mu(p)}{e_\mu}\right](1 + o(1))\Delta(\sqrt{\mu})\,.$$

Now, it is an easy computation to see $|\hat{\varphi}(p) - \hat{\varphi}(q)| \le C\mu^{-1/2}|p - q|$ for all p, q. Thus

$$|\Delta(p)| \le C\left(1 + \mu^{\min(s^*,2)/2-1/2+\delta}|p - \sqrt{\mu}| + \mu^{\min(s^*,2)/4-\beta^*+1/2+\delta}\right)\Delta(\sqrt{\mu}) \tag{10.2.10}$$

for any $\delta > 0$, again by means of Lemma 10.2.6 and Lemma 10.2.7, assuming that V is admissible. So, we get the desired control on $\Delta(p)$ in terms of $\Delta(\sqrt{\mu})$.

The bound on $\eta_\mu(\sqrt{\mu})$ is effectively a bound on $\left\langle u \middle| \mathfrak{F}_\mu^\dagger V M_{\Delta,\mu}^{(\kappa)} V \mathfrak{F}_\mu \middle| u \right\rangle$. (This will be clear from the proof.) For sufficiently large μ we have

$$\left| \left\langle u \middle| \mathfrak{F}_\mu^\dagger V M_{\Delta,\mu}^{(\kappa)} V \mathfrak{F}_\mu \middle| u \right\rangle \right| \le C_\delta \mu^{-\beta^*-\min(s^*,2)/2+1/2+\delta} \tag{10.2.11}$$

for any $\delta > 0$. This will be of importance in the perturbation argument in Proposition 10.2.10.

We are now able to prove the second and third equality in Lemma 10.2.2.

Proposition 10.2.9. *Let V be an admissible potential. Then we have*

$$m_\mu^{(\kappa)}(\Delta) = \sqrt{\mu}\left(\log\frac{\mu}{\Delta(\sqrt{\mu})} - 2 + \kappa\frac{\pi}{2} + \log(8) + o(1)\right)$$

in the limit $\mu \to \infty$.

Proof. Computing the angular integral, and substituting $s = \pm\frac{p^2-\mu}{\mu}$ we get

$$
\begin{aligned}
m_\mu^{(\kappa)}(\Delta) = \frac{\sqrt{\mu}}{2}\Bigg[&\int_0^1 \left(\frac{\sqrt{1-s}-1}{\sqrt{s^2+x_-(s)^2}} + \frac{\sqrt{1+s}-1}{\sqrt{s^2+x_+(s)^2}} - \frac{\sqrt{1-s}}{1-s+\kappa^2} - \frac{\sqrt{1+s}}{1+s+\kappa^2} \right) \mathrm{d}s \\
&+ \int_0^1 \left(\frac{1}{\sqrt{s^2+x_+(s)^2}} + \frac{1}{\sqrt{s^2+x_-(s)^2}} \right) \mathrm{d}s \\
&+ \int_1^\infty \left(\frac{\sqrt{1+s}}{\sqrt{s^2+x_+(s)^2}} - \frac{\sqrt{1+s}}{1+s+\kappa^2} \right) \mathrm{d}s \Bigg],
\end{aligned}
$$

where $x_\pm(s) = \frac{\Delta(\sqrt{\mu}\sqrt{1\pm s})}{\mu}$. Now, using dominated convergence and $\|\Delta\|_{L^\infty} = o(\mu)$, it is easy to see that the first and last integrals converge to

$$
\int_0^1 \left(\frac{\sqrt{1-s}-1}{s} + \frac{\sqrt{1+s}-1}{s} - \frac{\sqrt{1-s}}{1-s+\kappa^2} - \frac{\sqrt{1+s}}{1+s+\kappa^2} \right) \mathrm{d}s
$$

and

$$
\int_1^\infty \left(\frac{\sqrt{1+s}}{s} - \frac{\sqrt{1+s}}{1+s+\kappa^2} \right) \mathrm{d}s\,,
$$

respectively, in the limit $\mu \to \infty$. For the middle integral we claim that

$$
\int_0^1 \left(\frac{1}{\sqrt{s^2+x_\pm(s)^2}} - \frac{1}{\sqrt{s^2+x_\pm(0)^2}} \right) \mathrm{d}s \to 0 \quad \text{as} \quad \mu \to \infty\,. \tag{10.2.12}
$$

As in [HS08b; Lau21] this is where we need both the Lipschitz–like bound on Δ (Lemma 10.2.4) and the bound controlling $\Delta(p)$ in terms of $\Delta(\sqrt{\mu})$ (Equation (10.2.10)). In terms of $x_\pm$, Lemma 10.2.4 reads

$$
|x_\pm(s) - x_\pm(0)| \le C\mu^{-\delta_r} s\,. \tag{10.2.13}
$$

In terms of $x_\pm$, Equation (10.2.10) reads

$$
x_\pm(s) \le C(1 + \mu^{\min(s^*,2)/2+\delta} s + \mu^{\min(s^*,2)/4-\beta^*+1/2+\delta}) x_\pm(0)\,. \tag{10.2.14}
$$

Now, the integrand in Equation (10.2.12) is bounded by

$$
\frac{|x_\pm(s)^2 - x_\pm(0)^2|}{\sqrt{s^2+x_\pm(s)^2}\sqrt{s^2+x_\pm(0)^2}\left(\sqrt{s^2+x_\pm(s)^2} + \sqrt{s^2+x_\pm(0)^2}\right)}\,.
$$

We introduce a cutoff $\rho \in (0,1)$ and compute the integrals $\int_\rho^1$ and $\int_0^\rho$. For the first integral we have

$$
\begin{aligned}
&\int_\rho^1 \frac{|x_\pm(s)^2 - x_\pm(0)^2|}{\sqrt{s^2+x_\pm(s)^2}\sqrt{s^2+x_\pm(0)^2}\left(\sqrt{s^2+x_\pm(s)^2} + \sqrt{s^2+x_\pm(0)^2}\right)} \mathrm{d}s \\
&\le C\mu^{-\delta_r} \int_\rho^1 \frac{1}{s} \frac{x_\pm(s) + x_\pm(0)}{\sqrt{s^2+x_\pm(s)^2} + \sqrt{s^2+x_\pm(0)^2}} \mathrm{d}s \\
&\le C\mu^{-\delta_r} |\log\rho|\,.
\end{aligned}
$$

which vanishes for any $\rho \gg \exp\left(-\mu^{\delta_r}\right)$, in particular for $\rho = \mu^{-N}$ for suitable $N > 0$, which we choose here. For the second integral we have

$$\begin{aligned}
&\int_0^\rho \frac{|x_\pm(s)^2 - x_\pm(0)^2|}{\sqrt{s^2 + x_\pm(s)^2}\sqrt{s^2 + x_\pm(0)^2}\left(\sqrt{s^2 + x_\pm(s)^2} + \sqrt{s^2 + x_\pm(0)^2}\right)}\, \mathrm{d}s \\
&\quad \le C \int_0^\rho \mu^{-\delta_r} \left(1 + \mu^{\min(s^*,2)/4-\beta^*+1/2+\delta} + \mu^{\min(s^*,2)/2+\delta} s\right) \\
&\quad\quad \times \frac{x_\pm(0)}{\sqrt{x_\pm(0)^2 + s^2}\left(s + \sqrt{x_\pm(0)^2 + s^2}\right)}\, \mathrm{d}s \\
&\quad \le C\mu^{\min(s^*,2)/4-\beta^*-\delta_r+1/2+\delta} \int_0^\rho \frac{x_\pm(0)}{\sqrt{x_\pm(0)^2 + s^2}\left(s + \sqrt{x_\pm(0)^2 + s^2}\right)}\, \mathrm{d}s \\
&\quad \le C\mu^{\min(s^*,2)/4-\beta^*-\delta_r+1/2+\delta} .
\end{aligned}$$

Note that for $r = 2$, we have $\delta_{r=2} = 3/20$ and thus $\beta^* - \min(s^*, 2)/4 - 1/2 + 3/20 > 0$ for any $s^* > 7/5$ (see Remark 10.1.2). Also, optimizing this expression in the allowed r's gives the assumption $r > f(s^*)$ given in Remark 10.1.2. Therefore, also this second integral vanishes as desired by choosing $0 < \delta < \beta^* - \min(s^*, 2)/4 - 7/20$. We conclude that

$$\begin{aligned}
m_\mu^{(\kappa)}(\Delta) = \frac{\sqrt{\mu}}{2}\Bigg[&\int_0^1 \left(\frac{\sqrt{1-s}-1}{s} + \frac{\sqrt{1+s}-1}{s} - \frac{\sqrt{1-s}}{1-s+\kappa^2} - \frac{\sqrt{1+s}}{1+s+\kappa^2}\right) \mathrm{d}s \\
&+ \int_0^1 \frac{2}{\sqrt{s^2 + \left(\frac{\Delta(\sqrt{\mu})}{\mu}\right)^2}}\, \mathrm{d}s + \int_1^\infty \left(\frac{\sqrt{1+s}}{s} - \frac{\sqrt{1+s}}{1+s+\kappa^2}\right) \mathrm{d}s + o(1)\Bigg].
\end{aligned}$$

This may be computed (perhaps most easily by adding and subtracting the corresponding integral with $\kappa = 0$) as

$$m_\mu^{(\kappa)} = \sqrt{\mu}\left(\log\frac{\mu}{\Delta(\sqrt{\mu})} - 2 + \log(8) + \kappa\frac{\pi}{2} + o(1)\right). \qquad \square$$

We conclude by showing the third equality of Lemma 10.2.2.

Proposition 10.2.10. *Let V be an admissible potential. Then*

$$\frac{m_\mu^{(\kappa)}(\Delta)}{\sqrt{\mu}} = -\frac{\pi}{2\sqrt{\mu} b_\mu^{(\kappa)}} + o(1) .$$

Proof. Recall that, by the Birman–Schwinger principle the lowest eigenvalue of $B_{\Delta,\mu}$ is -1. Using the decomposition in Equation (10.2.2) and the bound in Equation (10.2.7) we get that

$$-1 = \lim_{\mu\to\infty} m_\mu^{(\kappa)}(\Delta) \inf\operatorname{spec}\left(V^{1/2}\mathfrak{F}_\mu{}^\dagger\mathfrak{F}_\mu|V|^{1/2}\right) = \lim_{\mu\to\infty} m_\mu^{(\kappa)}(\Delta) e_\mu .$$

Now, since $s^* > 7/5$ we have that $|\sqrt{\mu}e_\mu| \le C\mu^{-2/5}$ by Lemma 10.2.6 (recall Equation (10.1.6) and Equation (10.2.9)). Thus, by Proposition 10.2.9 we conclude that $\Delta(\sqrt{\mu})$ is exponentially small (in some positive power of μ) as $\mu \to \infty$.

To obtain the next order in the expansion of $m_\mu(\Delta)$, we note that $1 + V^{1/2}M_{\Delta,\mu}^{(\kappa)}|V|^{1/2}$ is invertible for μ large enough by means of Equation (10.2.7). We can thus factorize the

Birman–Schwinger operator (10.2.2) as

$$1 + B_{\Delta,\mu} = \left(1 + V^{1/2} M_{\Delta,\mu}^{(\kappa)} |V|^{1/2}\right) \left(1 + \frac{m_\mu^{(\kappa)}(\Delta)}{1 + V^{1/2} M_{\Delta,\mu}^{(\kappa)} |V|^{1/2}} V^{1/2} \mathfrak{F}_\mu^\dagger \mathfrak{F}_\mu |V|^{1/2}\right).$$

Because $B_{\Delta,\mu}$ has -1 as its lowest eigenvalue by the Birman–Schwinger principle, we conclude that, for μ large enough, the self–adjoint operator

$$T_{\Delta,\mu} := m_\mu^{(\kappa)}(\Delta) \mathfrak{F}_\mu |V|^{1/2} \frac{1}{1 + V^{1/2} M_{\Delta,\mu}^{(\kappa)} |V|^{1/2}} V^{1/2} \mathfrak{F}_\mu^\dagger$$

acting on $L^2(\mathbb{S}^2)$ has -1 as its lowest eigenvalue since it is isospectral to the right–most operator above. (This follows from the fact that for operators A, B the operators AB and BA have the same spectrum apart from possibly at 0. See also the argument around Equation (33) in [Hen22] as well as around Equation (30) and Equation (47) in [HS08b].)

To highest order $T_{\Delta,\mu}$ is proportional to $\mathcal{V}_\mu$. Since the constant function $u(p) = (4\pi)^{-1/2}$ on $\mathbb{S}^2$ is the unique eigenvector of $\mathcal{V}_\mu$ with lowest eigenvalue, this is true also for $T_{\Delta,\mu}$ whenever μ is large enough.

To find the lowest eigenvalue (which is -1) we expand the geometric series to first order and employ first order perturbation theory. This is completely analogous to the arguments in [HS08b] and Equation (34) in [Hen22]. We obtain

$$\frac{1}{\sqrt{\mu}} m_\mu^{(\kappa)}(\Delta) = \frac{-1}{\mu^{1/2} e_\mu - \mu^{1/2} \left\langle u \middle| \mathfrak{F}_\mu V M_{\Delta,\mu}^{(\kappa)} V \mathfrak{F}_\mu^\dagger \middle| u \right\rangle + O(\mu^{-3\beta^* + 3/2 + \delta})} \tag{10.2.15}$$

for any $\delta > 0$ (recall Equations (10.2.7), (10.2.8) and (10.2.11)). The error term in Equation (10.2.15) is twofold. The first part comes from the expansion of the geometric series. The second part comes from first order perturbation theory using the bounds

$$|\sqrt{\mu} e_\mu| \geq c_\delta \mu^{-\min(s^*,2)/2 + 1/2 - \delta} \quad \text{and} \quad \left|\mu^{1/2} \left\langle u \middle| \mathfrak{F}_\mu V M_{\Delta,\mu}^{(\kappa)} V \mathfrak{F}_\mu^\dagger \middle| u \right\rangle\right| \leq C_\delta \mu^{-\beta^* - \min(s^*,2)/2 + 1 + \delta}$$

for any $\delta > 0$ from Lemma 10.2.7 and Equation (10.2.11). The error from the series expansion is of order $O(\mu^{-3\beta^* + 3/2 + \delta})$ and the error from the perturbation argument is of order $O(\mu^{-2\beta^* - \min(s^*,2)/2 + 3/2 + \delta})$ and is hence dominated by the expansion of the geometric series, since $\beta^* \leq \min(s^*, 2)/2$.

Now, we need to show that $\mathfrak{F}_\mu V M_{\Delta,\mu}^{(\kappa)} V \mathfrak{F}_\mu^\dagger$ is close to $\mathcal{W}_\mu^{(\kappa)}$, when evaluated in $\langle u | \cdots | u \rangle$. Therefore, considering their difference, we split the involved radial p–integral according to $|p| \leq \mu^N$ and $|p| > \mu^N$ for some large $N > 0$. The second part is clearly bounded by, e.g., $C\mu^{-N/2}$. For the first part, we have $\Delta(p) \leq C\mu^N \Delta(\sqrt{\mu})$ by Equation (10.2.10). Using this in combination with the fact that $\Delta(\sqrt{\mu})$ is exponentially small, we find, by dominated convergence and Lipschitz continuity of the involved angular integrals (cf. Equation (35) in [HS08b] and Equation (36) in [Hen22]), that this part is bounded by $C_D \mu^{-D}$ for any $D > 0$. Since $N > 0$ was arbitrary, we conclude that

$$\left|\left\langle u \middle| \mathfrak{F}_\mu V M_{\Delta,\mu}^{(\kappa)} V \mathfrak{F}_\mu^\dagger - \mathcal{W}_\mu^{(\kappa)} \middle| u \right\rangle\right| \leq C_D \mu^{-D} \tag{10.2.16}$$

for any $D > 0$. Thus, by combining Equation (10.2.11) and Equation (10.2.16) (recall Equation (10.1.9) and Equation (10.1.10)) we get

$$\left|\left\langle u \middle| \mathcal{W}_\mu^{(\kappa)} \middle| u \right\rangle\right| \leq C_\delta \mu^{-\beta^* - \min(s^*,2)/2 + 1/2 + \delta} \tag{10.2.17}$$

for any $\delta > 0$. (In particular $b_\mu^{(\kappa)} < 0$ for large μ. This was also shown in [Hen22].)

In particular, combining Equations (10.2.15), (10.2.16) and (10.2.17), we get again by a perturbation theory argument that

$$\frac{1}{\sqrt{\mu}} m_\mu^{(\kappa)}(\Delta) = -\frac{\pi}{2\sqrt{\mu} b_\mu^{(\kappa)}} + O(\mu^{-3\beta^* + \min(s^*,2)+1/2+\delta}),$$

for any $\delta > 0$. Since $3\beta^* - \min(s^*, 2) - 1/2 > 0$ we conclude the desired. □

10.2.2 Proofs of Auxiliary Lemmas

In this Subsection, we prove the auxiliary Lemmas 10.2.3, 10.2.4, and 10.2.8.

Proof of Lemma 10.2.3. First we show

$$\|\alpha\|_{H^1}^2 \le C\|\alpha\|_{L^2}^2 + C\mu^{3/2}. \tag{10.2.18}$$

Since $V \in L^{3/2}(\mathbb{R}^3)$ we have by Sobolev's inequality [LL01, Thm. 8.3] $\inf\operatorname{spec}\left(\frac{p^2}{2} + V\right) > -\infty$. Thus, using $\sqrt{1-4x^2} \le 1 - 2x^2$ and $\hat\alpha \le 1/2$ we get

$$\begin{aligned}
\mathcal{F}(\alpha) &= \frac{1}{2}\int_{\mathbb{R}^3} |p^2 - \mu|\left(1 - \sqrt{1 - 4\hat\alpha(p)^2}\right) \mathrm{d}p + \int_{\mathbb{R}^3} V(x)|\alpha(x)|^2 \,\mathrm{d}x \\
&\ge \int_{\mathbb{R}^3} (p^2 - \mu)\hat\alpha(p)^2 \,\mathrm{d}p + \int_{\mathbb{R}^3} V(x)|\alpha(x)|^2 \,\mathrm{d}x \\
&= \left\langle \alpha \middle| \frac{p^2}{2} + V \middle| \alpha \right\rangle + \int_{\mathbb{R}^3} \left(\frac{p^2}{2} - \mu\right)\hat\alpha(p)^2 \,\mathrm{d}p \\
&\ge \frac{1}{4}\|\alpha\|_{H^1}^2 - C\|\alpha\|_{L^2}^2 + \int_{\mathbb{R}^3}\left(\frac{p^2}{4} - \mu - \frac{1}{4}\right)\hat\alpha(p)^2 \,\mathrm{d}p \\
&\ge \frac{1}{4}\|\alpha\|_{H^1}^2 - C\|\alpha\|_{L^2}^2 - \frac{1}{4}\int_{\mathbb{R}^3}\left[\frac{p^2}{4} - \mu - \frac{1}{4}\right]_- \mathrm{d}p \\
&\ge \frac{1}{4}\|\alpha\|_{H^1}^2 - C\|\alpha\|_{L^2}^2 - C\mu^{3/2},
\end{aligned}$$

which gives the desired. Now we show that

$$\left\|\hat\alpha \mathbb{1}_{\{|p|<t\}}\right\|_{L^2} \le C\left\|\hat\alpha \mathbb{1}_{\{|p|>t\}}\right\|_{L^2} + C\mu^{2\delta-1}\|\alpha\|_{H^1}^2,$$

for $t = \mu^\delta$ and $0 < \delta < 1/2$.

