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

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A B S T R A C T

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 et al. (1971) [15].

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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 $|x| \leq r$ 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 $L_a^2(\Lambda^N) = \bigwedge^N L^2(\Lambda)$. We consider the ground state energy density in the thermodynamic limit

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

It is a result of Robinson [31] 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

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

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 behaviour 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 [6]. (How the length a_0 is related to the effective range appearing in [6] is perhaps not immediate. We discuss this below.) To order $a^3\rho^{8/3}$ the formula follows by truncating expansion formulas of Jastrow [22], Iwamoto and Yamada [21], Clark and Westhaus [5,35] or Gaudin, Gillespie and Ripka [15]. Additionally the formula (to order $a^3\rho^{8/3}$) is claimed by Efimov and Amus'ya [8,9], see also [34] 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 [15].

For the dilute Fermi gas one can also study the setting where different spins are present. This is studied in [10,17,25], see also [16]. This system is realized by having the Hamiltonian H_N act on a definite spin-sector $L_a^2(\Lambda^{N_\uparrow}) \otimes L_a^2(\Lambda^{N_\downarrow})$, 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 [25] and later in [10,17] using different methods. The next correction is conjectured to be the Huang–Yang term [20] of order $a_s^2\rho^{7/3}$, see [16,17]. 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 $L_s^2(\Lambda^N) = L^2(\Lambda)^{\otimes_{\text{sym}} N}$ 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 [7] for an upper bound and Lieb and Yngvason [26] for the lower bound. The next correction, known as the Lee–Huang–Yang correction [24], was shown as an upper bound in [3,36] and as a lower bound in [12,13]. 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 [25], where the leading correction to the kinetic energy is shown. Recently also the bosonic problem has been studied in [11]. We show that for the spin-polarized setting in 2 dimensions we have the upper bound

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

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

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

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

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 [27, Appendix A]; [32].)

Definition 1.1. The *p-wave scattering length* a of the interaction v is defined by the minimization problem

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

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 2.1. We define the length a_0 as follows.

Definition 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 1.1. The normalization is chosen so that a hard core interaction of radius R_0 has $a_0 = a = R_0$, see Remark 2.3. (If v has a hard core we interpret $v(x)\,\mathrm{d}x$ as a measure as in Definition 1.1.)

We can now state our main theorem.

Theorem 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*

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

The essential steps in the proof are as follows.

(1) Show the absolute convergence of the formal cluster expansion formulas of [15] 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 2.2, as an approximation to the Fermi ball. The formulas of [15] are computed in Sections 3.0.1, 3.0.2, 3.0.3 and 3.0.4 and stated in Theorem 3.4. The absolute convergence is proven in Section 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 4.9 and proven in Appendix B. The computation of the energy of such a Jastrow-type trial state is given in Section 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 4.1.

Remark 1.4. The term of order $a^3 a_0^2 \rho^{10/3}$ is in fact the same as is claimed in [6]. 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

$$k^3 \cot \delta(k) = -\frac{3}{a^3} - \frac{1}{2R_{\text{eff}}} k^2 + \text{higher order in } k \qquad k \to 0 \tag{1.1}$$

for the phase shift $\delta(k)$ of low energy p-wave scattering. A formula for the effective range is found in [19, Equation (56)]. With this we find

Proposition 1.5. *The effective range is given by*

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

Using this formula we recover the formula [6, Equation (15)] to order $\rho^{10/3}$. The formula of [6] reads

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

with $k_F = (6\pi^2 \rho)^{1/3}$ the Fermi momentum. We give the proof of Proposition 1.5 in Section 2.1 below.

Remark 1.6 *(Numerical investigation).* The validity of the formula in Theorem 1.3 is investigated numerically in [4] using Quantum Monte Carlo simulations. We plot their findings in Fig. 1.1 and compare them to the formula in Theorem 1.3 and the claimed formula to order $\rho^{11/3}$ of [6, Equation (15)].

Remark 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 3.1 and 4 and that the "stability condition" of the tree-graph bound [30, Proposition 6.1]; [33] used in Section 3.1 is satisfied.

Remark 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 Theorem 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 1.3 arises from bounding the tail of the Gaudin-Gillespie-Ripka-expansion. Exact calculations 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 [2]. We shall discuss this further in Remark 4.10.
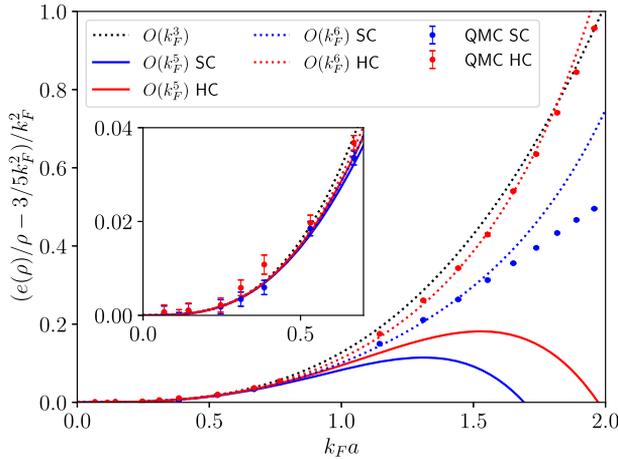
Fig. 1.1. Energies of dilute Fermi gasses. The curves and points labelled HC are for a *Hard Core* interaction of radius a. The curves and points labelled SC are for a *Soft Core* interaction of radius $2a$ and strength V_0 chosen so that it's scattering length is a. (Meaning $v(x) = V_0 \chi_{|x| \leq 2a}$, χ being the characteristic function.) The points (labelled QMC) are *Quantum Monte Carlo* simulations from [4]. The curves include the (conjectured) corrections up to the labelled order in $k_F = (6\pi^2 \rho)^{1/3}$.

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

Definition 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 1.3.

Theorem 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 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 1.11. The (1-dimensional) *p-wave scattering length* a of the interaction v is defined by the minimization problem

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

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

We show in Proposition 5.12 that Definition 1.11 agrees with the (seemingly different) definition of the scattering length in [1]. With this, we may state the 1-dimensional analogue of Theorem 1.3.

Theorem 1.12 *(One dimension). Suppose that $v \geq 0$ is even and compactly supported. Suppose moreover that $\int \left(\frac{1}{2} v f_0^2 + |\partial f_0|^2 \right) \, dx < \infty$, 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 [1] 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 [1].

Remark 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 $\int \left(\frac{1}{2} v f_0^2 + |\partial f_0|^2 \right) \, dx < \infty$, see Propositions 5.13 and 5.14.

We sketch in Section 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 2 we give some preliminary computations and in particular we introduce the "Fermi polyhedron", a polyhedral approximation to the Fermi ball. In Section 3 we introduce the fermionic cluster expansion of Gaudin, Gillespie and Ripka [15] and we find conditions on absolute convergence of the resulting formulas. In the subsequent Section 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 5 we sketch how to adapt the argument to the lower-dimensional settings. In Appendix A we give computations of "small diagrams" needed for some bounds in Sections 4 and 5.2 and in Appendix B we give the proof of Lemma 4.9, an important lemma used in Section 4.

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 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 [22] trial state (also known as a Bijl-Dingle-Jastrow-type trial state)

$$\psi_N = \frac{1}{\sqrt{C_N}} \prod_{i<j} f(x_i - x_j) D_N(x_1, \ldots, x_N), \tag{2.1}$$

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,

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

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

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 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 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 $A \leq CB$. 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

$$
\begin{aligned}
\langle \psi_N | H_N | \psi_N \rangle &= E_0 + 2 \sum_{j<k} \left\langle \psi_N \left| \left| \frac{\nabla f(x_j - x_k)}{f(x_j - x_k)} \right|^2 + \frac{1}{2} v(x_j - x_k) \right| \psi_N \right\rangle \\
&\quad + 6 \sum_{i<j<k} \left\langle \psi_N \left| \frac{\nabla f_{ij} \nabla f_{jk}}{f_{ij} f_{jk}} \right| \psi_N \right\rangle \\
&= E_0 + \iint \rho_{\text{Jas}}^{(2)}(x_1, x_2) \left(\left| \frac{\nabla f(x_1 - x_2)}{f(x_1 - x_2)} \right|^2 + \frac{1}{2} v(x_1 - x_2) \right) \, \mathrm{d}x_1 \, \mathrm{d}x_2 \\
&\quad + \iiint \rho_{\text{Jas}}^{(3)}(x_1, x_2, x_3) \frac{\nabla f_{12} \nabla f_{23}}{f_{12} f_{23}} \, \mathrm{d}x_1 \, \mathrm{d}x_2 \, \mathrm{d}x_3,
\end{aligned}
\tag{2.2}
$$

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

$$\rho_{\text{Jas}}^{(n)}(x_1, \ldots, x_n) = N(N-1)\cdots(N-n+1) \int \cdots \int |\psi_N(x_1, \ldots, x_N)|^2 \, \mathrm{d}x_{n+1} \ldots \mathrm{d}x_N,$$

$$n = 1, \ldots, N. \tag{2.3}$$

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 $\rho_{\text{Jas}}^{(2)}$ and bound $\rho_{\text{Jas}}^{(3)}$. Before we start on this endeavour we first recall some properties of the scattering function.

2.1. The scattering function

The scattering function f_0 is defined by the minimization problem in Definition 1.1, see also [27, Appendix A]; [32]. 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 equation reads

$$-\partial_r^2 f_0 - \frac{4}{r}\partial_r f_0 + \frac{1}{2}v f_0 = 0, \tag{2.4}$$

where ∂_r denotes the derivative in the radial direction. This is the same equation as for s-wave scattering in 5 dimensions, see [27, 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 2.2 ([27, 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 (2.4) we have $\partial_r(r^4 \partial_r f_0) = v r^4 f_0/2 \geq 0$. Denote by $f_{\mathrm{hc}} = \left[1 - \frac{a^3}{|x|^3}\right]_+$ the solution for a hard core potential of range a. Then

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

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

Remark 2.3. A hard core interaction of range $R_0 > 0$,

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

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

Finally, we give the

Proof of Proposition 1.5. Let R_0 denote the range of the interaction. Then the effective range is given by [19, Equation (56)]

$$-R_{\mathrm{eff}}^{-1} = -\frac{2}{R} - \frac{2R^2}{a^3} + \frac{2R^5}{5a^6} - 2\int_0^R u(r)^2 \, dr, \qquad \text{for } R \geq R_0 \tag{2.5}$$

where u solves [19, 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 (2.4). For $r \geq R_0$ we find using [19, Equation (27)] and Equation (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 (2.5) reads

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

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 1.5. $\quad\square$

2.2. The "Fermi polyhedron"

We introduce a polyhedral approximation P_F of the Fermi ball $B_F = \{k \in \frac{2\pi}{L}\mathbb{Z}^3 : |k| \leq k_F\}$. The main properties we will need of the polyhedral approximation are given in Lemmas 2.12, 2.13 and 4.9. We discuss why we need such a polyhedral approximation in Remark 3.5. The problem is that

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

for large N (see [14,28] 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 $\frac{1}{L^3} \int \sum_{k \in B(k_F) \cap \frac{2\pi}{L}\mathbb{Z}^3} e^{ikx} \, dx = 1$.

This type of quantity is referred to as the *Lebesgue constant* [14,28] of some domain Ω,

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

These kinds of integrals appear in estimates in Sections 3.1 and 4. For an overview of such Lebesgue constants, see [14,28]. 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 [23, Theorem 4.1] it is shown that for any fixed convex polyhedron P' of s vertices

$$\mathcal{L}(RP') = \frac{1}{(2\pi)^3} \int\limits_{[0,2\pi]^3} \left| \sum_{q \in RP' \cap \mathbb{Z}^3} e^{iqu} \right| du \leq Cs(\log R)^3 + C(s)(\log R)^2 \qquad (2.6)$$

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 $C(s) \leq Cs$. This is the content of Lemma 2.12 below. We first give an almost correct definition of the polyhedron P.

"Definition" 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 $d \geq cs^{-1/2}$ and $\inf_j |k - \kappa_j| \leq Cs^{-1/2}$.
- 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 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 2.6. For all purposes apart from the technical argument in Appendix B one may take this as the definition. In particular, the convergence criterion of the cluster expansion formulas of Gaudin, Gillespie and Ripka [15], given in Theorem 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 2.9 we give a few comments and in Remark 2.10 we give a short motivation.

Definition 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

$$Q^{-1/4} \leq Cs^{-1}, \qquad N^{4/3} \ll Q \leq CN^C$$

  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, $d \geq cs^{-1/2}Q^{-3/4}$ and $\inf_j \left| k - \kappa_j^{\mathbb{R}} \right| \leq Cs^{-1/2}Q^{-3/4}$ for some constants $c, C > 0$.
- Find points $\kappa_1, \ldots, \kappa_s$ of the form

$$\kappa_j = \left(\frac{p_j^1}{Q_1}, \frac{p_j^2}{Q_2}, \frac{p_j^3}{Q_3} \right), \qquad p_j^\mu \in \mathbb{Z}, \quad \mu = 1, 2, 3, \quad j = 1, \ldots, s, \qquad (2.7)$$

  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, $\tilde{P} = \text{conv}\{\kappa_1, \ldots, \kappa_s\}$.
- Define P as $\sigma\tilde{P}$, where σ is chosen such that $\text{Vol}(P) = 4\pi/3$. 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 $P^{\mathbb{R}} = \sigma \text{conv}\{\kappa_1^{\mathbb{R}}, \ldots, \kappa_s^{\mathbb{R}}\}$ 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 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 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 Appendix 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" 2.4.

- By choosing the points $\kappa_1, \ldots, \kappa_s$ as in Equation (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 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

$$
\frac{\alpha_1}{Q_2 Q_3} k^1 + \frac{\alpha_2}{Q_1 Q_3} k^2 + \frac{\alpha_3}{Q_1 Q_2} k^3 = \gamma \in \mathbb{Q}, \tag{2.8}
$$

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 (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 differs 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 Appendix B and will be explained there.

Remark 2.10 *(Motivation of construction).* The purpose of the construction is twofold. Firstly we avoid a casework argument as in the proof of [23, Lemma 3.5] of whether the coefficients of the planes are rational or not. The argument in Lemmas B.6 and B.7 is heavily inspired by [23, 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 Appendix B for the details).

These are technical details only needed in Appendix B. We reiterate, that apart from the arguments in Appendix B, the reader may have the simpler "Definition" 2.4 in mind instead.

As mentioned in Remark 2.9 the Fermi polyhedron is almost symmetric under permutation of the axes. This is formalized as follows.

Lemma 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 2.7 and χ denotes the indicator function.

Proof. Note that

$$\sum_{k \in \frac{2\pi}{L}\mathbb{Z}^3} \left| \chi_{(k \in P_F)} - \chi_{(k \in F_{\mu\nu}(P_F))} \right| t(k)$$

$$\leq \sum_{k \in \frac{2\pi}{L}\mathbb{Z}^3} \left| \chi_{(k \in P_F)} - \chi_{(k \in P_F^{\mathbb{R}})} \right| t(k) + \sum_{k \in \frac{2\pi}{L}\mathbb{Z}^3} \left| \chi_{(k \in F_{\mu\nu}(P_F))} - \chi_{(k \in F_{\mu\nu}(P_F^{\mathbb{R}}))} \right| t(k) \quad (2.9)$$

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 $\{\kappa_j\}_{j=1,\dots,s}$ only differ from $\{\kappa_j^{\mathbb{R}}\}_{j=1,\dots,s}$ by at most $\sim Q^{-1}$ thus the points $\{\sigma\kappa_j\}_{j=1,\dots,s}$ (the corners of P) only differ from the points $\{\sigma\kappa_j^{\mathbb{R}}\}_{j=1,\dots,s}$ 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,

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

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

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

The spacing between the k's in $\frac{2\pi}{L}\mathbb{Z}^3$ is $\sim L^{-1}$ and any k with $\mathrm{dist}(k, \partial(k_F P)) \lesssim k_F Q^{-1/4}$ 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 (2.9). We conclude the desired. $\quad\square$

We now improve on Equation (2.6) for our polyhedron.

Lemma 2.12. *The Lebesgue constant of the Fermi polyhedron satisfies*

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

The proof is (almost) the same as given in [23, 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 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 [23, Theorem 4.1] by the inclusion–exclusion principle we have

$$\mathcal{L}(RP) = \frac{1}{(2\pi)^3} \int \left| \sum_j \sum_{q \in T_j \cap \mathbb{Z}^3} e^{iqu} - \sum_{j<j'} \sum_{q \in T_j \cap T_{j'} \cap \mathbb{Z}^3} e^{iqu} + \cdots \right| du$$

$$\leq \sum_{\ell=1}^m \sum_{j_1 < \ldots < j_\ell} \mathcal{L}(T_{j_1} \cap \ldots \cap T_{j_\ell}).$$

In [23, 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 $Ck_F^2 N^{2/3}$. That is,

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

The integrals can be computed in spherical coordinates,

$$\int_{k_F P} |k|^2 \, dk - \int_{B(k_F)} |k|^2 \, dk = \int_{\mathbb{S}^2} \left(\int_0^{k_F R(\omega)} r^4 \, dr - \int_0^{k_F} r^4 \, dr \right) d\omega$$

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 2.9. Expanding the powers of R we thus get

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

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

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

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

$$\sum_{k \in P_F} |k|^2 = \sum_{k \in B_F} |k|^2 \left(1 + O(N^{-1/3}) + O(s^{-2}) \right)$$

$$= \frac{3}{5} (6\pi)^{2/3} \rho^{2/3} N \left(1 + O(N^{-1/3}) + O(s^{-2}) \right).$$

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

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

Completely analogously one can show that

$$\sum_{k\in P_F}|k|^4=\frac{18\pi^2}{7}(6\pi)^{1/3}\rho^{4/3}N\left(1+O(N^{-1/3})+O(s^{-2})\right).\tag{2.10}$$

We need this formula for Lemma 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

$$\sum_{k\in P_F}|k^1|^4=\frac{18\pi^2}{35}(6\pi)^{1/3}\rho^{4/3}N\left(1+O(N^{-1/3})+O(s^{-1})\right).\tag{2.11}$$

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

$$\sum_{k\in P_F}|k^1|^4-\sum_{k\in B_F}|k^1|^4$$

$$=\frac{L^3}{(2\pi)^3}\int\limits_0^{2\pi}\mathrm{d}\theta\int\limits_0^\pi\mathrm{d}\phi\cos(\phi)^4\left(\int\limits_0^{k_F(1+\varepsilon(\phi,\theta))}r^6\,\mathrm{d}r-\int\limits_0^{k_F}r^6\,\mathrm{d}r\right)+O(k_F^4 N^{2/3})$$

$$=O(k_F^4 N s^{-1})+O(k_F^4 N^{2/3}),$$

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.

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

$$\rho^{(2)}(x_1, x_2) = \frac{(6\pi^2)^{2/3}}{5} \rho^{8/3} |x_1 - x_2|^2 \left(1 - \frac{3(6\pi^2)^{2/3}}{35} \rho^{2/3} |x_1 - x_2|^2 \right.$$

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

This follows from a Taylor expansion akin to the argument in [1, Lemma 11].

