THE FRÖHLICH POLARON AT STRONG COUPLING: PART II — ENERGY-MOMENTUM RELATION AND EFFECTIVE MASS

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ABSTRACT

We study the Fröhlich polaron model in $\mathbf{R}^3$, and prove a lower bound on its ground state energy as a function of the total momentum. The bound is asymptotically sharp at large coupling. In combination with a corresponding upper bound proved earlier (Mitrouskas et al. in Forum Math. Sigma 11:1–52, 2023), it shows that the energy is approximately parabolic below the continuum threshold, and that the polaron's effective mass (defined as the semi-latus rectum of the parabola) is given by the celebrated Landau–Pekar formula. In particular, it diverges as α^4 for large coupling constant α.

1. Introduction and main results

This is the second part of a study of the Fröhlich polaron [5] in the regime of strong coupling between the electron and the phonons, which are the optical modes of a polar crystal. Our goal is to quantify the heuristic picture that the mass of an electron in a polarizable medium effectively increases due to an emerging phonon cloud attached to it. We are going to verify that the energy-momentum relation of a polaron is asymptotically given by the semi-classical formula $\mathrm{E}(\mathrm{P}) - \mathrm{E}(0) = \frac{|\mathrm{P}|^2}{2\alpha^4 m}$, which agrees with the energy-momentum relation of a particle having mass $\alpha^4 m$, where $\alpha^4 m$ is the asymptotic formula conjectured by Landau and Pekar [7] for the mass of a polaron in the regime where the coupling parameter α goes to infinity.

Following the notation of the first part [1], where a second order expansion for the absolute ground state energy of a polaron was verified, we are going to use creation and annihilation operators satisfying the semi-classical rescaled canonical commutation relations $[a(f), a^\dagger(g)] = \alpha^{-2}\langle f|g\rangle$ for $f, g \in \mathrm{L}^2(\mathbf{R}^3)$, in order to introduce the Fröhlich Hamiltonian acting on the Fock space $\mathrm{L}^2(\mathbf{R}^3) \otimes \mathcal{F}(\mathrm{L}^2(\mathbf{R}^3))$ as

$$\mathbf{H} := -\Delta_x - a(w_x) - a^\dagger(w_x) + \mathcal{N},$$

where $w_x(x') := \pi^{-\frac{3}{2}}|x' - x|^{-2}$ and the (rescaled) particle number operator $\mathcal{N}$ equals $\mathcal{N} := \sum_{n=1}^\infty a^\dagger(\varphi_n)a(\varphi_n)$ for an orthonormal basis $\{\varphi_n : n \in \mathbf{N}\}$ of $\mathrm{L}^2(\mathbf{R}^3)$. The Fröhlich Hamiltonian $\mathbf{H}$ commutes with the components $(\mathbf{P}_1, \mathbf{P}_2, \mathbf{P}_3)$ of the total momentum operator

$$\mathbf{P} := \frac{1}{i}\nabla + \alpha^2 \int_{\mathbf{R}^3} k\, a_k^\dagger a_k \mathrm{d}k\,,$$

where we use the standard notation $\int_{\mathbf{R}^3} f(k) a_k^\dagger a_k \mathrm{d}k$ as a symbolic expression for the operator $\sum_{n,m=1}^\infty \langle\varphi_n|f(\frac{1}{i}\nabla)|\varphi_m\rangle a^\dagger(\varphi_n)a(\varphi_m)$. Hence we can study their joint spectrum $\sigma(\mathbf{P}, \mathbf{H}) \subseteq \mathbf{R}^4$, and define the ground state energy $\mathrm{E}_\alpha(\mathrm{P})$ of $\mathbf{H}$ at total momentum P