To see this, we split the integrals in the functional $\mathcal{F}$ according to small or large momentum p and compute

$$\begin{aligned}
\mathcal{F}(\alpha) &= \frac{1}{2}\int_{\mathbb{R}^3} |p^2 - \mu|\left(1 - \sqrt{1 - 4\hat\alpha(p)^2}\right) \mathrm{d}p + \int_{\mathbb{R}^3} V(x)|\alpha(x)|^2 \,\mathrm{d}x \\
&\ge \int_{|p|<t} |p^2 - \mu|\hat\alpha(p)^2 \,\mathrm{d}p + \int_{|p|>t} |p^2 - \mu|\hat\alpha(p)^2 \,\mathrm{d}p \\
&\qquad + \frac{1}{(2\pi)^{3/2}}\iint_{\mathbb{R}^3\times\mathbb{R}^3} \hat\alpha(p)\hat V(p-q)\hat\alpha(q)\,\mathrm{d}p\,\mathrm{d}q \\
&\ge \mu\left\|\hat\alpha\mathbb{1}_{\{|p|<t\}}\right\|_{L^2}^2 - \left\|p^2\hat\alpha\mathbb{1}_{\{|p|<t\}}\right\|_{L^2}^2 + \left\langle \hat\alpha\mathbb{1}_{\{|p|>t\}}\middle| p^2 + V \middle| \hat\alpha\mathbb{1}_{\{|p|>t\}}\right\rangle - \mu\left\|\hat\alpha\mathbb{1}_{\{|p|>t\}}\right\|_{L^2}^2 \\
&\quad + \frac{1}{(2\pi)^{3/2}}\left[\iint_{|p|,|q|<t} \hat\alpha(p)\hat V(p-q)\hat\alpha(q)\,\mathrm{d}p\,\mathrm{d}q + 2\iint_{|p|<t,|q|>t} \hat\alpha(p)\hat V(p-q)\hat\alpha(q)\,\mathrm{d}p\,\mathrm{d}q\right].
\end{aligned}$$

Note that, again by Sobolev's inequality [LL01, Thm. 8.3], we have

$$\left\langle \hat{\alpha}\mathbb{1}_{\{|p|>t\}} \middle| p^2 + V \middle| \hat{\alpha}\mathbb{1}_{\{|p|>t\}} \right\rangle \geq -C \left\| \hat{\alpha}\mathbb{1}_{\{|p|>t\}} \right\|_{L^2}^2 .$$

Moreover, by application of Young's inequality [LL01, Thm. 4.2] we obtain

$$\begin{aligned}\int_{|p|<t} \int_{|q|<t} \hat{\alpha}(p)\hat{V}(p-q)\hat{\alpha}(q)\, \mathsf{d}p\, \mathsf{d}q &\geq -\left\| \hat{V} \right\|_{L^3} \left\| \hat{\alpha}\mathbb{1}_{\{|p|<t\}} \right\|_{L^{6/5}}^2 \\ &\geq -C \left(t^3\right)^{2\cdot(5/6-1/2)} \left\| \hat{\alpha}\mathbb{1}_{\{|p|<t\}} \right\|_{L^2}^2 \\ &= -C\mu^{2\delta} \left\| \hat{\alpha}\mathbb{1}_{\{|p|<t\}} \right\|_{L^2}^2\end{aligned}$$

and

$$\begin{aligned}\int_{|p|<t} \int_{|q|>t} \hat{\alpha}(p)\hat{V}(p-q)\hat{\alpha}(q)\, \mathsf{d}p\, \mathsf{d}q &\geq -\left\| \hat{\alpha}\mathbb{1}_{\{|p|<t\}} \right\|_{L^1} \left\| \hat{V} \right\|_{L^3} \left\| \hat{\alpha}\mathbb{1}_{\{|p|>t\}} \right\|_{L^{3/2}} \\ &\geq -Ct^{3/2} \left\| \alpha \right\|_{H^1} \left\| \hat{\alpha}\mathbb{1}_{\{|p|<t\}} \right\|_{L^2} \\ &= -C\mu^{3\delta/2} \left\| \alpha \right\|_{H^1} \left\| \hat{\alpha}\mathbb{1}_{\{|p|<t\}} \right\|_{L^2} ,\end{aligned}$$

where we used that $\|\hat{g}\|_{L^{3/2}} \leq C \|g\|_{H^1}$. Thus we arrive at

$$\mathcal{F}(\alpha) \geq c\mu \left\| \hat{\alpha}\mathbb{1}_{\{|p|<t\}} \right\|_{L^2}^2 - C_1\mu^{3\delta/2} \left\| \alpha \right\|_{H^1} \left\| \hat{\alpha}\mathbb{1}_{\{|p|<t\}} \right\|_{L^2} - C_2\mu \left\| \hat{\alpha}\mathbb{1}_{\{|p|>t\}} \right\|_{L^2}^2 ,$$

where we absorbed all non-leading terms in these. This is a second degree polynomial in $\left\| \hat{\alpha}\mathbb{1}_{\{|p|<t\}} \right\|_{L^2}$ and thus the value of $\left\| \hat{\alpha}\mathbb{1}_{\{|p|<t\}} \right\|_{L^2}$ lies between the roots, i.e.

$$\begin{aligned}\left\| \hat{\alpha}\mathbb{1}_{\{|p|<t\}} \right\|_{L^2} &\leq \frac{C_1\mu^{3\delta/2} \left\| \alpha \right\|_{H^1} + \sqrt{C_1^2\mu^{3\delta} \left\| \alpha \right\|_{H^1}^2 + 4c\, C_2\mu^2 \left\| \hat{\alpha}\mathbb{1}_{\{|p|>t\}} \right\|_{L^2}^2}}{2c\mu} \\ &\leq C \left\| \hat{\alpha}\mathbb{1}_{\{|p|>t\}} \right\|_{L^2} + C\mu^{3\delta/2-1} \left\| \alpha \right\|_{H^1} .\end{aligned}$$

From the estimate

$$\left\| \hat{\alpha}\mathbb{1}_{\{|p|>t\}} \right\|_{L^2}^2 = \int_{|p|>t} \hat{\alpha}(p)^2\, \mathsf{d}p \leq \int_{|p|>t} \hat{\alpha}(p)^2 \frac{1+p^2}{1+t^2}\, \mathsf{d}p \leq \frac{1}{1+t^2} \left\| \alpha \right\|_{H^1}^2 \leq C\mu^{-2\delta} \left\| \alpha \right\|_{H^1}^2 ,$$

we conclude that

$$\left\| \alpha \right\|_{L^2}^2 = \left\| \hat{\alpha}\mathbb{1}_{\{|p|<t\}} \right\|_{L^2}^2 + \left\| \hat{\alpha}\mathbb{1}_{\{|p|>t\}} \right\|_{L^2}^2 \leq C \left(\mu^{-2\delta} + \mu^{3\delta-2}\right) \left\| \alpha \right\|_{H^1}^2 .$$

Choosing the optimal $\delta = 2/5$ we get $\|\alpha\|_{L^2} \leq C\mu^{-2/5} \|\alpha\|_{H^1}$, which, in combination with Equation (10.2.18), yields

$$\left\| \alpha \right\|_{H^1}^2 \leq C\mu^{-4/5} \left\| \alpha \right\|_{H^1}^2 + \mu^{3/2}.$$

Hence $\|\alpha\|_{H^1} \leq C\mu^{3/4}$ and thus also $\|\alpha\|_{L^2} \leq C\mu^{-2/5} \|\alpha\|_{H^1} \leq C\mu^{7/20}$ for sufficiently large μ. □

We now turn to the proof of Lemma 10.2.4.

Proof of Lemma 10.2.4. Let $t = \frac{5}{2} - \frac{3}{r}$. Then we have

$$\|\Delta\|_{L^\infty} \leq C\,\|V\alpha\|_{L^1} \leq C\,\|V\|_{L^r}\,\|\alpha\|_{L^{r'}} \leq C\,\|\alpha\|_{L^2}^t\,\|\alpha\|_{L^6}^{1-t} \leq C\mu^{\frac{15-8t}{20}} = C\mu^{\frac{24-5r}{20r}}$$

by Sobolev's inequality [LL01, Thm. 8.3]. For the difference note that $\Delta(p) - \Delta(q)$ is (proportional to) the Fourier transform of $V(x)\left(1 - e^{i(p-q)\cdot x}\right)\alpha(x)$. Then

$$\left\|V(x)\left(1 - e^{i(p-q)x}\right)\right\|_{L^r}^r = \int_{\mathbb{R}^3} |V(x)|^r \left|1 - e^{i(p-q)\cdot x}\right|^r \mathrm{d}x \leq C\int_{\mathbb{R}^3} |V(x)|^r |p-q|^r |x|^r \,\mathrm{d}x.$$

Using radiality of Δ, the same argument as before gives the desired. $\square$

Finally, we give the proof of Lemma 10.2.8.

Proof of Lemma 10.2.8. Recall from the factorization of the Birman–Schwinger operator in the proof of Proposition 10.2.10, that the self–adjoint operator

$$m_\mu^{(\kappa)}(\Delta)\mathfrak{F}_\mu|V|^{1/2}\frac{1}{1 + V^{1/2}M_{\Delta,\mu}^{(\kappa)}|V|^{1/2}}V^{1/2}\mathfrak{F}_\mu^\dagger$$

acting on $L^2(\mathbb{S}^2)$ has -1 as its lowest eigenvalue and $u(p) = (4\pi)^{-1/2}$ is the unique eigenvector with lowest eigenvalue for μ large enough. Hence, one can easily see that

$$\frac{1}{1 + V^{1/2}M_{\Delta,\mu}^{(\kappa)}|V|^{1/2}}V^{1/2}\mathfrak{F}_\mu^\dagger u$$

is an eigenvector of $B_{\Delta,\mu}$ for the lowest eigenvalue and thus proportional to $V^{1/2}\alpha$. By expanding $\frac{1}{1+x} = 1 - \frac{x}{1+x}$ we conclude that $\Delta = f(\mu)[\hat{\varphi} + \eta_\mu]$, where

$$\eta_\mu = -\sqrt{4\pi}\mathfrak{F}|V|^{1/2}\frac{V^{1/2}M_{\Delta,\mu}^{(\kappa)}|V|^{1/2}}{1 + V^{1/2}M_{\Delta,\mu}^{(\kappa)}|V|^{1/2}}V^{1/2}\mathfrak{F}_\mu^\dagger u\,,$$

which can easily be bounded as

$$\|\eta_\mu\|_{L^\infty} \leq C\,\|V\|_{L^1}^{1/2}\left\|V^{1/2}M_{\Delta,\mu}^{(\kappa)}|V|^{1/2}\right\|_{\mathrm{op}}\left\|V^{1/2}\mathfrak{F}_\mu^\dagger u\right\|_{L^2}\,.$$

For $|p| = \sqrt{\mu}$, we first note that $\hat{\varphi}(\sqrt{\mu}) = \sqrt{4\pi}\mathfrak{F}_\mu V\mathfrak{F}_\mu^\dagger u(1) = e_\mu$. Similarly, since η_μ is radial, we have that

$$\eta_\mu(\sqrt{\mu}) = \frac{1}{4\pi}\int_{\mathbb{S}^2}\eta_\mu(\sqrt{\mu}q)\,\mathrm{d}\omega(q) = -\left\langle u\middle|\mathfrak{F}_\mu|V|^{1/2}\frac{V^{1/2}M_{\Delta,\mu}^{(\kappa)}|V|^{1/2}}{1 + V^{1/2}M_{\Delta,\mu}^{(\kappa)}|V|^{1/2}}V^{1/2}\mathfrak{F}_\mu^\dagger\middle|u\right\rangle$$

and we can thus bound

$$|\eta_\mu(\sqrt{\mu})| \leq C\left\|V^{1/2}M_{\Delta,\mu}^{(\kappa)}|V|^{1/2}\right\|_{\mathrm{op}}\left\||V|^{1/2}\mathfrak{F}_\mu^\dagger u\right\|_{L^2}^2\,.$$

It remains to check that

$$\begin{aligned}\left\||V|^{1/2}\mathfrak{F}_\mu^\dagger u\right\|_{L^2}^2 &= C\int_{\mathbb{R}^3}|V(x)|\left|\int_{\mathbb{S}^2}e^{i\sqrt{\mu}p\cdot x}\frac{1}{\sqrt{4\pi}}\,\mathrm{d}\omega(p)\right|^2\mathrm{d}x \\ &= C\int_{\mathbb{R}^3}|V(x)|\left(\frac{\sin\sqrt{\mu}|x|}{\sqrt{\mu}|x|}\right)^2\mathrm{d}x\,.\end{aligned}$$

Now the claim follows by application of Equations (10.2.7) and (10.2.9). $\square$

Chapter 11

Universal behaviour of the BCS energy gap

This chapter contains the paper

[AllTemp] J. Henheik and A. B. Lauritsen. "Universal behavior of the BCS energy gap". arXiv: 2312.11310 [cond-mat, physics:math-ph]. 2023. DOI: `10.48550/arXiv.2312.11310`.

Abstract. We consider the BCS energy gap $\Xi(T)$ (essentially given by $\Xi(T) \approx \Delta(T, \sqrt{\mu})$, the BCS order parameter) at all temperatures $0 \leq T \leq T_c$ up to the critical one, T_c, and show that, in the limit of weak coupling, the ratio $\Xi(T)/T_c$ is given by a universal function of the relative temperature T/T_c. On the one hand, this recovers a recent result by Langmann and Triola (Phys. Rev. B 108.10 (2023)) on three-dimensional s-wave superconductors for temperatures bounded uniformly away from T_c. On the other hand, our result lifts these restrictions, as we consider arbitrary spatial dimensions $d \in \{1, 2, 3\}$, discuss superconductors with non-zero angular momentum (primarily in two dimensions), and treat the perhaps physically most interesting (due to the occurrence of the superconducting phase transition) regime of temperatures close to T_c.

Contents

11.1 Introduction

The Bardeen–Cooper–Schrieffer (BCS) [BCS57] theory of superconductivity exhibits many interesting features. Notably it predicts, for s-wave superconductors (i.e. those for which the gap function has angular momentum $\ell = 0$, i.e. is radially symmetric), that the superconducting energy gap Ξ (essentially given by $\Xi \approx \Delta(\sqrt{\mu})$, the BCS order parameter) is proportional to the critical temperature T_c with a universal proportionality constant independent of the microscopic details of the electronic interactions, i.e. the specific superconductor. At zero temperature, the claimed universality is the (approximate) formula $\Xi/T_c \approx \pi e^{-\gamma} \approx 1.76$ with $\gamma \approx 0.57$ the Euler–Mascheroni constant, a property which is well-known in the physics literature [BCS57; NS85]. More recently, based on the variational formulation of BCS theory first introduced by Leggett [Leg80] and later developed on mostly by Hainzl and Seiringer with others [FHNS07; HHSS08; HS16; HS08c], it has been put on rigorous grounds in various (physically quite different) limiting regimes [FHNS07; HS08a; HS08b; Hen22; Lau21], [Chapters 9 and 10] (see Section 11.1.2.1 for details). The general picture in all these works is that the universal behavior appears in a limit where "superconductivity is weak", meaning that T_c is small.

The predicted universality at *positive* temperature is notably less studied. It is expected that the ratio $\Xi(T)/T_c$ is given by some universal function of the relative temperature T/T_c [LT23; Leg06], see Figure 11.1.1. For three-dimensional superconductors,[1] this has recently been shown in [LT23] (building on ideas of [LTB19]) for temperatures uniformly in an interval $[0,(1-\varepsilon)T_c]$ for any $\varepsilon > 0$ in an appropriate limit where T_c is small. The perhaps most interesting regime of temperatures, however, are those close to the critical temperature, due to the phase transition occurring there. For such temperatures one expects[2] the behavior [Tin04, Eq. (3.54)]

$$\Xi(T)/T_c \approx C_{\mathsf{univ}}\sqrt{1-T/T_c}, \qquad C_{\mathsf{univ}} = \sqrt{\frac{8\pi^2}{7\zeta(3)}} \approx 3.06. \tag{11.1.1}$$

Notably, the critical exponent $1/2$ (i.e. the order parameter $\Delta(\sqrt{\mu}) \approx \Xi$ vanishing as a square root) agrees with the prediction from the phenomenological Landau theory [Lan37] for second order phase transitions (not to be confused with *Ginzburg*-Landau theory of superconductivity [De 66; GL50; Gor59]) in mean-field systems.

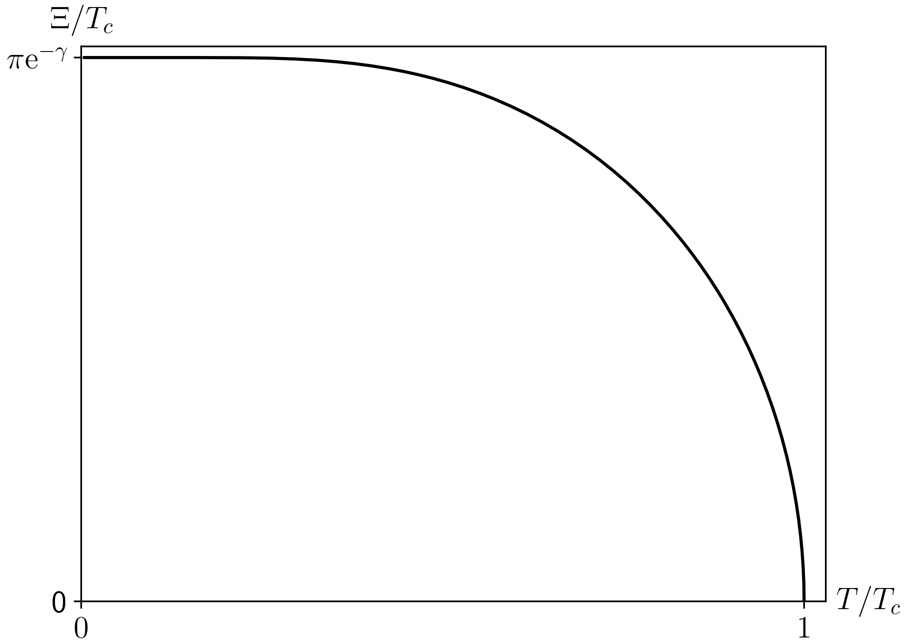


Figure 11.1.1: The ratio of the BCS energy gap and the critical temperature, Ξ/T_c, is well approximated by a *universal function* of the relative temperature T/T_c, which is given by $\mathsf{f}_{\mathsf{BCS}}(\sqrt{1-T/T_c})$ with $\mathsf{f}_{\mathsf{BCS}}$ defined in (11.2.9) below. At $T=0$, it approaches the well-known constant $\pi e^{-\gamma} \approx 1.76$, with $\gamma \approx 0.57$ being the Euler-Mascheroni constant.

In this paper we extend the previously shown universality in three important directions: Firstly, we consider all spatial dimensions $d \in \{1,2,3\}$. Secondly, we treat the full range of

[1] In [LT23], only the three-dimensional case is considered explicitly. However, their arguments seem to be easily extendable to handle also the cases of one- and two-dimensional superconductors.

[2] Historically, the first article suggesting the square root behavior near T_c is by Buckingham [Buc56]. In [BCS57, Eq. (3.31)], BCS verified this in their original model, however, with the numerical constant given by 3.2 instead of $C_{\mathsf{univ}} \approx 3.06$.

temperatures $0 \leq T \leq T_c$. Thirdly, we extend the result to the case of non-zero angular momentum in two dimensions, in particular proving the formula in (11.1.1). Interestingly the case of non-zero angular momentum in two dimensions has the exact same universal behavior as s-wave superconductors in any dimensions: Independently of the angular momentum we find the same universal function describing the ratio $\Xi(T)/T_c$. This is substantially different from the three-dimensional case, where one still expects some sort of universal behavior to occur, only the universal function strongly depends on the angular momentum, see, e.g., [PFCP07] and Remark 11.2.15 below.

One of the central ideas in the analysis of temperatures close to the critical temperature is the use of Ginzburg-Landau (GL) theory. In the physics literature it is well-known that for temperatures close to the critical BCS theory is well-approximated by GL theory [Gor59]. This correspondence has been studied, and put on rigorous grounds, quite recently in the mathematical physics literature [DHM23a; DHM23b; FHSS12b; FL16]. See Section 11.1.2.2 for more details.

11.1.1 Mathematical formulation of BCS theory

We consider a gas of fermions in $\mathbb{R}^d$ for $d = 1, 2, 3$ at temperature $T > 0$ and chemical potential $\mu > 0$. The interaction is described by a two-body, real-valued and reflection-symmetric potential $V \in L^1(\mathbb{R}^d)$, for which we assume the following.

Assumption 11.1.1. We have that $V \in L^{p_V}(\mathbb{R}^d)$ for $p_V = 1$ if $d = 1$, $p_V \in (1, \infty)$ if $d = 2$, or $p_V = 3/2$ if $d = 3$.

A BCS state Γ is given by a pair of functions (γ, α) and can be conveniently represented as a 2×2 matrix valued Fourier multiplier on $L^2(\mathbb{R}^d) \oplus L^2(\mathbb{R}^d)$ of the form

$$\hat{\Gamma}(p) = \begin{pmatrix} \hat{\gamma}(p) & \hat{\alpha}(p) \\ \overline{\hat{\alpha}(p)} & 1 - \hat{\gamma}(p) \end{pmatrix} \tag{11.1.2}$$

for all $p \in \mathbb{R}^d$. Here, $\hat{\gamma}(p)$ denotes the Fourier transform of the one particle density matrix and $\hat{\alpha}(p)$ is the Fourier transform of the Cooper pair wave function. We require reflection symmetry of $\hat{\alpha}$, i.e. $\hat{\alpha}(-p) = \hat{\alpha}(p)$, as well as $0 \leq \hat{\Gamma}(p) \leq 1$ as a matrix. Recall the definition of the BCS free energy functional [HHSS08; Leg80], which is given by

$$\mathcal{F}_T[\Gamma] := \int_{\mathbb{R}^d} (p^2 - \mu)\hat{\gamma}(p)\, \mathrm{d}p - TS[\Gamma] + \int_{\mathbb{R}^d} V(x)|\alpha(x)|^2\, \mathrm{d}x\,, \tag{11.1.3}$$

where the entropy per unit volume is defined as

$$S[\Gamma] = -\int_{\mathbb{R}^d} \mathrm{Tr}_{\mathbb{C}^2}\left[\hat{\Gamma}(p)\log\hat{\Gamma}(p)\right] \mathrm{d}p\,.$$

The variational problem associated with the BCS functional is studied on

$$\mathcal{D} := \left\{\Gamma \text{ as in (11.1.2)} : 0 \leq \hat{\Gamma} \leq 1\,,\ \hat{\gamma} \in L^1(\mathbb{R}^d, (1+p^2)\, \mathrm{d}p)\,,\ \alpha \in H^1_{\mathsf{sym}}(\mathbb{R}^d)\right\}.$$

The following proposition provides the foundation for studying this problem.

Proposition 11.1.2 ([HHSS08], see also [HS16])**.** *Under Assumption 11.1.1 on V, the BCS free energy is bounded below on $\mathcal{D}$ and attains its minimum.*

However, in general, the minimizer is not necessarily unique. This potential non-uniqueness shall not bother us at this stage but will be of importance later on (see Sections 11.1.1.1 and 11.2.3). The Euler–Lagrange equation for α associated with the minimization problem is the celebrated *BCS gap equation*

$$\Delta(p) = -\frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \hat{V}(p-q) \frac{\Delta(q)}{K_T^\Delta(q)} \, \mathrm{d}q \,, \tag{11.1.4}$$

satisfied by $\Delta(p) = -2\,(2\pi)^{-d/2}(\hat{V} \star \hat{\alpha})(p)$, where α is the off–diagonal entry of a minimizing $\Gamma \in \mathcal{D}$ of (11.1.3), see [HHSS08; HS16]. Here, $\hat{V}(p) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} V(x) e^{-ipx} \, \mathrm{d}x$ denotes the Fourier transform of V, and we have introduced the notation

$$K_T^\Delta(p) = \frac{E^\Delta(p)}{\tanh\left(\frac{E_\Delta(p)}{2T}\right)} \qquad \text{with} \qquad E_\Delta(p) = \sqrt{(p^2-\mu)^2 + |\Delta(p)|^2} \,.$$

The gap equation can equivalently be written as

$$(K_T^\Delta + V)\alpha = 0 \,, \tag{11.1.5}$$

where $K_T^\Delta(p)$ is understood as a multiplication operator in momentum space and $V(x)$ is understood as a multiplication operator in position space. The Euler–Lagrange equation for γ (see [HHSS08; HS16]) is given by

$$\hat{\gamma}(p) = \frac{1}{2} - \frac{p^2-\mu}{2K_T^\Delta(p)} \,. \tag{11.1.6}$$

Remark 11.1.3 (Log-divergence)**.** For $T = \Delta = 0$ we have $K_{T=0}^{\Delta=0}(p) = |p^2 - \mu|$. This gives rise to a logarithmic divergence in Equation (11.1.4). Understanding how to treat this $\log$-divergence was one of the key insights of Langmann and Triola [LT23].