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

$$\rho^{(2)}(x_1, x_2) = \rho^{(1)}(x_1)\rho^{(1)}(x_2) - \gamma_N^{(1)}(x_1; x_2)\gamma_N^{(1)}(x_2, x_1), \tag{2.12}$$

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 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

$$\gamma_N^{(1)}(x_1; x_2)$$

$$= \frac{1}{L^3} \sum_{k \in P_F} \left(1 - \frac{1}{2}(k \cdot (x_1 - x_2))^2 + \frac{1}{24}(k \cdot (x_1 - x_2))^4 + O(|k|^6 |x_1 - x_2|^6) \right)$$

$$= \rho - \frac{1}{2L^3} \sum_{k \in P_F} \left[|k^1|^2 |x_{12}^1|^2 + |k^2|^2 |x_{12}^2|^2 + |k^3|^2 |x_{12}^3|^2 \right]$$

$$+ \frac{1}{24L^3} \left(\sum_{k \in P_F} \left[|k^1|^4 |x_{12}^1|^4 + |k^2|^4 |x_{12}^2|^4 + |k^3|^4 |x_{12}^3|^4 \right] \right.$$

$$\left. + 6 \sum_{k \in P_F} \left[|k^1|^2 |k^2|^2 |x_{12}^1|^2 |x_{12}^2|^2 + |k^1|^2 |k^3|^2 |x_{12}^1|^2 |x_{12}^3|^2 + |k^2|^2 |k^3|^2 |x_{12}^2|^2 |x_{12}^3|^2 \right] \right)$$

$$+ O(\rho^3 |x_1 - x_2|^6).$$

By Lemma 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

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

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

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

Using Lemma 2.13 and Equations (2.10) and (2.11) we get that

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

Plugging this into Equation (2.12) we conclude the desired. $\square$

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

Lemma 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. $\square$

3. Gaudin-Gillespie-Ripka-expansion

We now present the cluster expansion of Gaudin, Gillespie and Ripka [15]. The argument given here is essentially the same as in [15], only we give sufficient conditions for

the formulas [15, Equations (3.19), (4.9) and (8.4)], given in Theorem 3.4, to hold, i.e., for absolute convergence of the expansion.

Recall the definition of the trial state ψ_N in Equation (2.1). We calculate the normalization constant C_N and the reduced densities $\rho_{\mathrm{Jas}}^{(1)}, \rho_{\mathrm{Jas}}^{(2)}$ and $\rho_{\mathrm{Jas}}^{(3)}$ defined in Equation (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.

3.0.1. 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

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

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

$$\rho^{(p)} = \det \left[\gamma_N^{(1)}(x_i; x_j) \right]_{1 \le i,j \le p} = \det \left[\sum_{k \in P_F} \overline{u_k(x_i)} u_k(x_j) \right]_{1 \le i,j \le p} = \det[S_p^* S_p],$$
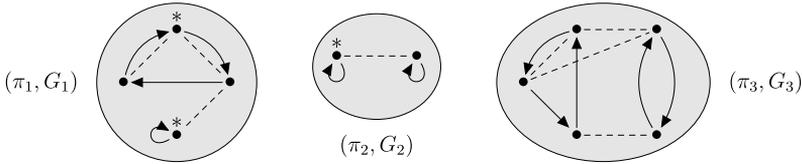
Fig. 3.1. A diagram $(\pi, G) \in \mathcal{D}_8^3$ decomposed into linked components. The dashed lines denote g-edges and the arrows (i, j) denote that $\pi(i) = j$. Vertices labelled with $*$ denote external vertices.

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 3.1. 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 $G \in \mathcal{G}_p^q$ (Fig. 3.1). 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 $\Gamma_{\pi,G} = \Gamma_{\pi,G}^0$ and $\mathcal{D}_p = \mathcal{D}_p^0$.

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 $\mathcal{L}_p^q$. For $q = 0$ we write $\mathcal{L}_p = \mathcal{L}_p^0$.

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

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

$$\frac{C_N}{N!}$$

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

$$\tag{3.1}$$

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 3.2 below. We conclude that if the assumptions of Lemma 3.2 are satisfied then

$$\frac{C_N}{N!} = 1 + \sum_{k=1}^{\infty} \frac{1}{k!} \sum_{p_1\geq 2} \cdots \sum_{p_k\geq 2} \sum_{(\pi_1,G_1)\in\mathcal{L}_{p_1}} \cdots \sum_{(\pi_k,G_k)\in\mathcal{L}_{p_k}} \frac{\Gamma_{\pi_1,G_1}}{p_1!} \cdots \frac{\Gamma_{\pi_k,G_k}}{p_k!}$$

$$= 1 + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\sum_{p=2}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p} \Gamma_{\pi,G} \right)^k = \exp\left(\sum_{p=2}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p} \Gamma_{\pi,G} \right).$$

$$\tag{3.2}$$

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 $\rho^{(1)}_{\text{Jas}} = \rho^{(1)} = \rho$. We nonetheless compute it here, as we need the formula in terms of (linked) diagrams. We have similarly as before

$$\rho^{(1)}_{\text{Jas}}(x_1) = \frac{N}{C_N} \int \cdots \int \prod_{2\leq i\leq N} f_{1i}^2 \prod_{2\leq i<j\leq N} f_{ij}^2 |D_N|^2 \, dx_2 \ldots dx_N$$

$$= \frac{N!}{C_N} \left[\rho^{(1)}(x_1) + \sum_{p=1}^{\infty} \frac{1}{p!} \int \cdots \int X_p^1 \rho^{(p+1)} \, dx_2 \ldots dx_{p+1} \right],$$

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 3.1. 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 $\rho_{\mathrm{Jas}}^{(1)}$ in terms of diagrams is

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

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 (3.1) we thus get for any $p \geq 0$

$$\frac{1}{p!} \sum_{(\pi,G) \in \mathcal{D}_p^1} \Gamma_{\pi,G}^1 = \sum_{(\pi_*,G_*) \in \mathcal{L}_p^1} \frac{\Gamma_{\pi_*,G_*}^1}{p!}$$

$$+ \left[\sum_{k=1}^{\infty} \frac{1}{k!} \sum_{p_* \geq 0} \sum_{p_1 \geq 2} \cdots \sum_{p_k \geq 2} \chi_{(\sum_{\ell \in \{*,1,\ldots,k\}} p_\ell = p)} \sum_{(\pi_*,G_*) \in \mathcal{L}_{p_*}^1} \frac{\Gamma_{\pi_*,G_*}^1}{p_*!} \right.$$

$$\left. \times \sum_{(\pi_1,G_1) \in \mathcal{L}_{p_1}} \cdots \sum_{(\pi_k,G_k) \in \mathcal{L}_{p_k}} \frac{\Gamma_{\pi_1,G_1}}{p_1!} \cdots \frac{\Gamma_{\pi_k,G_k}}{p_k!} \right],$$

where the superscript 1 refers to the slightly modified structure as described in Definition 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

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

then we have, as for the normalization in Equation (3.2), that

$$\rho_{\text{Jas}}^{(1)} = \frac{N!}{C_N} \sum_{p=0}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{D}_p^1} \Gamma_{\pi,G}^1$$

$$= \frac{N!}{C_N} \left[\sum_{p_*\geq 0} \sum_{(\pi_*,G_*)\in\mathcal{L}_{p_*}} \frac{\Gamma_{\pi_*,G_*}^1}{p_*!} \right] \times \left[\sum_{k=0}^{\infty} \frac{1}{k!} \left(\sum_{p\geq 2} \sum_{(\pi,G)\in\mathcal{L}_p} \frac{\Gamma_{\pi,G}}{p!} \right)^k \right]$$

$$= \sum_{p\geq 0} \sum_{(\pi,G)\in\mathcal{L}_p^1} \frac{\Gamma_{\pi,G}^1}{p!} = \rho^{(1)} + \sum_{p\geq 1} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p^1} \Gamma_{\pi,G}^1,$$

where we used Equation (3.2) and that the $p = 0$ term just gives the 1-particle density of the Slater determinant. Thus, by translation invariance, we have

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

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

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

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

$$\rho_{\text{Jas}}^{(2)}(x_1,x_2) = f_{12}^2 \left(\underbrace{\sum_{p_1,p_2\geq 0} \sum_{\substack{(\pi_1,G_1)\in\mathcal{L}_{p_1}^1 \\ (\pi_2,G_2)\in\mathcal{L}_{p_2}^1}} \frac{\Gamma_{\pi_1,G_1}^1(x_1)\Gamma_{\pi_2,G_2}^1(x_2)}{p_1!p_2!}}_{\{1\} \text{ and } \{2\} \text{ in different linked components}} \right.$$

$$\left. + \underbrace{\sum_{p_{12}\geq 0} \sum_{(\pi_{12},G_{12})\in\mathcal{L}_{p_{12}}^2} \frac{\Gamma_{\pi_{12},G_{12}}^2(x_1,x_2)}{p_{12}!}}_{\{1\} \text{ and } \{2\} \text{ in same linked component}} \right)$$

$$= f_{12}^2 \left(\rho_{\text{Jas}}^{(1)}(x_1)\rho_{\text{Jas}}^{(1)}(x_2) + \sum_{p_{12}\geq 0} \frac{1}{p_{12}!} \sum_{(\pi_{12},G_{12})\in\mathcal{L}_{p_{12}}^2} \Gamma_{\pi_{12},G_{12}}^2(x_1,x_2) \right)$$

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

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

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

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

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

$$\rho_{\mathrm{Jas}}^{(3)}(x_1, x_2, x_3)$$
$$= f_{12}^2 f_{13}^2 f_{23}^2 \left[\rho^3 + \rho \sum_{p \geq 0} \frac{1}{p!} \sum_{(\pi,G) \in \mathcal{L}_p^2} \left(\Gamma_{\pi,G}^2(x_1, x_2) + \Gamma_{\pi,G}^2(x_1, x_3) + \Gamma_{\pi,G}^2(x_2, x_3) \right) \right.$$
$$\left. + \sum_{p \geq 0} \frac{1}{p!} \sum_{(\pi,G) \in \mathcal{L}_p^3} \Gamma_{\pi,G}^3(x_1, x_2, x_3) \right].$$

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

3.0.5. Summarising the results

For the absolute convergence we have

Lemma 3.2. *There exists a constant $c > 0$ such that if $sa^3 \rho \log(b/a)(\log N)^3 < c$, then*

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

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

Remark 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 [30, Proposition 6.1]; [33] and $\hat{\gamma}(k) := \int_\Lambda \gamma(x)e^{-ikx} \, \mathrm{d}x$.

We give the proof of Lemma 3.2 in Section 3.1. Thus, we have the following.

Theorem 3.4. *There exists a constant $c > 0$ such that if $sa^3\rho \log(b/a)(\log N)^3 < c$, then*

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

$$\rho_{\mathrm{Jas}}^{(1)} = \rho^{(1)} + \sum_{p=1}^\infty \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p^1} \Gamma_{\pi,G}^1,$$

$$\rho_{\mathrm{Jas}}^{(2)} = f_{12}^2 \left[\rho^{(2)} + \sum_{p=1}^\infty \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p^2} \Gamma_{\pi,G}^2\right],$$

$$\rho_{\mathrm{Jas}}^{(3)} = f_{12}^2 f_{13}^2 f_{23}^2 \left[\rho^{(3)} + \rho \sum_{p\geq 1} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p^2} \left(\Gamma_{\pi,G}^2(x_1,x_2) + \Gamma_{\pi,G}^2(x_1,x_3) + \Gamma_{\pi,G}^2(x_2,x_3)\right)\right.$$

$$\left. + \sum_{p\geq 1} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p^3} \Gamma_{\pi,G}^3\right].$$

$$(3.3)$$

The first three formulas are the same as those of [15, 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 3.5. The factor $s(\log N)^3$ results from the bound in Lemma 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 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 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 2.13) is smaller than the claimed energy contribution from the interaction ($\sim Na^3\rho^{5/3}$, see Theorem 1.3). For this reason we need the polyhedron of Section 2.2.

Remark 3.6. The formulas for $\rho_{\mathrm{Jas}}^{(2)}$ and $\rho_{\mathrm{Jas}}^{(3)}$ only hold for periodic boundary conditions, since in this case $\rho_{\mathrm{Jas}}^{(1)} = \rho^{(1)} = \rho$. For different boundary conditions, one has to take into account that this equality is not valid. In general one has for $\rho_{\mathrm{Jas}}^{(2)}$ that

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

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 3.7. 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 3.2, to any q, only one may have to change the constant $c > 0$ to depend on q.

3.1. Absolute convergence

We now prove Lemma 3.2, i.e. that the appropriate sums are absolutely convergent.

Proof of Lemma 3.2. We consider the four sums $\sum_{p \geq 0} \frac{1}{p!} \left| \sum_{(\pi,G) \in \mathcal{L}_p^q} \Gamma_{\pi,G}^q \right|$, $q = 0, 1, 2, 3$ one by one.

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* (Fig. 3.2). (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 $p \geq 2$)
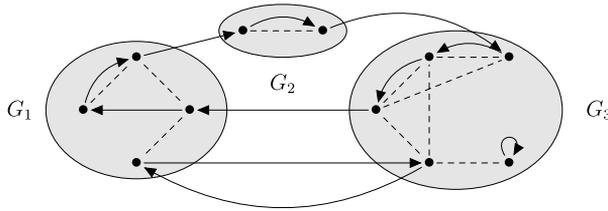
Fig. 3.2. A linked diagram $(\pi, G) \in \mathcal{L}_{11}$ decomposed into clusters G_1, G_2, G_3. Dashed lines denote g-edges, and arrows (i, j) denote that $\pi(i) = j$.

$$\frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p} \Gamma_{\pi,G} = \sum_{k=1}^{\infty} \frac{1}{k!} \sum_{\substack{n_1,\ldots,n_k \geq 2}} \frac{1}{n_1! \cdots n_k!} \chi_{(\sum n_\ell = p)} \sum_{\substack{G_1,\ldots,G_k \\ G_\ell \in \mathcal{C}_{n_\ell}}} \sum_{\pi \in \mathcal{S}_p} (-1)^\pi \chi_{((\pi,\cup G_\ell)\in\mathcal{L}_p)}$$

$$\times \int \cdots \int \prod_{\ell=1}^{k} \prod_{e\in G_\ell} g_e \prod_{j=1}^{p} \gamma_N^{(1)}(x_j; x_{\pi(j)}) \, \mathrm{d}x_1 \ldots \mathrm{d}x_p,$$

where $\mathcal{C}_n$ denotes the set of connected graphs on n (labelled) vertices. The factorial factors are similar to those of Equation (3.1). 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.

For the analysis we will need the following.

Definition 3.8. Let $A_1, \ldots, A_k$ denote disjoint non-empty sets. The *truncated* correlation function is

$$\rho_{\mathrm{t}}^{(A_1,\ldots,A_k)} := \sum_{\pi \in \mathcal{S}_{\cup_\ell A_\ell}} (-1)^\pi \chi_{((\pi,\cup G_\ell) \text{ linked})} \prod_{j\in\cup_\ell A_\ell} \gamma_N^{(1)}(x_j; x_{\pi(j)}), \tag{3.4}$$

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,

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

The truncated correlation functions are also sometimes referred to as *connected* correlation functions [18, Appendix D].

Remark 3.9. We write the characteristic function in Equation (3.4) as $\chi_{((\pi,\cup G_\ell) \text{ linked})}$ for ease of generalizability to the cases in Sections 3.1.2 and 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 $0 \leq f \leq 1$ we have $-1 \leq g \leq 0$. Thus, by the tree-graph bound [30, Proposition 6.1]; [33] we have

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

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

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

$$
\leq \sum_{k=1}^{\infty} \frac{1}{k!} \sum_{n_1,\ldots,n_k \geq 2} \frac{1}{n_1! \cdots n_k!} \int \cdots \int \sum_{\substack{T_1,\ldots,T_k \\ T_\ell \in \mathcal{T}_{n_\ell}}} \prod_{\ell=1}^{k} \prod_{e \in T_\ell} |g_e| \left| \rho_{\mathrm{t}}^{(n_1,\ldots,n_k)} \right| \, \mathrm{d}x_1 \ldots \mathrm{d}x_{\sum n_\ell}.
$$

$$(3.5)$$

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

$$
\rho_{\mathrm{t}}^{(A_1,\ldots,A_k)} = \sum_{\tau \in \mathcal{A}^{(A_1,\ldots,A_k)}} \prod_{(i,j) \in \tau} \gamma_N^{(1)}(x_i; x_j) \int \mathrm{d}\mu_\tau(r) \det \mathcal{N}(r), \tag{3.6}
$$

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 (Fig. 3.3). The measure μ_τ is a probability measure on $\{(r_{\ell\ell'})_{1 \leq \ell \leq \ell' \leq k} : 0 \leq r_{\ell\ell'} \leq 1\} = [0,1]^{k(k-1)/2}$ 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

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

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

From [18, 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 [18, Lemma D.2] slightly. We sketch the argument here.

Lemma 3.10 (*[18, 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 $r \in [0,1]^{k(k-1)/2}$.*
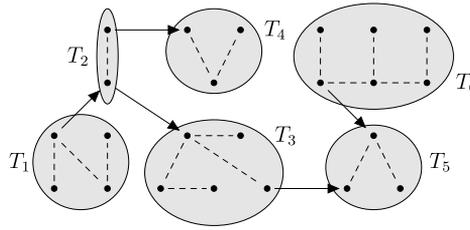
Fig. 3.3. An anchored tree τ (arrows) and trees $T_1, \ldots, T_6$ (dashed lines).

Proof. First we bound $\rho^{(p)} = \det[\gamma_N^{(1)}(x_i; x_j)]_{1 \leq i,j \leq p}$ following the strategy of [18, Lemma D.2]. This is done by writing (as in [18, 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 Gram-Hadamard inequality [18, 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 [18, Lemma D.6] and noting that $r_{\ell\ell'} \leq 1$ one concludes the desired. $\square$

Remark 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 (4.16).

In particular one concludes the bound

$$\left| \rho_{\mathrm{t}}^{(n_1,\ldots,n_k)} \right| \leq \rho^{\sum n_\ell - (k-1)} \sum_{\tau \in \mathcal{A}^{(n_1,\ldots,n_k)}} \prod_{(i,j) \in \tau} \left| \gamma_N^{(1)}(x_i; x_j) \right|. \tag{3.7}$$

Plugging this into Equation (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 2.2

$$\int |g(x)| \, dx = \int \left(1 - f(x)^2\right) \, dx$$

$$\leq \frac{4\pi}{(1 - a^3/b^3)^2} \int_a^b \left(\left(1 - \frac{a^3}{b^3}\right)^2 - \left(1 - \frac{a^3}{r^3}\right)^2\right) r^2 \, dr \leq Ca^3 \log \frac{b}{a}.$$

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 2.12 as

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

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 $\{j\}$ 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

$$\int \cdots \int \, dx_1 \ldots dx_{\sum n_\ell} \prod_{\ell=1}^k \prod_{e \in T_\ell} |g_e| \prod_{(i,j) \in \tau} \left|\gamma_N^{(1)}(x_i; x_j)\right|$$

$$\leq \left(Ca^3 \log(b/a)\right)^{\sum n_\ell - k} \left(Cs(\log N)^3\right)^{k-1} L^3.$$

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 [18, Appendix D.5] $\#\mathcal{A}^{(n_1,\ldots,n_k)} \leq k! 4^{\sum n_\ell}$. Thus, we get

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

$$\leq CNa^3\rho\log(b/a) \sum_{k=1}^{\infty} \left[Csa^3\rho\log(b/a)(\log N)^3\right]^{k-1}$$

$$\leq CNa^3\rho\log(b/a) < \infty,$$

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.