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as $E_\alpha(P) := \inf\{E : (P, E) \in \sigma(\mathbf{P}, \mathbf{H})\}$. Our main result below is the proof of the asymptotic energy-momentum relation

$$(\mathbf{1.1}) \qquad E_\alpha(P) = E_\alpha(0) + \min\left\{\frac{|P|^2}{2\alpha^4 m}, \alpha^{-2}\right\} + O_{\alpha\to\infty}\big(\alpha^{-(2+\epsilon)}\big),$$

where $\epsilon > 0$ is a suitable constant and m is the conjectured constant by Landau and Pekar. In order to provide an explicit expression for m, let us first define the Pekar functional $\mathcal{F}^{\mathrm{Pek}}(\varphi) := \|\varphi\|^2 + \inf \sigma(-\Delta + V_\varphi)$ for $\varphi \in L^2(\mathbf{R}^3)$, where we define the potential $V_\varphi := -2(-\Delta)^{-\frac{1}{2}}\mathfrak{Re}\,\varphi$. If follows from the analysis in [9] that there exists a unique radial minimizer φ^{Pek} of the functional $\mathcal{F}^{\mathrm{Pek}}$. With this minimizer at hand, we can introduce the constant $m := \frac{2}{3}\|\nabla\varphi^{\mathrm{Pek}}\|^2$ in Eq. (1.1).

In order to formulate our main Theorem 1.1, let us further introduce the minimal Pekar energy $e^{\mathrm{Pek}} := \inf_\varphi \mathcal{F}^{\mathrm{Pek}}(\varphi)$ as well as the Hessian H^{Pek} of $\mathcal{F}^{\mathrm{Pek}}$ at the minimizer φ^{Pek} restricted to real-valued functions $\varphi \in L^2_{\mathbf{R}}(\mathbf{R}^3)$, i.e. we define H^{Pek} as the unique self-adjoint operator on $L^2(\mathbf{R}^3)$ satisfying

$$\langle\varphi|H^{\mathrm{Pek}}|\varphi\rangle = \lim_{\epsilon\to 0}\frac{1}{\epsilon^2}\big(\mathcal{F}^{\mathrm{Pek}}\big(\varphi^{\mathrm{Pek}} + \epsilon\varphi\big) - e^{\mathrm{Pek}}\big)$$

for all $\varphi \in L^2_{\mathbf{R}}(\mathbf{R}^3)$. With this notation at hand, we can state our main new result in Theorem 1.1. It provides a sharp asymptotic lower bound on the ground state energy $E_\alpha(P)$ of the operator $\mathbf{H}$ as a function of the total momentum $\mathbf{P}$.

Theorem **1.1.** — *There exists a constant* $\epsilon > 0$ *such that*

$$(\mathbf{1.2}) \qquad E_\alpha(P) \geq e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\Big[1 - \sqrt{H^{\mathrm{Pek}}}\Big] + \min\left\{\frac{|P|^2}{2\alpha^4 m}, \alpha^{-2}\right\} - \alpha^{-(2+\epsilon)}$$

for all $P \in \mathbf{R}^3$ *and for all* $\alpha \geq \alpha_0$, *where* α_0 *is a suitable constant.*

That the lower bound in Eq. (1.2) is indeed sharp follows from the corresponding asymptotic upper bound established in [10], given by

$$(\mathbf{1.3}) \qquad E_\alpha(P) \leq e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\Big[1 - \sqrt{H^{\mathrm{Pek}}}\Big] + \min\left\{\frac{|P|^2}{2\alpha^4 m}, \alpha^{-2}\right\} + C_\kappa\alpha^{-\frac{5}{2}+\kappa},$$

where $\kappa > 0$ is arbitrary and C_κ a suitable constant. In combination with Eq. (1.2) this shows that

$$E_\alpha(P) = e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\Big[1 - \sqrt{H^{\mathrm{Pek}}}\Big] + \min\left\{\frac{|P|^2}{2\alpha^4 m}, \alpha^{-2}\right\} + O_{\alpha\to\infty}\big(\alpha^{-(2+\epsilon)}\big)$$

for all $P \in \mathbf{R}^3$, which in particular proves Eq. (1.1). Note that α^{-2} corresponds to the continuum threshold; i.e., $\sigma(\mathbf{P}, \mathbf{H}) \supset \mathbf{R}^3 \times [E_\alpha(0) + \alpha^{-2}, \infty)$, the latter corresponding to states describing free phonons on top of the polaron ground state [6, 11].