11.1.1.1 Critical temperature and energy gap

The system described by $\mathcal{F}_T$ is *superconducting* if and only if any minimizer Γ of $\mathcal{F}_T$ has off–diagonal entry $\alpha = \Gamma_{12} \not\equiv 0$ (or, equivalently, (11.1.4) has a solution $\Delta \not\equiv 0$). The question, whether a system is superconducting or not can be reduced to a linear criterion involving the pseudo–differential operator with symbol

$$K_T(p) \equiv K_T^0(p) = \frac{p^2-\mu}{\tanh\left(\frac{p^2-\mu}{2T}\right)} \,.$$

In fact, as shown in [HHSS08], the system is superconducting if and only if the operator $K_T + V$ has at least one negative eigenvalue. Moreover, there exists a unique *critical temperature* $T_c \geq 0$ being defined as

$$\boxed{T_c := \inf\{T > 0 : K_T + V \geq 0\}} \,, \tag{11.1.7}$$

for which $K_{T_c} + V \geq 0$ and $\inf \operatorname{spec}(K_T + V) < 0$ for all $T < T_c$. By Assumption 11.1.1 and the asymptotic behavior $K_{T_c}(p) \sim p^2$ for $|p| \to \infty$ the critical temperature is well-defined by Sobolev's inequality [LL01, Thm. 8.3]. Note that, for $T \geq T_c$ the BCS functional (11.1.3) is uniquely minimized by the normal state $\Gamma_{\mathsf{FD}} \equiv (\gamma_{\mathsf{FD}}, 0)$, where

$$\hat{\gamma}_{\mathsf{FD}}(p) = \frac{1}{1 + e^{\frac{1}{T}(p^2-\mu)}} \tag{11.1.8}$$

is the usual Fermi-Dirac distribution. In contrast, for temperatures $0 \leq T < T_c$ strictly below the critical temperature, the normal state Γ_{FD} is not a minimizer of (11.1.3) and it is a priori not clear whether or not the minimizer of (11.1.3) is unique.

In this paper we deal with two different cases. In the case of s-wave superconductivity we will assume properties of V such that the minimizer is unique and in the case of 2-dimensional non-zero angular momentum we will assume properties of V such that there are at most 2 minimizers, see Section 11.2.3.

For the s-wave case we assume the following.

Assumption 11.1.4. Let the (real valued) interaction potential $V \in L^1(\mathbb{R}^d)$ be *radially symmetric* and assume that V is of *negative type*, i.e. $\hat{V} \leq 0$ and $\hat{V}(0) < 0$.

As shown in [HS08b], Assumption 11.1.4 implies that, in particular, the critical temperature is non-zero, i.e. $T_c > 0$.[3] Moreover, as already indicated above, it ensures that the minimizer of (11.1.3) is unique. While this fact is already known at zero temperature [HS08b, Lemma 2], we are not aware of any place in the literature where the extension to positive temperature is given. As we will need this extension, we formulate it in the following proposition and give a proof in Section 11.A.1.

Proposition 11.1.5 (Uniqueness of minimizers for potentials of negative type)**.** *Let V satisfy Assumptions 11.1.1 and 11.1.4, and consider the BCS functional* (11.1.3)*. Then we have the following:*

(i) For $0 \leq T < T_c$, let $\Gamma \equiv (\gamma, \alpha)$ be a minimizer of the BCS functional (11.1.3) *(which exists by means of Proposition 11.1.2). Then the operator $K_T^{\Delta} + V$ from* (11.1.5) *is non–negative and α is its unique ground state with eigenvalue zero 0.*

(ii) The minimizer $\Gamma =: \Gamma_* \equiv (\gamma_*, \alpha_*)$ of (11.1.3) *is unique up to a phase of α_* and can be chosen to have strictly positive Fourier transform $\hat{\alpha}_*$. Moreover, both γ_* and α_* are radial functions.*

In particular, under Assumption 11.1.4, we have that the *energy gap*

$$\boxed{\Xi(T) := \inf_{p \in \mathbb{R}^d} \sqrt{(p^2 - \mu)^2 + |\Delta(p)|^2}}\,, \tag{11.1.9}$$

for Δ being the (up to multiplication by a constant phase) unique non-zero solution of (11.1.4) and temperatures $0 \leq T < T_c$, is well-defined.

In case there is more than one solution Δ of the BCS gap equation (11.1.4) (i.e. more than one minimizer of the BCS functional) we may for each such Δ define the energy gap Ξ as in Equation (11.1.9). In the case of two dimensions with (definite) non-zero angular momentum we shall prove that there exist exactly two (up to multiplication of either by a constant phase) such functions, $\Delta_{\pm}$. They however satisfy $|\Delta_+| = |\Delta_-|$ and so the energy gap Ξ is also here uniquely defined. For the details see Section 11.2.3.

Remark 11.1.6. The energy gap is essentially the same as the order parameter $\left|\Delta(\sqrt{\mu})\right|$ as we show in Equations (11.3.18) and (11.3.29) below. In particular, one may replace Ξ with $\left|\Delta(\sqrt{\mu})\right|$ in our main results, Proposition 11.2.1 and Theorems 11.2.4 and 11.2.11.

[3] To be precise, the arguments in [HS08b] cover only the case $d = 3$, but, as already noted in [FHSS12b], they are immediately transferable to the cases $d = 1, 2$.

11.1.1.2 Weak coupling

We consider here the weak–coupling limit where the interaction is of the form λV for a $\lambda > 0$ and we consider the limit $\lambda \to 0$. In the weak–coupling limit an important role is played by the (rescaled) operator $\mathcal{V}_\mu : L^2(\mathbb{S}^{d-1}) \to L^2(\mathbb{S}^{d-1})$ [CM21; HS08b; HS10], [Chapter 9]. This operator, which is defined as

$$(\mathcal{V}_\mu u)(p) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{S}^{d-1}} \hat{V}(\sqrt{\mu}(p-q))u(q) \, \mathrm{d}\omega(q)\,, \tag{11.1.10}$$

where $\mathrm{d}\omega$ denotes the uniform (Lebesgue) measure on the unit sphere $\mathbb{S}^{d-1}$, measures the strength of the interaction potential $\hat{V}$ on the Fermi surface. The pointwise evaluation of $\hat{V}$ (and in particular on a $\operatorname{codim}-1$ submanifold) is well-defined since we assume that $V \in L^1(\mathbb{R}^d)$.

The lowest eigenvalue $e_\mu = \inf \operatorname{spec} \mathcal{V}_\mu$ is of particular importance. Note, that $\mathcal{V}_\mu$ is a trace-class operator (see the argument above [FHNS07, Equation (3.2)]) with

$$\operatorname{tr}(\mathcal{V}_\mu) = \frac{|\mathbb{S}^{d-1}|}{(2\pi)^d} \int_{\mathbb{R}^d} V(x) \, \mathrm{d}x = \frac{|\mathbb{S}^{d-1}|}{(2\pi)^{d/2}} \hat{V}(0)\,.$$

For radial potentials one sees that the eigenfunctions of $\mathcal{V}_\mu$ are the spherical harmonics.

For potentials of negative type we have $\hat{V}(0) < 0$ and so $e_\mu < 0$. This corresponds to an attractive interaction between (some) electrons on the Fermi sphere. Further, one easily sees that the constant function $u(p) = (|\mathbb{S}^{d-1}|)^{-1/2}$ is an eigenfunction of $\mathcal{V}_\mu$, which, since $\hat{V} \leq 0$ by Assumption 11.1.4, is in fact the ground state by the Perron–Frobenius theorem, i.e.

$$e_\mu = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{S}^{d-1}} \hat{V}(\sqrt{\mu} - q\sqrt{\mu}) \, \mathrm{d}\omega(q)\,. \tag{11.1.11}$$

In two dimensions the spherical harmonics take the form $u_{\pm\ell}(p) = (2\pi)^{-1/2} e^{\pm i\ell\varphi}$ with φ denoting the angle of $p \in \mathbb{R}^2$ in polar coordinates. In this case the ground state space of $\mathcal{V}_\mu$ is spanned by $\{u_{\pm\ell}\}_{\ell\in\mathcal{L}}$ for some set of angular momenta $\mathcal{L}$. If $\ell_0 \neq 0$ for some $\ell_0 \in \mathcal{L}$ then the ground state is at least twice degenerate, since then both $u_{\pm\ell_0}$ are eigenfunctions with this lowest eigenvalue.

11.1.2 Previous mathematical results

So far, all mathematical results on solutions of the BCS gap equation (11.1.4) focused either on zero temperature, $T = 0$, or the regime close to the critical one, $T \approx T_c$, where the transition from superconducting to normal behavior is described by Ginzburg-Landau theory.

11.1.2.1 BCS theory in limiting regimes: Universality at $T = 0$

At zero temperature it is expected, that the ratio of the energy gap and the critical temperature is given by a universal constant,

$$\frac{\Xi(T=0)}{T_c} \approx \pi e^{-\gamma}\,, \tag{11.1.12}$$

with $\gamma \approx 0.577$ the Euler–Mascheroni constant in a limiting regime where "superconductivity is weak", meaning that T_c is small.

In the literature three such limits have been studied: Historically, the first regime, which has been considered is the *weak coupling limit* in three spatial dimensions [FHNS07; HS08b], which we recently extended to one and two dimensions in Chapter 9. The critical temperature in the *low density limit* in three dimensions was studied in [HS08a] and later complemented by a study of the energy gap by one of us in [Lau21], thus, in combination, yielding the above-mentioned universal behavior. Finally, we considered the *high density limit*, again in three dimension, in [Hen22] and Chapter 10 and proved (11.1.12) in this regime.

11.1.2.2 Superconductors close to T_c: Ginzburg-Landau theory

For temperatures close to the critical BCS theory is well-approximated by Ginzburg-Landau (GL) theory. In contrast to the microscopic BCS model, GL theory is a phenomenological model, which describes the superconductor on a macroscopic scale. Moreover, as suggested by Equation (11.1.1) a natural parameter measuring "closeness to T_c" is the parameter $h = \sqrt{1 - T/T_c}$. A rigorous analysis of various aspects of BCS theory in the limit $h \to 0$ was then studied in [FHSS12b; FHSS16; FL16], very recently also allowing for general external fields [DHM23a; DHM23b]. Of particular interest to us is the fact that any minimizer of the BCS functional (γ, α) has $\alpha \approx h\psi\mathfrak{a}_0$ with $\mathfrak{a}_0 \in \ker(K_{T_c} + \lambda V)$ fixed and $\psi \in \mathbb{C}$ a minimizer of the corresponding GL functional, see [FL16, Theorem 2.10].

11.1.3 Outline of the paper

The rest of this paper is structured as follows. In Section 11.2 we present our main result, starting with the prototypical universality in the original BCS model (Section 11.2.1). Afterwards, in Sections 11.2.2 and 11.2.3 we describe our results on universality for s-wave superconductors in arbitrary dimension $d \in \{1, 2, 3\}$, and for two-dimensional superconductors having pure angular momentum, respectively. The proofs of these results are given in Section 11.3, while several additional proofs are deferred to Appendix 11.A.

11.2 Main Result

We next describe the main results of the paper. We first consider the example of an interaction as considered by BCS [BCS57]. The reason for doing this is twofold:

1. It highlights, how the universal function $\Xi(h)/T_c \approx \mathsf{f}_{\mathrm{BCS}}(h)$ appears.
2. A central idea in the proof of removing the $\log$-divergence is already present in the BCS gap equation (11.1.4). (Recall Remark 11.1.3.)

11.2.1 Energy gap in the original BCS approximation [BCS57]

In their seminal work [BCS57], Bardeen–Cooper–Schrieffer modeled the interaction by a so called *separable potential* $V(x, y)$ (i.e. factorizing and depending not only on the relative coordinate $x - y$), whose Fourier transform $\hat{V}(p, q)$ is a product of two *radial single variable* functions, that are compactly supported in the shell

$$\mathcal{S}_\mu(T_D) := \{p \in \mathbb{R}^d : |p^2 - \mu| \le T_D\} \tag{11.2.1}$$

around the Fermi surface $\{p \in \mathbb{R}^d : p^2 = \mu\}$, the only (material dependent) parameter being the so-called *Debye temperature* $0 < T_D < \mu$. Switching from momentum p to energy $\varepsilon = p^2 - \mu$, the just mentioned single variable functions are chosen in such a way, that[4]

$$\hat{V}(\varepsilon, \varepsilon')N(\varepsilon') = -\lambda_{\mathsf{BCS}}\, \theta(1 - |\varepsilon/T_D|)\theta(1 - |\varepsilon'/T_D|)\,, \qquad \lambda_{\mathsf{BCS}} > 0\,, \tag{11.2.2}$$

where the electronic density of states (DOS) is denoted by $N(\varepsilon) \sim (\varepsilon + \mu)^{(d-2)/2}$ and θ is the Heaviside function. ($\theta(t) = 1$ for $t > 0$ and $\theta(t) = 0$ otherwise.)

In this case, the (unique non-negative) solution to the BCS gap equation (11.1.4) is given by

$$\Delta(\varepsilon) = \Delta \cdot \theta(1 - |\varepsilon/T_D|) \tag{11.2.3}$$

for some temperature dependent constant $\Delta \geq 0$, which is determined by the scalar gap equation (cf. [BCS57, Eq. (3.27)])

$$\frac{1}{\lambda_{\mathsf{BCS}}} = \int_0^{T_D} \frac{\tanh\left(\frac{\sqrt{\varepsilon^2+\Delta^2}}{2T}\right)}{\sqrt{\varepsilon^2 + \Delta^2}} \mathrm{d}\varepsilon \tag{11.2.4}$$

for any temperature $0 \leq T < T_c$. In turn, the critical temperature $T_c > 0$ is determined by (11.2.4) with $\Delta = 0$, i.e.

$$\frac{1}{\lambda_{\mathsf{BCS}}} = \int_0^{T_D} \frac{\tanh\left(\frac{\varepsilon}{2T_c}\right)}{\varepsilon} \mathrm{d}\varepsilon\,. \tag{11.2.5}$$

In case of a small BCS coupling parameter, $\lambda_{\mathsf{BCS}} \ll 1$,[5] it holds that T_c is exponentially small in λ_{BCS}, i.e. $T_c \sim e^{-1/\lambda_{\mathsf{BCS}}}$ (see [BCS57, Eq. (3.29)]). Moreover, it is easily checked that Δ as a function of temperature is monotonically decreasing in the interval $[0, T_c]$ and satisfies $\Delta(T = 0) \sim e^{-1/\lambda_{\mathsf{BCS}}}$, similarly to the critical temperature.

Next, changing variables as $x := \varepsilon/T_c$ and setting $\delta := \Delta/T_c$ as well as[6]

$$h := \sqrt{1 - \frac{T}{T_c}} \quad \text{for} \quad 0 \leq T \leq T_c\,, \tag{11.2.6}$$

we can subtract (11.2.4) and (11.2.5) to find

$$\int_0^{T_D/T_c} \left\{ \frac{\tanh\left(\frac{\sqrt{x^2+\delta^2}}{2(1-h^2)}\right)}{\sqrt{x^2+\delta^2}} - \frac{\tanh\left(\frac{x}{2}\right)}{x} \right\} \mathrm{d}x = 0\,. \tag{11.2.7}$$

Note that this difference formula (11.2.7) removes the divergences of (11.2.4)–(11.2.5) as $\lambda_{\mathsf{BCS}} \to 0$.

The proof of the following proposition is given in Section 11.3.1. (In the statement of Proposition 11.2.1, one may replace Ξ by the order parameter $\Delta(\sqrt{\mu})$, see Remark 11.1.6 above.)

[4]Assuming that $\hat{V}$ is constant throughout the energy shell (11.2.1) (as done in [BCS57]), the BCS coupling parameter emerges as $\lambda_{\mathsf{BCS}} = -\hat{V}(0,0)N(0)$.

[5]This can happen for various reasons. One example is that V itself is scaled by a coupling parameter $\lambda > 0$, i.e. $V \to \lambda V$, and one considers the limit $\lambda \to 0$, as done in Sections 11.2.2–11.2.3.

[6]As mentioned above, the parameter h is commonly used (see, e.g., [FHSS12b; FL16]) in the context of Ginzburg-Landau theory, where it served as a 'semiclassical' small parameter in the derivation this theory.

Proposition 11.2.1 (Energy gap in the original BCS model [BCS57])**.** *Let $\mu > 0$, fix a Debye temperature $0 < T_D < \mu$ and let $\lambda_{\mathsf{BCS}} > 0$ be the BCS coupling parameter as above. Let the critical temperature T_c and the gap function $\Delta(p)$ be defined via* (11.2.3)–(11.2.5)*.*

Then the energy gap Ξ (defined in (11.1.9)*) as a function of $h = \sqrt{1 - T/T_c}$ for $0 \le T \le T_c$ (recall* (11.2.6)*) is given by*

$$\Xi(h) = T_c \, \mathsf{f}_{\mathsf{BCS}}(h) \left(1 + O(e^{-1/\lambda_{\mathsf{BCS}}})\right) \tag{11.2.8}$$

uniformly in $h \in [0,1]$, where the function $\mathsf{f}_{\mathsf{BCS}} : [0,1] \to [0,\infty)$ is implicitly defined via

$$\int_{\mathbb{R}} \left\{ \frac{\tanh \frac{\sqrt{s^2 + \mathsf{f}_{\mathsf{BCS}}(h)^2}}{2(1-h^2)}}{\sqrt{s^2 + \mathsf{f}_{\mathsf{BCS}}(h)^2}} - \frac{\tanh \frac{s}{2}}{s} \right\} \mathrm{d}s = 0 \tag{11.2.9}$$

and plotted in Figure 11.2.1.

This means that, independent of the material dependent Debye temperature $T_D > 0$ and the chemical potential $\mu > 0$, the energy gap Ξ within the original BCS approximation [BCS57], follows a universal curve, described by (11.2.8), in the limit of weak BCS coupling. A similar formula for $\mathsf{f}_{\mathsf{BCS}}$ like (11.2.9) (but as a function of $x := 1 - h^2$) also appeared in the monograph of Leggett [Leg06, Eq. (5.5.21)]. We now list a few basic properties of $\mathsf{f}_{\mathsf{BCS}}$, whose proofs we omit, as they can be obtained by means of the implicit function theorem and further elementary tools (see also [LT23, Lemma 1] as well as Lemmas 11.3.1 and 11.3.13 below). Almost all of these properties become apparent from Figure 11.2.1.

Lemma 11.2.2 (Properties of $\mathsf{f}_{\mathsf{BCS}}$)**.** *There exists a unique implicitly defined solution function $\mathsf{f}_{\mathsf{BCS}} : [0,1] \to [0,\infty)$ of* (11.2.9)*. Moreover, $\mathsf{f}_{\mathsf{BCS}}$ has the following properties:*

(i) It is strictly monotonically increasing in $[0,1]$.

(ii) It is C^1 in $(0,1)$ and has continuous one-sided derivatives at the boundaries 0 and 1.

(iii) It has the boundary values $\mathsf{f}_{\mathsf{BCS}}(0) = 0$, $\mathsf{f}'_{\mathsf{BCS}}(0) = C_{\mathsf{univ}}$ and $\mathsf{f}_{\mathsf{BCS}}(1) = \pi e^{-\gamma} \approx 1.76$, $\mathsf{f}'_{\mathsf{BCS}}(1) = 0$. Here, $\gamma \approx 0.57$ is the Euler-Mascheroni constant and

$$C_{\mathsf{univ}} := \sqrt{\frac{8\pi^2}{7\zeta(3)}} \approx 3.06\,, \tag{11.2.10}$$

where $\zeta(s)$ denotes Riemann's ζ-function.

Remark 11.2.3 (Contact interactions)**.** Our proof of Proposition 11.2.1 can easily be generalized to all BCS models, in which the energy gap is constant (at least near the Fermi surface).

(a) In case of a delta potential, $V(x) = -\delta(x)$ in one spatial dimension, $d = 1$, the gap function solving (11.1.4) is given by a constant (simply because here $\hat{V}$ is constant). This setting can be analyzed similarly (in a weak coupling limit, i.e. replacing $V \to \lambda V$ and taking $\lambda \to 0$) as done in Proposition 11.2.1 for the original BCS model [BCS57].

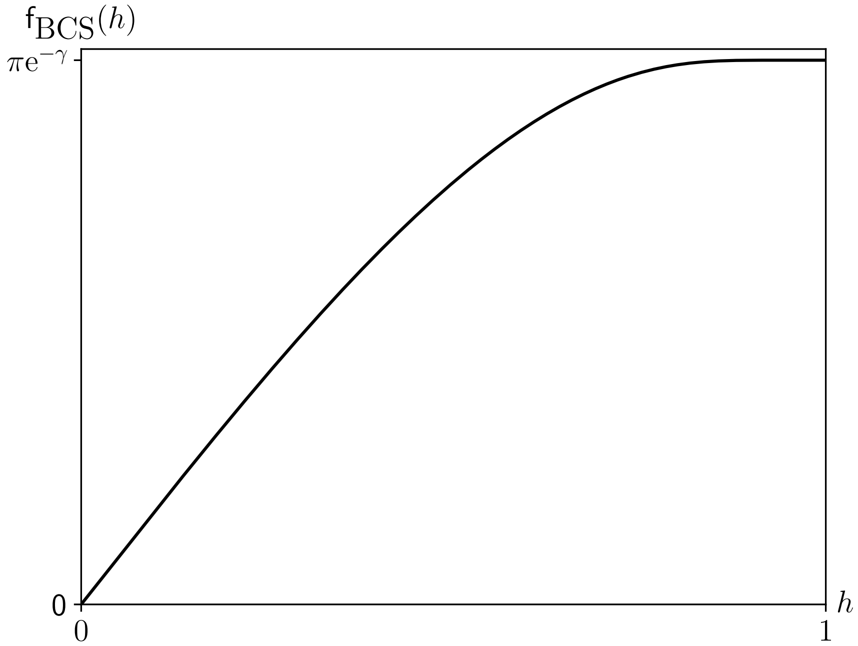


Figure 11.2.1: Sketch of the function f_{BCS} obtained via the implicit relation (11.2.9).

(b) Also for contact interactions in three spatial dimensions, $d = 3$, the situation is similar. This setting is studied in [BHS14a; BHS14b], where it is shown that for a suitable sequence of potentials V_ℓ converging to a point interaction with scattering length $a < 0$, the gap function Δ_ℓ converges (uniformly on compact sets, see [BHS14a, Eq. (14)]) to a constant Δ solving the gap equation

$$-\frac{1}{4\pi a} = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left(\frac{1}{K_T^\Delta(p)} - \frac{1}{p^2} \right) \mathrm{d}p \, .$$

Replacing the limit of weak coupling by a small scattering length limit, $a \to 0$, one can obtain a result similar to Proposition 11.2.1.