3.1.2. Absolute convergence of the Γ^1-sum

Consider now $\frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p^1} \Gamma_{\pi,G}^1$. 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 $\sum_{(\pi,G)\in\mathcal{L}_0^1} \Gamma_{\pi,G}^1 = \rho$)

$$\frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p^1} \Gamma_{\pi,G}^1(x_1)$$

$$= \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{n_*\geq 0} \sum_{n_1,\ldots,n_k\geq 2} \frac{1}{n_*!n_1!\cdots n_k!} \chi\big(\textstyle\sum_{\ell\{*,1,\ldots,k\}} n_\ell=p\big) \sum_{\substack{G_1\in\mathcal{C}_{n_1},\ldots,G_k\in\mathcal{C}_{n_k} \\ G_*\in\mathcal{C}_{n_*+1}}} \sum_{\pi\in\mathcal{S}_{p+1}} (-1)^\pi$$

$$\times \chi_{\big((\pi,\cup_{\ell\in\{*,1,\ldots,k\}}G_\ell)\in\mathcal{L}_p^1\big)} \int \cdots \int \prod_{\ell\in\{*,1,\ldots,k\}} \prod_{e\in G_\ell} g_e \prod_{j=1}^{p+1} \gamma_N^{(1)}(x_j;x_{\pi(j)}) \,dx_2\ldots\,dx_{p+1}.$$

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

$$\sum_{G_*\in\mathcal{C}_{p+1}} \sum_{\pi\in\mathcal{S}_{p+1}} (-1)^\pi \int \cdots \int \prod_{e\in G_*} g_e \prod_{j=1}^{p+1} \gamma_N^{(1)}(x_j;x_{\pi(j)}) \,dx_2\ldots\,dx_{p+1},$$

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 3.9) to get

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

$$\leq \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{n_* \geq 0} \sum_{n_1,\ldots,n_k \geq 2} \frac{1}{n_*! n_1! \cdots n_k!} \sum_{\substack{T_1 \in \mathcal{T}_{n_1}, \ldots, T_k \in \mathcal{T}_{n_k} \\ T_* \in \mathcal{T}_{n_*+1}}}$$

$$\times \int \cdots \int \prod_{\ell \in \{*,1,\ldots,k\}} \prod_{e \in T_\ell} |g_e| \left| \rho_{\mathrm{t}}^{(n_*+1,n_1,\ldots,n_k)} \right| \, \mathrm{d}x_2 \ldots \mathrm{d}x_{\sum_{\ell \in \{*,1,\ldots,k\}} n_\ell + 1}.$$

To bound this we use the same bound, Equation (3.7), on the truncated correlations as before. It reads

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

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 $\#\mathcal{A}^{(n_*+1,n_1,\ldots,n_k)} \leq (k+1)! 4^{\sum_{\ell \in \{*,1,\ldots,k\}} n_\ell + 1}$. Thus, uniformly in x_1

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

$$\leq C\rho \left(\sum_{n_*=0}^{\infty} \left[Ca^3 \rho \log(b/a) \right]^{n_*} \right) \left(\sum_{k=0}^{\infty} (k+1) \left[Cs(\log N)^3 \right]^k \left[\sum_{n=2}^{\infty} (Ca^3 \rho \log(b/a))^{n-1} \right]^k \right)$$

$$\leq C\rho < \infty,$$

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.

3.1.3. 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

$$\frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p^2} \Gamma_{\pi,G}^2 = \Sigma_{\text{different}} + \Sigma_{\text{same}}, \tag{3.8}$$

where

$$\Sigma_{\text{different}} = \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{n_*,n_{**}\geq 0} \sum_{n_1,\ldots,n_k\geq 2} \frac{1}{\prod_\ell n_\ell!} \chi_{(\sum n_\ell=p)} \sum_{\substack{G_1\in\mathcal{C}_{n_1},\ldots,G_k\in\mathcal{C}_{n_k} \\ G_*\in\mathcal{C}_{n_*+\{1\}} \\ G_{**}\in\mathcal{C}_{n_{**}+\{2\}}}}$$

$$\times \int \cdots \int \prod_\ell \prod_{e\in G_\ell} g_e \rho_{\text{t}}^{(n_*+\{1\},n_{**}+\{2\},n_1,\ldots,n_k)} \, \mathrm{d}x_3\ldots\mathrm{d}x_{p+2},$$

$$\Sigma_{\text{same}} = \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{n_*\geq 1} \sum_{n_1,\ldots,n_k\geq 2} \frac{1}{\prod_\ell n_\ell!} \chi_{(\sum n_\ell=p)} \sum_{\substack{G_1\in\mathcal{C}_{n_1},\ldots,G_k\in\mathcal{C}_{n_k} \\ G_*\in\mathcal{C}_{n_*+\{1,2\}} \\ (1,2)\notin G_*}}$$

$$\times \int \cdots \int \prod_\ell \prod_{e\in G_\ell} g_e \rho_{\text{t}}^{(n_*+\{1,2\},n_1,\ldots,n_k)} \, \mathrm{d}x_3\ldots\mathrm{d}x_{p+2}. \tag{3.9}$$

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 (3.7). The latter reads

$$\left|\rho_{\text{t}}^{(n_*+\{1\},n_{**}+\{2\},n_1,\ldots,n_k)}\right|$$

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

The integration procedure is slightly modified compared to that of Section 3.1.2. 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)

$$
\begin{aligned}
|\Sigma_{\text{different}}| \leq C\rho^2 &\left(\sum_{n_*=0}^{\infty} \left[Ca^3\rho\log(b/a) \right]^{n_*} \right)^2 \\
&\times \left(\sum_{k=0}^{\infty} (k^2+1)\left[Cs(\log N)^3 \right]^k \left[\sum_{n=2}^{\infty} (Ca^3\rho\log(b/a))^{n-1} \right]^k \right) \\
\leq &\ C\rho^2 < \infty.
\end{aligned}
\tag{3.10}
$$

Now we consider the case where $\{1\}$ and $\{2\}$ are in the same distinguished cluster. Here we may readily apply the bound in Equation (3.7) 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

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

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)

$$|\Sigma_{\text{same}}| \le C\rho^2 \left(\sum_{n_*=1}^{\infty} \left[Ca^3 \rho \log(b/a) \right]^{n_*} \right)$$

$$\times \left(\sum_{k=0}^{\infty} (k+1) \left[Cs(\log N)^3 \right]^k \left[\sum_{n=2}^{\infty} (Ca^3 \rho \log(b/a))^{n-1} \right]^k \right) \tag{3.11}$$

$$\le Ca^3 \rho^3 \log(b/a) < \infty.$$

We conclude that

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

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

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 3.2. $\quad\square$

4. Energy of the trial state

In this section we bound the energy of the trial state ψ_N defined in Equation (2.1). Recall Equation (2.2). By Theorem 3.4 we have (for $sa^3 \rho \log(b/a)(\log N)^3$ sufficiently small)

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

We can expand $\rho^{(2)}$ in $x_1 - x_2$ using Lemma 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 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*

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

$$
\leq Ca^6\rho^4 (\log(b/a))^2 \left[s^3 a^6 \rho^2 (\log b/a)^2 (\log N)^9 + 1 \right]
$$

$$
+ Ca^3\rho^{3+2/3}|x_1 - x_2|^2 \left[s^5 a^{12}\rho^4 (\log(b/a))^5 (\log N)^{16} + b^2\rho^{2/3} + \log(b/a) \right].
$$

Lemma 4.2. *There exists a constant $c > 0$ such that if $sa^3\rho\log(b/a)(\log N)^3 < c$, then*

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

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

We give the proof of these lemmas in Sections 4.2 and 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 2.15. Combining now Lemmas 2.13, 2.14, 4.1 and 4.2, Theorem 3.4 and Equation (2.2) we thus get (for $sa^3\rho\log(b/a)(\log N)^3$ sufficiently small and N sufficiently large)

$$
\langle \psi_N | H_N | \psi_N \rangle
$$

$$
= \frac{3}{5}(6\pi)^{2/3}\rho^{2/3}N \left(1 + O(N^{-1/3}) + O(s^{-2}) \right)
$$

$$
+ L^3 \int dx \left(|\nabla f(x)|^2 + \frac{1}{2}v(x)f(x)^2 \right)
$$

$$
\times \left[\frac{(6\pi^2)^{2/3}}{5}\rho^{8/3}|x|^2 \left(1 - \frac{3(6\pi^2)^{2/3}}{35}\rho^{2/3}|x|^2 \right. \right.
$$

$$
\left. + O(N^{-1/3}) + O(s^{-2}) + O(N^{-1/3}\rho^{2/3}|x|^2) + O(\rho^{4/3}|x|^4) \right) \tag{4.1}
$$

$$
+ O\left(a^6\rho^4(\log(b/a))^2 \left[s^3 a^6\rho^2(\log b/a)^2(\log N)^9 + 1 \right] \right)
$$

$$
\left. + O\left(a^3\rho^{3+2/3}|x|^2 \left[s^5 a^{12}\rho^4(\log(b/a))^5(\log N)^{16} + b^2\rho^{2/3} + \log(b/a) \right] \right) \right]
$$

$$
+ \iiint dx_1\, dx_2\, dx_3 f_{12}\nabla f_{12} f_{23}\nabla f_{23} f_{13}^2 \left[O(\rho^{3+4/3}|x_1-x_2|^2|x_2-x_3|^2) \right.
$$

$$
\left. + O\left(a^3\rho^4\log(b/a) \left[s^3 a^6\rho^2(\log(b/a))^2(\log N)^9 + 1 \right] \right) \right].
$$

We will choose N (really L, see Remark 2.8) some large negative power of $a^3\rho$, so errors with $N^{-1/3}$ are subleading. We may compute

$$\int dx \left(|\nabla f(x)|^2 + \frac{1}{2} v(x) f(x)^2 \right) |x|^2$$

$$= \frac{1}{(1 - a^3/b^3)^2} \int_{|x| \leq b} dx \left(|\nabla f_0(x)|^2 + \frac{1}{2} v(x) f_0(x)^2 \right) |x|^2 \qquad (4.2)$$

$$\leq 12\pi a^3 \left(1 + O(a^3/b^3) \right),$$

by Definition 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 $|\nabla f_0| \leq |\nabla f_{\mathrm{hc}}| = \frac{3a^3}{|x|^4}$ for $|x| \geq a$ by Lemma 2.2. Then we have (for $n = 4, 6$)

$$\int dx \left(|\nabla f(x)|^2 + \frac{1}{2} v(x) f(x)^2 \right) |x|^n$$

$$= \frac{1}{(1 - a^3/b^3)^2} \int_{|x| \leq b} dx \left(|\nabla f_0(x)|^2 + \frac{1}{2} v(x) f_0(x)^2 \right) |x|^n$$

$$\leq \frac{1}{2} R_0^{n-2} \int v |f_0|^2 |x|^2 \, dx + \int_{|x| \geq a} \left(\frac{3a^3}{|x|^4} \right)^2 |x|^n \, dx + a^{n-2} \int_{|x| \leq a} |\nabla f_0|^2 |x|^2 \, dx \qquad (4.3)$$

$$\lesssim C R_0^{n-2} a^3.$$

For $n = 4$ we have more precisely

$$\int dx \left(|\nabla f(x)|^2 + \frac{1}{2} v(x) f(x)^2 \right) |x|^4$$

$$\leq \int dx \left(|\nabla f_0(x)|^2 + \frac{1}{2} v(x) f_0(x)^2 \right) |x|^4 \left(1 + O(a^3 b^{-3}) \right)$$

$$= 36\pi a^3 a_0^2 + O(a^6 a_0^2 b^{-3}).$$

For the lower moment, we have by Equation (2.4)

$$\int dx \left(|\nabla f(x)|^2 + \frac{1}{2} v(x) f(x)^2 \right) = 4\pi \int_0^b \left(|\partial_r f|^2 r^2 + r^2 f \partial_r^2 f + 4 r f \partial_r f \right) dr$$

$$= \frac{12\pi a^3/b^2}{1 - a^3/b^3} + 8\pi \int_0^b r f \partial_r f \, dr \qquad (4.4)$$

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 2.2 we have

$$2\int\limits_0^b rf\partial_r f\,\mathrm{d}r = b - \int\limits_0^b f^2\,\mathrm{d}r \le b - \frac{1}{(1-a^3/b^3)^2}\int\limits_a^b\left(1-\frac{a^3}{r^3}\right)^2\mathrm{d}r \le Ca. \qquad (4.5)$$

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 (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,

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

Using integration by parts and Lemma 2.2, we have that

$$\frac{1}{4\pi}\int |x|^n f\partial_r f\,\mathrm{d}x = \int\limits_0^b r^{n+2}f\partial_r f\,\mathrm{d}r = \frac{b^{n+2}}{2} - \frac{n+2}{2}\int\limits_0^b r^{n+1}f^2\,\mathrm{d}r$$

$$\le \frac{b^{n+2}}{2} - \frac{n+2}{2}\int\limits_a^b r^{n+1}\left(\frac{1-a^3/r^3}{1-a^3/b^3}\right)^2\mathrm{d}r \le \begin{cases} Ca^2 & n=0, \\ Ca^3 b & n=2. \end{cases} \qquad (4.6)$$

Plugging all this into Equation (4.1) we thus get for the energy density

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

$$+ O\left(a^6\rho^{3+2/3}\left[s^5 a^{12}\rho^4(\log(b/a))^5(\log N)^{16} + b^2\rho^{2/3} + \log(b/a)\right]\right)$$

$$+ O\left(a^6 b^2\rho^{3+4/3}\right) + O\left(a^7\rho^4 \log(b/a)\left[s^3 a^6\rho^2(\log(b/a))^3(\log N)^9 + 1\right]\right). \tag{4.7}$$

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

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

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.

$$\frac{\langle\psi_N|H_N|\psi_N\rangle}{L^3}$$
$$= \frac{3}{5}(6\pi)^{2/3}\rho^{5/3} \tag{4.8}$$
$$+ \frac{12\pi}{5}(6\pi^2)^{2/3}a^3\rho^{8/3}\left[1 - \frac{9}{35}(6\pi^2)^{2/3}a_0^2\rho^{2/3} + O((a^3\rho)^{2/3+1/21}|\log(a^3\rho)|^6)\right]$$

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 $N^{4/3} \ll Q \le CN^C$ satisfies the condition $Q^{-1/4} \le Cs^{-1}$ of Definition 2.7.

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 [3,11,25,36]. 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 [31, Lemmas 2.1.12 and 2.1.13]. We present a slightly modified version in [29, Section C].

Lemma 4.3 ([29,31]). *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 $H^{\mathrm{per}}_{N,L} = \sum_{j=1}^N -\Delta^{\mathrm{per}}_{j,L} + \sum_{i<j} v_{\mathrm{per}}(x_i - x_j)$ denote the N-particle Hamiltonian with periodic boundary conditions on a box of sides L, with the interaction $v_{\mathrm{per}}(x) = \sum_{n \in \mathbb{Z}^3} v(x + nL)$, the periodized interaction.*

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

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

Proof. This is a trivial modification of [29, Lemma 4], noting that the explicitly constructed V respects the anti-symmetry. $\square$

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 (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 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

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

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

$$e(\tilde{\rho}) \leq \liminf_{M \to \infty} \frac{\left\langle \Psi_N \Big| H^D_{N,M(\ell+2d+b)} \Big| \Psi_N \right\rangle}{M^3(\ell + 2d + b)^3} = \frac{\left\langle V\psi_n \Big| H^D_{n,\ell+2d} \Big| V\psi_N \right\rangle}{(\ell + 2d + b)^3}$$

$$\leq \frac{\left\langle \psi_n \Big| H^{\mathrm{per}}_{n,\ell} \Big| \psi_n \right\rangle}{\ell^3} \left[1 + O(d/\ell) + O(b/\ell) \right] + O(\rho d^{-2}). \tag{4.9}$$

Choosing $d = a(a^3\rho)^{-5}$ and using Equation (4.8) we conclude that for $a^3\rho$ sufficiently small

$$e(\tilde{\rho}) \leq \frac{3}{5}(6\pi)^{2/3}\rho^{5/3}$$

$$+ \frac{12\pi}{5}(6\pi^2)^{2/3}a^3\rho^{8/3}\left[1 - \frac{9}{35}(6\pi^2)^{2/3}a_0^2\rho^{2/3} + O\left((a^3\rho)^{2/3+1/21}|\log(a^3\rho)|^6\right)\right]$$

$$= \frac{3}{5}(6\pi)^{2/3}\tilde{\rho}^{5/3}$$

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

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 1.3.

It remains to give the proofs of Lemmas 4.1 and 4.2.

4.2. Subleading 2-particle diagrams (proof of Lemma 4.1)

In this section we give the proof of Lemma 4.1. Before doing this, we first discuss why we don't just use the bounds of these terms from the proof of Lemma 3.2.

Remark 4.4 (*Why not use bounds of Lemma 3.2?*). Inspecting the proof of Lemma 3.2 (more precisely Equations (3.10) and (3.11) of Section 3.1.3) we can extract the following bound

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

This is immediate by considering the bounds Equations (3.10) and (3.11) and noting that since we have $p \geq 1$ 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 $k \geq 1$ or $n_* \geq 1$ or $n_{**} \geq 1$. 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 4, using Lemma 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 1.3.

Similarly, by following the proof of Lemma 3.2 one could get the bound

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

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 4.2 in order to get a better error bound in Theorem 1.3.

Proof of Lemma 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 (3.8) and (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 3.2.) Then we define

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

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

$$G = \quad \begin{matrix} * \\ \bullet \\ 1 \end{matrix} \qquad \left.\begin{matrix} \bullet\text{-}\text{-}\text{-}\text{-}\bullet \\ \vdots \quad\quad \vdots \\ \vdots \quad\quad \vdots \\ \bullet\text{-}\text{-}\text{-}\text{-}\bullet \end{matrix}\right\}k \quad \begin{matrix} * \\ \bullet \\ 2 \end{matrix}.$$
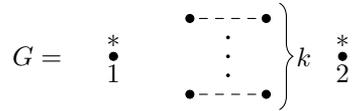
Then $\nu + \nu^*$ is the number of (internal) vertices a diagram has more than this lowest number.

By following the bound in Equations (3.10) and (3.11) we see that for $p = \nu_0 + 2k_0$

$$\left| \frac{1}{p!} \sum_{\substack{(\pi,G)\in\mathcal{L}_p^2 \\ \nu(\pi,G)+\nu^*(\pi,G)=\nu_0 \\ k(\pi,G)=k_0}} \Gamma_{\pi,G}^2 \right| \le C\rho^2 (Cs(\log N)^3)^{k_0} (Ca^3\rho\log(b/a))^{k_0+\nu_0}. \tag{4.10}$$

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 4.5. Here "large" and "small" should be interpreted in the sense of how many vertices appear in the diagram. Equation (4.10) describes 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 (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 $a^3 a_0^2 \rho^{10/3}$ 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 (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 (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 Fig. A.1 in Appendix A.1. We then write

$$\sum_{p=1}^{\infty} \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p^2} \Gamma_{\pi,G}^2 = \xi_{\text{small},0} + \xi_{\text{small},\geq 1} + \xi_0 + \xi_{\geq 1}, \tag{4.11}$$

where $\xi_{\text{small},0}$ is the contribution of all small diagrams of types (A) and (B), $\xi_{\text{small},\geq 1}$ 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 $\xi_{\text{small},0}$) and the small diagrams of type (C) somewhat similar to the large diagrams in

$\xi_{\geq 1}$ (hence the notation $\xi_{\mathrm{small},\geq 1}$). Indeed, we will do a Taylor expansion of $\xi_{\mathrm{small},0}$ and ξ_0 but not of $\xi_{\mathrm{small},\geq 1}$ or $\xi_{\geq 1}$.