In particular, $E_\alpha(P)$ has an approximate parabolic shape below the continuum threshold, i.e., for $|P| < \sqrt{2m}\alpha$. The Landau–Pekar formula for the effective mass appears in the limit $\alpha \to \infty$ as the semi-latus rectum of the parabola, in the sense that for any $0 < |P| < \sqrt{2m}$

$$m = \lim_{\alpha \to \infty} \alpha^{-4} \frac{|\alpha P|^2}{2(E_\alpha(\alpha P) - E_\alpha(0))}. \tag{1.4}$$

It is common the define the polaron's effective mass for fixed α as

$$M_{\text{eff}}(\alpha) := \lim_{P \to 0} \frac{|P|^2}{2(E_\alpha(P) - E_\alpha(0))}.$$

The quantity on the right hand side of Eq. (1.4) is clearly related to the large α limit of $\alpha^{-4} M_{\text{eff}}(\alpha)$, with the difference being that the limit $P \to 0$ is taken before the limit $\alpha \to \infty$. While it is not clear at this point how to obtain the lower bound $\lim_{\alpha\to\infty} \alpha^{-4} M_{\text{eff}}(\alpha) \geq m$, we can make use of the inequality $E_\alpha(P) \leq E_\alpha(0) + \frac{|P|^2}{2M_{\text{eff}}(\alpha)}$ recently proved in [14] in order to verify the upper bound $\lim_{\alpha\to\infty} \alpha^{-4} M_{\text{eff}}(\alpha) \leq m$. In fact, by applying Eq. (1.1) in the special case of P satisfying $|P| = \sqrt{2m}\alpha$ we have

$$E_\alpha(0) + \frac{1}{\alpha^2} + O_{\alpha\to\infty}\left(\alpha^{-(2+\epsilon)}\right) = E_\alpha(P) \leq E_\alpha(0) + \frac{m\alpha^2}{M_{\text{eff}}(\alpha)},$$

which yields the claimed upper bound on $M_{\text{eff}}(\alpha)$. We formulate it as the subsequent Corollary.

Corollary **1.2.** — *There exists a constant* $\epsilon > 0$ *such that*

$$M_{\text{eff}}(\alpha) \leq \alpha^4 m + O_{\alpha\to\infty}\left(\alpha^{4-\epsilon}\right).$$

The remainder of this paper contains the proof of Theorem 1.1. In order to guide the reader, we start with a short explanation of the main strategy.

Proof strategy of Theorem 1.1. — Since $(P, E_\alpha(P))$ is an element of the joint spectrum of the operator pair $(\mathbf{P}, \mathbf{H})$, there clearly exist states Ψ_α satisfying $\mathbf{P}\Psi_\alpha \approx P\Psi_\alpha$ and $\mathbf{H}\Psi_\alpha \approx E_\alpha(P)\Psi_\alpha$. In order to verify Theorem 1.1, it is therefore enough to show that $\langle \Psi_\alpha | \mathbf{H} | \Psi_\alpha \rangle$ is bounded from below by the right hand side of Eq. (1.2). For this to hold it is crucial to use the additional information $\mathbf{P}\Psi_\alpha \approx P\Psi_\alpha$ on the momentum, since in general $\mathbf{H}$, as an operator, is not bounded from below by the right hand side of Eq. (1.2). It is not possible to transform the constrained minimization problem to a global one by the usual method of Lagrange multipliers, since the operators $\mathbf{P}$ are not bounded relative to $\mathbf{H}$. More precisely, while clearly

$$\mathrm{E}_\alpha(\mathrm{P}) \geq \inf \sigma\left(\mathbf{H} + \lambda(\mathrm{P} - \mathbf{P})\right) \tag{1.5}$$

for any $\lambda \in \mathbf{R}^3$, such a bound is insufficient as the right hand side is $-\infty$ for $\lambda \neq 0$, which follows easily from the fact that $\mathrm{E}_\alpha(\mathrm{P})$ is bounded uniformly in P (compare with Eq. (1.1)).