11.2.2 Universal behavior of the s-wave BCS energy gap

After having discussed the prototypical universality in the seminal BCS paper [BCS57], we can now formulate our main result on general s-wave superconductors with local interactions. The proof of Theorem 11.2.4 is presented in Sections 11.3.2–11.3.4, while the main ideas are briefly described in Remark 11.2.7 below. (We remark that, in the statement of Theorem 11.2.4, one may replace Ξ by the order parameter $\Delta(\sqrt{\mu})$, see Remark 11.1.6 above.)

Theorem 11.2.4 (BCS energy gap for s-wave superconductors). *Let $d \in \{1, 2, 3\}$, $\mu > 0$, $\lambda > 0$ and let V satisfy Assumptions 11.1.1 and 11.1.4. Let T_c and Ξ be as in* (11.1.7) *and* (11.1.9) *with interaction λV and Δ the unique non-zero solution the BCS gap equation* (11.1.4) *with interaction λV.*

Then, with $f_{BCS}(h), h = \sqrt{1 - T/T_c}$ being the function defined via (11.2.9)*, we have the following:*

(a) *Assuming additionally that* $|\cdot|^2 V \in L^1(\mathbb{R}^d)$, *it holds that*

$$\Xi(h) = T_c \, \mathsf{f}_{\mathsf{BCS}}(h) \left(1 + O(h^{-1} e^{-c/\lambda})\right) \tag{11.2.11}$$

for some constant $c > 0$ *independent of* λ *and* h.

(b) *Assuming additionally that* $(1 + |\cdot|)V \in L^2(\mathbb{R}^d)$, *it holds that*

$$\Xi(h) = T_c \, \mathsf{f}_{\mathsf{BCS}}(h) \left(1 + O(h e^{c'/\lambda}) + o_{\lambda \to 0}(1)\right) \tag{11.2.12}$$

for some constant $c' > 0$ *independent of* λ *and* h *and where* $o_{\lambda \to 0}(1)$ *vanishes as* $\lambda \to 0$ *uniformly in* h.

For the special case $h = 1$, i.e. $T = 0$, (11.2.11) reproduces the results from [HS08b] (for $d = 3$) and Chapter 9 (for $d = 1, 2$), which state the universality

$$\lim_{\lambda \to 0} \frac{\Xi(T = 0)}{T_c} = \frac{\pi}{e^\gamma}$$

at $T = 0$. Moreover, by (11.2.11) again, we find that, uniformly in temperatures bounded away from T_c, i.e. $h \in [\varepsilon, 1]$ for some fixed $\varepsilon > 0$,

$$\lim_{\lambda \to 0} \frac{\Xi(h)}{T_c} = \mathsf{f}_{\mathsf{BCS}}(h) \,,$$

recovering the universality result in [LT23] (for $d = 3$), with an exponential speed $O(e^{-c/\lambda})$ of convergence. In the complementary case, for temperatures very close to the critical temperature, $T \approx T_c$, the question of universality is (i) physically more interesting due to the phase transition from superconducting to normal behavior and (ii) mathematically more delicate than in the previous scenarios. This is because now there are *two* small parameters λ and h, instead of λ only, and the error term in (11.2.11) might actually be large compared to one. However, now involving both, (11.2.11) *and* (11.2.12), we find that

$$\lim_{\substack{\lambda, h \to 0 \\ e^{-c/\lambda} \ll h}} \frac{\Xi(h)}{T_c \, h} = C_{\mathsf{univ}} \quad \text{and} \quad \lim_{\substack{\lambda, h \to 0 \\ h \ll e^{-c'/\lambda}}} \frac{\Xi(h)}{T_c \, h} = C_{\mathsf{univ}} \tag{11.2.13}$$

with the aid of Lemma 11.2.2 (iii). In particular, the ratio $\Xi(h)/(T_c h)$ converges to the *same* universal constant C_{univ} (recall (11.2.10)) in both orders of limits, $\lim_{\lambda \to 0} \lim_{h \to 0}$ and $\lim_{h \to 0} \lim_{\lambda \to 0}$.

Remark 11.2.5 (Joint limit)**.** A careful inspection of the proof reveals that the constants c, c' satisfy $c < c'$. In particular, the proof does *not* allow the two regimes considered in (11.2.13) to be overlapping and we cannot prove that $\lim_{\lambda, h \to 0} \frac{\Xi(h)}{T_c h} = C_{\mathsf{univ}}$ in any joint limit. We expect this to hold in any joint limit, however, as we saw for the particular example from [BCS57] in Proposition 11.2.1

Remark 11.2.6 (Comparison of assumptions with [LT23])**.** Compared to the similar result in [LT23] our assumptions hold for a slightly different class of potentials. The assumptions of [LT23] are essentially on the smoothness of the interaction V (formulated via some regularity/decay assumption on the Fourier transform $\hat{V}$). Our assumptions on the other hand are on the regularity/decay of V. In particular, our assumptions cover the examples of [LT23, Table I] which are *not* covered by the assumptions of [LT23]. These are (in three dimensions)

$$V_{\mathsf{Yukawa}}(x) = \frac{e^{-|x|}}{4\pi|x|}, \qquad V_{a\mathsf{Y}+b\mathsf{E}}(x) = \frac{(2a + b|x|)e^{-|x|}}{8\pi|x|}, \qquad V_{x\text{-}\mathsf{box}}(x) = \frac{3\theta(1 - |x|)}{4\pi} \,.$$

Remark 11.2.7 (On the proof)**.** The main ideas in the proof of Theorem 11.2.4 are the following.

(a) For part (a), we crucially use that both, $K_T^{\Delta}+\lambda V$ and $K_{T_c}+\lambda V$, have lowest eigenvalue zero. We then consider their corresponding Birman-Schwinger (BS) operators and use that, for λ small enough, two naturally associated operators on the Fermi sphere both have the *same* ground state. Evaluating the difference of these two associated operators in this common ground state, we find that a *difference* of two logarithmically divergent integrals, similarly to (11.2.9), vanishes up to exponentially small errors $O(\mathrm{e}^{-c/\lambda})$.

The removal of the $\log$-divergence in this way (which – in a similar fashion – was the major insight in [LT23]) is the key idea to (i) access also non-zero temperatures and (ii) obtain extremely precise error estimates (compared to all the previous results mentioned in Section 11.1.2.1).

(b) For part (b), we employ Ginzburg-Landau (GL). The principal realm of GL theory is to describe superconductors and superfluids close to their critical temperature T_c. In this regime, when superconductivity is weak, the main idea is that the prime competitor for developing a small off-diagonal component $\hat{\alpha}$ for a BCS minimizer, is the *normal state* $\Gamma_{\mathsf{FD}} = (\gamma_{\mathsf{FD}}, 0)$, with γ_{FD} given by the usual Fermi-Dirac distribution (recall (11.1.8)). Moreover, to leading order, the off-diagonal component $\hat{\alpha}$ lies in the kernel (which agrees with the ground state space) of the operator $K_{T_c}+\lambda V$.

The main input, which we use, is that every minimizer (γ, α) of the BCS functional has $\alpha \approx h\psi\mathfrak{a}_0$ with $\mathfrak{a}_0 \in \ker(K_{T_c}+\lambda V)$ fixed and $\psi \in \mathbb{C}$ minimizing the corresponding GL functional [FL16, Theorem 2.10]. Taking the convolution of $\hat{\mathfrak{a}}_0$ with $\hat{V}$, we find the universal constant (11.2.10) appearing in $\Xi/(T_c h) \approx C_{\mathsf{univ}}$.

Moreover, the “additional assumptions" in Theorem 11.2.4 are not quite rigid, meaning that they can be weakened in the following sense.

(a) In case that $|\cdot|^{2\alpha}V \in L^1$ for a $0<\alpha\leq 1$ the error term in Equation (11.2.11) should instead be $O(h^{-1}e^{-c\alpha/\lambda})$ with the constant c then being independent also of α.

(b) In case that $(1+|\cdot|)V \in L^p(\mathbb{R}^d)$ for $p<2$, the factor h in the first error term in (11.2.12) would not appear raised to the first power but with exponent

$$(3p-4)/p \quad \text{for} \quad d=1, \quad (3p-4)/p-\varepsilon \quad \text{for} \quad d=2, \quad \text{and} \quad (4p-6)/p \quad \text{for} \quad d=3.$$

Remark 11.2.8 (Other limits)**.** Although, in this paper, we considered only the weak coupling limit, we expect the relation $\Xi(h) \approx T_c \mathsf{f}_{\mathsf{BCS}}(h)$ to hold also in other limiting regimes in which “superconductivity is weak", that is, e.g., the low-[7] and high-density limit, that were studied in [HS08a; Lau21] and [Hen22] and Chapter 10, respectively. This idea is already contained in [LT23], where the authors considered a “universal" parameter λ in [LT23, Eq. (7)], which can be small for various physical situations.

Remark 11.2.9 (Non-universality)**.** We recover also the formula [LT23, Equation (16)]

$$\frac{\Delta(p)}{\Delta(\sqrt{\mu})} = F(p) + O(e^{-c/\lambda}) \tag{11.2.14}$$

[7] For dimensions $d=1,2$, the same caveats mentioned in Remark 9.2.8 apply.

for some function F not depending on the temperature and some constant $c > 0$. The function F depends on the interaction V however. For this reason (11.2.14) is called a "non-universal" feature in [LT23]. The proof of (11.2.14) is given in Section 11.3.3.

11.2.3 The case of pure angular momentum for $d = 2$

In this section, we generalize Theorem 11.2.4 from s-wave superconductors to two-dimensional systems which have a definite (or *pure*) angular momentum $\ell_0 \in \mathbb{N}_0$, which can differ from 0.

Assumption 11.2.10 (Pure angular momentum)**.** Let $V \in L^1(\mathbb{R}^2)$ be radially symmetric and *attractive on the Fermi sphere*, i.e. the lowest eigenvalue e_μ of $\mathcal{V}_\mu$ is strictly negative (recall (11.1.10)–(11.1.11)). Moreover, suppose that for all $\lambda > 0$ small enough the lowest eigenvalue of $K_{T_c} + \lambda V$ is at most twice degenerate, i.e. $\dim\ker(K_{T_c} + \lambda V) \in \{1, 2\}$.

Since K_{T_c} commutes with the Laplacian, Assumption 11.2.10 ensures the ground state of $K_{T_c} + \lambda V$ to have definite angular momentum. More precisely, it holds that

$$\ker(K_{T_c} + \lambda V) = \mathrm{span}\{\rho\} \otimes \mathcal{S}_{\ell_0} \quad \text{with} \quad \mathcal{S}_\ell := \mathrm{span}\Big\{\mathrm{e}^{\pm \mathrm{i}\ell\varphi}\Big\} \subset L^2(\mathbb{S}^1) \quad \text{for some} \quad \ell_0 \in \mathbb{N}_0\,, \tag{11.2.15}$$

where $\rho \in L^2((0,\infty); r\,\mathrm{d}r)$ is a (λ-dependent) radial function.[8]

We can now formulate our main result in the case of pure angular momentum for $d = 2$. (We again remark that, in the statement of Theorem 11.2.11, one may replace Ξ by the order parameter $|\Delta(\sqrt{\mu})|$, see Remark 11.1.6 above.)

Theorem 11.2.11 (BCS energy gap for $2d$ pure angular momentum)**.** *Let $d = 2$, $\mu > 0$ and let V satisfy Assumptions 11.1.1 and 11.2.10. Define the critical temperature T_c and energy gap Ξ as in* (11.1.7) *and* (11.1.9) *with interaction λV for a $\lambda > 0$ and Δ being* any (arbitrary!) *non-zero solution the BCS gap equation* (11.1.4) *with interaction λV.*

Then, with $\mathsf{f}_{\mathsf{BCS}}(h), h = \sqrt{1 - T/T_c}$ being the function defined via (11.2.9)*, we have the following:*

(a) Assume additionally that $V \in L^2(\mathbb{R}^2)$, $\hat{V} \in L^r(\mathbb{R}^2)$ for some $1 \le r < 2$ and that $|\cdot|^2 V \in L^1(\mathbb{R}^d)$. Then there exists $0 \le \tilde{T} < T_c$ with $\tilde{T}/T_c \le \mathrm{e}^{-\mathfrak{c}/\lambda}$ for some $\mathfrak{c} > 0$, such that for all temperatures $T \in (\tilde{T}, T_c)$ it holds that

$$\Xi(h) = T_c\, \mathsf{f}_{\mathsf{BCS}}(h) \left(1 + O(h^{-1} e^{-c/\lambda})\right) \tag{11.2.16}$$

for some constant $c > 0$ independent of λ and h.

(b) Assuming additionally that $(1 + |\cdot|)V \in L^2(\mathbb{R}^d)$, it holds that

$$\Xi(h) = T_c\, \mathsf{f}_{\mathsf{BCS}}(h) \left(1 + O(h e^{c'/\lambda}) + o_{\lambda\to 0}(1)\right) \tag{11.2.17}$$

for some constant $c' > 0$ independent of λ and h and where $o_{\lambda\to 0}(1)$ vanishes as $\lambda \to 0$ uniformly in h.

The proof of Theorem 11.2.11 is given in Section 11.3.5.

[8] In fact, the angular momentum of the kernel of $K_{T_c} + \lambda V$ must be *even*, i.e. $\ell_0 \in 2\mathbb{N}_0$. This is because BCS theory is formulated for reflection symmetric α, whence $K_{T_c} + \lambda V$ is naturally defined on the space of reflection symmetric functions only.

Remark 11.2.12 (On the assumptions)**.** The additional assumptions in part (a) here compared to Theorem 11.2.4 (namely $V \in L^2$ and $\hat{V} \in L^r$) are those of [DGHL18, Theorem 2.1]. The proof of Equation (11.2.16) centrally uses this result. As discussed in [DGHL18, Remark 2.3] these additional assumptions are expected to be of a technical nature.

Remark 11.2.13 (The temperature $\tilde{T}$)**.** The presence of the temperature $\tilde{T}$ in Theorem 11.2.11 (a) arises from the first excited eigenvalue of $K_{T_c}+\lambda V$, see [DGHL18, Remark 2.2]. As discussed in the proof, the temperatures $T_c, \tilde{T}$ are given by $T_c = T_c(\ell_0)$ and $\tilde{T} = T_c(\ell_1)$, the critical temperatures restricted to angular momenta ℓ_0 and ℓ_1, for some angular momenta $\ell_0 \neq \ell_1$, see also [DGHL18, Remark 2.2]. For temperatures $T \in (\tilde{T}, T_c)$ the BCS minimizer(s) then have angular momentum ℓ_0 [DGHL18, Theorem 2.1]. For temperatures $T < \tilde{T}$ however, we do not in general know whether the BCS minimizer(s) have angular momentum ℓ_0. The proof crucially uses that the minimizer(s) have a definite angular momentum. If we however know a priori, that the BCS minimizer(s) have angular momentum ℓ_0 for some larger ranger of temperatures (T_1, T_c), then the formula in Equation (11.2.16) holds in this larger range of temperatures.

Remark 11.2.14 (Nodes of the gap function)**.** As already mentioned in Section 11.1.1.1, we establish during the proof, that any solution Δ of the BCS gap equation (11.1.4) has a radially symmetric absolute value, $|\Delta(p)|$, which is, moreover, independent of the particular solution Δ. In particular, every solution Δ of the BCS gap equation (11.1.4) does *not* have nodes on the Fermi surface. This contrasts many examples of d-wave superconductors in the physics literature, where a (necessarily) non-radial interaction V leads to a gap function Δ with nodes on the Fermi surface, see, e.g., [BH94; Fle+09; MW96; Zha+12].

Remark 11.2.15 (Non-extension to three dimensions)**.** The formula $\Xi(h) \approx T_c \mathsf{f}_{\mathsf{BCS}}(h)$ is *not* expected to hold in three dimensions for non-zero angular momentum, see for instance [PFCP07, Figure 14.6]. More precisely, we have the following:

(i) For non-zero angular momentum in three dimensions, our method of proving Theorem 11.2.11 (a) breaks down. In fact, we crucially use that $K_T^\Delta + \lambda V \geq 0$ for $\Delta = -2\lambda\widehat{V\alpha}$ with α a minimizer of the BCS functional. However, as shown in [DGHL18, Proposition 2.11] this implies that $|\hat{\alpha}|$ is a radial function. In particular, in three dimensions, α (and therefore also Δ) cannot have a definite non-zero angular momentum.

(ii) *Assume* that we know *a priori* that a solution of the BCS gap equation (11.1.4) (in spherical coordinates) satisfies $\Delta(p,\omega) = \Delta_0(p) Y_\ell^m(\omega)$ — at least to leading order.[9] Here, Y_ℓ^m is the usual L^2-normalized (complex) spherical harmonic with $\ell \in \mathbb{N}_0$ and $m \in \{-\ell, ..., \ell\}$. Then, by application of [FL16, Theorem 2.10], following very similar arguments to Sections 11.3.4 and 11.3.5.2, we find that the radial part of the gap function is given by
$$|\Delta_0(\sqrt{\mu})| \approx c_{\ell,m} C_{\mathsf{univ}} h T_c \tag{11.2.18}$$
on the Fermi sphere $\{p^2 = \mu\}$. Here C_{univ} was defined in (11.2.10) and we denoted
$$\begin{aligned} c_{\ell,m} &:= \left(\int_{\mathbb{S}^2} |Y_\ell^m(\omega)|^4 \, \mathrm{d}\omega \right)^{-1/2} \\ &= \left(\sum_{L=0}^{2\ell} \frac{(2\ell+1)^2}{4\pi(2L+1)} |\langle \ell,\ell;0,0|L;0\rangle|^2 \, |\langle \ell,\ell;m,m|L;2m\rangle|^2 \right)^{-1/2} \end{aligned} \tag{11.2.19}$$

[9] If one models the interaction V by a rank one projection $V = |\chi\rangle\langle\chi|$ (similarly to (11.2.2)), instead of a multiplication operator, such a form of Δ can easily be enforced by taking $\chi(p,\omega) = \chi_0(p) Y_\ell^m(\omega)$.

with $\langle \ell_1, \ell_2; m_1, m_2 | L; M\rangle$ being the well tabulated Clebsch-Gordan coefficients (see, e.g., [CDL91, p. 1046]). The relation (11.2.19) shows that, in particular, even in the subspace of fixed angular momentum $\ell \neq 0$, the behavior (11.2.18) is non-universal due to a non-trivial dependence on $m \in \{-\ell, ..., \ell\}$, as, for example (see [FL16, Eq. (6.8)]),

$$c_{2,0} = \sqrt{\frac{28\pi}{15}} \quad \text{and} \quad c_{2,\pm 1} = c_{2,\pm 2} = \sqrt{\frac{14\pi}{5}}\,.$$

For temperatures $0 \leq T \leq T_c$ and $h := \sqrt{1 - T/T_c}$, we expect (11.2.18) to generalize to

$$|\Delta_0(\sqrt{\mu})| \approx T_c\, \mathsf{f}_{\mathsf{BCS}}^{(\ell,m)}(h)$$

with $\mathsf{f}_{\mathsf{BCS}}^{(\ell,m)} : [0,1] \to [0,\infty)$ being implicitly defined via

$$\int_0^\infty \mathrm{d}s \int_{\mathbb{S}^2} \mathrm{d}\omega \left\{ \frac{\tanh \frac{\sqrt{s^2 + \left(\mathsf{f}_{\mathsf{BCS}}^{(\ell,m)}(h)\right)^2 |Y_\ell^m(\omega)|^2}}{2(1-h^2)}}{\sqrt{s^2 + \left(\mathsf{f}_{\mathsf{BCS}}^{(\ell,m)}(h)\right)^2 |Y_\ell^m(\omega)|^2}} - \frac{\tanh \frac{s}{2}}{s} \right\} |Y_\ell^m(\omega)|^2 = 0\,, \quad (11.2.20)$$

similarly to [PFCP07, Eq. (14.33)]. For $\ell = m = 0$, (11.2.20) yields that $\mathsf{f}_{\mathsf{BCS}}^{(0,0)} = (4\pi)^{1/2}\mathsf{f}_{\mathsf{BCS}}$ with $\mathsf{f}_{\mathsf{BCS}}$ from (11.2.9) due to the L^2-normalization of the spherical harmonics (recall $\Delta(p,\omega) = \Delta_0(p) Y_\ell^m(\omega)$).

A detailed analysis of the three-dimensional case with non-zero angular momentum is deferred to future work.

11.3 Proofs of the main results

This section contains the proofs of our main results formulated in Section 11.2.

11.3.1 Proof of Proposition 11.2.1

For ease of notation, we shall henceforth write λ instead of λ_{BCS}. From the explicit form (11.2.3) it is clear that $\Xi = \Delta$ and $\delta(h) \equiv \delta = \Delta/T_c$ is determined through (11.2.7). Hence, the goal is to show that $\delta(h)/\mathsf{f}_{\mathsf{BCS}}(h) = 1 + O(\mathrm{e}^{-1/\lambda})$ uniformly in $h \in [0,1]$. The proof of this is conducted in three steps.

11.3.1.1 A priori bound on δ

We shall prove the following lemma.

Lemma 11.3.1. *For $\delta = \delta(h)$ defined through* (11.2.7) *and $\lambda > 0$ small enough, it holds that*

$$\delta(h) \leq Ch\,. \quad (11.3.1)$$

Proof. First, we note that $\delta(h) \leq C$ uniformly for $h \in [0,1]$. This easily follows from observing that $\delta(h)$ is strictly monotonically increasing (as follows from elementary monotonicity properties of the integrand in (11.2.7)) and $\delta(1)$ is necessarily bounded.