Using the bound in Equation (4.10) and the absolute convergence (Lemma 3.2) we get

$$
\begin{aligned}
|\xi_{\geq 1}(x_1, x_2)| &\leq \underbrace{C\rho^2 (s(\log N)^3)^3 (a^3 \rho \log(b/a))^4}_{\text{type } (A) \text{ diagrams}} + \underbrace{C\rho^2 (a^3 \rho \log(b/a))^2}_{\text{type } (B) \text{ diagrams}} \\
&\leq Ca^6 \rho^4 (\log(b/a))^2 \left[s^3 (\log N)^9 a^6 \rho^2 (\log(b/a))^2 + 1 \right]
\end{aligned}
\tag{4.12}
$$

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

Lemma 4.6. *For the small diagrams of type (C) we have the bound*

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

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

Remark 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 of 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 $\xi_{\mathrm{small},0}$ and ξ_0 to second order around the diagonal. We first claim that

$$
\xi_{\mathrm{small},0}(x_2, x_2) + \xi_0(x_2, x_2) + \xi_{\mathrm{small},\geq 1}(x_2, x_2) + \xi_{\geq 1}(x_2, x_2) = 0
\tag{4.13}
$$

Indeed by Theorem 3.4 we have

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

(Formally to do the division by f in the first equality in case $f = 0$ somewhere one uses Theorem 3.4 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 (4.13). We may thus bound the zeroth order term of $\xi_{\mathrm{small},0}$ and ξ_0 by

$$|\xi_{\text{small},0}(x_2, x_2) + \xi_0(x_2, x_2)|$$
$$\leq |\xi_{\text{small},\geq 1}(x_2, x_2)| + |\xi_{\geq 1}(x_2, x_2)| \tag{4.14}$$
$$\leq C a^6 \rho^4 (\log(b/a))^2 \left[s^3 (\log N)^9 a^6 \rho^2 (\log(b/a))^2 + 1 \right].$$

Since both $\xi_{\text{small},0}$ 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 $\xi_{\text{small},0}$ we have

Lemma 4.8. *For any $\mu, \nu = 1, 2, 3$ we have*

$$\left| \partial_{x_1}^\mu \partial_{x_1}^\nu \xi_{\text{small},0} \right| \leq C a^3 \rho^{3+2/3} \log(b/a)$$

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

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

Next we consider $\partial_{x_1}^\mu \partial_{x_1}^\nu \xi_0$. We write ξ_0 in terms of truncated densities as in Equation (3.9), i.e.

$$\xi_0 = \sum_{k=0}^\infty \frac{1}{k!} \sum_{n_1, \ldots, n_k \geq 2} \chi_{(k \geq 5, n_\ell = 2 \text{ or } k \geq 1, \sum n_\ell = 2k+1)} \frac{1}{\prod_\ell n_\ell!} \sum_{\substack{G_1, \ldots, G_k \\ G_\ell \in \mathcal{C}_{n_\ell}}}$$

$$\times \int \cdots \int \prod_\ell \prod_{e \in G_\ell} g_e \rho_{\text{t}}^{(\{1\}, \{2\}, n_1, \ldots, n_k)} \, \mathrm{d}x_3 \ldots \mathrm{d}x_{p+2}.$$

Since we consider terms with $n_* = n_{**} = 0$, there are no g-factors that depend on x_1 and thus all derivatives are of $\rho_{\text{t}}^{(\{1\}, \{2\}, n_1, \ldots, n_k)}$. We thus need to calculate $\partial_{x_1}^\mu \partial_{x_1}^\nu \rho_{\text{t}}^{(\{1\}, \{2\}, n_1, \ldots, n_k)}$. For this we use the definition in Equation (3.4) rather than the formula in Equation (3.6). In Equation (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 $p = 2 + \sum_\ell n_\ell$)

$$\partial_{x_1}^\mu \partial_{x_1}^\nu \rho_{\text{t}}^{(\{1\}, \{2\}, n_1, \ldots, n_k)}$$

$$= \partial_{x_1}^\mu \partial_{x_1}^\nu \sum_{\pi \in \mathcal{S}_p} (-1)^\pi \chi_{((\pi, \cup G_\ell) \in \mathcal{L}_p)} \prod_{j=1}^p \gamma_N^{(1)}(x_j; x_{\pi(j)})$$

$$= \sum_{\pi \in \mathcal{S}_p} (-1)^\pi \chi_{((\pi, \cup G_\ell) \in \mathcal{L}_p)} \prod_{j \neq 1, j \neq \pi^{-1}(1)} \gamma_N^{(1)}(x_j; x_{\pi(j)})$$

$$\times \left[2 \partial_{x_1}^\mu \partial_{x_1}^\nu \gamma_N^{(1)}(x_1; x_{\pi(1)}) \gamma_N^{(1)}(x_{\pi^{-1}(1)}; x_1) + 2 \partial_{x_1}^\mu \gamma_N^{(1)}(x_1; x_{\pi(1)}) \partial_{x_1}^\nu \gamma_N^{(1)}(x_{\pi^{-1}(1)}; x_1) \right]. \tag{4.15}$$

With this formula we may then redo the computation of [18, 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 [18, Equation (D.9)] how to modify Lemma 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 3.10. Since we may bound $|k| \leq C\rho^{1/3}$ for $k \in P_F$ we get

$$\left| \det \tilde{\mathcal{N}}(r) \right| \leq \begin{cases} \rho^{\sum n_\ell + 2 - (k+2-1)} & \text{if no derivatives end up in } \mathcal{N}, \\ C\rho^{\sum n_\ell + 2 - (k+2-1)+1/3} & \text{if one derivative ends up in } \mathcal{N}, \\ C\rho^{\sum n_\ell + 2 - (k+2-1)+2/3} & \text{if two derivatives end up in } \mathcal{N}, \end{cases} \tag{4.16}$$

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 give the same factor $\gamma_N^{(1)}(x_1; x_j)$. A simple calculation (essentially just undoing the product rule) then shows that

$$\partial_{x_1}^\mu \partial_{x_1}^\nu \rho_\text{t}^{(\{1\},\{2\},n_1,\ldots,n_k)}$$

$$= \sum_{\partial \in \{1, \partial_{x_1}^\mu, \partial_{x_1}^\nu, \partial_{x_1}^\mu \partial_{x_1}^\nu\}} \left[\sum_{\substack{\tau \in \mathcal{A}^{(\{1\},\{2\},n_1,\ldots,n_k)} \\ \text{two edges to/from } \{1\}}} \partial \left[\gamma_N^{(1)}(x_{j_2}, x_1) \gamma_N^{(1)}(x_1; x_{j_1}) \right] \right. \tag{4.17}$$

$$\left. + \sum_{\substack{\tau \in \mathcal{A}^{(\{1\},\{2\},n_1,\ldots,n_k)} \\ \text{one edge to/from } \{1\}}} \partial \gamma_N^{(1)}(x_1; x_{j_1}) \right] \prod_{\substack{(i,j) \in \tau \\ i,j \neq 1}} \gamma_N^{(1)}(x_i; x_j) \int d\mu_\tau(r) \det \tilde{\mathcal{N}}_\partial(r),$$

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 (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 (4.17) to $\partial_{x_1}^\mu \partial_{x_1}^\nu \xi_0$ by $(\partial_{x_1}^\mu \partial_{x_1}^\nu \xi_0)^{\rightarrow \bullet \rightarrow}$ and $(\partial_{x_1}^\mu \partial_{x_1}^\nu \xi_0)^{\bullet \rightarrow}$ respectively.

We first deal with the second term of Equation (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 3.2. We give a sketch here. Using Equation (4.16) we get the bound

$$
\leq C \sum_{\partial \in \{1, \partial_{x_1}^{\mu}, \partial_{x_1}^{\nu}, \partial_{x_1}^{\mu} \partial_{x_1}^{\nu}\}} \rho^{(2 - \#\partial)/3} \sum_{\tau \in \mathcal{A}^{(\{1\}, \{2\}, n_1, \ldots, n_k)}} \left| \partial \gamma_N^{(1)}(x_1; x_{j_1}) \right|
$$
$$
\times \prod_{\substack{(i,j) \in \tau \\ i, j \neq 1}} \left| \gamma_N^{(1)}(x_i; x_j) \right| \rho^{(\sum_\ell n_\ell + 2) - (k + 2 - 1)}, \tag{4.18}
$$

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 3.2, Section 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 3.1.3. We conclude the bound

$$
\int \cdots \int \prod_{\ell=1}^{k} \prod_{e \in T_\ell} |g_e| \left| \partial \gamma_N^{(1)}(x_1; x_{j_1}) \right| \prod_{\substack{(i,j) \in \tau \\ i, j \neq 1}} \left| \gamma_N^{(1)}(x_i; x_j) \right| \, dx_3 \ldots dx_{\sum n_\ell + 2}
$$
$$
\leq \rho^{1 + \#\partial/3} \left(Ca^3 \log(b/a) \right)^{\sum n_\ell - k} \left(Cs(\log N)^3 \right)^k.
$$

Again, as in the proof of Lemma 3.2 we have by Cayley's formula that $\#\mathcal{T}_n = n^{n-2} \leq C^n n!$ and by [18, 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 (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

$$
\left| (\partial_{x_1}^{\mu} \partial_{x_1}^{\nu} \xi_0)^{\bullet \to} \right| \leq C\rho^{2 + 2/3} \bigg[\underbrace{(s(\log N)^3)^5 (a^3 \rho \log(b/a))^5}_{\text{type } (A) \text{ diagrams}} + \underbrace{s(\log N)^3 (a^3 \rho \log(b/a))^2}_{\text{type } (B) \text{ diagrams}} \bigg]
$$
$$
\leq Ca^6 \rho^{4 + 2/3} (\log(b/a))^2 s(\log N)^3 \left[s^4 (\log N)^{12} a^9 \rho^3 (\log(b/a))^3 + 1 \right] \tag{4.19}
$$

uniformly in x_1, x_2.

Next consider the first term of Equation (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 (4.19) we should replace one factor $Cs\rho^{1/3}(\log N)^3$ with $\int |\partial^{\mu} \gamma_N^{(1)}| \, dx$.

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 (4.19) we should replace one factor $Cs\rho^{2/3}(\log N)^3$ with $\int |\partial^\mu \partial^\nu \gamma_N^{(1)}| \, dx$.

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

$$
\leq C\rho^2 \left(\rho^{2/3} s(\log N)^3 + \rho^{1/3} \int_\Lambda \left| \partial^\mu \gamma_N^{(1)} \right| \, dx + \rho^{1/3} \int_\Lambda \left| \partial^\nu \gamma_N^{(1)} \right| \, dx + \int_\Lambda \left| \partial^\mu \partial^\nu \gamma_N^{(1)} \right| \, dx \right)
$$

$$
\times \left[(s(\log N)^3)^4 (a^3 \rho \log(b/a))^5 + (a^3 \rho \log(b/a))^2 \right]
$$

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

$$
\left| (\partial_{x_1}^\mu \partial_{x_1}^\nu \xi_0)^{\rightarrow \bullet \rightarrow} \right|
$$

$$
\leq C\rho^2 \left(\rho^{2/3} s(\log N)^3 + \rho^{1/3} \int_\Lambda \left| \partial^\mu \gamma_N^{(1)} \right| \, dx + \rho^{1/3} \int_\Lambda \left| \partial^\nu \gamma_N^{(1)} \right| \, dx + \int_\Lambda \left| \partial^\mu \partial^\nu \gamma_N^{(1)} \right| \, dx \right)
$$

$$
\times \left[(s(\log N)^3)^4 (a^3 \rho \log(b/a))^5 + (a^3 \rho \log(b/a))^2 \right] \tag{4.20}
$$

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

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

and

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

Here we have

Lemma 4.9. *The polyhedron P from Definition 2.7 satisfies for any $\mu, \nu = 1, 2, 3$ that*

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

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

for sufficiently large N.

The proof of Lemma 4.9 is a long and technical computation, which we give in Appendix B. Applying the lemma we conclude that

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

By combining this with Equations (4.19) and (4.20) we get

$$\left| \partial_{x_1}^\mu \partial_{x_1}^\nu \xi_0 \right| \leq C a^6 \rho^{4+2/3} (\log(b/a))^2 s (\log N)^4 \left[s^4 (\log N)^{12} a^9 \rho^3 (\log(b/a))^3 + 1 \right] \qquad (4.21)$$

uniformly in x_1, x_2. Combining Lemmas 4.6 and 4.8 and Equations (4.12), (4.14) and (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. $\quad\square$

Remark 4.10 *(Treating more diagrams as small).* One can improve the error bound in Theorem 1.3 slightly by treating more diagrams as small, i.e. calculating their values more precisely. This is similar to what is done in [2] for the dilute Bose gas. (In [2] 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 [2]], which if chosen sufficiently large yields the bounds of [2].) 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 (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 Appendix A and conclude that their contributions are as given in Appendix 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 1.3.

4.3. Subleading 3-particle diagrams (proof of Lemma 4.2)

Proof of Lemma 4.2. Recall the formula for $\rho_{\mathrm{Jas}}^{(3)}$ of Theorem 3.4. In this formula there are terms like $\rho \sum_{p \geq 1} \frac{1}{p!} \sum_{(\pi, G) \in \mathcal{L}_p^2} \Gamma_{\pi, G}^2(x_2, x_3)$. We have $\rho = \rho_{\mathrm{Jas}}^{(1)}(x_1) = \sum_{p' \geq 1} \frac{1}{p'!} \sum_{(\pi', G') \in \mathcal{L}_{p'}^1} \Gamma_{\pi', G'}^1(x_1)$ by translation invariance. Joining the two diagrams $(\pi, G) \in \mathcal{L}_p^2$ and $(\pi', G') \in \mathcal{L}_{p'}^1$ we get a new (no longer linked) diagram $(\pi'', G'') \in \mathcal{D}_{p+p'}^3$ 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

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

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 $\rho_{\text{Jas}}^{(3)}$ of Theorem 3.4 reads (assuming that $sa^3\rho\log(b/a)(\log N)^3$ is sufficiently small)

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

We split the diagrams in $\tilde{\mathcal{L}}_p^3$ into two groups, large and small similarly to the proof of Lemma 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 3.2.) Then we define

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

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 3.1.2 and 3.1.3.) We may still think of $\nu + \nu^*$ as the "number of added vertices". As for Equation (4.10) we have (for $p = 2k_0 + \nu_0$)

$$\left| \frac{1}{p!} \sum_{\substack{(\pi,G)\in\tilde{\mathcal{L}}_p^3 \\ \nu(\pi,G)+\nu^*(\pi,G)=\nu_0 \\ k(\pi,G)=k_0}} \Gamma_{\pi,G}^3 \right| \leq C\rho^3 (Cs(\log N)^3)^{k_0} (Ca^3\rho\log(b/a))^{k_0+\nu_0}. \qquad (4.22)$$

The main difference compared to Equation (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 3.1.3) 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 3.1.3. 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 4.2, the splitting is motivated by counting powers in Equation (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 (4.12) we may bound, using Equation (4.22)

$$|\xi_{\text{large}}^3| \leq \underbrace{C\rho^3 (s(\log N)^3)^3 (a^3 \rho \log(b/a))^3}_{\text{type } (A) \text{ diagrams}} + \underbrace{C\rho^3 a^3 \rho \log(b/a)}_{\text{type } (B) \text{ diagrams}}$$

$$\leq Ca^3 \rho^4 \log(b/a) \left[s^3 a^6 \rho^2 (\log(b/a))^2 (\log N)^9 + 1 \right].$$

For the small diagrams we have

Lemma 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 4.8, the proof is simply a computation, which we give in Appendix A.2. We conclude the desired. $\square$

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 2, 3 and 4 the relevant 1- and 2-dimensional analogues.

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

$$-\partial_r^2 f_0 - \frac{3}{r} \partial_r f_0 + \frac{1}{2} v f_0 = 0, \tag{5.1}$$

see Section 2.1 and recall Definition 1.9. Thus, it is the same as the s-wave scattering function in 4 dimensions. In particular it satisfies the bound

Lemma 5.1 ([27, Lemma A.1], Lemma 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 2.7.)

Definition 5.2. The polygon P is defined as follows.

- First pick Q, satisfying

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

  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 $\text{Vol}(P) = \pi$.
- 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 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 2.9.) Moreover, P_F is almost symmetric under the map $(k^1, k^2) \mapsto (k^2, k^1)$ similarly to Lemma 2.11.

Lemma 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 5.2.

The analogue of Lemma 2.12 is then

Lemma 5.4. *The Lebesgue constant of the Fermi polygon satisfies*

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

We can again compute the kinetic energy of the Slater determinant analogously to Lemma 2.13 and its 2-particle reduced density analogously to Lemma 2.14.

Lemma 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 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 make no reference to the dimension and are thus also valid in dimension $d = 2$. For the absolute convergence in Section 3.1 and Lemma 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 5.1 and 5.4)

$$\int_\Lambda |g| \lesssim a^2 + \frac{1}{(1 - a^2/b^2)^2} \int_a^b \left[\left(1 - \frac{a^2}{b^2} \right)^2 - \left(1 - \frac{a^2}{x^2} \right)^2 \right] x \, \mathrm{d}x \lesssim a^2 \log(b/a),$$

$$(5.2)$$

$$\int_\Lambda |\gamma_N^{(1)}| \lesssim s (\log N)^2.$$

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 3.4 reads

Theorem 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) hold (with $\rho_{\mathrm{Jas}}^{(n)}$ and $\Gamma_{\pi,G}^n$ interpreted as appropriate in the two-dimensional setting).*

The analogues of Lemmas 4.1 and 4.2 read

Lemma 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*

$$\left| \sum_{p=1}^{\infty} \frac{1}{p!} \sum_{(\pi,G) \in \mathcal{L}_p^2} \Gamma_{\pi,G}^2 \right| \leq C a^4 \rho^4 (\log(b/a))^2 \left[s^3 a^4 \rho^2 (\log b/a)^2 (\log N)^6 + 1 \right]$$

$$+ C a^2 \rho^4 |x_1 - x_2|^2 \left[s^5 a^8 \rho^4 (\log(b/a))^5 (\log N)^{11} + b^2 \rho + \log(b/a) \right],$$

and

$$\rho_{\mathrm{Jas}}^{(3)} \leq C f_{12}^2 f_{13}^2 f_{23}^2 \left[\rho^5 |x_1 - x_2|^2 |x_2 - x_3|^2 \right.$$

$$\left. + a^2 \rho^4 \log(b/a) \left[s^3 a^4 \rho^2 (\log(b/a))^2 (\log N)^6 + 1 \right] \right].$$

The proof is again similar to the 3-dimensional case replacing the bounds on $\int |g|$ and $\int |\gamma_N^{(1)}|$ as in Equation (5.2) above. Apart from this, there are two main changes. The first is in the proof of the analogue of Lemma 4.6, namely Equation (A.1), where one bounds $\int |x|^2 |1 - f^2|$. In two dimensions this bound is, using Lemma 5.1,

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

The other main difference is for the analogue of Lemma 4.9. Here the 2-dimensional analogue reads

Lemma 5.9. *The polygon P from Definition 5.2 satisfies for any $\mu, \nu = 1, 2$ that*

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

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

for sufficiently large N.

The proof is similar to that of Lemma 4.9 given in Appendix B only one skips Appendix B.2 and notes that $R = \frac{Lk_F}{2\pi} \sim N^{1/2}$.

Putting together the formulas in Theorem 5.7 with the bounds in Lemmas 5.5, 5.6 and 5.8 we easily find the analogue of Equation (4.1). We then need to bound a few terms. Following the type of arguments of Section 4, namely Equations (4.2), (4.3), (4.4), (4.5) and (4.6) and using Lemma 5.1 we get the bounds

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

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

Plugging this into the analogue of Equation (4.1) we get the analogue of Equation (4.7),

$$\begin{aligned}
\frac{\langle \psi_N | H_N | \psi_N \rangle}{L^2} &= 2\pi\rho^2 + 4\pi^2 a^2 \rho^3 \\
&\quad + O\left(s^{-4}\rho^2\right) + O\left(N^{-1/2}\rho^2\right) \\
&\quad + O\left(a^4 b^{-2}\rho^3\right) + O\left(a^4\rho^4 \log(b/a)\right) + O\left(R_0^2 a^2 \rho^4\right) \\
&\quad + O\left(a^4\rho^4 (\log(b/a))^2 \left[s^3 a^4 \rho^2 (\log b/a)^2 (\log N)^6 + 1\right]\right) \\
&\quad + O\left(a^4\rho^4 \left[s^5 a^8 \rho^4 (\log(b/a))^5 (\log N)^{11} + b^2\rho + \log(b/a)\right]\right) \\
&\quad + O\left(a^4 b^2 \rho^5\right) + O\left(a^4\rho^4 \log(b/a) \left[s^3 a^4 \rho^2 (\log(b/a))^3 (\log N)^6 + 1\right]\right).
\end{aligned}$$
$$(5.3)$$

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

$$\frac{\langle \psi_N | H_N | \psi_N \rangle}{L^3} = 2\pi\rho^2 + 4\pi^2 a^2 \rho^3 \left[1 + O\left(a^2\rho |\log(a^2\rho)|^2\right)\right] \tag{5.4}$$

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 $N^{3/2} \ll Q \le CN^C$ satisfies the condition $Q^{-1/2} \le Cs^{-2}$ of Definition 5.2.

The extension to the thermodynamic limit of Section 4.1 is readily generalized. We thus conclude the proof of Theorem 1.10.