In order to improve the lower bound in Eq. (1.5), we introduce a wavenumber cut-off Λ in the Hamiltonian $\mathbf{H}$ as well as in the momentum operator $\mathbf{P}$, leading to the study of the ground state energy $\mathrm{E}_{\alpha,\Lambda}(\mathrm{P})$ of the truncated Hamiltonian $\mathbf{H}_\Lambda$ as a function of the truncated momentum $\mathbf{P}_\Lambda$. As we will show in the subsequent Section 2, it is enough to prove Eq. (1.2) for the modified energy $\mathrm{E}_{\alpha,\Lambda}(\mathrm{P})$ in order to verify our main Theorem 1.1. By introducing the cut-off we manually exclude the radiative regime where a single phonon carries the total momentum, which is responsible for the (approximately) flat energy-momentum relation $\mathrm{E}_\alpha(\mathrm{P})$ above the threshold $|\mathrm{P}| = \sqrt{2m}\alpha$ and the resulting collapse of the quadratic approximation $\mathrm{E}_\alpha(\mathrm{P}) - \mathrm{E}_\alpha(0) \approx \frac{|\mathrm{P}|^2}{2\alpha^4 m}$ above this threshold.

In contrast, in the presence of the cut-off, it turns out that we can apply the method of Lagrange multipliers. We shall follow the strategy developed in the first part [1], and construct approximate eigenstates Ψ_α to the joint eigenvalue $(\mathrm{P}, \mathrm{E}_{\alpha,\Lambda}(\mathrm{P}))$ of the operator pair $(\mathbf{P}_\Lambda, \mathbf{H}_\Lambda)$, which in addition satisfy (complete) Bose–Einstein condensation with respect to the minimizer φ^{Pek} of the Pekar functional $\mathcal{F}^{\mathrm{Pek}}$. In this context we call Ψ_α an approximate eigenstate in case

$$\langle \Psi_\alpha \big| (\mathbf{P}_\Lambda - \mathrm{P})^2 \big| \Psi_\alpha \rangle = \mathrm{O}_{\alpha\to\infty}\left(\alpha^{2-r}\right),$$
$$\mathrm{E}_{\alpha,\Lambda}(\mathrm{P}) \geq \langle \Psi_\alpha | \mathbf{H}_\Lambda | \Psi_\alpha \rangle + \mathrm{O}_{\alpha\to\infty}\left(\alpha^{-(2+r)}\right)$$

for some $r > 0$. In order to verify that $\mathrm{E}_{\alpha,\Lambda}(\mathrm{P})$ is bounded from below by the right hand side of Eq. (1.2), it is consequently enough to show that

$$\left\langle \Psi \middle| \mathbf{H}_\Lambda + \lambda(\mathrm{P} - \mathbf{P}_\Lambda) \middle| \Psi \right\rangle \geq e^{\mathrm{Pek}} - \frac{1}{2\alpha^2} \mathrm{Tr}\left[1 - \sqrt{\mathrm{H}^{\mathrm{Pek}}}\right] + \lambda \mathrm{P} - \frac{\alpha^4 m |\lambda|^2}{2} - \alpha^{-(2+\epsilon)} \tag{1.6}$$

for all states Ψ satisfying (complete) Bose–Einstein condensation with respect to the minimizer φ^{Pek}, providing the desired lower bound for the optimal choice $\lambda = \frac{\mathrm{P}}{m\alpha^4}$, with the term $\frac{\alpha^4 m |\lambda|^2}{2}$ in Eq. (1.6) arising naturally as the Legendre transformation of the quadratic approximation $\frac{|\mathrm{P}|^2}{2\alpha^4 m}$.