In order to show (11.3.1), we employ the implicit function theorem to derive an asymptotic ODE for $\delta(h)$. For this purpose, we now introduce the function (recalling $T_c \sim \mathrm{e}^{-1/\lambda}$)

$$G_\lambda : [0,1] \times [0,\infty) \to \mathbb{R}\,, (h,\delta) \mapsto \int_0^{T_D/T_c} \left\{ \frac{\tanh\left(\frac{\sqrt{x^2+\delta^2}}{2(1-h^2)}\right)}{\sqrt{x^2+\delta^2}} - \frac{\tanh\left(\frac{x}{2}\right)}{x} \right\} \mathrm{d}x$$

and trivially note that (11.2.7) is equivalent to $G_\lambda(h,\delta(h)) = 0$. Since G_λ is C^1 (away from the boundary) in δ and h (this easily follows from dominated convergence), we can apply the implicit function theorem to obtain the differential equation

$$\frac{\partial \delta(h)}{\partial h} = \frac{(1-h^2)h}{\delta(h)} \left(\int_0^{T_D/T_c} \frac{1}{\cosh^2\left(\frac{\sqrt{x^2+\delta^2}}{2(1-h^2)}\right)} \,\mathrm{d}x \Big/ \int_0^{T_D/T_c} \frac{g_1\left(\frac{\sqrt{x^2+\delta^2}}{1-h^2}\right)}{\frac{\sqrt{x^2+\delta^2}}{1-h^2}} \,\mathrm{d}x \right) , \qquad (11.3.2)$$

where we introduced the auxiliary functions

$$g_0(z) := \frac{\tanh(z/2)}{z}\,, \qquad g_1(z) := -g_0'(z) = z^{-1} g_0(z) - \frac{1}{2} z^{-1} \frac{1}{\cosh^2(z/2)}\,. \qquad (11.3.3)$$

It is elementary to check that the even function $z \mapsto g_1(z)/z$ is (strictly) positive and (strictly) decreasing for $z \in [0,\infty)$. In combination with $\delta(h) \le C$ and $T_c \sim \mathrm{e}^{-1/\lambda}$, one can thus bound the denominator on the r.h.s. of (11.3.2) from below. Together with an upper bound on the integral in the numerator (obtained by using elementary monotonicity properties of the hyperbolic cosine), we find that

$$\frac{\partial \delta(h)}{\partial h} \le C' \frac{h}{\delta(h)} \left(\int_0^\infty \frac{1}{\cosh^2(x)} \,\mathrm{d}x \Big/ \int_0^C \frac{g_1\left(\sqrt{x^2+C^2}\right)}{\sqrt{x^2+C^2}} \,\mathrm{d}x \right) \le C'' \frac{h}{\delta(h)} \qquad (11.3.4)$$

for $h > 0$ and $\lambda > 0$ small enough (to ensure $T_D/T_c \ge C$).

Finally, the differential inequality (11.3.4) can be integrated using the boundary condition $\delta(0) = 0$ to conclude the desired.[10] □

11.3.1.2 Uniform error estimate

Having Lemma 11.3.1 as an input, we shall now prove the following.

Lemma 11.3.2. *For $\delta = \delta(h)$ defined through (11.2.7), it holds that*

$$\int_{T_D/T_c}^\infty \left| \frac{\tanh\left(\frac{\sqrt{x^2+\delta^2}}{2(1-h^2)}\right)}{\sqrt{x^2+\delta^2}} - \frac{\tanh\left(\frac{x}{2}\right)}{x} \right| \mathrm{d}x \le C\, h^2\, \mathrm{e}^{-2/\lambda}\,. \qquad (11.3.5)$$

[10] Strictly speaking, this requires to extend the function $\delta(h)$ in $(0,1)$, obtained via the implicit function theorem for G_λ, to the boundary points 0. In order to do so, note that, for $h \in (0,1/2)$, (11.3.2) yields

$$\frac{\partial \delta(h)}{\partial h} \sim \frac{h}{\delta(h)}\,,$$

from which we immediately conclude that $|\partial_h \delta(h)| \le C$, uniformly in $(0,1/2)$. Hence, $\delta(h)$ continuously extends to 0. The same is true for its derivative by means of (11.3.2) again. We remark that by a similar argument, $\delta(h)$ can be extended to 1 as well.

Proof. First, we add and subtract $\tanh(x/2)/\sqrt{x^2+\delta^2}$ in (11.3.5). Then, we employ $T_c \sim \mathrm{e}^{-1/\lambda}$ and Lemma 11.3.1 to estimate

$$\int_{T_D/T_c}^{\infty} \left| \frac{\tanh\left(\frac{\sqrt{x^2+\delta^2}}{2(1-h^2)}\right)}{\sqrt{x^2+\delta^2}} - \frac{\tanh\left(\frac{x}{2}\right)}{\sqrt{x^2+\delta^2}} \right| \mathrm{d}x \le C\,h^2 \int_{T_D/T_c}^{\infty} \frac{1}{\cosh^2(x/2)} \mathrm{d}x \le C\,h^2\,\mathrm{e}^{-2/\lambda}$$

and

$$\int_{T_D/T_c}^{\infty} \left| \frac{\tanh\left(\frac{x}{2}\right)}{\sqrt{x^2+\delta^2}} - \frac{\tanh\left(\frac{x}{2}\right)}{x} \right| \mathrm{d}x \le C\,h^2 \int_{T_D/T_c}^{\infty} \frac{1}{x^3} \mathrm{d}x \le C\,h^2\,\mathrm{e}^{-2/\lambda}\,.$$

Combining these bounds yields the claim by means of the triangle inequality. □

From Lemma 11.3.2 and Equation (11.2.7), we immediately conclude that

$$\int_{\mathbb{R}} \left\{ \frac{\tanh\left(\frac{\sqrt{x^2+\delta^2}}{2(1-h^2)}\right)}{\sqrt{x^2+\delta^2}} - \frac{\tanh\left(\frac{x}{2}\right)}{x} \right\} \mathrm{d}x = O(h^2\,\mathrm{e}^{-2/\lambda})\,. \tag{11.3.6}$$

11.3.1.3 Comparison with $\mathsf{f}_{\mathsf{BCS}}$

Given (11.3.6), the remaining task is to show that, because δ approximately *solves* the defining equation of $\mathsf{f}_{\mathsf{BCS}}$, it is *actually* close to $\mathsf{f}_{\mathsf{BCS}}$. This is the content of the following lemma.

Lemma 11.3.3. *Fix $h \in [0,1]$. If $\phi \in [0,\infty)$ satisfies*[11]

$$\int_{\mathbb{R}} \left\{ \frac{\tanh\left(\frac{\sqrt{x^2+\phi^2}}{2(1-h^2)}\right)}{\sqrt{x^2+\phi^2}} - \frac{\tanh\left(\frac{x}{2}\right)}{x} \right\} \mathrm{d}x = R \tag{11.3.7}$$

for some $|R| \le C$, then

$$\phi = \mathsf{f}_{\mathsf{BCS}}(h) + O(|R|^{1/2}) \tag{11.3.8}$$

with $\mathsf{f}_{\mathsf{BCS}}$ defined in (11.2.9).

Hence, combining (11.3.6) with (11.3.8) and invoking Lemma 11.2.2 (iii), we find that

$$\delta(h) = \mathsf{f}_{\mathsf{BCS}}(h) + O(h\mathrm{e}^{-1/\lambda}) = \mathsf{f}_{\mathsf{BCS}}(h)\left(1 + O(\mathrm{e}^{-1/\lambda})\right).$$

This concludes the proof of Proposition 11.2.1.

Proof of Lemma 11.3.3. First, we note that, given $h \in [0,1]$, (11.3.7) has a solution $\phi \in [0,\infty)$ if and only if $R \le \log\left(1/(1-h^2)\right)$. Then, as in the proof of [LT23, Lemma 6] (see [LT23, Equation (C50)]) we find that

$$\phi = \mathrm{e}^{-R}\mathsf{f}_{\mathsf{BCS}}\left(\sqrt{h^2 + (1-h^2)(1-e^R)}\right). \tag{11.3.9}$$

Taylor expanding in R around 0, using regularity of $\mathsf{f}_{\mathsf{BCS}}$ from Lemma 11.2.2, we get

$$\mathrm{e}^R\phi = \mathsf{f}_{\mathsf{BCS}}(h) + \int_0^1 \mathsf{f}_{\mathsf{BCS}}'\left(\sqrt{h^2+(1-h^2)(1-\mathrm{e}^{tR})}\right) \frac{-(1-h^2)R\mathrm{e}^{tR}}{2\sqrt{h^2+(1-h^2)(1-\mathrm{e}^{tR})}}\,\mathsf{d}t\,.$$

[11] We follow the convention that, if $h = 1$, we replace $\tanh(...)$ by the constant function 1.

To bound the integral we change variables to $s = h^2+(1-h^2)(1-e^{tR})$ and bound $|\mathsf{f}'_{\mathsf{BCS}}(h)| \leq C$ by Lemma 11.2.2. We split into cases depending on the sign of R.

$\underline{R > 0:}$ For $R > 0$ the integral is bounded by

$$\int_{h^2-(1-h^2)(\mathrm{e}^R-1)}^{h^2} \frac{\mathrm{d}s}{2\sqrt{s}} = h - \sqrt{h^2-(1-h^2)(\mathrm{e}^R-1)} = \frac{(1-h^2)(\mathrm{e}^R-1)}{\sqrt{h^2-(1-h^2)(\mathrm{e}^R-1)}+h}.$$

Noting that $\frac{\delta}{\sqrt{\varepsilon-\delta}+\sqrt{\varepsilon}} \leq \sqrt{\delta}$ and that $(1-h^2)(\mathrm{e}^R-1) \leq CR$ we find that the integral is bounded by $\sqrt{R}$.

$\underline{R < 0:}$ For $R < 0$ the integral is similarly bounded by

$$\int_{h^2}^{h^2+(1-h^2)(1-\mathrm{e}^R)} \frac{\mathrm{d}s}{2\sqrt{s}} = \sqrt{h^2+(1-h^2)(1-\mathrm{e}^R)} - h \leq C\sqrt{|R|}\,.$$

Plugging these bounds into (11.3.9), we conclude the desired. $\square$

11.3.2 Proof of Theorem 11.2.4(a)

We give here the proof of Theorem 11.2.4(a). The argument is divided into several steps.

11.3.2.1 A priori spectral information

For any temperature T we have by Proposition 11.1.5 that there exists a unique (up to a constant global phase) minimizer (γ_*, α_*) of the BCS functional. The function α_* is radial and has $\hat{\alpha}_* > 0$. Moreover, the operator $K_T^\Delta + \lambda V$ has lowest eigenvalue 0 and α_* is the unique eigenfunction with this eigenvalue.

11.3.2.2 Weak a priori bound on Δ

From the proof of Proposition 11.1.2 in [HS16] we have the following bound on the minimising (γ_*, α_*) of the BCS functional [HS16, Eqn. 3.12]

$$\begin{aligned}\int (1+p^2)(|\hat{\alpha}_*(p)|^2 + \hat{\gamma}_*(p))\,\mathrm{d}p \\ \leq 8T\int \log\left(1+e^{-(p^2-\mu)/4T}\right)\mathrm{d}p + 8\int \left[p^2/4 - 1 + C_2(\lambda)\right]_-\,\mathrm{d}p \leq C_\lambda\end{aligned}$$

with $C_2(\lambda) = \inf\operatorname{spec}(p^2/4+\lambda V) \leq 0$ and thus C_λ uniformly bounded for λ small enough. In particular $\|\alpha_*\|_{H^1} \leq C$ uniformly for λ small enough. By Sobolev's inequality [LL01, Thm 8.3] we then have

$$\begin{aligned}\|\alpha\|_{L^\infty}^2 &\leq C\,\|\nabla\alpha\|_{L^2}\,\|\alpha\|_{L^2} \leq C && (d=1)\\ \|\alpha\|_{L^q}^2 &\leq C\,\|\nabla\alpha\|_{L^2}\,\|\alpha\|_{L^2} \leq C && (d=2)\\ \|\alpha\|_{L^6}^2 &\leq C\,\|\nabla\alpha\|_{L^2}^2 \leq C && (d=3)\end{aligned}$$

for any $2 \leq q < \infty$. Thus,

$$\|\Delta\|_{L^\infty} \leq 2\lambda\,\|V\alpha\|_{L^1} \leq \begin{cases} 2\lambda\,\|V\|_{L^1}\,\|\alpha\|_{L^\infty} & d=1 \\ 2\lambda\,\|V\|_{L^p}\,\|\alpha\|_{L^2}^{(2pq-2q-2p)/(pq-2p)}\,\|\alpha\|_{L^q}^{(2q-pq)/(pq-2p)} & d=2 \\ 2\lambda\,\|V\|_{L^{3/2}}\,\|\alpha\|_{L^2}^{1/2}\,\|\alpha\|_{L^6}^{1/2} & d=3 \end{cases} \leq C\lambda \tag{11.3.10}$$

uniformly for λ small enough (for any $1 < p < \min\{2, p_V\}$ by choosing q large enough in dimension $d = 2$). In particular we see that $\Delta(p) \to 0$ as $\lambda \to 0$.

11.3.2.3 Birman–Schwinger principle

Next, by the Birman–Schwinger principle [FHNS07; HHSS08; HS16] the fact that $K_T^\Delta + \lambda V$ has lowest eigenvalue 0 with α_* being the unique eigenvector is equivalent to the Birman–Schwinger operator

$$B_{T,\Delta} := \lambda V^{1/2} \frac{1}{K_T^\Delta} |V|^{1/2}$$

having -1 as its lowest eigenvalue and $\phi = V^{1/2}\alpha_*$ being the unique eigenfunction corresponding to this eigenvalue. Here we use the convention $V^{1/2}(x) = \operatorname{sgn}(V(x))|V(x)|^{1/2}$. We decompose the Birman–Schwinger operator into a dominant singular term and an error term. For this purpose we define the (rescaled) Fourier transform restricted to the sphere $\mathfrak{F}_\mu : L^1(\mathbb{R}^d) \to L^2(\mathbb{S}^{d-1})$ by

$$\mathfrak{F}_\mu \psi(p) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \psi(x) e^{-\mathrm{i}\sqrt{\mu} p \cdot x} \, \mathrm{d}x,$$

which is well-defined by the Riemann–Lebesgue Lemma. Define then

$$m(T,\Delta) = \frac{1}{|\mathbb{S}^{d-1}|} \int_{|p| \le \sqrt{2\mu}} \frac{1}{K_T^\Delta(p)} \, \mathrm{d}p \tag{11.3.11}$$

and decompose

$$B_{T,\Delta} = \lambda m(T,\Delta) V^{1/2} \mathfrak{F}_\mu^\dagger \mathfrak{F}_\mu |V|^{1/2} + \lambda V^{1/2} M_{T,\Delta} |V|^{1/2},$$

with $M_{T,\Delta}$ defined such that this holds. Analogously to [FHNS07, Lemma 2] and Lemma 9.3.5 we have the following lemma, the proof of which (it is analogous to the one of Lemma 9.3.5) is given in Section 11.A.2.1.

Lemma 11.3.4. *We have $\left\| V^{1/2} M_{T,\Delta} |V|^{1/2} \right\|_{\mathsf{HS}} \le C$ for small λ uniformly in T and Δ, where $\| \cdot \|_{\mathrm{HS}}$ denotes the Hilbert-Schmidt norm of an operator.*

We conclude that $1 + \lambda V^{1/2} M_{T,\Delta} |V|^{1/2}$ is invertible for sufficiently small λ and thus, analogously to [HS08b, Lemma 4] and Lemma 10.2.8 and Proposition 10.2.10 the fact that $B_{T,\Delta}$ has lowest eigenvalue -1 is equivalent to the fact that the operator

$$S_{T,\Delta} := \lambda m(T,\Delta) \mathfrak{F}_\mu |V|^{1/2} \frac{1}{1 + \lambda V^{1/2} M_{T,\Delta} |V|^{1/2}} V^{1/2} \mathfrak{F}_\mu^\dagger \tag{11.3.12}$$

acting on $L^2(\mathbb{S}^{d-1})$ has lowest eigenvalue -1. Moreover, the function $\mathfrak{F}_\mu |V|^{1/2} \phi = \mathfrak{F}_\mu V \alpha_*$ is the unique eigenfunction of $S_{T,\Delta}$ corresponding to the eigenvalue -1.

11.3.2.4 A priori bounds on Δ

For the analysis of the integral $m(T,\Delta)$ we need some a priori bounds on Δ. Analogously as in Chapter 9 and [HS08b] we need some control of $\Delta(p)$ in terms of $\Delta(\sqrt{\mu})$ and some type of Lipschitz-continuity of Δ. These are collected in the following lemma.

Lemma 11.3.5. *The function Δ satisfies the bounds*

$$\Delta(p) \le C\Delta(\sqrt{\mu}), \tag{11.3.13}$$

$$|\Delta(p) - \Delta(q)| \le C\Delta(\sqrt{\mu})|p-q| \tag{11.3.14}$$

for sufficiently small λ.

Proof. As noted above, the function $\mathfrak{F}_\mu |V|^{1/2}\phi = \mathfrak{F}_\mu V\alpha$ is the eigenfunction of $S_{T,\Delta}$ corresponding to the lowest eigenvalue -1.

Further, to leading order, $S_{T,\Delta}$ is proportional to $\mathcal{V}_\mu = \mathfrak{F}_\mu V \mathfrak{F}_\mu^\dagger$. Since the constant function $u = \left|\mathbb{S}^{d-1}\right|^{-1/2} \in L^2(\mathbb{S}^{d-1})$ is the ground state of $\mathcal{V}_\mu$ (see the argument around (11.1.11)), the same is also true for $S_{T,\Delta}$ whenever λ is small enough. Hence, one can easily see that

$$\frac{1}{1+\lambda V^{1/2} M_{T,\Delta}|V|^{1/2}} V^{1/2}\mathfrak{F}_\mu^\dagger u$$

is an eigenvector of $B_{T,\Delta}$ corresponding to the eigenvalue -1 and thus proportional to $\phi = V^{1/2}\alpha_*$. Thus, with $\mathfrak{F}$ denoting the usual Fourier transform, by expanding $\frac{1}{1+x} = 1 - \frac{x}{1+x}$ we have

$$\begin{aligned}\Delta &= -2\lambda \mathfrak{F}|V|^{1/2}\phi = f(\lambda)\mathfrak{F}|V|^{1/2}\frac{1}{1+\lambda V^{1/2} M_{T,\Delta}|V|^{1/2}} V^{1/2}\mathfrak{F}_\mu^\dagger u \\ &= f(\lambda)\left(\int_{\mathbb{S}^{d-1}} \hat{V}(p-\sqrt{\mu}q)\,\mathrm{d}\omega(q) + \lambda\eta_\lambda(p)\right)\end{aligned}$$

for some constant $f(\lambda)$ (where we absorbed the factor $|\mathbb{S}^{d-1}|^{-1/2}(2\pi)^{-d/2}$ into $f(\lambda)$). One easily verifies that

$$\eta_\lambda = -(2\pi)^{d/2}\mathfrak{F}|V|^{1/2}\frac{V^{1/2}M_{T,\Delta}|V|^{1/2}}{1+\lambda V^{1/2} M_{T,\Delta}|V|^{1/2}} V^{1/2}\mathfrak{F}_\mu^\dagger u$$

has $\|\eta_\lambda\|_\infty \le C$ uniformly in $\lambda < \lambda_0$ for some λ_0 by Lemma 11.3.4. By evaluating at $p = \sqrt{\mu}$ we find $|f(\lambda)| \le C\Delta(\sqrt{\mu})$ for small λ and thus the global bound (11.3.13). Moreover, we have the Lipschitz-bound:

$$\begin{aligned}|\Delta(p)-\Delta(q)| &\le |f(\lambda)||p-q| \left\| |x||V|^{1/2}\frac{1}{1+\lambda V^{1/2} M_{T,\Delta}|V|^{1/2}} V^{1/2}\mathfrak{F}_\mu^\dagger u\right\|_{L^1} \\ &\le C\Delta(\sqrt{\mu})|p-q| \left\||x|^2 V\right\|_{L^1}^{1/2} \frac{1}{1-\lambda \left\|V^{1/2} M_{T,\Delta}|V|^{1/2}\right\|} \left\|V^{1/2}\mathfrak{F}_\mu^\dagger u\right\|_{L^2} \\ &\le C\Delta(\sqrt{\mu})|p-q|\end{aligned}$$

for sufficiently small λ. □

11.3.2.5 First order

Expanding the resolvent in Equation (11.3.12) to first order in a geometric series we see that $S_{T,\Delta}$ to leading order is proportional to the operator $\mathcal{V}_\mu$ (defined in (11.1.10) above). Moreover, we have

$$\begin{aligned}-1 &= \lambda m(T,\Delta) \inf\operatorname{spec}\left(\mathfrak{F}_\mu |V|^{1/2}\frac{1}{1+\lambda V^{1/2} M_{T,\Delta}|V|^{1/2}} V^{1/2}\mathfrak{F}_\mu^\dagger\right) \\ &= \lambda m(T,\Delta)\inf\operatorname{spec}\mathcal{V}_\mu(1+O(\lambda)) = \lambda e_\mu m(T,\Delta)(1+O(\lambda)).\end{aligned}$$

In particular $m(T,\Delta) = \frac{-1}{\lambda e_\mu}(1+O(\lambda)) \to \infty$ as $\lambda \to 0$.

11.3.2.6 Exponential vanishing of Δ

Pointwise we may bound $K_T^\Delta \geq E_\Delta$. Thus, by the first–order analysis above, we have

$$\begin{aligned}\frac{-1}{\lambda e_\mu}(1+O(\lambda)) = m(T,\Delta) &= \frac{1}{|\mathbb{S}^{d-1}|}\int_{|p|<\sqrt{2\mu}} \frac{1}{K_T^\Delta}\,\mathrm{d}p \\ &\leq \frac{1}{|\mathbb{S}^{d-1}|}\int_{|p|<\sqrt{2\mu}} \frac{1}{\sqrt{|p^2-\mu|^2+|\Delta(p)|^2}}\,\mathrm{d}p\end{aligned}$$

The latter integral is calculated in Chapter 9 and [HS08b]. The same calculation is valid here by the bounds (11.3.13) and (11.3.14) and the fact that $\Delta(p)\to 0$ by (11.3.10). That is

$$\frac{-1}{\lambda e_\mu} \leq \mu^{d/2-1}\left(\log\frac{\mu}{\Delta(\sqrt{\mu})} + O(1)\right)$$

in the limit $\lambda\to 0$. We conclude that $\Delta(\sqrt{\mu}) \lesssim e^{-c/\lambda}$ as $\lambda \to 0$ (with $c = -1/e_\mu \mu^{d/2-1}$).

The constant c shall henceforth be used generically and its precise value might change from line to line.