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)

$$-\partial^2 f_0 - \frac{2}{r}\partial f_0 + \frac{1}{2}vf_0 = 0, \tag{5.5}$$

see Section 2.1 and recall Definition 1.11. Thus, it is the same as the s-wave scattering function in 3 dimensions. In particular it satisfies the bound

Lemma 5.10 ([27, Lemma A.1], Lemma 2.2). *The scattering function satisfies* $\left[1 - \frac{a}{|x|}\right]_+$ $\le f_0(x) \le 1$ *for all* x *and* $|\partial f_0(x)| \le \frac{a}{|x|^2}$ *for* $|x| > a$.

Before giving the proof of Theorem 1.12 we first compare our definition of the scattering length to that of [1]. In [1] the following definition is given.

Definition 5.11 ([1, Section 1.3]). The *odd-wave scattering length* a_{odd} is given by

$$\frac{4}{R - a_{\mathrm{odd}}} = \inf\left\{\int\limits_{-R}^{R} \left(2|\partial h|^2 + v|h|^2\right)\,\mathrm{d}x : h(R) = -h(-R) = 1\right\}$$

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 5.12. *The p-wave scattering length a defined in Definition 1.11 and the odd-wave scattering length a_{odd} defined in Definition 5.11 agree, i.e. $a = a_{\mathrm{odd}}$.*

Proof. Note first that $h \mapsto \mathcal{E}(h) = \int_{-R}^{R}\left(2|\partial h|^2 + v|h|^2\right)\,\mathrm{d}x$ is convex, so by replacing h by $(h(x) - h(-x))/2$ we can only lower its value. Thus, we have

$$\frac{4}{R - a_{\mathrm{odd}}} = \inf\left\{\int\limits_{-R}^{R} \left(2|\partial h|^2 + v|h|^2\right)\,\mathrm{d}x : h(x) = -h(-x), h(R) = 1\right\}.$$

Any h we write as $h(x) = \frac{xf(x)}{R}$. Using this and integration by parts we get

$$\frac{4}{R - a_{\mathrm{odd}}}$$

$$= \frac{1}{R^2} \inf \left\{ \int_{-R}^{R} \left(2|f|^2 + 4xf\partial f + 2|x|^2|\partial f|^2 + v|f|^2|x|^2 \right) \mathrm{d}x : f(x) = f(-x),\ f(R) = 1 \right\}$$

$$= \frac{4}{R} + \frac{2}{R^2} \inf \left\{ \int_{-R}^{R} \left(|\partial f|^2 + \frac{1}{2}v|f|^2 \right) |x|^2 \mathrm{d}x : f(x) = f(-x),\ f(R) = 1 \right\}.$$

That is,

$$2R \left(\frac{1}{1 - a_{\mathrm{odd}}/R} - 1 \right) = \inf \left\{ \int_{-R}^{R} \left(|\partial f|^2 + \frac{1}{2}v|f|^2 \right) |x|^2 \mathrm{d}x : f(x) = f(-x),\ f(R) = 1 \right\}.$$

Taking $R \to \infty$ in this we recover the definition of a. We conclude that $a = a_{\mathrm{odd}}$. □

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 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

$$\int \left(\frac{1}{2}vf_0^2 + |\partial f_0|^2 \right) \mathrm{d}x \leq \frac{1}{x_2^2} \int_{|x| \geq x_2} \left(\frac{1}{2}vf_0^2 + |\partial f_0|^2 \right) |x|^2 \mathrm{d}x = 2ax_2^{-2} < \infty. □$$

Proposition 5.14. *Suppose that $v \geq 0$ is even, compactly supported and smooth. 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. For smooth v also the scattering function f_0 is smooth. Recall the scattering equation (5.5). Then a simple calculation using integration by parts shows that

$$\int \left(\frac{1}{2}vf_0^2 + |\partial f_0|^2 \right) \mathrm{d}x = 2 \int_0^\infty \left(f_0\partial^2 f_0 + \frac{2f_0\partial f_0}{x} + (\partial f_0)^2 \right) \mathrm{d}x$$

$$= 2 \int_0^\infty \frac{f_0(x)^2 - f_0(0)^2}{x^2} \mathrm{d}x.$$

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 1.12. We consider the trial state given in Equation (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

$$
D_N(x_1, \ldots, x_N) = \det[u_k(x_i)]_{\substack{1 \leq i \leq N \\ k \in \bar{B}_F}}, \qquad u_k(x) = \frac{1}{L^{1/2}} e^{ikx}, \qquad N = \#B_F.
$$

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 [23, Lemma 3.2] or Lemma B.11)

Lemma 5.15. *The Lebesgue constant of the Fermi ball satisfies*

$$
\int_{-L/2}^{L/2} \frac{1}{L} \left| \sum_{k \in B_F} e^{ikx} \right| \, \mathrm{d}x = \frac{1}{2\pi} \int_0^{2\pi} \left| \sum_{q \in \left(B\left(\frac{Lk_F}{2\pi}\right)\right) \cap \mathbb{Z}^2} e^{iqu} \right| \, \mathrm{d}u \leq C \log N.
$$

As for the 2-dimensional setting one easily generalizes the computation of the kinetic energy in Lemma 2.13 and the calculation of the 2-particle reduced density for a Slater determinant in Lemma 2.14. That is,

Lemma 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 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 5.10 and 5.15)

$$\int_\Lambda |g| \lesssim a \log(b/a), \qquad \int_\Lambda |\gamma_N^{(1)}| \lesssim \log N. \tag{5.6}$$

Then, the 1-dimensional analogue of Theorem 3.4 reads

Theorem 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) hold (with $\rho_{\mathrm{Jas}}^{(n)}$ and $\Gamma_{\pi,G}^n$ interpreted as appropriate for the 1-dimensional setting).*

For the analogues of Lemmas 4.1 and 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 $\left|\Gamma_{\pi,G}^3\right| \leq Ca\rho^4 \log(b/a) \log N$ (see Section 4.3 and Appendix A.2) for any subleading diagram (π, G), i.e. for $(\pi, G) \in \tilde{\mathcal{L}}_p^3$ with $p \geq 1$.)

Remark 5.19 *(Why this was not a problem for dimensions $d = 2, 3$).* In dimensions $d = 1, 2, 3$ the analogous bound reads $\left|\Gamma_{\pi,G}^3\right| \leq Csa^d\rho^4 \log(b/a)(\log N)^d$ (if $d = 1$ then there is no s) for any subleading diagram, see Equation (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 4.1. We have the bounds

Lemma 5.20. *There exists a constant $c > 0$ such that if $a\rho \log(b/a) \log N < c$, then*

$$\left|\sum_{p=1}^\infty \frac{1}{p!} \sum_{(\pi,G)\in\mathcal{L}_p^2} \Gamma_{\pi,G}^2\right| \leq Ca^2\rho^4 \left[a\rho(\log(b/a))^3(\log N)^3 + b^4\rho^4\right]$$

$$+ Ca\rho^5|x_1 - x_2|^2 \left[b^2\rho^2 + Nab^4\rho^5 + \log(b/a)\right]$$

and

$$\rho_{\mathrm{Jas}}^{(3)} \leq Cf_{12}^2 f_{13}^2 f_{23}^2 \left[\rho^7|x_1 - x_2|^2|x_2 - x_3|^2 + a^2\rho^5(\log(b/a))^2(\log N)^2 \right.$$

$$\left. + a\rho^6 \left((b^2\rho^2 + \log(b/a))\right) \left[|x_1 - x_2|^2 + |x_1 - x_3|^2 + |x_2 - x_3|^2\right]\right].$$

The proof is similar to that of Lemmas 4.1 and 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 4.1. With this we get the analogue of Equation (4.1) in 1 dimension,

$$\langle \psi_N | H_N | \psi_N \rangle$$

$$= \frac{\pi^2}{3} \rho^2 N \left(1 + O(N^{-1}) \right) + L \int dx \left(|\partial f(x)|^2 + \frac{1}{2} v(x) f(x)^2 \right)$$

$$\times \left[\frac{\pi^2}{3} \rho^4 |x|^2 \left(1 + O(N^{-1}) + O(\rho^2 |x|^2) \right) + O \left(a\rho^5 |x|^2 \left[b^2 \rho^2 + Nab^4 \rho^5 + \log(b/a) \right] \right) \right.$$

$$\left. + O \left(a^2 \rho^4 \left[a\rho (\log b/a)^3 (\log N)^3 + b^4 \rho^4 \right] \right) \right]$$

$$+ \iiint dx_1 \, dx_2 \, dx_3 \, f_{12} \partial f_{12} f_{23} \partial f_{23} f_{13}^2$$

$$\times \left[O(\rho^7 |x_1 - x_2|^2 |x_2 - x_3|^2) + O \left(a^2 \rho^5 (\log(b/a))^2 (\log N)^2 \right) \right.$$

$$\left. + O \left(a\rho^6 \left[b^2 \rho^2 + \log(b/a) \right] \left[|x_1 - x_2|^2 + |x_1 - x_3|^2 + |x_2 - x_3|^2 \right] \right) \right].$$

$$(5.7)$$

For the 2-body error terms we may follow the type of arguments of Section 4, namely Equations (4.2), (4.3), (4.4), (4.5) and (4.6) exactly as for the 2-dimensional case. By using Lemma 5.10 we get the bounds

$$\int \left(|\partial f(x)|^2 + \frac{1}{2} v(x) f(x)^2 \right) |x|^n \, dx \leq \begin{cases} 2a, & n = 2, \\ Ca^2 b, & n = 4, \end{cases}$$

$$\int |x|^n f \partial f \, dx \leq \begin{cases} C, & n = 0, \\ Ca \log(b/a), & n = 1, \\ Cab, & n = 2. \end{cases}$$

Define a_0 by

$$\frac{1}{2a_0} = \int \left(|\partial f(x)|^2 + \frac{1}{2} v(x) f(x)^2 \right) dx$$

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 4. For the first term we bound $f_{13} \leq 1$. By the translation invariance one integration gives a volume (i.e. length) factor L. That is,

$$\iiint dx_1 \, dx_2 \, dx_3 \, \left| f_{12} \partial f_{12} f_{23} \partial f_{23} f_{13}^2 \right|$$

$$\times \left[O(\rho^7 |x_1 - x_2|^2 |x_2 - x_3|^2) + O \left(a^2 \rho^5 (\log(b/a))^2 (\log N)^2 \right) \right.$$

$$+ O\left(a\rho^6 \left[b^2\rho^2 + \log(b/a)\right]\left[|x_1 - x_2|^2 + |x_1 - x_3|^2 + |x_2 - x_3|^2\right]\right)\Bigg]$$

$$\leq CN\rho^6 \left(\int_0^b |x|^2 f\partial f \,\mathrm{d}x\right)^2 + CNa^2\rho^4(\log(b/a))^2(\log N)^2 \left(\int_0^b f\partial f\right)^2$$

$$+ CNa\rho^5 \left[b^2\rho^2 + \log(b/a)\right]\left[\left(\int_0^b |x|^2 f\partial f \,\mathrm{d}x\right)\left(\int_0^b f\partial f \,\mathrm{d}x\right) + \left(\int_0^b |x| f\partial f \,\mathrm{d}x\right)^2\right]$$

$$\leq CNa^2\rho^4 \left[b^2\rho^2 + (\log(b/a))^2(\log N)^2 + b\rho\left[b^2\rho^2 + \log(b/a)\right]\right].$$

We conclude the analogue of Equation (4.7) in dimension 1

$$
\begin{aligned}
\frac{\langle\psi_N|H_N|\psi_N\rangle}{L} &= \frac{\pi^2}{3}\rho^3 + \frac{2\pi^2}{3}a\rho^4 + O\left(N^{-1}\rho^3\right) + O\left(a^2 b^{-1}\rho^4\right) + O\left(a^2 b\rho^6\right) \\
&\quad + O\left(a^2\rho^4 a_0^{-1}\left[a\rho(\log(b/a))^3(\log N)^3 + b^4\rho^4\right]\right) \\
&\quad + O\left(a^2\rho^5\left[b^2\rho^2 + Nab^4\rho^5 + \log(b/a)\right]\right) \\
&\quad + O\left(a^2\rho^5\left[b^2\rho^2 + (\log(b/a))^2(\log N)^2 + b\rho\left[b^2\rho^2 + \log(b/a)\right]\right]\right).
\end{aligned}
\tag{5.8}
$$

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

$$
\begin{aligned}
\frac{\langle\psi_N|H_N|\psi_N\rangle}{L} &= \frac{\pi^2}{3}\rho^3 + \frac{2\pi^2}{3}a\rho^4 + O\left(N^{-1}\rho^3\right) + O\left(a^2 b^{-1}\rho^4\right) + O\left(a^2 a_0^{-1}b^2\rho^6\right) \\
&\quad + O\left(Na^3 b^4\rho^{10}\right).
\end{aligned}
\tag{5.9}
$$

Using the box method similarly as in Section 4.1 we also have to be careful with how we choose the parameter d. As in Equation (4.9) we get

$$
\begin{aligned}
e(\tilde\rho) &\leq \frac{\langle\psi_n|H_n|\psi_n\rangle}{\ell}\left[1 + O(d/\ell) + O(b/\ell)\right] + O\left(\rho d^{-2}\right) \\
&\leq \frac{\pi^2}{3}\rho^3 + \frac{2\pi^2}{3}a\rho^4 + O\left(n^{-1}\rho^3\right) + O\left(a^2 b^{-1}\rho^4\right) + O\left(a^2 a_0^{-1}b^2\rho^6\right) + O\left(na^3 b^4\rho^{10}\right) \\
&\quad + O\left(d\ell^{-1}\rho^3\right) + O\left(b\ell^{-1}\rho^3\right) + O\left(\rho d^{-2}\right).
\end{aligned}
$$

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

$$\alpha = \frac{33}{13}, \qquad \beta = \frac{9}{13}, \qquad \delta = \frac{24}{13} \tag{5.10}$$

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 1.12.

It remains to give the

Proof of Lemma 5.20. Note first that, completely analogously to Equations (4.10) and (4.22), we have

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

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

$$\tag{5.11}$$

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 $1 \leq k + \nu + \nu^* \leq 2$, $\{1\}$ and $\{2\}$ in different clusters
   (A) and $k \geq 1$,
   (B) and $k = 0, \nu^* = 1$.
2. Small diagrams with $1 \leq k + \nu + \nu^* \leq 2$ 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 $k + \nu + \nu^* \geq 3$.

We then split

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

where $\xi_{\text{small},0}$ is the contribution of all small diagram in the first group, $\xi_{\text{small},\geq 1}$ is the contribution of all small diagrams in the second group and $\xi_{\geq 1}$ is the contribution of all large diagrams. We will then do a Taylor expansion of $\xi_{\text{small},0}$ 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 $k + \nu + \nu^* \geq 2$.

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 (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 (5.11) that

$$|\xi_{\geq 1}| \leq Ca^3 \rho^5 (\log(b/a))^3 (\log N)^3, \qquad |\xi_{\geq 1}^3| \leq Ca^2 \rho^5 (\log(b/a))^2 (\log N)^2. \qquad (5.12)$$

Similarly as in the proof of Lemma 4.1 we have for $x_1 = x_2$

$$\xi_{\text{small},0}(x_2, x_2) + \xi_{\text{small},\geq 1}(x_2, x_2) + \xi_{\geq 1}(x_2, x_2) = 0,$$
$$\xi_{\text{small},0}^3(x_2, x_2, x_3) + \xi_{\text{small},\geq 1}^3(x_2, x_2, x_3) + \xi_{\geq 1}^3(x_2, x_2, x_3) = 0.$$

Hence we may bound the zeroth order by

$$|\xi_{\text{small},0}(x_2, x_2)| \le |\xi_{\text{small},\ge 1}(x_2, x_2)| + |\xi_{\ge 1}(x_2, x_2)|,$$
$$\left|\xi^3_{\text{small},0}(x_2, x_2, x_3)\right| \le \left|\xi^3_{\text{small},\ge 1}(x_2, x_2, x_3)\right| + \left|\xi^3_{\ge 1}(x_2, x_2, x_3)\right|.$$

For the diagrams in $\xi_{\text{small},0}$ and $\xi^3_{\text{small},0}$ we have similarly to Lemma 4.8 that

$$\left|\partial^2_{x_1} \xi_{\text{small},0}\right| \le C a \rho^5 \log(b/a), \qquad \left|\partial^2_{x_1} \xi^3_{\text{small},0}\right| \le C a \rho^6 \log(b/a) \qquad (5.13)$$

uniformly in x_1, x_2, x_3. For the diagrams in $\xi_{\text{small},\ge 1}$ and $\xi^3_{\text{small},\ge 1}$ the analysis is somewhat similar to the proof of Lemma 4.6. We have

Lemma 5.21. *For the small diagrams in $\xi_{\text{small},\ge 1}$ and $\xi^3_{\text{small},\ge 1}$ we have the bounds*

$$|\xi_{\text{small},\ge 1}| \le C a^2 b^4 \rho^8 + C a b^2 \rho^7 |x_1 - x_2|^2 \left[1 + N a b^2 \rho^3\right], \qquad (5.14)$$

$$\left|\xi^3_{\text{small},\ge 1}\right| \le C a b^2 \rho^8 \left(|x_1 - x_2|^2 + |x_1 - x_3|^2 + |x_2 - x_3|^2\right) \qquad (5.15)$$

uniformly in x_1, x_2, x_3.

We give the proof of Lemma 5.21 in Appendix A.3. Combining Lemma 5.21 and Equations (5.12) and (5.13) concludes the proof of Lemma 5.20. □

Data availability

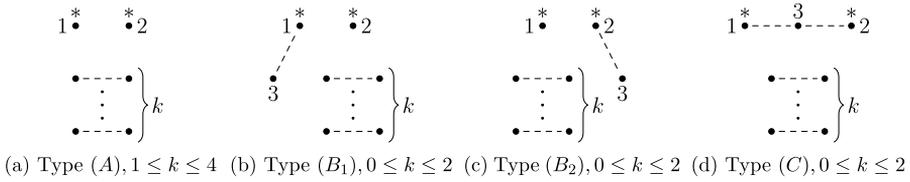No data was used for the research described in the article.

Acknowledgments

Appendix A. Small diagrams

In this appendix we compute the contributions of all the small diagrams of Lemmas 4.6, 4.8, 4.11 and 5.21. We first consider those of Lemmas 4.6 and 4.8.

(a) Type $(A), 1 \le k \le 4$ (b) Type $(B_1), 0 \le k \le 2$ (c) Type $(B_2), 0 \le k \le 2$ (d) Type $(C), 0 \le k \le 2$

Fig. 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.

A.1. Small 2-particle diagrams (proof of Lemmas 4.6 and 4.8)

Recall from the proof of Lemma 4.1, Section 4.2 that

$$\xi_{\text{small},0} + \xi_{\text{small}, \ge 1} = \sum_{p=1}^{\infty} \frac{1}{p!} \sum_{\substack{(\pi,G) \in \mathcal{L}_p^2 \\ (\pi,G) \text{ small}}} \Gamma_{\pi,G}^2.$$

The criterion for being small is defined in the proof of Lemma 4.1 around Equation (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 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 Fig. A.1.

(A) $\{1\}$ and $\{2\}$ in different clusters and $1 \le k \le 4, \nu = 0, \nu^* = 0$,
(B) $\{1\}$ and $\{2\}$ in different clusters and $0 \le k \le 2, \nu = 0, \nu^* = 1$,
    (B_1) and $n_* = 1, n_{**} = 0$,
    (B_2) and $n_* = 0, n_{**} = 1$,
(C) $\{1\}$ and $\{2\}$ in the same cluster and $0 \le k \le 2, \nu = 0, \nu^* = 1$.