11.3.2.7 Infinite order

Recall that, for small λ, the unique eigenfunction of $S_{T,\Delta}$ corresponding to the eigenvalue -1 is given by the constant function u. Thus, for small λ we have

$$-1 = \lambda m(T,\Delta)\left\langle u\middle|\mathfrak{F}_\mu|V|^{1/2}\frac{1}{1+\lambda V^{1/2}M_{T,\Delta}|V|^{1/2}}V^{1/2}\mathfrak{F}_\mu^\dagger\middle|u\right\rangle.$$

Combining this for the temperatures T and T_c we find

$$\begin{aligned}&m(T,\Delta)-m(T_c,0)\\ &=\frac{-1}{\lambda}\left[\frac{1}{\left\langle u\middle|\mathfrak{F}_\mu|V|^{1/2}\frac{1}{1+\lambda V^{1/2}M_{T,\Delta}|V|^{1/2}}V^{1/2}\mathfrak{F}_\mu^\dagger\middle|u\right\rangle}-\frac{1}{\left\langle u\middle|\mathfrak{F}_\mu|V|^{1/2}\frac{1}{1+\lambda V^{1/2}M_{T_c,0}|V|^{1/2}}V^{1/2}\mathfrak{F}_\mu^\dagger\middle|u\right\rangle}\right]\\ &=\frac{-1}{\lambda e_\mu^2}(1+O(\lambda))\left\langle u\middle|\mathfrak{F}_\mu|V|^{1/2}\left(\frac{1}{1+\lambda V^{1/2}M_{T,\Delta}|V|^{1/2}}-\frac{1}{1+\lambda V^{1/2}M_{T_c,0}|V|^{1/2}}\right)V^{1/2}\mathfrak{F}_\mu^\dagger\middle|u\right\rangle\end{aligned} \tag{11.3.15}$$

for small enough λ by expanding to first order in the denominator and noting that $\inf\operatorname{spec}\mathcal{V}_\mu = e_\mu$. The proof of the following lemma (which is somewhat analogous to the proof of Lemma 11.3.4) is given in Section 11.A.2.2.

Lemma 11.3.6. *There exists $\lambda_0>0$ such that for $0<\lambda<\lambda_0$*

$$\left\|V^{1/2}(M_{T,\Delta}-M_{T_c,0})|V|^{1/2}\right\|_{\mathsf{HS}} \leq Ce^{-c/\lambda}$$

for some constants $C,c>0$ uniformly in λ.

Having Lemma 11.3.6 at hand, we write the difference as a telescoping sum

$$
\begin{aligned}
&\frac{1}{1+\lambda V^{1/2}M_{T,\Delta}|V|^{1/2}} - \frac{1}{1+\lambda V^{1/2}M_{T_c,0}|V|^{1/2}} \\
&\quad = \sum_{k=1}^{\infty}(-\lambda)^k \left[\left(V^{1/2}M_{T,\Delta}|V|^{1/2}\right)^k - \left(V^{1/2}M_{T_c,0}|V|^{1/2}\right)^k\right] \\
&\quad = \sum_{k=1}^{\infty}(-\lambda)^k \sum_{\ell=0}^{k-1}\left(V^{1/2}M_{T,\Delta}|V|^{1/2}\right)^{k-1-\ell} V^{1/2}(M_{T,\Delta}-M_{T_c,0})|V|^{1/2}\left(V^{1/2}M_{T_c,0}|V|^{1/2}\right)^{\ell}.
\end{aligned}
$$

Thus, by Lemmas 11.3.4 and 11.3.6 we have

$$
\begin{aligned}
\left\|\frac{1}{1+\lambda V^{1/2}M_{T,\Delta}|V|^{1/2}} - \frac{1}{1+\lambda V^{1/2}M_{T_c,0}|V|^{1/2}}\right\|_{\mathsf{HS}} &\le \sum_{k=1}^{\infty}\lambda^k \sum_{\ell=0}^{k-1} C^{k-1-\ell}\times Ce^{-c/\lambda}\times C^{\ell} \\
&\le \sum_{k=1}^{\infty} k\lambda^k C^k e^{-c/\lambda} \le C\lambda e^{-c/\lambda}.
\end{aligned}
$$

We conclude that

$$
|m(T,\Delta)-m(T_c,0)| \le Ce^{-c/\lambda}. \tag{11.3.16}
$$

11.3.2.8 Calculation of the integral $m(T,\Delta)-m(T_c,0)$

To extract the asymptotics in (11.2.11) from the bound in (11.3.16) we calculate the difference $m(T,\Delta)-m(T_c,0)$ and show that it is essentially the left-hand-side of (11.2.9). The argument is essentially given in [LT23, Appendix C.4]. For completeness, we give the argument here.

By changing variables to $s=(p^2-\mu)/\mu$ and defining $x(s)=\Delta(\sqrt{\mu(1+s)})/\mu$ we get

$$
\begin{aligned}
m(T,\Delta)-m(T_c,0) &= \int_0^{\sqrt{2\mu}}\left(\frac{1}{K_T^{\Delta}}-\frac{1}{K_{T_c}}\right)p^{d-1}\,\mathsf{d}p \\
&= \frac{\mu^{d/2-1}}{2}\int_{-1}^{1}\left(\frac{\tanh\left(\frac{\sqrt{s^2+x(s)^2}}{2T/\mu}\right)}{\sqrt{s^2+x(s)^2}} - \frac{\tanh\frac{s}{2T_c/\mu}}{s}\right)(1+s)^{d/2-1}\,\mathsf{d}s.
\end{aligned}
$$

This is of the form where we can use [LT23, Lemma 5].

Lemma 11.3.7 ([LT23, Lemma 5])**.** *Let g,G be functions with $g(0)=G(0)=1$ and $g\in L^\infty$ and let $\tau,\tau_c,\delta>0$. Assume that $\tilde g(s):=(g(s)-1)/s$ and $\tilde G(s):=(G(s)-1)/s$ satisfy $\tilde g,\tilde G\in L^\infty(\mathbb{R})$. Let $s_1>0$ such that $g(s)>1/2$ for $|s|<s_1$ and define*

$$
\begin{aligned}
J_{\tau,\delta,\tau_c}(g,G) &= \int_{\mathbb{R}}\left\{\frac{\tanh\frac{\sqrt{s^2+g(s)^2\delta^2}}{2\tau}}{\sqrt{s^2+g(s)^2\delta^2}} - \frac{\tanh\frac{s}{2\tau_c}}{s}\right\}G(s)\,\mathsf{d}s, \\
J^{(0)}_{\tau,\delta,\tau_c} = J_{\tau,\delta,\tau_c}(1,1) &= \int_{\mathbb{R}}\left\{\frac{\tanh\frac{\sqrt{s^2+\delta^2}}{2\tau}}{\sqrt{s^2+\delta^2}} - \frac{\tanh\frac{s}{2\tau_c}}{s}\right\}\mathsf{d}s.
\end{aligned}
$$

Then

$$
\begin{aligned}
&\left|J_{\tau,\delta,\tau_c}(g,G) - J^{(0)}_{\tau,\delta,\tau_c}\right| \\
&\quad\le \left\|\tilde G\right\|_{L^\infty}\left(4\tau+4\tau_c+\pi\delta\|g\|_{L^\infty}\right) + 4\delta\|\tilde g\|_{L^\infty}\left(1+\|g\|_{L^\infty}\right)\left(1+\frac{\delta}{2s_1}\right).
\end{aligned}
$$

To apply this lemma we write

$$x(s)=\frac{\Delta(\sqrt{\mu(1+s)})}{\Delta(\sqrt{\mu})}\frac{\Delta(\sqrt{\mu})}{\mu}=g(s)\delta.$$

Then $g\in L^\infty$ uniformly in λ by (11.3.13) and $\tilde{g}\in L^\infty$ uniformly in λ by (11.3.14). Finally, clearly $G(s)=(1+s)^{d/2-1}\chi_{|s|\le 1}$ has $\tilde{G}\in L^\infty$. We conclude that

$$m(T,\Delta)-m(T_c,0)=\frac{\mu^{d/2-1}}{2}\int_{\mathbb{R}}\left\{\frac{\tanh\frac{\sqrt{s^2+(\Delta(\sqrt{\mu})/\mu)^2}}{2T/\mu}}{\sqrt{s^2+(\Delta(\sqrt{\mu})/\mu)^2}}-\frac{\tanh\frac{s}{2T_c/\mu}}{s}\right\}\mathrm{d}s+O(e^{-c/\lambda}).$$

Writing $T=T_c(1-h^2)$, recalling the bound in (11.3.16) and changing variables we find

$$\int_{\mathbb{R}}\left\{\frac{\tanh\frac{\sqrt{s^2+(\Delta(\sqrt{\mu})/T_c)^2}}{2(1-h^2)}}{\sqrt{s^2+(\Delta(\sqrt{\mu})/T_c)^2}}-\frac{\tanh\frac{s}{2}}{s}\right\}\mathrm{d}s=R,$$

with $R=O(e^{-c/\lambda})$. Hence, by Lemma 11.3.3, we find that

$$\frac{\Delta(\sqrt{\mu})}{T_c}=\mathsf{f}_{\mathsf{BCS}}(h)+O(|R|^{1/2})=\mathsf{f}_{\mathsf{BCS}}(h)(1+O(h^{-1}e^{-c/\lambda}))\tag{11.3.17}$$

since $\mathsf{f}_{\mathsf{BCS}}(h)\sim h$ for small h by Lemma 11.2.2.

11.3.2.9 Comparing $\Delta(\sqrt{\mu})$ and Ξ

We finally prove that Ξ is essentially given by $\Delta(\sqrt{\mu})$.

Clearly $\Xi=\inf_p E_\Delta(p)\le E_\Delta(\sqrt{\mu})=\Delta(\sqrt{\mu})$. To show a corresponding lower bound consider p with $|p^2-\mu|\le\Xi\le\Delta(\sqrt{\mu})$. Then by Equation (11.3.14) and the bound $\Delta(\sqrt{\mu})=O(e^{-c/\lambda})$ we have

$$\Delta(p)\ge\Delta(\sqrt{\mu})-C\Delta(\sqrt{\mu})|p-\sqrt{\mu}|\ge\Delta(\sqrt{\mu})\,(1-C\Delta(\sqrt{\mu}))\ge\Delta(\sqrt{\mu})(1+O(e^{-c/\lambda})).$$

We conclude that

$$\Xi=\Delta(\sqrt{\mu})\left(1+O(e^{-c/\lambda})\right).\tag{11.3.18}$$

Together with (11.3.17) this concludes the proof of Theorem 11.2.4(a).

11.3.3 Non-universal property of Δ: Proof of Equation (11.2.14)

From the Birman–Schwinger argument (Section 11.3.2.3) we have that $\phi=V^{1/2}\alpha_*$ is the (unique) eigenvector of

$$\frac{\lambda m(T,\Delta)}{1+\lambda V^{1/2}M_{T,\Delta}|V|^{1/2}}V^{1/2}\mathfrak{F}_\mu^\dagger\mathfrak{F}_\mu|V|^{1/2}$$

corresponding to the eigenvalue -1. Recalling that $\Delta=-2\lambda\mathfrak{F}V\alpha_*$ we thus get the equation

$$\Delta=-\mathfrak{F}|V|^{1/2}\frac{\lambda m(T,\Delta)}{1+\lambda V^{1/2}M_{T,\Delta}|V|^{1/2}}V^{1/2}\mathfrak{F}_\mu^\dagger\Delta(\sqrt{\mu}\,\cdot)$$

with $\Delta(\sqrt{\mu}\,\cdot)$ being the constant function on the unit sphere of value $\Delta(\sqrt{\mu})$. Recall that $-1 = \lambda m(T,\Delta)\left\langle u\middle|\mathfrak{F}_\mu|V|^{1/2}\frac{1}{1+\lambda V^{1/2}M_{T,\Delta}|V|^{1/2}}V^{1/2}\mathfrak{F}_\mu^\dagger\middle|u\right\rangle$ for small enough λ. By the same argument as in Section 11.3.2.7 we may replace $M_{T,\Delta}$ by $M_{0,0}$, its corresponding value at $T=\Delta=0$, up to errors of order $e^{-c/\lambda}$. (Concretely one can define $M_{0,0}$ via the representation of its kernel as given in Equations (11.A.3), (11.A.4), (11.A.5), (11.A.8) and (11.A.9), setting $T=\Delta=0$.) Hence, for sufficiently small λ,

$$\frac{\Delta}{\Delta(\sqrt{\mu})} = \frac{|\mathbb{S}^{d-1}|^{1/2}\mathfrak{F}|V|^{1/2}\frac{1}{1+\lambda V^{1/2}M_{0,0}|V|^{1/2}}V^{1/2}\mathfrak{F}_\mu^\dagger u}{\left\langle u\middle|\mathfrak{F}_\mu|V|^{1/2}\frac{1}{1+\lambda V^{1/2}M_{0,0}|V|^{1/2}}V^{1/2}\mathfrak{F}_\mu^\dagger\middle|u\right\rangle} + O(e^{-c/\lambda}) = F + O(e^{-c/\lambda}).$$

Clearly, the function F does not depend on the temperature T.

11.3.4 Ginzburg-Landau theory: Proof of Theorem 11.2.4(b)

As mentioned above, the proof of Theorem 11.2.4(b) builds on Ginzburg–Landau (GL) theory. For convenience of the reader, we recall the main input from GL theory for the purpose of the present paper in Proposition 11.3.9 below. More general and detailed statements can be found in the original papers [DHM23a; DHM23b; FHSS12b; FL16]. In particular, these works allow for external fields or ground state degeneracy (cf. Lemma 11.3.8 below), respectively.

As a preparation for Proposition 11.3.9, we have the following lemma.

Lemma 11.3.8 (Ground state of $K_{T_c}+\lambda V$)**.** *Let V satisfy Assumptions 11.1.1 and 11.1.4. Then $K_{T_c}+\lambda V$ has 0 as a non-degenerate ground state eigenvalue and its $L^2(\mathbb{R}^d)$-normalized ground state $\mathfrak{a}_0$ can be chosen to have strictly positive Fourier transform. Moreover, it holds that $\hat{\mathfrak{a}}_0 \in L^\infty(\mathbb{R}^d)$.*

Proof. Since $T_c>0$ (recall the discussion below Assumption 11.1.4), we first note that the Fourier multiplier K_{T_c} is strictly positive. Then using $\hat{V}\le 0$, the claim follows from a Perron-Frobenius type argument (see also [HS08b] and [FHSS12b, Assumption 2]). The fact that $\hat{\mathfrak{a}}_0 \in L^\infty(\mathbb{R}^d)$ follows from [FHSS12b, Proposition 2] by invoking Assumption 11.1.1. □

We can now formulate the main results from GL theory, needed for the present paper.

Proposition 11.3.9 (Ginzburg-Landau theory, see [FL16, Theorem 2.10])**.** *Let V be a function satisfying Assumptions 11.1.1 and 11.1.4 and suppose that $0\le T<T_c$. Then, using the notations from Proposition 11.1.5 and Lemma 11.3.8, we have that*

$$\mathcal{F}_T[\Gamma_*] - \mathcal{F}_T[\Gamma_{\mathsf{FD}}] = h^4\mathcal{E}_{\mathsf{GL}}(\psi_{\mathsf{GL}}) + \mathcal{O}(h^6) \quad \textit{as} \quad h\to 0\,,$$

where $\psi_{\mathsf{GL}}\neq 0$ minimizes the Ginzburg-Landau "functional" $\mathcal{E}_{\mathsf{GL}}:\mathbb{C}\to\mathbb{R}$,

$$\begin{aligned}\mathcal{E}_{\mathsf{GL}}(\psi) =&|\psi|^4\left[\frac{1}{T_c^3}\int_{\mathbb{R}^d}\frac{g_1((p^2-\mu)/T_c)}{(p^2-\mu)/T_c}|K_{T_c}(p)|^4|\hat{\mathfrak{a}}_0(p)|^4\,\mathsf{d}p\right]\\ &-|\psi|^2\left[\frac{1}{2T_c}\int_{\mathbb{R}^d}\frac{1}{\cosh^2\left((p^2-\mu)/(2T_c)\right)}|K_{T_c}(p)|^2|\hat{\mathfrak{a}}_0(p)|^2\,\mathsf{d}p\right].\end{aligned} \tag{11.3.19}$$

Here we used the auxiliary function g_1 from (11.3.3)*. Moreover, we can decompose the off–diagonal element $\hat{\alpha}_*$ of Γ_* as*

$$\hat{\alpha}_* = h|\psi_0|\hat{\mathfrak{a}}_0 + \hat{\xi} \tag{11.3.20}$$

where $\|\xi\|_{L^2} = \mathcal{O}(h^2)$ *and* $\psi_0 \neq 0$ *approximately minimizes* (11.3.19), *i.e.*

$$\mathcal{E}_{\mathsf{GL}}(\psi_0) \leq \mathcal{E}_{\mathsf{GL}}(\psi_{\mathsf{GL}}) + \mathcal{O}(h^2)\,. \tag{11.3.21}$$

Remark 11.3.10. We emphasize that all error terms in the above proposition (and also the implicit constants hidden in $\hat{\mathfrak{a}}_0 \in L^\infty(\mathbb{R}^d)$) are *not* uniform in λ. This crucially limits the applicability of our GL theory based method for temperatures slightly away from the critical one with $\mathrm{e}^{-c'/\lambda} \ll h \ll 1$ (cf. the error bound in (11.2.12)). Indeed, a careful examination of the proofs in [FHSS12b; FL16] reveals that the hidden dependencies on the critical temperature T_c are at most inverse polynomially and hence exponential in λ, i.e. $e^{c/\lambda}$ for some $c > 0$ (independent of λ and h).

11.3.4.1 Minimizing the Ginzburg-Landau functional

Given the inputs from GL theory, Theorem 11.2.4(b) is based on the following Proposition 11.3.11, the proof of which we postpone after finishing the proof of Theorem 11.2.4(b).

Proposition 11.3.11. *The (up to a phase unique) minimizer* ψ_{GL} *of the GL functional* (11.3.19) *satisfies*

$$|\psi_{\mathsf{GL}}| = C_{\mathsf{univ}}\,\frac{T_c}{\Delta_0(\sqrt{\mu})}\Big(1 + o_{\lambda\to 0}(1)\Big)\,, \tag{11.3.22}$$

where $\Delta_0 := -2(2\pi)^{-d/2}\lambda\hat{V} \star \hat{\mathfrak{a}}_0$,[12] *the constant* C_{univ} *is given in* (11.2.10), *and the error is uniform in* h.

The fact that $|\psi_0| > 0$ approximately minimizes (11.3.19) (see (11.3.21)), implies that (recalling Remark 11.3.10)

$$|\psi_0| = |\psi_{\mathsf{GL}}| + O\Big(he^{c/\lambda}\Big)\,.$$

Therefore, by means of (11.3.20) in combination with Proposition 11.3.11, we infer

$$\hat{\alpha}_* = C_{\mathsf{univ}}\,T_c\,h\,\frac{\hat{\mathfrak{a}}_0}{\Delta_0(\sqrt{\mu})}\Big(1 + o_{\lambda\to 0}(1) + O\Big(he^{c/\lambda}\Big)\Big) + \hat{\xi}\,.$$

Thus, after taking the convolution with $\lambda\hat{V}$,

$$\Delta = C_{\mathsf{univ}}\,T_c\,h\,\frac{\Delta_0}{\Delta_0(\sqrt{\mu})}\Big(1 + o_{\lambda\to 0}(1) + O\Big(he^{c/\lambda}\Big)\Big) + \Delta_\xi\,, \tag{11.3.23}$$

where $\Delta > 0$ is the unique solution of the BCS gap equation (11.1.4) (see Proposition 11.1.5) and we denoted $\Delta_\xi := -2(2\pi)^{-d/2}\lambda\hat{V} \star \hat{\xi}$.

11.3.4.2 A priori bounds on Δ_0

For the proof of Theorem 11.2.4(b) we need some a priori bounds on Δ_0 analogously to those of Section 11.3.2.4. The bounds follow from the following lemma, the proof of which is analogous to the argument of Sections 11.3.2.3 and 11.3.2.4 and given in Section 11.A.2.3.

[12] Note that Δ_0 was denoted by t in [FHSS12b; FL16]. We also remark that $\Delta_0(\sqrt{\mu}) \neq 0$ as follows from $\hat{\mathfrak{a}}_0 > 0$ (by Lemma 11.3.8) and $\hat{V} \leq 0$ (by Assumption 11.1.4).

Lemma 11.3.12 (c.f. [HS08b, Lemma 4] and Lemma 10.2.8)**.** *Let $\mathfrak{a}_0 \in H^1(\mathbb{R}^d)$ with $\hat{\mathfrak{a}}_0 > 0$ be the unique $H^1(\mathbb{R}^d)$-normalized ground state of $K_{T_c} + \lambda V$ from Lemma 11.3.8. Moreover, let $u(p) = (|\mathbb{S}^{d-1}|)^{-1/2}$ be the constant function on the sphere $\mathbb{S}^{d-1}$ and let*

$$\hat{\varphi}(p) = -\frac{1}{(2\pi)^{d/2}} \int_{\mathbb{S}^{d-1}} \hat{V}(p - \sqrt{\mu} q) \, \mathrm{d}\omega(q) \,. \tag{11.3.24}$$

Then $\Delta_0 = -2(2\pi)^{-d/2} \lambda \hat{V} \star \hat{\mathfrak{a}}_0$ can be expanded as

$$\Delta_0(p) = f(\lambda)[\hat{\varphi}(p) + \lambda \eta_\lambda(p)] \tag{11.3.25}$$

for some positive function $f(\lambda)$ and $\|\eta_\lambda\|_{L^\infty(\mathbb{R}^d)}$ bounded uniformly in $\lambda > 0$.

After realizing $\hat{\varphi}(\sqrt{\mu}) = -e_\mu$ by (11.1.11), we conclude for small enough $\lambda > 0$ that

$$\Delta_0(p) - \Delta_0(\sqrt{\mu}) = \frac{[\hat{\varphi}(p) - \hat{\varphi}(\sqrt{\mu})] + \lambda[\eta_\lambda(p) - \eta_\lambda(\sqrt{\mu})]}{-e_\mu + \lambda \eta_\lambda(\sqrt{\mu})} \Delta_0(\sqrt{\mu}) \,.$$

Now it is an easy computation to see $|\hat{\varphi}(p) - \hat{\varphi}(q)| \le C \min\Big\{ ||p| - |q||, 1 \Big\}$ for all $p, q \in \mathbb{R}^d$. Thus,

$$\Big| \Delta_0(p) - \Delta_0(\sqrt{\mu}) \Big| \le C \, \Big(\min\Big\{ \Big| |p| - \sqrt{\mu} \Big|, 1 \Big\} + \lambda \Big) \, \Delta_0(\sqrt{\mu}) \,. \tag{11.3.26}$$

11.3.4.3 A priori bounds on Δ_ξ

For the following arguments, we need two estimates on $\Delta_\xi = -2(2\pi)^{-d/2} \lambda \hat{V} \star \hat{\xi}$.

- First, it is a simple consequence of Young's inequality and $\|\hat{\xi}\|_{L^2} = \|\xi\|_{L^2} = O\Big(h^2 e^{c/\lambda}\Big)$, that
$$\|\Delta_\xi\|_{L^\infty} = \|V\|_{L^2} \, O\Big(h^2 e^{c/\lambda}\Big) \,. \tag{11.3.27}$$
- Second, we note that $\Delta_\xi(p) - \Delta_\xi(q)$ is (proportional to) the Fourier transform of $V(x)\Big(1 - e^{i(p-q)\cdot x}\Big)\xi(x)$, and thus
$$\Big\| V(x) \Big(1 - e^{i(p-q)\cdot x}\Big) \Big\|_{L^2}^2 = \int_{\mathbb{R}^d} |V(x)|^2 \left| 1 - e^{i(p-q)\cdot x} \right|^2 \mathrm{d}x$$
$$\le C|p-q|^2 \int_{\mathbb{R}^d} |V(x)|^2 |x|^2 \, \mathrm{d}x \,.$$

  Using radiality of Δ and Δ_0, we conclude the radiality of Δ_ξ and therefore
$$|\Delta_\xi(p) - \Delta_\xi(q)| \le \Big| |p| - |q| \Big| \; \| | \cdot | V \|_{L^2} \; O\Big(h^2 e^{c/\lambda}\Big) \,. \tag{11.3.28}$$

Recall that $\|(1 + |\cdot|)V\|_{L^2} < \infty$ by assumption.

11.3.4.4 Comparing $\Delta(\sqrt{\mu})$ and Ξ

We aim at proving

$$\Xi = \Delta(\sqrt{\mu}) \left(1 + O\Big(\lambda + h^2 e^{c/\lambda}\Big) \right) \,. \tag{11.3.29}$$

In order to see this, we note that clearly $\Xi = \sqrt{(p^2 - \mu)^2 + |\Delta(p)|^2} \le \Delta(\sqrt{\mu})$. For the reverse inequality, let $p \in \mathbb{R}^d$ with $|p^2 - \mu| \le \Xi \le \Delta(\sqrt{\mu})$. Then

$$|\Delta(p) - \Delta(\sqrt{\mu})| \le C \, T_c \, h \Big(1 + o_{\lambda \to 0}(1) + O(h e^{c/\lambda})\Big) \cdot \Big(\Big| |p| - \sqrt{\mu} \Big| + \lambda \Big) + C \Big| |p| - \sqrt{\mu} \Big| \, h^2 e^{c/\lambda}$$

by application of (11.3.26) and (11.3.28). Using that $\Delta(\sqrt{\mu}) \sim T_c h$, as a consequence of (11.3.23) for h small enough (meaning $h e^{c/\lambda} \ll 1$), we then conclude

$$|\Delta(p) - \Delta(\sqrt{\mu})| \leq C\left(\lambda + h^2 e^{c/\lambda}\right)\Delta(\sqrt{\mu})$$

In combination with the upper bound, this proves (11.3.29).

11.3.4.5 Conclusion: Proof of Theorem 11.2.4(b)

We evaluate (11.3.23) at $p = \sqrt{\mu}$, such that we find

$$\Xi = \left[C_{\mathsf{univ}}\, T_c\, h\left(1 + o_{\lambda\to 0}(1) + O\Big(h e^{c/\lambda}\Big)\right) + O\Big(h^2 e^{c/\lambda}\Big)\right] \cdot \Big(1 + O\Big(\lambda + h^2 e^{c/\lambda}\Big)\Big)$$

with the aid of (11.3.27) and (11.3.29). Collecting all the error terms leaves us with

$$\Xi = C_{\mathsf{univ}}\, T_c\, h\Big(1 + o_{\lambda\to 0}(1) + O\Big(h e^{c/\lambda}\Big)\Big)\,. \tag{11.3.30}$$

Hence, using $\mathsf{f}_{\mathsf{BCS}}(h) = C_{\mathsf{univ}} h + O(h^2)$, by Lemma 11.2.2, we arrive at Theorem 11.2.4(b). $\square$

11.3.4.6 Proof of Proposition 11.3.11

In the following estimates, we use the shorthand notations (recall the definition of the auxiliary function g_1 from (11.3.3))

$$f_4(p) := \frac{g_1((p^2-\mu)/T_c)}{(p^2-\mu)/T_c} \qquad f_2(p) := \frac{1}{\cosh^2\left((p^2-\mu)/(2T_c)\right)}\,, \tag{11.3.31}$$

such that the absolute value of the minimizer ψ_{GL} of (11.3.19) is given by

$$|\psi_{\mathsf{GL}}| = T_c\left(\frac{\int_{\mathbb{R}^d} f_2(p)|K_{T_c}(p)|^2|\hat{\mathfrak{a}}_0(p)|^2\,\mathsf{d}p}{4\int_{\mathbb{R}^d} f_4(p)|K_{T_c}(p)|^4|\hat{\mathfrak{a}}_0(p)|^4\,\mathsf{d}p}\right)^{1/2} = T_c\left(\frac{\int_{\mathbb{R}^d} f_2(p)|\Delta_0(p)|^2\,\mathsf{d}p}{\int_{\mathbb{R}^d} f_4(p)|\Delta_0(p)|^4\,\mathsf{d}p}\right)^{1/2}.$$

We denoted $\Delta_0 = -2(2\pi)^{-d/2}\lambda\hat{V} \star \hat{\mathfrak{a}}_0$ (as in Proposition 11.3.11) and used that $\mathfrak{a}_0 \in \ker\Big(K_{T_c} + \lambda V\Big)$. Note that, $\Delta_0 = |\Delta_0|$ by means of Proposition 11.1.5 and $\hat{V} \leq 0$ from Assumption 11.1.4.

Next, we add and subtract $|\Delta_0(\sqrt{\mu})|^2$ (resp. $|\Delta_0(\sqrt{\mu})|^4$) in the integral in the numerator (resp. denominator). The terms involving $|\Delta_0(\sqrt{\mu})|^j$ are evaluated as follows.

Lemma 11.3.13 (Emergence of C_{univ} in GL theory)**.** *Let $\mu > 0$. In the limit $T_c/\mu \to 0$ we have that (recall C_{univ} from* (11.2.10)*)*

$$\left(\int_{\mathbb{R}^d} \frac{1}{\cosh^2\left(\frac{p^2-\mu}{2T_c}\right)}\,\mathsf{d}p \Bigg/ \int_{\mathbb{R}^d} \frac{g_1((p^2-\mu)/T_c)}{(p^2-\mu)/T_c}\,\mathsf{d}p\right)^{1/2} \longrightarrow C_{\mathsf{univ}} \tag{11.3.32}$$

for all $d = 1, 2, 3$.

Proof. Since the integrands are both radial, we switch to spherical coordinates and neglect the common $|\mathbb{S}^{d-1}|$–factor in numerator and denominator. By splitting the remaining radial integration according to $p^2 \leq \mu$ and $p^2 \geq \mu$ and changing the integration variables from $(p^2-\mu)/2T_c$ to $-t$ resp. t we find the numerator of (11.3.32) being equal to

$$2T_c\mu^{(d-2)/2}\left[\int_0^{\mu/2T_c}\Big(1 - 2\tfrac{T_c}{\mu}t\Big)^{(d-2)/2} + \int_0^\infty \Big(1 + 2\tfrac{T_c}{\mu}t\Big)^{(d-2)/2}\right]\left(\frac{1}{\cosh^2(t)}\right)\mathsf{d}t\,. \tag{11.3.33}$$

Similarly, we find the denominator of (11.3.32) to equal

$$\frac{2T_c\mu^{(d-2)/2}}{8}\left[\int_0^{\mu/2T_c}\left(1-2\tfrac{T_c}{\mu}t\right)^{(d-2)/2}+\int_0^\infty\left(1+2\tfrac{T_c}{\mu}t\right)^{(d-2)/2}\right]\left[\frac{\tanh(t)}{t^3}-\frac{1}{t^2\cosh^2(t)}\right]\mathrm{d}t. \tag{11.3.34}$$

We now take the ratio of (11.3.33) and (11.3.34) and send $T_c/\mu \to 0$. By means of the dominated convergence theorem (note that the integrand in (11.3.34) behaves as t^{-3} for large t) we thus find the limit being given as the ratio of

$$\int_0^\infty \frac{1}{\cosh^2(t)}\,\mathrm{d}t \qquad \text{and} \qquad \frac{1}{8}\int_0^\infty\left(\frac{\tanh(t)}{t^3}-\frac{1}{t^2\cosh^2(t)}\right)\mathrm{d}t\,.$$

While the former is easily evaluated as being equal to one, the latter is given by $\frac{7\zeta(3)}{8\pi^2}$ (see, e.g., [GR07, p. 3.333.3]). This proves the claim. □

With the aid of (11.3.26) and noting $f_j > 0$, the resulting differences (from adding and subtracting $|\Delta_0(\sqrt{\mu})|^j$) can be estimated as

$$\begin{aligned}&\left|\int_{\mathbb{R}^d} f_j(p)\Big(|\Delta_0(p)|^j-|\Delta_0(\sqrt{\mu})|^j\Big)\,\mathrm{d}p\right|\\ &\quad\le C\,|\Delta_0(\sqrt{\mu})|^j\int_{\mathbb{R}^d} f_j(p)\Big(\min\Big(\Big||p|-\sqrt{\mu}\Big|,1\Big)+\lambda\Big)\,\mathrm{d}p\end{aligned}$$

for $j = 2, 4$. These integrals can be treated analogously to (11.3.33) and (11.3.34) in Lemma 11.3.13 (for the $\big||p|-\sqrt{\mu}\big|$-term, note that f_j essentially concentrates around $|p| \approx \sqrt{\mu}$) and we find them to be smaller than the corresponding leading term $\int_{\mathbb{R}^d} f_j(p)|\Delta_0(\sqrt{\mu})|^j\,\mathrm{d}p$ in the limit $\lambda \to 0$ (and hence $T_c \to 0$). Therefore,

$$|\psi_{\mathsf{GL}}| = \frac{T_c}{\Delta_0(\sqrt{\mu})}\left(\frac{\int_{\mathbb{R}^d} f_2(p)\,\mathrm{d}p}{\int_{\mathbb{R}^d} f_4(p)\,\mathrm{d}p}\right)^{1/2}\cdot\Big(1+o_{\lambda\to 0}(1)\Big) = C_{\mathsf{univ}}\,\frac{T_c}{\Delta_0(\sqrt{\mu})}\cdot\Big(1+o_{\lambda\to0}(1)\Big)\,,$$

where we used Lemma 11.3.13 in the last step. As the GL functional (11.3.19) is entirely independent of the relative difference to the critical temperature $(T_c - T)/T_c = h^2$, it is clear that all the errors here hold uniform in the parameter h. This finishes the proof of Proposition 11.3.11. □

11.3.5 Pure angular momentum for $d = 2$: Proof of Theorem 11.2.11

11.3.5.1 Part (a)

The proof of Theorem 11.2.11 (a) is mostly the same as that of Theorem 11.2.4 (a). We sketch the argument here, highlighting the few differences.

The operator $\mathcal{V}_\mu$. Using the Birman–Schwinger principle on the operator $K_{T_c} + \lambda V$ (as is done in [FHNS07; HS08b]) we find that, for sufficiently small λ, the lowest eigenvalue e_μ of $\mathcal{V}_\mu$ (recall (11.1.10)) is an eigenvalue for angular momentum ℓ_0, since this is the angular momentum of the ground state(s) of $K_{T_c} + \lambda V$ by assumption. Further, since V is radial, the eigenfunctions of $\mathcal{V}_\mu$ all have a definite angular momentum. In particular the first excited state has some angular momentum $\ell_1 \neq \ell_0$:

$$e_\mu^{(1)} = \inf_{u \perp u_{\pm \ell_0}} \langle u | \mathcal{V}_\mu | u \rangle = \langle u_{\pm \ell_1} | \mathcal{V}_\mu | u_{\pm \ell_1} \rangle \,,$$

with $u_{\pm\ell}(p) = (2\pi)^{-1/2} e^{\pm i \ell \varphi}$ the eigenfunctions of angular momentum ℓ. Here φ denotes the angle of $p \in \mathbb{R}^2$ in polar coordinates. Note that $e_\mu^{(1)} \leq 0$ since $\mathcal{V}_\mu$ is a compact operator on an infinite-dimensional space.

A priori spectral information. It is proved in [DGHL18, Theorem 2.1] that there exists a temperature $\tilde{T}$ such that for temperatures $\tilde{T} < T < T_c$ the minimizers of the BCS functional are given by

$$\hat{\alpha}_\pm(p) = e^{\pm i \ell_0 \varphi} \hat{\alpha}_0(p)$$

where φ denotes the angle of $p \in \mathbb{R}^2$ in polar coordinates, $\hat{\alpha}_0$ is a radial function, and ℓ_0 is the angular momentum given by Equation (11.2.15). The BCS gap functions are then $\Delta_\pm(p) = \Delta_0(p) e^{\pm i \ell_0 \varphi}$, with Δ_0 a radial function.[13] Further, we have $K_T^{\Delta_0} + \lambda V \geq 0$ for temperatures $T \in (\tilde{T}, T_c)$ [DGHL18, Proposition 4.3] and $\ker(K_T^{\Delta_0} + \lambda V) = \mathrm{span}\{\alpha_+, \alpha_-\}$.

The temperature $\tilde{T}$. As discussed in [DGHL18, Remark 2.6] the temperature $\tilde{T}$ is given by $\tilde{T} = T_c(\ell_1)$, the critical temperature when restricted to angular momentum ℓ_1. Following the argument in [FHNS07] (see also [HS10, Theorem 1]) we find

$$\tilde{T} \leq \begin{cases} C e^{1/\lambda e_\mu^{(1)}} & e_\mu^{(1)} < 0, \\ C e^{-c/\lambda^2} & e_\mu^{(1)} = 0. \end{cases}$$

Recalling that $T_c \sim e^{1/\lambda e_\mu}$ and that $e_\mu < e_\mu^{(1)} \leq 0$ then clearly $\tilde{T}/T_c \leq C e^{-\mathfrak{c}/\lambda}$ for some $\mathfrak{c} > 0$.

Weak a priori bound on $\Delta_\pm$. Exactly as in Equation (11.3.10) we have $\|\Delta_\pm\|_{L^\infty} \leq C\lambda$.

Birman–Schwinger principle. Analogously to Section 11.3.2.3 we have by the Birman–Schwinger principle that

$$B_{T,\Delta_0} = V^{1/2} \frac{1}{K_T^{\Delta_0}} |V|^{1/2}$$

has -1 as its lowest eigenvalue, only the eigenspace is spanned by the two vectors $\phi_\pm = V^{1/2} \alpha_\pm$. By a completely analogous argument is in Section 11.3.2.3 we find that

$$S_{T,\Delta_0} = \lambda m(T, \Delta_0) \mathfrak{F}_\mu |V|^{1/2} \frac{1}{1 + \lambda V^{1/2} M_{T,\Delta_0} |V|^{1/2}} V^{1/2} \mathfrak{F}_\mu^\dagger$$

has -1 as its lowest eigenvalue with corresponding eigenspace spanned by $\mathfrak{F}_\mu V \alpha_\pm$.

A priori bounds on $\Delta_\pm$. Analogously to Lemma 11.3.5 we claim

Lemma 11.3.14. *The functions $\Delta_\pm$ satisfy the bounds (with slight abuse of notation, recall that Δ_0 is a radial function)*

$$|\Delta_\pm(p)| \leq C |\Delta_0(\sqrt{\mu})|, \qquad |\Delta_\pm(p) - \Delta_\pm(q)| \leq C |\Delta_0(\sqrt{\mu})| |p - q| \,.$$

[13] This should not be confused with the function Δ_0 used in Section 11.3.4.

Proof. The proof is analogous to that of Lemma 11.3.5. First we note that $\mathcal{V}_\mu = \mathfrak{F}_\mu V \mathfrak{F}_\mu^\dagger$ has eigenfunctions of lowest eigenvalue $u_{\pm\ell_0}(p) = (2\pi)^{-1/2} e^{\pm i\ell_0\varphi}$ and that the operator S_{T,Δ_0} preserves the angular momentum. Analogously to the proof of Lemma 11.3.5 we find

$$\Delta_\pm(p) = f_\pm(\lambda)\left(\int_{\mathbb{S}^1} \hat{V}(p - \sqrt{\mu}q) u_{\pm\ell_0}(q)\,\mathrm{d}\omega(q) + \lambda\eta_{\lambda\pm}(p)\right)$$

with $\|\eta_{\lambda\pm}\|_{L^\infty} \leq C$ uniformly in λ. Evaluating on the Fermi surface $\{p^2 = \mu\}$ we get (recall that $\inf\operatorname{spec}\mathcal{V}_\mu = e_\mu$)

$$\Delta_\pm(\sqrt{\mu}p/|p|) = f_\pm(\lambda)\left(e_\mu u_{\pm\ell_0}(p/|p|) + \lambda\eta_{\lambda\pm}(\sqrt{\mu}p/|p|)\right).$$

In particular, we conclude that $\left|\Delta_0(\sqrt{\mu})\right| = \left|\Delta_\pm(\sqrt{\mu}p/|p|)\right| > 0$ for λ small enough and that $|f_\pm(\lambda)| \leq C\left|\Delta_0(\sqrt{\mu})\right|$. We conclude the rest of the proof exactly as for Lemma 11.3.5. $\square$

The remaining parts of the argument (first order analysis of m, the exponential vanishing of $\Delta_\pm$, infinite order analysis of m, calculation of the integral $m(T,\Delta_0) - m(T_c, 0)$ and comparing $\Delta_\pm$ on the Fermi surface with Ξ) are exactly as in Sections 11.3.2.5, 11.3.2.6, 11.3.2.7, 11.3.2.8 and 11.3.2.9 only replacing Δ and u by $\Delta_\pm$ and $u_{\pm\ell_0}$, respectively. This concludes the proof of Theorem 11.2.11 (a).

11.3.5.2 Part (b)

Again, we highlight only the main differences compared to the proof of Theorem 11.2.4 (b).

Ginzburg-Landau functional Since every function $\hat{\mathfrak{a}}_0$ in kernel of $K_{T_c} + \lambda V$ can be written (in polar coordinates) as

$$\hat{\mathfrak{a}}_0(p,\varphi) = \hat{\rho}(p)\left[\psi_+ \mathrm{e}^{\mathrm{i}\ell_0\varphi} + \psi_- \mathrm{e}^{-\mathrm{i}\ell_0\varphi}\right]$$

for an appropriate normalized $\hat{\rho} \in L^2((0,\infty); p\,\mathrm{d}p)$ and $\psi_\pm \in \mathbb{C}$ by Assumption 11.2.10 (cf. (11.2.15)), the analog of the Ginzburg-Landau functional (11.3.19) becomes [FL16, Theorems 2.10 and 3.5]

$$\begin{aligned}
&\mathcal{E}_{\mathsf{GL}}(\psi_+,\psi_-) \\
&\quad = \left[|\psi_+|^4 + |\psi_-|^4 + 4|\psi_+|^2|\psi_-|^2\right] \times \left[\frac{2\pi}{T_c^3}\int_0^\infty \frac{g_1((p^2-\mu)/T_c)}{(p^2-\mu)/T_c} |K_{T_c}(p)|^4 |\hat{\rho}(p)|^4\, p\ \mathrm{d}p\right] \\
&\qquad - \left[|\psi_+|^2 + |\psi_-|^2\right] \times \left[\frac{\pi}{T_c}\int_0^\infty \frac{1}{\cosh^2\left((p^2-\mu)/(2T_c)\right)} |K_{T_c}(p)|^2 |\hat{\rho}(p)|^2\, p\ \mathrm{d}p\right].
\end{aligned} \tag{11.3.35}$$

Minimizers of the GL functional In contrast to (11.3.19), the functional (11.3.35) now has *two* (up to a phase unique) minimizers. This follows from observing that $\mathcal{E}_{\mathsf{GL}}(\psi_+,\psi_-) = \mathcal{E}_{\mathsf{GL}}(\psi_-,\psi_+)$ and that one of the $\psi_\pm$ is necessarily zero for any minimizer of (11.3.35). In fact, these minimizers are

$$(|\psi_{\mathsf{GL}}|, 0) \quad \text{and} \quad (0, |\psi_{\mathsf{GL}}|)$$

with $|\psi_{\mathsf{GL}}|$ given in (11.3.22) but with $\Delta_0 := -2(2\pi)^{-d/2}\lambda\hat{V} \star \hat{\rho}$, where $\hat{\rho}$ is understood as a radial function in $L^2(\mathbb{R}^2)$.[14] Hence, using the notation from Proposition 11.3.9 (see also

[14]The fact that $\Delta_0(\sqrt{\mu}) \neq 0$ can be seen in a similar way as in the proof of Lemma 11.3.14.

[FL16, Theorem 2.10], which provides a general analog of (11.3.20)–(11.3.21), valid also for the concrete functional (11.3.35)) and (11.3.23), we find that (up to a constant phase) *every* non-zero solution of the BCS gap equation (11.1.4) can be written as

$$\Delta_\pm(p,\varphi) = C_{\mathsf{univ}}|\,T_c\,h\,\frac{\Delta_0(p)}{\Delta_0(\sqrt{\mu})}\mathrm{e}^{\pm\mathrm{i}\ell_0\varphi}\Big(1 + o_{\lambda\to 0}(1) + O\Big(he^{c/\lambda}\Big)\Big) + \Delta_\xi(p,\varphi)\,.$$

The rest of the argument (a priori bounds on $\Delta_0(p)\mathrm{e}^{\pm\mathrm{i}\ell_0\varphi}$ and Δ_ξ, comparison of $|\Delta_\pm|$ on the Fermi surface with Ξ) works completely analogously to Section 11.3.4 with similar adjustments as explained in Section 11.3.5.1. This concludes the proof of Theorem 11.2.11 (b). □

11.A Additional proofs

11.A.1 Uniqueness of the minimizer: Proof of Proposition 11.1.5

Finally, we present the proof of Proposition 11.1.5.