We first give the

Proof of Lemma 4.6. Consider first all diagrams of type (C) of smallest size, i.e. with g-graph

$$G_0 = \quad 1 \overset{*}{\bullet} ----- \bullet ----- \overset{*}{\bullet} 2$$

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 2.15. Now we bound $|g_{23}| \leq 1$. Thus
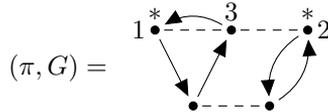
$$\left| \sum_{\pi \in \mathcal{S}_3:(\pi,G_0)\in\mathcal{L}_1^2} \Gamma^2_{\pi,G_0} \right| \leq C\rho^{3+4/3}|x_1 - x_2|^2 \int \left(1 - f(x)^2\right)|x|^2 \, \mathrm{d}x.$$

Recalling Lemma 2.2 we may bound

$$\int \left(1 - f(x)^2\right)|x|^2 \, \mathrm{d}x \leq Ca^5 + \frac{C}{(1 - a^3/b^3)^2} \int_a^b \left[\left(1 - \frac{a^3}{b^3}\right)^2 - \left(1 - \frac{a^3}{r^3}\right)^2 \right] r^4 \, \mathrm{d}r \leq Ca^3b^2.$$

$$\tag{A.1}$$

We conclude that all diagrams of smallest size contribute $\leq Ca^3b^2\rho^{3+4/3}|x_1 - x_2|^2$.
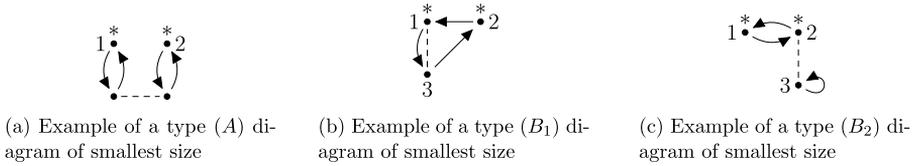
For the larger diagrams, we consider an example diagram

$$(\pi, G) = \qquad$$

For this diagram we have

$$\Gamma^2_{\pi,G} = (-1)^\pi \iiint \gamma_N^{(1)}(x_1; x_4)\gamma_N^{(1)}(x_4; x_3)\gamma_N^{(1)}(x_3; x_1)\gamma_N^{(1)}(x_2; x_5)\gamma_N^{(1)}(x_5; x_2)g_{13}g_{23}g_{45} \, \mathrm{d}x_3 \, \mathrm{d}x_4 \, \mathrm{d}x_5$$

$$= \frac{-1}{L^{15}} \sum_{k_1,\dots,k_5 \in P_F} \iiint e^{ik_1(x_1-x_4)}e^{ik_2(x_4-x_3)}e^{ik_3(x_3-x_1)}e^{ik_4(x_2-x_5)}e^{ik_5(x_5-x_2)}g_{13}g_{23}g_{45} \, \mathrm{d}x_3 \, \mathrm{d}x_4 \, \mathrm{d}x_5$$

$$= \frac{-1}{L^{15}} \sum_{k_1,\dots,k_5 \in P_F} e^{i(k_1-k_3)x_1}e^{i(k_4-k_5)x_2} \int \mathrm{d}x_3\, e^{i(k_3-k_2)x_3}g(x_1 - x_3)g(x_2 - x_3)$$

$$\times \int \mathrm{d}x_4 \left[e^{i(k_2-k_1+k_5-k_4)x_4} \int \mathrm{d}x_5\, e^{-i(k_5-k_4)(x_4-x_5)}g(x_4 - x_5) \right]$$

$$= \frac{-1}{L^{12}} \sum_{k_1,\dots,k_5 \in P_F} e^{i(k_1-k_3)x_1}e^{i(k_4-k_5)x_2} \int \mathrm{d}x_3\, e^{i(k_3-k_2)x_3}g(x_1 - x_3)g(x_2 - x_3)$$

$$\times \chi_{(k_2-k_1=k_4-k_5)}\hat{g}(k_5 - k_4),$$

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 $\hat{g}(k_i - k_j)$

(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

Fig. 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.

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. $\quad\square$

Proof of Lemma 4.8. As with the larger diagrams of type (C) we only give calculations for a few example diagrams and explain how the calculations for the remaining diagrams are similar. We consider the examples in Fig. A.2.

The contribution of the diagram in Fig. A.2a to $\partial_{x_1}^\mu \partial_{x_1}^\nu \xi_{\text{small}}$ is

$$
\frac{1}{2} \partial_{x_1}^\mu \partial_{x_1}^\nu \Gamma_{\pi,G}^2
$$

$$
= \frac{-1}{2L^{12}} \sum_{k_1,\ldots,k_4 \in P_F} (k_1^\mu - k_2^\mu)(k_1^\nu - k_2^\nu) \iint e^{ik_1(x_1 - x_3)} e^{ik_2(x_3 - x_1)} e^{ik_3(x_2 - x_4)} e^{ik_4(x_4 - x_2)} g_{34} \, dx_3 \, dx_4
$$

$$
= \frac{-1}{2L^{12}} \sum_{k_1,\ldots,k_4 \in P_F} (k_1^\mu - k_2^\mu)(k_1^\nu - k_2^\nu) e^{i(k_1 - k_2)x_1} e^{i(k_3 - k_4)x_2}
$$

$$
\times \iint e^{-i(k_4 - k_3)(x_3 - x_4)} e^{i(k_2 - k_1 + k_4 - k_3)x_3} g(x_3 - x_4) \, dx_3 \, dx_4
$$

$$
= \frac{-1}{2L^9} \sum_{k_1,\ldots,k_4 \in P_F} (k_1^\mu - k_2^\mu)(k_1^\nu - k_2^\nu) e^{i(k_1 - k_2)x_1} e^{i(k_3 - k_4)x_2} \chi_{(k_2 - k_1 = k_3 - k_4)} \hat{g}(k_4 - k_3)
$$

$$
= O(\rho^{3 + 2/3} a^3 \log(b/a))
$$

using that $\hat{g}(k) = \int_\Lambda g(x) e^{-ikx} \, dx$ satisfies $|\hat{g}(k)| \le \int |g| \le Ca^3 \log(b/a)$. The same type of computation is valid for all other diagrams of type (A).

Consider now the diagram in Fig. A.2c of type (B_2). This contributes

$$
\partial_{x_1}^\mu \partial_{x_1}^\nu \frac{-1}{L^9} \sum_{k_1,k_2,k_3 \in P_F} \int e^{ik_1(x_1 - x_2)} e^{ik_2(x_2 - x_1)} g(x_2 - x_3) \, dx_3
$$

$$
= \frac{1}{L^9} \sum_{k_1,k_2,k_3 \in P_F} (k_1^\mu - k_2^\mu)(k_1^\nu - k_2^\nu) e^{i(k_1 - k_2)x_1} e^{i(k_2 - k_1)x_2} \int g(x_2 - x_3) \, dx_3
$$

$$
= O(\rho^{3 + 2/3} a^3 \log(b/a))
$$

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 Fig. A.2b of type (B_1). Here we have

$$\partial_{x_1}^\mu \partial_{x_1}^\nu \Gamma_{\pi,G}^2$$

$$= \partial_{x_1}^\mu \partial_{x_1}^\nu \frac{1}{L^9} \sum_{k_1,k_2,k_3 \in P_F} \int e^{ik_1(x_1-x_3)} e^{ik_2(x_3-x_2)} e^{ik_3(x_2-x_1)} g(x_1-x_3) \, dx_3$$

$$= \partial_{x_1}^\mu \partial_{x_1}^\nu \frac{1}{L^9} \sum_{k_1,k_2,k_3 \in P_F} e^{i(k_2-k_3)x_1} e^{i(k_3-k_2)x_2} \int e^{-i(k_2-k_1)(x_1-x_3)} g(x_1-x_3) \, dx_3$$

$$= \frac{-1}{L^9} \sum_{k_1,k_2,k_3 \in P_F} (k_2^\mu - k_3^\mu)(k_2^\nu - k_3^\nu) e^{i(k_2-k_3)x_1} e^{i(k_3-k_2)x_2} \hat{g}(k_2-k_1)$$

$$= O(\rho^{3+2/3} a^3 \log(b/a)).$$

All larger diagrams of type (B_1) may be bounded similarly. We conclude the desired.   □

A.2. Small 3-particle diagrams (proof of Lemma 4.11)

We now give the

Proof of Lemma 4.11. Recall that

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

where "small" refers to diagrams with G-graph
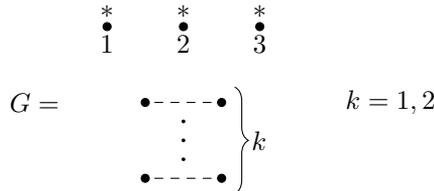
and permutation π such that (π,G) has at most two linked components, both of which contain at least one external vertex. As in the proof of Lemmas 4.6 and 4.8 in Appendix A.1 we compute the value of a few examples and explain how to compute the value of the remaining diagrams. We consider the examples of Fig. 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

Fig. A.3. Exemplary small diagrams in $\tilde{\mathcal{L}}_2^3$.

The contribution of the diagram in Fig. A.3a is

$$
\Gamma_{\pi,G}^3
$$
$$
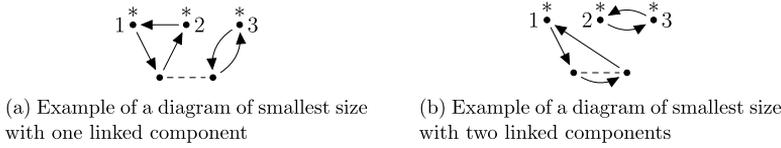= \frac{-1}{L^{15}} \sum_{k_1,\ldots,k_5 \in P_F} \iint e^{ik_1(x_1-x_4)} e^{ik_2(x_4-x_2)} e^{ik_3(x_2-x_1)} e^{ik_4(x_3-x_5)} e^{ik_5(x_5-x_3)} g_{45} \, \mathrm{d}x_4 \, \mathrm{d}x_5
$$
$$
= \frac{-1}{L^{12}} \sum_{k_1,\ldots,k_5 \in P_F} e^{i(k_1-k_3)x_1} e^{i(k_3-k_2)x_2} e^{i(k_4-k_5)x_3} \chi_{(k_2-k_1=k_4-k_5)} \hat{g}(k_5 - k_4)
$$
$$
= O(a^3 \rho^4 \log(b/a)).
$$

Similarly, the contribution of the diagram in Fig. A.3b is

$$
\Gamma_{\pi,G}^3
$$
$$
= \frac{-1}{L^{15}} \sum_{k_1,\ldots,k_5 \in P_F} \iint e^{ik_1(x_1-x_4)} e^{ik_2(x_4-x_5)} e^{ik_3(x_5-x_1)} e^{ik_4(x_2-x_3)} e^{ik_5(x_3-x_2)} g_{45} \, \mathrm{d}x_4 \, \mathrm{d}x_5
$$
$$
= \frac{-1}{L^{12}} \sum_{k_1,\ldots,k_5 \in P_F} e^{i(k_1-k_3)x_1} e^{i(k_4-k_5)x_2} e^{i(k_5-k_4)x_3} \chi_{(k_2-k_1=k_2-k_3)} \hat{g}(k_3 - k_2)
$$
$$
= O(a^3 \rho^4 \log(b/a)).
$$

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. □

A.3. Small diagrams in 1 dimension (proof of Lemma 5.21)

We now give the

Proof of Lemma 5.21. We first give the proof of Equation (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) $n_* = 1, n_{**} = 1$.

(a) Type (A_1) (b) Type (A_2) (c) Type (B_1) (d) Type (B_2)
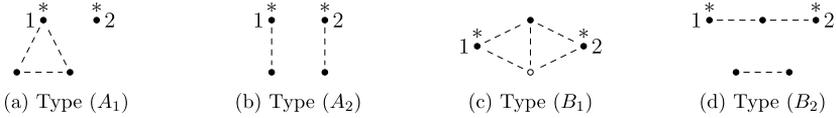
Fig. A.4. g-graphs of small diagrams of different types. For each diagram only the graph G is drawn. The relevant diagrams come with permutations π such that the diagrams are linked. The diagrams of type (A_1) and (B_1) may have some of the drawn g-edges not present, but the same connected components. 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.

(B) $\{1\}$ and $\{2\}$ in the same cluster and $1 \leq k + \nu + \nu^* \leq 2$,

   (B_1) $k = 0$,
   (B_2) $k = 1$.

See also Fig. A.4.

We will consider some examples of diagrams. Namely those drawn in Fig. 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

$$G_0 = \quad 1 \overset{*}{\bullet}\text{----}\bullet\text{----}\overset{*}{\bullet} 2 \tag{A.2}$$

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 (3.4). 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,

$$\rho_t^{(A_1,\ldots,A_k)} = \sum_{\pi \in \mathcal{S}_{\cup A_\ell}} (-1)^\pi \prod_{j \in \cup A_\ell} \gamma_N^{(1)}(x_j; x_{\pi(j)})$$
$$- \sum_{\pi \in \mathcal{S}_{\cup A_\ell}} (-1)^\pi \chi((\pi, \cup G_\ell) \text{ not linked}) \prod_{j \in \cup A_\ell} \gamma_N^{(1)}(x_j; x_{\pi(j)}).$$

For our case we only need to consider cases where there are at most two clusters. If there is just one cluster then $\rho_t^{(A)} = \rho^{(|A|)}((x_j)_{j \in A})$. 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,

$$\rho_t^{(A_1,A_2)}((x_j)_{j \in A_1 \cup A_2})$$
$$= \sum_{\pi \in \mathcal{S}_{A_1 \cup A_2}} (-1)^\pi \prod_{j \in A_1 \cup A_2} \gamma_N^{(1)}(x_j; x_{\pi(j)})$$

$$- \sum_{\pi_1 \in \mathcal{S}_{A_1}} (-1)^{\pi_1} \prod_{j \in A_1} \gamma_N^{(1)}(x_j; x_{\pi_1(j)}) \sum_{\pi_2 \in \mathcal{S}_{A_2}} (-1)^{\pi_2} \prod_{j \in A_2} \gamma_N^{(1)}(x_j; x_{\pi_2(j)})$$

$$= \rho^{(|A_1|+|A_2|)}((x_j)_{j \in A_1 \cup A_2}) - \rho^{(|A_1|)}((x_j)_{j \in A_1}) \rho^{(|A_2|)}((x_j)_{j \in A_2}). \tag{A.3}$$

We now consider the diagrams in Figs. A.4a, A.4b and A.4d and (A.2). We get

$$\text{Type } (A_1): \quad \sum_{\pi \in \mathcal{S}_4 : (\pi, G_0) \in \mathcal{L}_2^2} \Gamma_{\pi, G_0}^2 = \iint g_{13} g_{14} g_{34} \rho_{\mathrm{t}}^{(\{1,3,4\},\{2\})} \, \mathrm{d}x_3 \, \mathrm{d}x_4,$$

$$\text{Type } (A_2): \quad \sum_{\pi \in \mathcal{S}_4 : (\pi, G_0) \in \mathcal{L}_2^2} \Gamma_{\pi, G_0}^2 = \iint g_{13} g_{24} \rho_{\mathrm{t}}^{(\{1,3\},\{2,4\})} \, \mathrm{d}x_3 \, \mathrm{d}x_4,$$

$$\text{Type } (B_1): \quad \sum_{\pi \in \mathcal{S}_3 : (\pi, G_0) \in \mathcal{L}_1^2} \Gamma_{\pi, G_0}^2 = \int g_{13} g_{23} \rho^{(3)} \, \mathrm{d}x_3,$$

$$\text{Type } (B_2): \quad \sum_{\pi \in \mathcal{S}_5 : (\pi, G_0) \in \mathcal{L}_3^2} \Gamma_{\pi, G_0}^2 = \iiint g_{13} g_{23} g_{45} \rho_{\mathrm{t}}^{(\{1,2,3\},\{4,5\})} \, \mathrm{d}x_3 \, \mathrm{d}x_4 \, \mathrm{d}x_5. \tag{A.4}$$

Using Equation (A.3) and (the 1-dimensional versions of) Lemmas 2.14 and 2.15 and similar bounds for the 4- and 5-particle reduced densities we get the bounds on the truncated correlations

$$(A_1) \qquad \left| \rho_{\mathrm{t}}^{(\{1,3,4\},\{2\})} \right| \leq \rho^{(4)}(x_1, \ldots, x_4) + \rho^{(3)}(x_1, x_3, x_4) \rho^{(1)}(x_2)$$

$$\leq C \rho^8 |x_1 - x_3|^2 |x_1 - x_4|^2,$$

$$(A_2) \qquad \left| \rho_{\mathrm{t}}^{(\{1,3\},\{2,4\})} \right| \leq \rho^{(4)}(x_1, \ldots, x_4) + \rho^{(2)}(x_1, x_3) \rho^{(2)}(x_2, x_4)$$

$$\leq C \rho^8 |x_1 - x_3|^2 |x_2 - x_4|^2,$$

$$(B_1) \qquad \rho^{(3)} \leq C \rho^7 |x_1 - x_2|^2 |x_1 - x_3|^2,$$

$$(B_2) \qquad \left| \rho_{\mathrm{t}}^{(\{1,2,3\},\{4,5\})} \right| \leq \rho^{(5)}(x_1, \ldots, x_5) + \rho^{(3)}(x_1, x_2, x_3) \rho^{(2)}(x_4, x_5)$$

$$\leq C \rho^{11} |x_1 - x_2|^2 |x_1 - x_3|^2 |x_4 - x_5|^2.$$

Bounding moreover, $g_{34} \leq 1$ for the diagram of type (A_1) we thus get by the translation invariance

$$\left| \sum_{\substack{\pi \in \mathcal{S}_4 : (\pi, G_0) \in \mathcal{L}_2^2 \\ \text{type } (A_1)}} \Gamma_{\pi, G_0}^2 \right| \leq C \rho^8 \left(\int |g(x)| |x|^2 \, \mathrm{d}x \right)^2.$$

For the diagram of type (A_2) we get

$$\left| \sum_{\substack{\pi \in \mathcal{S}_4 : (\pi, G_0) \in \mathcal{L}_2^2 \\ \text{type } (A_2)}} \Gamma_{\pi, G_0}^2 \right| \leq C\rho^8 \left(\int |g(x)||x|^2 \, \mathrm{d}x \right)^2 .$$

For the diagram of type (B_1) we get by bounding $g_{23} \leq 1$ (as in the proof of Lemma 4.6)

$$\left| \sum_{\substack{\pi \in \mathcal{S}_3 : (\pi, G_0) \in \mathcal{L}_1^2 \\ \text{type } (B_1)}} \Gamma_{\pi, G_0}^2 \right| \leq C\rho^7 |x_1 - x_2|^2 \int |g(x)||x|^2 \, \mathrm{d}x .$$

Finally, for the diagram of type (B_2) we get in the same way

$$\left| \sum_{\substack{\pi \in \mathcal{S}_5 : (\pi, G_0) \in \mathcal{L}_3^2 \\ \text{type } (B_2)}} \Gamma_{\pi, G_0}^2 \right| \leq CN\rho^{10} |x_1 - x_2|^2 \left(\int |g(x)||x|^2 \, \mathrm{d}x \right)^2 .$$

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 (5.14).

To prove Equation (5.15) we recall that we consider all diagrams with g-graph

$$G_0 = \quad \overset{*}{\underset{1}{\bullet}} \text{---} \bullet \text{---} \overset{*}{\underset{2}{\bullet}} \quad \overset{*}{\underset{3}{\bullet}} \qquad \text{or} \qquad G_1 = \quad \overset{\overset{*}{\underset{2}{\bullet}}}{\underset{\overset{*}{\underset{1}{\bullet}}}{\diagdown}} \hspace{-0.3em} \searrow \bullet \text{---} \overset{*}{\underset{3}{\bullet}}$$

(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

$$\left| \sum_{\pi \in \mathcal{S}_4 : (\pi, G_0) \in \mathcal{L}_1^3} \Gamma_{\pi, G_0}^3 \right| \leq \int |g_{14}||g_{24}| \left| \rho_t^{(\{1,2,4\},\{3\})} \right| \, \mathrm{d}x_4 \leq Cab^2 \rho^8 |x_1 - x_2|^2$$

$$\left| \sum_{\pi \in \mathcal{S}_4 : (\pi, G_1) \in \mathcal{L}_1^3} \Gamma_{\pi, G_1}^3 \right| \leq \int |g_{14}||g_{24}||g_{34}| \rho^{(4)} \, \mathrm{d}x_4 \leq Cab^2 \rho^8 |x_1 - x_2|^2 .$$

Summing this over all the permutations of $\{1, 2, 3\}$ we conclude the proof of Equation (5.15). □

Appendix B. Derivative Lebesgue constants (proof of Lemma 4.9)

In this appendix we give the proof of Lemma 4.9. We recall the statement in slightly different notation for convenience.