Proof of Proposition 11.1.5. We remark that the argument has already partly been sketched in [DGHL18; HS16]. The key observation for our proof is, that, if $\hat{V} \le 0$, then

$$\Big\langle \hat{\alpha}|\hat{V}\star\hat{\alpha}\Big|\geq\Big\rangle\,\Big\langle|\hat{\alpha}|\,|\hat{V}\star|\hat{\alpha}|\Big|\,\Big\rangle\,. \tag{11.A.1}$$

Let $(\hat{\gamma},\hat{\alpha})$ minimize the BCS functional (11.1.3). Then, by means of (11.A.1), we have $\mathcal{F}_T[(\hat{\gamma},\hat{\alpha})] \ge \mathcal{F}_T[(\hat{\gamma},|\hat{\alpha}|)]$, hence also $(\hat{\gamma},|\hat{\alpha}|)$ is a minimizer. Consequently, the (inverse) Fourier transform of $|\hat{\alpha}|$ is an eigenvector of $K_T^\Delta + V$ with $\Delta = -2(2\pi)^{-d/2}\hat{V}\star|\hat{\alpha}|$ with the eigenvalue zero. Note that, using continuity of Δ and the BCS gap equation (11.1.4), we not only have $|\hat{\alpha}| \ge 0$ but also $|\hat{\alpha}| > 0$ everywhere (see [HS08b, Lemma 2.1]). By the observation (11.A.1) again, we find that for any ground state $\hat{\alpha}_{\mathsf{GS}}$ of $K_T^\Delta + V$ also $|\hat{\alpha}_{\mathsf{GS}}|$ is a ground state. But $|\hat{\alpha}_{\mathsf{GS}}|$ is non–orthogonal to $|\hat{\alpha}|$, which implies that zero has to be the lowest eigenvalue of $K_T^\Delta + V$, i.e.

$$K_T^\Delta + V \ge 0\,. \tag{11.A.2}$$

By writing out (11.A.1), we see that the inequality is actually an application of Cauchy-Schwarz and thus becomes strict, unless $\hat{\alpha}(p) = e^{i\phi}\,|\hat{\alpha}(p)|$ for some fixed $\phi\in\mathbb{R}$. Therefore, by repeating the above arguments, we find that the ground state of (11.A.2) is non–degenerate and we have proven item (i).

In order to prove item (ii), let $\Gamma_i \equiv (\gamma_i,\alpha_i)$, $i=1,2$, be two (non–trivial) minimizers of the BCS functional (11.1.3) and denote the corresponding gap functions by Δ_1 resp. Δ_2. We now apply the relative entropy identity (see [FHSS12b] and [FL16, Prop. 5.2]) and a simple trace inequality (see [FHSS12b, Lemma 3] and [FL16, Lemma 5.7]) to find that

$$\mathcal{F}_T[\Gamma_1] - \mathcal{F}_T[\Gamma_2] \ge \Big\langle(\alpha_1-\alpha_2)\Big|K_T^{\Delta_1} + V\Big|(\alpha_1-\alpha_2)\Big\rangle \ge 0$$

(and the same inequality with indices 1 and 2 interchanged) by means of (11.A.2). Since $\mathcal{F}_T[\Gamma_1] = \mathcal{F}_T[\Gamma_2]$, this implies $(\alpha_1-\alpha_2)\in\ker(K_T^{\Delta_1}+V)$ and thus $\alpha_2 = \psi_{21}\alpha_1$ for some $\psi_{21}\in\mathbb{C}\setminus\{0\}$ (recall from (i) that $\ker(K_T^{\Delta_1}+V)$ is one–dimensional). From this we conclude

$$\Big(K_T^{\psi_{21}\Delta_1} + V\Big)\alpha_1 = 0\,.$$

Now, the pointwise strict monotonicity of $|\psi_{21}| \mapsto K_T^{\psi_{21}\Delta_1}(p)$ together with the fact that one can choose $|\hat{\alpha}_1|$ to be strictly positive, implies that $|\psi_{21}| = 1$ and we have shown uniqueness of minimizers up to a constant phase, which can be chosen in such a way that it ensures strict positivity of $\hat{\alpha}$. Finally, it is shown in [DGHL18, Proposition 2.9] that if α is not radial, then (11.A.2) is violated. Radiality of the corresponding γ follows from (11.1.6). This finishes the proof. □

11.A.2 Proofs of technical lemmas within the proof of Theorem 11.2.4

This section contains the proofs of Lemmas 11.3.4, 11.3.6, and 11.3.12.

11.A.2.1 Proof of Lemma 11.3.4

The argument is slightly different in dimensions $d = 1, 2, 3$. The case $d = 3$ is similar to [FHNS07; HS08b] and the case $d = 1, 2$ is similar to Chapter 9.

The case $d = 3$: We write

$$\begin{aligned} V^{1/2} M_{T,\Delta} |V|^{1/2} = V^{1/2} \frac{1}{p^2} |V|^{1/2} + V^{1/2} \left(M_{T,\Delta} - \frac{1}{p^2} \chi_{|p| > \sqrt{2\mu}} \right) |V|^{1/2} \\ - V^{1/2} \frac{1}{p^2} \chi_{|p| \leq \sqrt{2\mu}} |V|^{1/2}. \end{aligned} \tag{11.A.3}$$

The first term in Equation (11.A.3) has kernel (proportional to)

$$V(x)^{1/2} \frac{1}{|x-y|} |V(y)|^{1/2} \in L^2(\mathbb{R}^3 \times \mathbb{R}^3) \tag{11.A.4}$$

by the Hardy–Littlewood–Sobolev inequality [LL01, Theorem 4.3]. The kernel of the second term in Equation (11.A.3) is given by

$$\begin{aligned} V(x)^{1/2} |V(y)|^{1/2} \frac{1}{(2\pi)^3} \Bigg[\int_{|p| < \sqrt{2\mu}} \frac{1}{K_T^{\Delta}(p)} \left(e^{ip(x-y)} - e^{i\sqrt{\mu} p/|p| (x-y)} \right) \mathrm{d}p \\ + \int_{|p| > \sqrt{2\mu}} \left(\frac{1}{K_T^{\Delta}(p)} - \frac{1}{p^2} \right) e^{ip(x-y)} \, \mathrm{d}p \Bigg]. \end{aligned} \tag{11.A.5}$$

We compute the angular integral first. In the first term the integral is

$$4\pi \int_0^{\sqrt{2\mu}} \frac{1}{K_T^{\Delta}(p)} \left[\frac{\sin |p||x-y|}{|p||x-y|} - \frac{\sin \sqrt{\mu} |x-y|}{\sqrt{\mu} |x-y|} \right] |p|^2 \, \mathrm{d}|p|. \tag{11.A.6}$$

Here we bound $\left| \frac{\sin a}{a} - \frac{\sin b}{b} \right| \leq C \frac{|a-b|}{a+b}$ for $a, b > 0$. Thus we get the bound

$$|(11.A.6)| \leq C \int_0^{\sqrt{2\mu}} \frac{1}{K_T^{\Delta}(p)} \frac{\left| p - \sqrt{\mu} \right|}{p + \sqrt{\mu}} p^2 \, \mathrm{d}p \leq C \int_0^{\sqrt{2\mu}} \frac{1}{|p^2 - \mu|} \frac{\left| p - \sqrt{\mu} \right|}{p + \sqrt{\mu}} p^2 \, \mathrm{d}p \leq C.$$

In the second term the integral is (bounded by)

$$4\pi \int_{\sqrt{2\mu}}^{\infty} \left| \frac{1}{K_T^{\Delta}(p)} - \frac{1}{p^2} \right| \frac{|\sin |p||x-y||}{|p||x-y|} |p|^2 \, \mathrm{d}|p| \leq \frac{4\pi}{|x-y|} \int_{\sqrt{2\mu}}^{\infty} \left| \frac{1}{K_T^{\Delta}(p)} - \frac{1}{p^2} \right| p \, \mathrm{d}p.$$

To bound the remaining integral we bound

$$\left|\frac{1}{K_T^{\Delta}(p)}-\frac{1}{p^2}\right| \leq \frac{\left|\tanh\frac{\sqrt{|p^2-\mu|^2+\Delta(p)^2}}{2T}-1\right|}{\sqrt{|p^2-\mu|^2+\Delta(p)^2}}+\left|\frac{1}{\sqrt{|p^2-\mu|^2+\Delta(p)^2}}-\frac{1}{|p^2-\mu|}\right| \\ +\left|\frac{1}{|p^2-\mu|}-\frac{1}{p^2}\right|.$$

Note first that $|\tanh x-1|\leq 2e^{-2x}$. Thus, we have

$$\begin{aligned}\int_{\sqrt{2\mu}}^{\infty}\frac{\left|\tanh\frac{\sqrt{|p^2-\mu|^2+\Delta(p)^2}}{2T}-1\right|}{\sqrt{|p^2-\mu|^2+\Delta(p)^2}}p\,\mathsf{d}p &\leq 2\int_{\sqrt{2\mu}}^{\infty}e^{-\sqrt{|p^2-\mu|^2+\Delta(p)^2}/T}\frac{1}{\sqrt{|p^2-\mu|^2+\Delta(p)^2}}p\,\mathsf{d}p\\ &\leq 2\int_{\sqrt{2\mu}}^{\infty}e^{-|p^2-\mu|/T}\frac{p}{|p^2-\mu|}\,\mathsf{d}p\leq CT.\end{aligned}$$

Next, we estimate

$$\begin{aligned}&\left|\frac{1}{\sqrt{|p^2-\mu|^2+\Delta(p)^2}}-\frac{1}{|p^2-\mu|}\right|\\ &=\frac{1}{|p^2-\mu|}\frac{\Delta(p)^2}{\sqrt{|p^2-\mu|^2+\Delta(p)^2}\left(|p^2-\mu|+\sqrt{|p^2-\mu|^2+\Delta(p)^2}\right)}\\ &\leq\frac{1}{|p^2-\mu|}\frac{\|\Delta\|_{L^\infty}^2}{\sqrt{|p^2-\mu|^2+\|\Delta\|_{L^\infty}^2}\left(|p^2-\mu|+\sqrt{|p^2-\mu|^2+\|\Delta\|_{L^\infty}^2}\right)}\leq\frac{\|\Delta\|_{L^\infty}^2}{2|p^2-\mu|^3},\end{aligned} \tag{11.A.7}$$

using pointwise monotonicity in $\Delta(p)$. Thus, changing variables to $u=p^2-\mu$ we have

$$\int_{\sqrt{2\mu}}^{\infty}\left|\frac{1}{\sqrt{|p^2-\mu|^2+\Delta(p)^2}}-\frac{1}{|p^2-\mu|}\right|p\,\mathsf{d}p\leq\frac{1}{4}\|\Delta\|_{L^\infty}^2\int_{\mu}^{\infty}\frac{1}{u^3}\,\mathsf{d}u\leq C\|\Delta\|_{L^\infty}^2.$$

Finally,

$$\int_{\sqrt{2\mu}}^{\infty}\left|\frac{1}{|p^2-\mu|}-\frac{1}{p^2}\right|p\,\mathsf{d}p\leq C.$$

We conclude that the kernel of the second term in Equation (11.A.3) is bounded by

$$|V(x)|^{1/2}\left(\frac{1+T+\|\Delta\|_{L^\infty}^2}{|x-y|}+1\right)|V(y)|^{1/2}\in L^2(\mathbb{R}^3\times\mathbb{R}^3).$$

Finally, the last term of Equation (11.A.3) has kernel

$$4\pi V(x)^{1/2}|V(y)|^{1/2}\int_0^{\sqrt{2\mu}}\frac{\sin p|x-y|}{p|x-y|}\,\mathsf{d}p\in L^2\left(\mathbb{R}^3\times\mathbb{R}^3\right) \tag{11.A.8}$$

since the integral is bounded by $\sqrt{2\mu}$.

The cases $d = 1$ and $d = 2$: The kernel of $M_{T,\Delta}$ is given by

$$M_{T,\Delta}(x,y) = \frac{1}{(2\pi)^d}\left[\int_{|p|<\sqrt{2\mu}} \frac{1}{K_T^\Delta}\left(e^{ip(x-y)} - e^{i\sqrt{\mu}p/|p|(x-y)}\right) + \int_{|p|>\sqrt{2\mu}} \frac{1}{K_T^\Delta} e^{ip(x-y)}\right] \tag{11.A.9}$$

Now, one may bound $K_T^\Delta \geq |p^2-\mu|$ uniformly in T, Δ. Then we may bound $M_{T,\Delta}$ exactly as in Lemma 9.3.5. That is, we have the bounds

$$\left\|V^{1/2}M_{T,\Delta}|V|^{1/2}\right\|_{\mathsf{HS}}^2 \lesssim \begin{cases} \|V\|_{L^1}^2 + \|V\|_{L^1}\int_{\mathbb{R}}|V(x)|\left[1+\log(1+\sqrt{\mu}|x|)\right]^2 \mathsf{d}x & d=1, \\ \|V\|_{L^1}^2 + \|V\|_{L^p}^2 & d=2 \end{cases}$$

for any $1 < p \leq 4/3$. This concludes the proof of Lemma 11.3.4. □

11.A.2.2 Proof of Lemma 11.3.6

To bound the difference, first note that by computing the angular integrals we have

$$\begin{aligned}\left[M_{T,\Delta} - M_{T_c,0}\right](x,y) = \frac{|\mathbb{S}^{d-1}|}{(2\pi)^d}&\left[\int_0^{\sqrt{2\mu}}\left[\frac{1}{K_T^\Delta} - \frac{1}{K_{T_c}}\right]\left[j_d(p|x-y|) - j_d(\sqrt{\mu}|x-y|)\right]p^{d-1}\,\mathsf{d}p\right. \\ &\left.+\int_{\sqrt{2\mu}}^\infty\left[\frac{1}{K_T^\Delta} - \frac{1}{K_{T_c}}\right]j_d(p|x-y|)p^{d-1}\,\mathsf{d}p\right]\end{aligned} \tag{11.A.10}$$

where

$$j_d(x) = \frac{1}{|\mathbb{S}^{d-1}|}\int_{\mathbb{S}^{d-1}} e^{ix\omega}\,\mathsf{d}\omega = \begin{cases}\cos x & d=1 \\ J_0(|x|) & d=2 \\ \frac{\sin|x|}{|x|} & d=3\end{cases}$$

with J_0 the zero'th Bessel function.

Bounding Equation (11.A.10) is similar in spirit to the proof of Lemma 11.3.4 above. We bound

$$\left|\frac{1}{K_T^\Delta} - \frac{1}{K_{T_c}}\right| \leq \frac{\left|\tanh\frac{E_\Delta}{2T} - 1\right|}{E_\Delta} + \left|\frac{1}{E_\Delta} - \frac{1}{|p^2-\mu|}\right| + \frac{\left|1-\tanh\frac{|p^2-\mu|}{2T_c}\right|}{|p^2-\mu|}.$$

We bound the first term as follows

$$\frac{\left|\tanh\frac{E_\Delta}{2T} - 1\right|}{E_\Delta} \leq 2e^{-E_\Delta/T}\frac{1}{E_\Delta} \leq 2e^{-|p^2-\mu|/T}\frac{1}{|p^2-\mu|} \leq 2e^{-|p^2-\mu|/T_c}\frac{1}{|p^2-\mu|}.$$

Similarly,

$$\frac{\left|1-\tanh\frac{|p^2-\mu|}{2T_c}\right|}{|p^2-\mu|} \leq 2e^{-|p^2-\mu|/T_c}\frac{1}{|p^2-\mu|}.$$

Finally, we estimate, exactly as in (11.A.7) in the course of proving Lemma 11.3.4,

$$\begin{aligned}\left|\frac{1}{E_\Delta} - \frac{1}{|p^2-\mu|}\right| &\leq \frac{1}{|p^2-\mu|}\frac{\|\Delta\|_{L^\infty}^2}{\sqrt{|p^2-\mu|^2+\|\Delta\|_{L^\infty}^2}\left(|p^2-\mu| + \sqrt{|p^2-\mu|^2+\|\Delta\|_{L^\infty}^2}\right)} \\ &\leq \frac{\|\Delta\|_{L^\infty}^2}{2|p^2-\mu|^3}.\end{aligned}$$

We will use the first bound for the first integral in Equation (11.3.13) and the second bound for the second integral in Equation (11.3.13). Note further that $\frac{1}{\sqrt{x^2+A^2}\left(x+\sqrt{x^2+A^2}\right)}$ is decreasing in x and $|p^2-\mu| \geq \sqrt{\mu}|p-\sqrt{\mu}|$. That is, we have the bound

$$\left|\frac{1}{K_T^{\Delta}} - \frac{1}{K_{T_c}}\right| \leq 4e^{-|p^2-\mu|/T_c} \frac{1}{|p^2-\mu|} + \chi_{|p|>\sqrt{2\mu}} \frac{\|\Delta\|_{L^\infty}^2}{2|p^2-\mu|^3}$$
$$+\chi_{|p|<\sqrt{2\mu}} \frac{1}{\sqrt{\mu}|p-\sqrt{\mu}|} \frac{\|\Delta\|_{L^\infty}^2}{\sqrt{\mu|p-\sqrt{\mu}|^2+\|\Delta\|_{L^\infty}^2}\left(\sqrt{\mu}|p-\sqrt{\mu}|+\sqrt{\mu|p-\sqrt{\mu}|^2+\|\Delta\|_{L^\infty}^2}\right)}. \tag{11.A.11}$$

In the first integral in Equation (11.A.10) we bound $|j_d(a)-j_d(b)| \leq C|a-b|$. Then the contribution of the first term of Equation (11.A.11) to the first integral in Equation (11.A.10) is bounded by (changing variables to $s = \sqrt{\mu}|p-\sqrt{\mu}|/T_c$)

$$\int_0^{\sqrt{2\mu}} e^{-|p^2-\mu|/T_c} \frac{1}{|p^2-\mu|} |p-\sqrt{\mu}||x-y|p^{d-1} \, \mathrm{d}p \leq C|x-y| \int_0^{\sqrt{2\mu}} e^{-\sqrt{\mu}|p-\sqrt{\mu}|/T_c} \, \mathrm{d}p$$
$$\leq T_c|x-y| \int_0^{\mu/T_c} e^{-s} \, \mathrm{d}s \leq CT_c|x-y|.$$

Next, the contribution of the last term of Equation (11.A.11) is bounded by (changing variables to $s = \sqrt{\mu}|p-\sqrt{\mu}|/\left\|\Delta\right\|_{L^\infty}$)

$$\int_0^{\sqrt{2\mu}} \frac{\|\Delta\|_{L^\infty}^2}{\sqrt{\mu|p-\sqrt{\mu}|^2+\|\Delta\|_{L^\infty}^2}\left(|p-\sqrt{\mu}|\sqrt{\mu}+\sqrt{\mu|p-\sqrt{\mu}|^2+\|\Delta\|_{L^\infty}^2}\right)} \frac{|p-\sqrt{\mu}||x-y|p^{d-1}}{|p-\sqrt{\mu}|\sqrt{\mu}} \, \mathrm{d}p$$
$$\leq C\left\|\Delta\right\|_{L^\infty}|x-y| \int_0^{\mu/\|\Delta\|_{L^\infty}} \frac{1}{\sqrt{s^2+1}(s+\sqrt{s^2-1})} \, \mathrm{d}s \leq C\left\|\Delta\right\|_{L^\infty}|x-y|.$$

Next we estimate the last integral of Equation (11.A.10). Here we note that $|j_d(a)| \leq C$. Then the contributions of the first and second term in Equation (11.A.11) to Equation (11.A.10) is bounded by

$$\int_{\sqrt{2\mu}}^{\infty} e^{-|p^2-\mu|/T_c} \frac{1}{|p^2-\mu|} p^{d-1} \, \mathrm{d}p \leq C \int_{\sqrt{2\mu}}^{\infty} e^{-|p^2-\mu|/T_c} |p^2-\mu|^{d/2-2} p \, \mathrm{d}p \leq CT_c e^{-\mu/T_c} \leq CT_c$$

and $$\int_{\sqrt{2\mu}}^{\infty} \frac{\|\Delta\|_{L^\infty}^2}{|p^2-\mu|^3} p^{d-1} \, \mathrm{d}p \leq C\left\|\Delta\right\|_{L^\infty}^2 .$$

We conclude that (using $\left\|\Delta\right\|_{L^\infty} \leq CT_c$)

$$\left\|V^{1/2}(M_{T,\Delta}-M_{T_c,0})|V|^{1/2}\right\|_{\mathsf{HS}}^2 \leq CT_c^2 \iint |V(x)||V(y)|(\mu|x-y|^2+1) \, \mathrm{d}x \, \mathrm{d}y$$
$$\leq CT_c^2\left(\mu\left\||\cdot|^2 V\right\|_1 \|V\|_1 + \|V\|_1^2\right) \leq Ce^{-c/\lambda}$$

by assumption on V. This finishes the proof of Lemma 11.3.6. □

11.A.2.3 Proof of Lemma 11.3.12

The proof is very similar to the ones of [HS08b, Lemma 4] and Lemma 10.2.8 and follows from a Birman–Schwinger argument analogously to Sections 11.3.2.3 and 11.3.2.4.

First of all, recall from Proposition 11.1.5 (ii), that $K_{T_c} + \lambda V$ has 0 as a (non-degenerate) ground state eigenvalue, which, by the Birman–Schwinger principle, is equivalent to the fact that the Birman-Schwinger operator $B_{T_c} := \lambda V^{1/2} K_{T_c}^{-1} |V|^{1/2}$ has -1 as its (non-degenerate) ground state eigenvalue. As in Section 11.3.2.3, defining $m(T_c) := m(T_c, 0)$ (recall (11.3.11)), we decompose B_{T_c} as

$$B_{T_c} = \lambda m(T_c) V^{1/2} \mathfrak{F}_\mu^\dagger \mathfrak{F}_\mu |V|^{1/2} + \lambda V^{1/2} M_{T_c} |V|^{1/2} \,,$$

where M_{T_c} is such that this holds. It has been shown in [FHNS07, Lemma 2] (for $d = 3$) and Lemma 9.3.5 (for $d = 1, 2$), that the Hilbert-Schmidt norm $\| V^{1/2} M_{T_c} |V|^{1/2} \|_{\mathsf{HS}}$ of the second term is uniformly bounded for small T_c (i.e. small λ).

Then, by an argument completely analogous to the one in the proof of Lemma 11.3.5 in Section 11.3.2.4 we find that $\Delta_0 = f(\lambda)\Big[\hat{\varphi} + \lambda \eta_\lambda\Big]$ with $\hat{\varphi}$ defined in (11.3.24) and η_λ has $\|\eta_\lambda\|_{L^\infty} \le C$ uniformly in small λ (cf. (11.3.25)). This concludes the proof of Lemma 11.3.12. $\square$

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