Lemma 4.9. *The polyhedron P from Definition 2.7 satisfies for any $\mu, \nu = 1, 2, 3$ that*

$$\int\limits_{[0,2\pi]^3} \left| \sum_{k \in RP \cap \mathbb{Z}^3} k^\mu e^{ikx} \right| \mathrm{d}x \leq CsR(\log R)^3,$$

$$\int\limits_{[0,2\pi]^3} \left| \sum_{k \in RP \cap \mathbb{Z}^3} k^\mu k^\nu e^{ikx} \right| \mathrm{d}x \leq CsR^2(\log R)^4$$

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 [23]. 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 [23].

Notation 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 2.11 and choosing $Q \gtrsim N^4$ in Definition 2.7 we have a symmetry of coordinates up to error-terms which are subleading compared to Lemma 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

$$\int\limits_{[0,2\pi]^3} \left| \sum_{k \in RP \cap \mathbb{Z}^3} t_j(k)e^{ikx} \right| dx \leq \begin{cases} CsR(\log R)^3 & j = 1, \\ CsR^2(\log R)^4 & j = 2,3. \end{cases}$$

As in the proof of Lemma 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 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 B.1. Then the tetrahedra are of the form

$$T = \left\{ k \in \mathbb{Z}^3 : [\lambda_1] \leq k^1 \leq [\Lambda_1], [\lambda_2(k^1)] \leq k^2 \leq [\Lambda_2(k^1)], [\lambda_3(k^1, k^2)] \leq k^3 \leq [\Lambda_3(k^1, k^2)] \right\},$$
$$(B.1)$$

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 (B.1), we need to bound

$$\int\limits_{[0,2\pi]^3} \left| \sum_{k \in T \cap \mathbb{Z}^3} t_j(k)e^{ikx} \right| dx \leq \begin{cases} CR(\log R)^3 & j = 1, \\ CR^2(\log R)^4 & j = 2,3. \end{cases} \qquad (B.2)$$

Gluing together tetrahedra as in Lemma 2.12 we conclude the desired bound, Lemma 4.9. The remainder of this section gives the proof of Equation (B.2).

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 $|\kappa| \leq CR$. For t_2 we have

$$\sum_{k \in T \cap \mathbb{Z}^3} (k^1)^2 e^{ikx} = \sum_{k \in (T - \kappa) \cap \mathbb{Z}^3} (k^1 + \kappa^1)^2 e^{ikx}$$

$$= \sum_{k \in (T - \kappa) \cap \mathbb{Z}^3} (k^1)^2 e^{ikx} + 2\kappa^1 \sum_{k \in (T - \kappa) \cap \mathbb{Z}^3} k^1 e^{ikx} + (\kappa^1)^2 \sum_{k \in (T - \kappa) \cap \mathbb{Z}^3} e^{ikx}.$$

A similar computation holds for t_1, t_3. We may bound $|\kappa| \leq CR$ and thus we may assume that $T \subset [0, CR]^3$. (Recall that $\int_{[0,2\pi]^3} \left| \sum_{k \in T \cap \mathbb{Z}^3} e^{ikx} \right| \, dx \leq C(\log R)^3$ by [23, Theorem 4.1], see the proof of Lemma 2.12.)

For any tetrahedron of the form (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 (B.1) each instance of $[\cdot]$ may be either of the definitions of Notation 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 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 $k^2 \leq \lambda_2(k^1)$. 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

$$\int_{[0,2\pi]^3} \left| \sum_{k^1=[\Lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1, k^2) \sum_{k^3=0}^{[\Lambda_3(k^1,k^2)]} e^{ikx} \right| \, dx \lesssim \begin{cases} R(\log R)^3 & j = 1, \\ R^2(\log R)^4 & j = 2, 3. \end{cases}$$

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 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 $R\sigma(p_j^1/Q_1, p_j^2/Q_2, p_j^3/Q_3), j = 1, 2, 3$ is given by

$$\frac{\alpha_1}{Q_2 Q_3} k^1 + \frac{\alpha_2}{Q_1 Q_3} k^2 + \frac{\alpha_3}{Q_1 Q_2} k^3 = R\sigma\gamma$$

where by construction of P, see Definition 2.7, we have

$$\sigma \notin \mathbb{Q}, \qquad \gamma \in \mathbb{Q}, \qquad \alpha_j \in \mathbb{Z}, \qquad |\alpha_j| \leq C\sqrt{Q}, \quad j = 1, 2, 3.$$

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 $\alpha_3 \neq 0$. 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

$$\Lambda_3(k^1, k^2) = n_3 - m^1 k^1 - m^2 k^2 = n_3 - \frac{Q_1 \alpha_1}{Q_3 \alpha_3} k^1 - \frac{Q_2 \alpha_2}{Q_3 \alpha_3} k^2,$$

$$n_3 \notin \mathbb{Q}, \quad |\alpha_j| \leq C\sqrt{Q}, j = 1, 2, 3. \tag{B.3}$$

Define for $j = 1, 2, 3$ the quantities

$$D_3^j(x) := \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1, k^2) \sum_{k^3=0}^{[\Lambda_3(k^1, k^2)]} e^{ik^{(3)}x^{(3)}},$$

$$\tilde{D}_2^j(x) := \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1, k^2) e^{ik^{(2)}x^{(2)}},$$

$$G_3^j(x) := \frac{1}{e^{ix^3} - 1} \left(e^{i(n_3+1)x^3} \tilde{D}_2^j(x^{(2)} - m^{(2)}x^3) - \tilde{D}_2^j(x^{(2)}) \right),$$

$$F_3^j(x) := \frac{e^{i(n_3+1)x^3}}{e^{ix^3} - 1} \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1, k^2) e^{ik^{(2)}(x^{(2)}-m^{(2)}x^3)} \left(e^{-i\left\langle \Lambda_3(k^{(2)}) \right\rangle x^3} - 1 \right),$$

$$\tag{B.4}$$

where $m^{(2)} = (m^1, m^2)$ is defined in Equation (B.3). We shall prove the following bound.

Lemma 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 $j = 1, 2, 3$*

$$\int\limits_{[0,2\pi]^3} \left| D_3^j(x^{(3)}) \right| \, \mathrm{d}x^{(3)}$$

$$\lesssim (\log R + \log Q) \int\limits_{[0,2\pi]^2} \left| \tilde{D}_2^j(x^{(2)}) \right| \, \mathrm{d}x^{(2)} + 1 + \int\limits_0^{2\pi} \left| \sum_{\tau=0}^{h} t_j \left(k_0^{(2)} + \tau \kappa^{(2)} \right) e^{i\tau |\kappa^{(2)}| x^1} \right| \, \mathrm{d}x^1.$$

As a first step, consider the case where both $\alpha_1 = \alpha_2 = 0$ in Equation (B.3). Then the k^3-sum and x^3-integral in Lemma B.3 factors out. Using [23, 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 B.8, but only then.)

A simple calculation shows that [23, Lemma 3.1]

$$D_3^j(x) = G_3^j(x) + F_3^j(x), \quad j = 1, 2, 3. \tag{B.5}$$

By a straightforward modification of the argument in [23, Lemma 3.3] (including the factor t_j) we have

Lemma B.4 *([23, Lemma 3.3]). For any $j = 1, 2, 3$ we have*

$$\int\limits_{[0,2\pi]^3} \left| G_3^j(x) \right| \, \mathrm{d}x \lesssim \log R \int\limits_{[0,2\pi]^2} \left| \tilde{D}_2^j(x^{(2)}) \right| \, \mathrm{d}x^{(2)}.$$

We thus want to bound the integral of F_3^j. Again, by a straightforward modification of the argument in [23, Lemma 3.7] (including the factor t_j) we have

Lemma B.5 *([23, Lemma 3.7]). For any $j = 1, 2, 3$ we have*

$$\int\limits_{[0,2\pi]^3} \left| F_3^j(x) \right| \, \mathrm{d}x$$

$$\lesssim \sum_{r=1}^{\infty} \frac{(2\pi)^r}{r!} \int\limits_{[0,2\pi]^2} \left| \sum_{k^1 = [\lambda_1]}^{[\Lambda_1]} \sum_{k^2 = [\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1, k^2) e^{ik^{(2)} x^{(2)}} \left\langle \Lambda_3(k^{(2)}) \right\rangle^r \right| \, \mathrm{d}x^{(2)}.$$

To bound the right hand side of Lemma B.5 we bound either definition of $\langle \cdot \rangle$ by the fractional part $\{\cdot\}$. This follows the strategy in [23]. In analogy with [23, Lemma 3.6] we have

Lemma B.6 *([23, Lemma 3.6]). For either definition of $\langle \cdot \rangle$ we have the bound*

$$\int\limits_{[0,2\pi]^2} \left| \sum_{k^1 = [\lambda_1]}^{[\Lambda_1]} \sum_{k^2 = [\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1, k^2) e^{ik^{(2)} x^{(2)}} \left\langle \Lambda_3(k^{(2)}) \right\rangle^r \right| \, \mathrm{d}x^{(2)}$$

$$\leq \int_{[0,2\pi]^2} \left| \tilde{D}_2^j(x^{(2)}) \right| \, dx^{(2)}$$

$$+ \sum_{\nu=1}^r \binom{r}{\nu} \int_{[0,2\pi]^2} \left| \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} \{\Lambda_3(k^{(2)})\}^\nu \right| \, dx^{(2)}$$

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

$$\sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} \left\langle \Lambda_3(k^{(2)}) \right\rangle^r$$

$$= \sum_{\nu=0}^r (-1)^{r-\nu} \binom{r}{\nu} \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} \{\Lambda_3(k^{(2)})\}^\nu$$

$$= (-1)^r \tilde{D}_2^j(x^{(2)}) + \sum_{\nu=1}^r (-1)^{r-\nu} \binom{r}{\nu} \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} \{\Lambda_3(k^{(2)})\}^\nu. \quad \square$$

We now bound the second summand of Lemma B.6 similarly to [23, 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 (B.3). By Dirichlet's approximation theorem we may for any Q_∞ find integers p, q with $1 \leq q \leq Q_\infty$ 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

$$\tilde{\Lambda}_3(k^{(2)}) = \Lambda_3(k^{(2)}) - \gamma_3 = \frac{p}{q} - \frac{Q_1 \alpha_1}{Q_3 \alpha_3} k^1 - \frac{Q_2 \alpha_2}{Q_3 \alpha_3} k^2. \tag{B.6}$$

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) $\{\tilde{\Lambda}_3(k^{(2)})\} \in \{0, \frac{1}{qQ_\infty}, \ldots, \frac{qQ_\infty-1}{qQ_\infty}\}$. Thus, since $|\gamma_3| < \frac{1}{qQ_\infty}$ we have

$$\{\Lambda_3(k^{(2)})\} = \gamma_3 + \{\tilde{\Lambda}_3(k^{(2)})\} + \begin{cases} 1 & \text{if } \gamma_3 < 0 \text{ and } \tilde{\Lambda}_3(k^{(2)}) \in \mathbb{Z}, \\ 0 & \text{otherwise.} \end{cases} \tag{B.7}$$

We claim that

Lemma B.7. *For N sufficiently large, we have uniformly in (integer) $r \geq 1$ that*

$$\int\limits_{[0,2\pi]^2} \left| \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} \{\Lambda_3(k^{(2)})\}^r \right| dx^{(2)}$$

$$\lesssim \log(rQ) \int\limits_{[0,2\pi]^2} \left| \tilde{D}_2^j(x^{(2)}) \right| dx^{(2)}$$

$$+ \int\limits_{[0,2\pi]^2} \left| \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{\substack{k^2=[\lambda_2(k^1)] \\ \tilde{\Lambda}_3(k^1,k^2)\in\mathbb{Z}}}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} \right| dx^{(2)} + 2^r$$

The proof differs from that of [23, Lemmas 3.8 and 3.9] in a few key location, so we give it here.

Proof. Using Equation (B.7) we have

$$\sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} \{\Lambda_3(k^{(2)})\}^r$$

$$= \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} \left(\gamma_3 + \{\tilde{\Lambda}_3(k^{(2)})\} \right)^r$$

$$+ \chi_{(\gamma_3<0)} \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{\substack{k^2=[\lambda_2(k^1)] \\ \tilde{\Lambda}_3(k^1,k^2)\in\mathbb{Z}}}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} + \text{mixed terms}.$$

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 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

$$\sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} \{\Lambda_3(k^{(2)})\}^r$$

$$= \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} \sum_{k^2=[\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1,k^2) e^{ik^{(2)}x^{(2)}} \{\tilde{\Lambda}_3(k^{(2)})\}^r \tag{B.8}$$

$$+ \chi_{(\gamma_3 < 0)} \sum_{\substack{k^1 = [\lambda_1]}}^{[\Lambda_1]} \sum_{\substack{k^2 = [\lambda_2(k^1)] \\ \tilde{\Lambda}_3(k^1, k^2) \in \mathbb{Z}}}^{[\Lambda_2(k^1)]} t_j(k^1, k^2) e^{ik^{(2)}x^{(2)}} + O(2^r),$$

where the error is $O(2^r)$ uniform in $x^{(2)}$. For the first summand we have by a simple modification of [23, Lemma 3.8] (including the factor t_j) that

$$\int\limits_{[0,2\pi]^2} \left| \sum_{k^1 = [\lambda_1]}^{[\Lambda_1]} \sum_{k^2 = [\lambda_2(k^1)]}^{[\Lambda_2(k^1)]} t_j(k^1, k^2) e^{ik^{(2)}x^{(2)}} \{\tilde{\Lambda}_3(k^{(2)})\}^r \right| \, dx^{(2)}$$

$$\lesssim \log(rqQ_\infty) \int\limits_{[0,2\pi]^2} \left| D_2^j(x^{(2)}) \right| \, dx^{(2)}.$$

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 one 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 [23, 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 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 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

$$\int\limits_{[0,2\pi]^2} \left| \sum_{\substack{k^1 = [\lambda_1]}}^{[\Lambda_1]} \sum_{\substack{k^2 = [\lambda_2(k^1)] \\ \tilde{\Lambda}_3(k^1, k^2) \in \mathbb{Z}}}^{[\Lambda_2(k^1)]} t_j(k^1, k^2) e^{ik^{(2)}x^{(2)}} \right| \, dx^{(2)} \lesssim \int\limits_0^{2\pi} \left| \sum_{\tau=0}^{h} t_j \left(k_0^{(2)} + \tau\kappa^{(2)} \right) e^{i\tau|\kappa^{(2)}|x} \right| \, dx.$$

$$(B.9)$$

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 (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 $|\alpha_j| \le C\sqrt{Q}$.) 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 $i \ne j$. (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 $\alpha_{12} \ne 0$ 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 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

$$\delta\tilde{\Lambda}_3(\kappa) := \tilde{\Lambda}_3(k_0^{(2)} + \kappa) - \tilde{\Lambda}_3(k_0^{(2)}) = \frac{-Q_1\alpha_1\kappa^1 - Q_2\alpha_2\kappa^2}{Q_3\alpha_3}. \tag{B.10}$$

Suppose first that either $\alpha_1 = 0$ or $\alpha_2 = 0$, say $\alpha_2 = 0$. Now, $Q_1 \ne Q_3$ and $|\alpha_j| \le C\sqrt{Q}$ 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 $\alpha_1 \ne 0$, $\alpha_2 \ne 0$. Varying $\kappa \in \mathbb{Z}^2$ we have by Bézout's lemma that the numerator in Equation (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 $\alpha_{12} \ge 1$ 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

$$\Gamma = \{a\kappa_1 + b\kappa_0 : a, b \in \mathbb{Z}\}, \qquad \tilde{\Lambda}_3(k_0^{(2)} + a\kappa_1 + b\kappa_0) = \tilde{\Lambda}_3(k_0^{(2)}) + a\alpha_{12}, \quad a, b \in \mathbb{Z}. \tag{B.11}$$

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 (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

$$I_0 = \{k_0^{(2)} + \tau\kappa_2 : \tau \in \{0, \ldots, h\}\}, \qquad \text{for some } h \in \mathbb{Z}, h \geq 0. \tag{B.12}$$

(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 (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 (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 (B.12)

$$\int\limits_{[0,2\pi]^2} \left| \sum_{k \in I_0} t_j(k^1, k^2) e^{ik^{(2)} x^{(2)}} \right| \mathrm{d}x^{(2)} \le \int\limits_{S_0} \left| \sum_{\tau=0}^{h} t_j \left(k_0^{(2)} + \tau \kappa^{(2)} \right) e^{i\tau\kappa^{(2)} x^{(2)}} \right| \mathrm{d}x^{(2)}.$$

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

$$\int\limits_{S_0} \left| \sum_{\tau=0}^{h} t_j \left(k_0^{(2)} + \tau \kappa^{(2)} \right) e^{i\tau\kappa^{(2)} x^{(2)}} \right| \mathrm{d}x^{(2)} = 32\pi \int\limits_0^{2\pi} \left| \sum_{\tau=0}^{h} t_j \left(k_0^{(2)} + \tau \kappa^{(2)} \right) e^{i\tau |\kappa^{(2)}| x} \right| \mathrm{d}x.$$

This concludes the proof. $\square$

Combining Lemmas B.5, B.6, B.7 and B.8 the r- and ν-sums in Lemmas B.5 and B.6 are readily bounded because of the factor $1/r!$ from Lemma B.5. We conclude that

$$\int\limits_{[0,2\pi]^3} \left| F_3^j(x) \right| \mathrm{d}x \lesssim \log Q \int\limits_{[0,2\pi]^2} \left| \tilde{D}_2^j(x) \right| \mathrm{d}x + 1 + \int\limits_0^{2\pi} \left| \sum_{\tau=0}^{h} t_j \left(k_0^{(2)} + \tau \kappa^{(2)} \right) e^{i\tau |\kappa^{(2)}| x^1} \right| \mathrm{d}x^1,$$

where $k_0^{(2)}$ and $\kappa^{(2)}$ are as in Lemma B.8. If the set I_0 from Lemma 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 B.4 and Equation (B.5) we prove the desired bound, Lemma B.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 Appendix B.2. We sketch the main differences.

As we did in Appendix 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 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 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 $k^1 \leq \lambda_1$ as in Remark 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

$$D_2^j(x) := \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} t_j(k^1) \sum_{k^2=0}^{[\Lambda_2(k^1)]} e^{ik^{(2)}x^{(2)}},$$

$$\tilde{D}_1^j(x) := \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} t_j(k^1) e^{ik^1 x^1},$$

$$G_2^j(x) := \frac{1}{e^{ix^2}-1}\left(e^{i(n_2+1)x^2}\tilde{D}_1^j(x^1-m_1x^2) - \tilde{D}_1^j(x^1)\right),$$

$$F_2^j(x) := \frac{e^{i(n_2+1)x^2}}{e^{ix^2}-1} \sum_{k^1=[\lambda_1]}^{[\Lambda_1]} t_j(k^1) e^{ik^1(x^1-m_1x^2)}\left(e^{-i\langle\Lambda_2(k^1)\rangle x^2}-1\right).$$

We claim the following inductive bound.

Lemma 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

$$\frac{p_1^1-p_2^1}{Q_2}k^1 + \frac{p_2^2-p_1^2}{Q_1}k^2 = \mathrm{const}.$$

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 [23, Lemma 3.2] we have that

$$\int\limits_{[0,2\pi]^2} \left| D_2^j(x^{(2)}) \right| \, \mathrm{d}x^{(2)} \le C \log R \int\limits_0^{2\pi} \left| \tilde{D}_1^j(x^1) \right| \, \mathrm{d}x^1.$$

Hence, this case yields the desired inductive bound, Lemma B.10. Suppose then $\alpha_1, \alpha_2 \ne 0$.

Then

$$\Lambda_2(k^1) = n_2 - m_1 k^1 = n_2 - \frac{Q_1 \alpha_1}{Q_2 \alpha_2} k^1, \qquad n_2 \notin \mathbb{Q}, \qquad |\alpha_j| \le C Q^{1/4}, \quad j = 1, 2.$$

Lemmas B.4, B.5 and B.6 are readily adapted and proven as before. The adaptation of Lemma B.7 is then mostly analogous. One chooses $Q_\infty = Q_2 \alpha_2$ and finds the rational approximation of Λ_2 as

$$\tilde{\Lambda}_2(k^1) = \Lambda_2(k^1) - \gamma_2 = \frac{p}{q} - \frac{Q_1 \alpha_1}{Q_2 \alpha_2} k^1, \qquad |\gamma_2| < \frac{1}{q Q_\infty} \le Q^{-1}.$$

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.

$$\left| \sum_{\substack{k^1 = [\lambda_1] \\ \tilde{\Lambda}_2(k^1) \in \mathbb{Z}}}^{[\Lambda_1]} t_j(k^1) e^{ik^1 x^1} \right| \le \begin{cases} R & j = 1 \\ R^2 & j = 2 \end{cases}$$

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 $|\alpha_1| \le C Q^{1/4} \ll Q_2$, 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. □

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 B.3 and B.10. For $\tilde{D}_1^j$ we may assume that the lower bound of the summations is at 0 by the same procedure as in Appendix 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,

$$t_2 \left(k_0^{(2)} + \tau \kappa \right) = (k_0^1)^2 + 2 k_0^1 \kappa^1 \tau + (\kappa^1)^2 \tau^2.$$

Thus, bounding both the integrals amounts to bounding the following:

Lemma B.11. *Let $M \ge 2$ 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) $\displaystyle\int_0^{2\pi} \left| \sum_{k=0}^{M} k e^{ikx} \right| \, \mathrm{d}x \leq C M \log M,$

(3) $\displaystyle\int_0^{2\pi} \left| \sum_{k=0}^{M} k^2 e^{ikx} \right| \, \mathrm{d}x \leq C M^2 \log M.$

Proof. The bound (1) is elementary, see also [23, Lemma 3.2]. For any $M \in \mathbb{N}$ and $q \in \mathbb{C} \setminus \{1\}$ we have

$$\sum_{k=0}^{M} q^k = \frac{q^{M+1} - 1}{q - 1}$$

$$\sum_{k=0}^{M} k q^k = \frac{q}{(q-1)^2} \left[q^M (Mq - M - 1) + 1 \right] \tag{B.13}$$

$$\sum_{k=0}^{M} k^2 q^k = \frac{q}{(q-1)^3} \left[q^M \left(M^2 (q-1)^2 - 2M(q-1) + q + 1 \right) - q - 1 \right].$$

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 to whether $x \leq 1/M$ or $x \geq 1/M$. For $x \leq 1/M$ we have

$$\int_0^{1/M} \left| \sum_{k=0}^{M} k e^{ikx} \right| \, \mathrm{d}x \lesssim \int_0^{1/M} M^2 \, \mathrm{d}x \lesssim M,$$

$$\int_0^{1/M} \left| \sum_{k=0}^{M} k^2 e^{ikx} \right| \, \mathrm{d}x \lesssim \int_0^{1/M} M^3 \, \mathrm{d}x \lesssim M^2.$$

For $x \geq 1/M$ we use Equation (B.13) and note that $\left| e^{ix} - 1 \right| \geq cx$ for $x \leq \pi$. Expanding the exponentials $e^{ix} = 1 + O(x)$ we thus have

$$\int_{1/N}^{\pi} \left| \sum_{k=0}^{M} k e^{ikx} \right| \, \mathrm{d}x \lesssim \int_{1/M}^{\pi} \frac{1}{x^2} \left[M e^{iMx} (e^{ix} - 1) + 1 - e^{iMx} \right] \, \mathrm{d}x$$

$$\lesssim \int_{1/M}^{\pi} \left(\frac{M}{x} + \frac{1}{x^2} \right) \, \mathrm{d}x \lesssim M \log M$$

and

$$\int\limits_{1/N}^{\pi} \left| \sum_{k=0}^{M} k^2 e^{ikx} \right| \mathrm{d}x \lesssim \int\limits_{1/M}^{\pi} \frac{1}{x^3} \left[e^{iMx} \left(M^2 (e^{ix}-1)^2 - 2M(e^{ix}-1) + e^{ix} + 1 \right) - e^{ix} - 1 \right] \mathrm{d}x$$

$$\lesssim \int\limits_{1/M}^{\pi} \left(\frac{M^2}{x} + \frac{M}{x^2} + \frac{1}{x^3} \right) \mathrm{d}x \lesssim M^2 \log M.$$

This concludes the proof. $\quad\square$

With this we may thus bound for ($j = 2$, say)

$$\int\limits_{0}^{2\pi} \left| \sum_{\tau=0}^{h} t_2 \left(k_0^{(2)} + \tau\kappa \right) e^{i\tau|\kappa|x} \right| \mathrm{d}x$$

$$= \int\limits_{0}^{2\pi} \left| \sum_{\tau=0}^{h} \left((k_0^1)^2 + 2k_0^1 \kappa^1 \tau + (\kappa^1)^2 \tau^2 \right) e^{i\tau|\kappa|x} \right| \mathrm{d}x$$

$$\leq CR^2 \int\limits_{0}^{2\pi} \left| \sum_{\tau=0}^{h} e^{i\tau|\kappa|x} \right| \mathrm{d}x + CR|\kappa| \int\limits_{0}^{2\pi} \left| \sum_{\tau=0}^{h} \tau e^{i\tau|\kappa|x} \right| \mathrm{d}x + C|\kappa|^2 \int\limits_{0}^{2\pi} \left| \sum_{\tau=0}^{h} \tau^2 e^{i\tau|\kappa|x} \right| \mathrm{d}x.$$

Substituting $y = |\kappa|x$, using Lemma B.11 and recalling that $h|\kappa| \lesssim R$ and $|\kappa| \geq 1$ by Lemma B.8 we may bound this by $R^2 \log R$. An analogous bound holds for $j = 1$. This takes care of all the one-dimensional integrals. In combination with Lemmas B.3 and B.10 we get the bounds for $j = 1, 2$ of Equation (B.2). It remains to consider the two-dimensional integral for $j = 3$.

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 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 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 Appendix B.1 we may assume that the k^2-sum also starts at 0. That is, we need to evaluate the integral

$$\iint\limits_{[0,2\pi]^2} \left| \sum_{k=0}^{[\Lambda_1]} \sum_{\ell=0}^{[\Lambda_2(k)]} k\ell e^{ikx} e^{i\ell y} \right| \mathrm{d}x \, \mathrm{d}y,$$

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 Appendices B.2, B.3 and B.4. It is sufficiently different that we find it easier to do the arguments separately. We shall show the following.

Lemma B.12. *We have the following bound*

$$\iint\limits_{[0,2\pi]^2} \left| \sum_{k=0}^{[\Lambda_1]} \sum_{\ell=0}^{[\Lambda_2(k)]} k\ell e^{ikx} e^{i\ell y} \right| \, \mathrm{d}x \, \mathrm{d}y \leq CR^2 (\log R)^2 \log Q.$$

Combining then Lemmas B.3, B.10, B.11 and B.12 and choosing Q some sufficiently large power of N as required in Definition 2.7 we conclude the proof of Equation (B.2) and thus of Lemma 4.9. It remains to give the proof of Lemma 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 $m_1 \geq 0$. If $m_1 = 0$ the sum factors, and so does the integral into two one-dimensional sums/integrals. These may be bounded using Lemma B.11. In this case we get the bound $\leq CR^2(\log R)^2$ 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,

$$\sum_{k=0}^{M} \sum_{\ell=0}^{[\Lambda_2(k)]} = \sum_{k=0}^{M} \sum_{\ell=0}^{[n_2-m_1 M]} + \sum_{k=0}^{M} \sum_{\ell=[n_2-m_1 M]+1}^{[\Lambda_2(k)]} .$$

The first sum factors into one-dimensional integrals which we may bound using Lemma B.11 again. The second we may shift by a constant ℓ (again then using Lemma 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

$$\iint\limits_{[0,2\pi]^2} \left| \sum_{k=0}^{M} \sum_{\ell=0}^{[\Lambda(k)]} k\ell e^{ikx} e^{i\ell y} \right| \, \mathrm{d}x \, \mathrm{d}y,$$

where

$$\Lambda(k) = n - mk, \qquad M \leq R, \qquad mM = n + O(1), \qquad n \leq R.$$

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 (B.13). Recall that $[\Lambda(k)] = \Lambda(k) - \langle \Lambda(k) \rangle$. We thus have

$$\sum_{\ell=0}^{[\Lambda(k)]} \ell e^{i\ell y} = \frac{e^{iy}}{(e^{iy}-1)^2}\left[e^{i[\Lambda(k)]y}([\Lambda(k)]e^{iy}-[\Lambda(k)]-1)+1\right]$$

$$= \frac{e^{iy}}{(e^{iy}-1)^2}\left[\left(e^{i\Lambda(k)y}(\Lambda(k)e^{iy}-\Lambda(k)-1)+1\right)\right.$$

$$+ \left(e^{-i\langle\Lambda(k)\rangle y}-1\right)\left(e^{i\Lambda(k)y}(\Lambda(k)e^{iy}-\Lambda(k)-1)+1\right)$$

$$\left. - \left(\langle\Lambda(k)\rangle e^{i(\Lambda(k)-\langle\Lambda(k)\rangle)y}(e^{iy}-1)+(e^{-i\langle\Lambda(k)\rangle y}-1)\right)\right]$$

$$=: (\mathrm{I}) + (\mathrm{II}) + (\mathrm{III}).$$

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

$$\int_{-\pi}^{\pi} dx \int_0^{1/n} dy \frac{1}{y^2}\left|\sum_{k=0}^M ke^{ikx}\left[\langle\Lambda(k)\rangle\left(e^{i[\Lambda(k)]y}-1\right)y + O(y^2)\right]\right| \lesssim \frac{1}{n}M^2 n + \frac{1}{n}M^2 \lesssim R^2.$$

For $y \geq 1/n$ we bound $e^{i[\Lambda(k)]y} - 1 = O(1)$. We get

$$\int_{-\pi}^{\pi} dx \int_{1/n}^{\pi} dy \frac{1}{y^2}\left|\sum_{k=0}^M ke^{ikx}\left[\langle\Lambda(k)\rangle\left(e^{i[\Lambda(k)]y}-1\right)y + O(y^2)\right]\right|$$

$$\lesssim (\log n)M^2 + M^2 \lesssim R^2 \log R.$$

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

$$\frac{e^{iy}}{(e^{iy}-1)^2}\left(e^{-i\langle\Lambda(k)\rangle y}-1\right)\left(e^{i\Lambda(k)y}(\Lambda(k)e^{iy}-\Lambda(k)-1)+1\right) = O(\Lambda(k)^2 y) = O(n).$$

Hence this contributes the term

$$\int_{-\pi}^{\pi} dx \int_0^{1/n} dy\left|\sum_{k=0}^M ke^{ikx}O(\Lambda(k)^2 y)\right| \lesssim \frac{1}{n}M^2 n \lesssim R^2.$$

For $y \geq 1/n$ we write

$$\frac{e^{iy}}{(e^{iy}-1)^2}\left(e^{-i\langle\Lambda(k)\rangle y}-1\right)\left(e^{i\Lambda(k)y}(\Lambda(k)e^{iy}-\Lambda(k)-1)+1\right)$$

$$=\frac{e^{iy}}{(e^{iy}-1)^2}\sum_{\nu=1}^{\infty}\frac{(-iy)^{\nu}}{\nu!}\langle\Lambda(k)\rangle^{\nu}\left(e^{i\Lambda(k)y}(\Lambda(k)e^{iy}-\Lambda(k)-1)+1\right).$$

Again we bound the factor $\frac{e^{iy}}{(e^{iy}-1)^2}$ as $1/y^2$. We treat each summand similarly as in Lemmas B.6 and B.7 (or rather, the 2-dimensional version of these as used in Appendix B.3). Completely analogously to Lemma B.6 we see that for any integer $r \geq 1$ we have

$$\iint\left|\sum_{k=0}^{M}ke^{ikx}\frac{e^{i\Lambda(k)y}(\Lambda(k)e^{iy}-\Lambda(k)-1)+1}{y^2}\langle\Lambda(k)\rangle^{r}\right|\,\mathrm{d}x\,\mathrm{d}y$$

$$\leq\iint\left|\sum_{k=0}^{M}ke^{ikx}\frac{e^{i\Lambda(k)y}(\Lambda(k)e^{iy}-\Lambda(k)-1)+1}{y^2}\right|\,\mathrm{d}x\,\mathrm{d}y$$

$$+\sum_{\nu=1}^{r}\binom{r}{\nu}\iint\left|\sum_{k=0}^{M}ke^{ikx}\frac{e^{i\Lambda(k)y}(\Lambda(k)e^{iy}-\Lambda(k)-1)+1}{y^2}\{\Lambda(k)\}^{\nu}\right|\,\mathrm{d}x\,\mathrm{d}y,$$

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 B.7 is analogous to its use in Appendix 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 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.

$$\iint\left|\sum_{k}ke^{ikx}(\mathrm{II})\right|\,\mathrm{d}x\,\mathrm{d}y\lesssim\log Q\iint\left|\sum_{k}ke^{ikx}(\mathrm{I})\right|\,\mathrm{d}x\,\mathrm{d}y+R^2\log R.$$
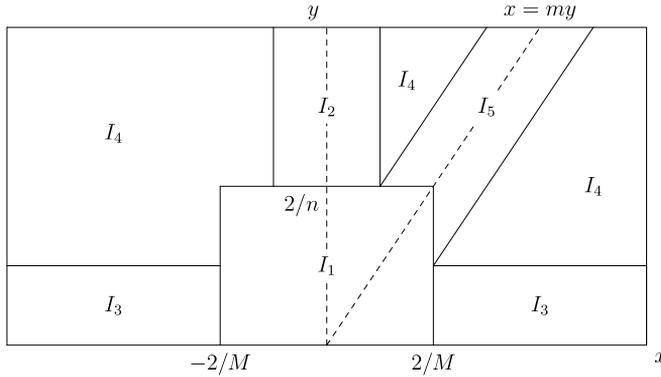
In particular

Fig. B.1. Decomposition of the domain $[-\pi, \pi] \times [0, \pi]$ into different regions.

$$
\iint\limits_{[0,2\pi]^2} \left| \sum_{k=0}^{M} \sum_{\ell=0}^{[\Lambda(k)]} k\ell e^{ikx} e^{i\ell y} \right| \mathrm{d}x\,\mathrm{d}y
$$

$$
\lesssim \log Q \int\limits_{-\pi}^{\pi} \mathrm{d}x \int\limits_{0}^{\pi} \mathrm{d}y \left| \sum_{k=0}^{M} k e^{ikx} \frac{e^{i\Lambda(k)y}(\Lambda(k)e^{iy} - \Lambda(k) - 1) + 1}{y^2} \right| + R^2 \log R. \tag{B.14}
$$

In order to evaluate the integral on the right-hand side, we split the integration domain into 5 regions, see Fig. B.1.

$$I_1 = \{|x| \leq 2/M, y \leq 2/n\}, \qquad I_2 = \{|x| \leq 1/M, y \geq 2/n\},$$
$$I_3 = \{y \leq 1/n, |x| \geq 2/M\}, \qquad I_4 = \{y \geq 1/n, |x| \geq 1/M, |x - my| \geq 1/M\},$$
$$I_5 = \{|x - my| \leq 1/M, (x, y) \notin I_1\}.$$

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

$$
(*) := \sum_{k=0}^{M} k e^{ikx} \frac{e^{i\Lambda(k)y}(\Lambda(k)e^{iy} - \Lambda(k) - 1) + 1}{y^2}
$$

(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

$$
I_1 \lesssim \int\limits_{-2/M}^{2/M} \mathrm{d}x \int\limits_{0}^{2/n} \mathrm{d}y M^2 n^2 \lesssim Mn \lesssim R^2.
$$

(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

$$
\begin{aligned}
(*) &= \frac{1}{y^2} \sum_{k=0}^{M} k e^{ikx} (e^{i\Lambda(k)y} (\Lambda(k) e^{iy} - \Lambda(k) - 1) + 1) \\
&= \frac{1}{y^2} \sum_{k=0}^{M} \left(k e^{ikx} + k e^{ik(x-my)} e^{iny} (n e^{iy} - n - 1) + k^2 e^{ik(x-my)} e^{iny} (m - m e^{iy}) \right) \\
&= \frac{1}{y^2} \left(-i\partial D(x) - i e^{iny} (n e^{iy} - n - 1) \partial D(x - my) + m e^{iny} (e^{iy} - 1) \partial^2 D(x - my) \right),
\end{aligned}
\tag{B.15}
$$

where we introduced $D(z) = \sum_{k=0}^{M} e^{ikz} = \frac{e^{i(M+1)z} - 1}{e^{iz} - 1}$. From Equation (B.13) we conclude that we may bound derivatives of D as

$$
|\partial D(z)| \lesssim \frac{M}{z} + \frac{1}{z^2}, \quad |\partial^2 D(z)| \lesssim \frac{M^2}{z} + \frac{M}{z^2} + \frac{1}{z^3}, \quad |\partial^3 D(z)| \lesssim \frac{M^3}{z} + \ldots + \frac{1}{z^4}. \tag{B.16}
$$

(I_3). We have $y \leq 1/n$ and $|x| \geq 2/M$. We expand Equation (B.15) to second order in y. Expanding first the exponentials and then derivatives of D where needed we get

$$
\begin{aligned}
\text{(B.15)} &= \frac{1}{y^2} \Big(-i\partial D(x) + i\partial D(x - my) + imy \partial^2 D(x - my) \\
&\quad + O(n^2 y^2 \partial D(x - my)) + O(nmy^2 \partial^2 D(x - my)) \Big) \\
&\lesssim n^2 \sup_y |\partial D(x - my)| + nm \sup_y |\partial^2 D(x - my)| + m^2 \sup_y |\partial^3 D(x - my)|.
\end{aligned}
$$

Now we use the bounds Equation (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

$$
|\text{(B.15)}| \leq \frac{|\partial D(x)|}{y^2} + \frac{n|\partial D(x - my)|}{y} + \frac{|\partial D(x - my)|}{y^2} + \frac{m|\partial^2 D(x - my)|}{y}.
$$

Using the bounds Equation (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

$$
|\text{(B.15)}| \leq \frac{|\partial D(x)|}{y^2} + \frac{n|\partial D(x - my)|}{y} + \frac{|\partial D(x - my)|}{y^2} + \frac{m|\partial^2 D(x - my)|}{y}.
$$

We use the bounds

$$|\partial D(z)| = \left| \sum_{k=0}^{M} k e^{ikz} \right| \le M^2, \qquad |\partial^2 D(z)| = \left| \sum_{k=0}^{M} k^2 e^{ikz} \right| \le M^3.$$

Thus

$$I_5 \lesssim \frac{1}{M} \int_{1/n}^{\pi} \frac{M^2}{y^2} + \frac{nM^2 + mM^3}{y} \, \mathrm{d}y \lesssim R^2 \log R.$$

We conclude that

$$\int_{-\pi}^{\pi} \mathrm{d}x \int_{0}^{\pi} \mathrm{d}y \left| \sum_{k=0}^{M} k e^{ikx} \frac{e^{i\Lambda(k)y}(\Lambda(k)e^{iy} - \Lambda(k) - 1) + 1}{y^2} \right| \lesssim R^2 (\log R)^2.$$

Together with Equation (B.14) this concludes the proof. □

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