Since Eq. (1.6) claims a global lower bound, i.e. there is no constraint on the momentum of Ψ, we can utilize the methods developed in the first part [1], where a lower bound on the total minimum $\mathrm{E}_\alpha = \inf \sigma(\mathbf{H})$ was established. The basic idea is that we can find, up to a unitary transformation, a lower bound on the operator $\mathbf{H}_\Lambda + \frac{\mathrm{P}}{m\alpha^4}(\mathrm{P} - \mathbf{P}_\Lambda)$ of the form

$$e^{\mathrm{Pek}} + \frac{|\mathrm{P}|^2}{2\alpha^4 m} + \mathbf{Q}_\Lambda + \mathrm{O}_{\alpha\to\infty}\big(\alpha^{-(2+r)}\big), \tag{1.7}$$

where $\mathbf{Q}_\Lambda$ is a system of harmonic oscillators, which holds when tested against states satisfying (complete) Bose–Einstein condensation. The operator $\mathbf{Q}_\Lambda$ is bounded from below in the presence of a (suitable) wavenumber cut-off Λ and the ground state energy of $\mathbf{Q}_\Lambda$ can be computed explicitly, giving rise to the quantum correction $-\frac{1}{2\alpha^2}\mathrm{Tr}[1 - \sqrt{\mathrm{H}^{\mathrm{Pek}}}\,]$ in Eq. (1.2).

Finally, we note that it would be a natural idea to study the right hand side of the following Eq. (1.8)

$$\mathrm{E}_\alpha(\mathrm{P}) \geq \inf \sigma\left(\mathbf{H} + \frac{\mu}{\alpha^4}(\mathrm{P} - \mathbf{P})^2\right), \tag{1.8}$$

in the limit $\mu \to \infty$, which, in contrast to Eq. (1.5), would be sharp enough to yield the desired lower bound even without a wavenumber cut-off Λ. However, in order to establish a lower bound on $\mathbf{H} + \frac{\mu}{\alpha^4}(\mathrm{P} - \mathbf{P})^2$ of the form

$$e^{\mathrm{Pek}} + \frac{|\mathrm{P}|^2}{2\alpha^4 m} + \mathbf{Q} + \mathrm{O}_{\alpha\to\infty}\big(\alpha^{-(2+r)}\big),$$

where $\mathbf{Q}$ is a semi-bounded system of harmonic oscillators, we believe it is still a necessity to include a wavenumber cut-off Λ. For technical reasons we therefore prefer to work with Eq. (1.5) due to the presence of the (typically) small parameter $\alpha^2\lambda = \frac{|\mathrm{P}|}{m\alpha^2}$ in front of the operator $\frac{1}{\alpha^2}(\mathrm{P} - \mathbf{P})$. □

Outline. The paper is structured as follows. In Section 2 we shall show that it is sufficient to prove Eq. (1.2) for a model including a suitable ultraviolet wavenumber cut-off in order to verify our main Theorem 1.1. In the subsequent Section 3, we will construct approximate eigenstates for the truncated model defined in Section 2, which in addition satisfy (complete) Bose–Einstein condensation with respect to the state φ^{Pek}. Section 4 is then devoted to the proof of our main technical Theorem 2.1, where we use the method of Lagrange multipliers in order to get rid of the momentum constraint. Finally, Appendix A contains auxiliary results on commutator estimates as well as properties of the Pekar minimizer φ^{Pek}, which get used in the proof.

2. Reduction to bounded wavenumbers

In this section we shall introduce the truncated Hamiltonian $\mathbf{H}_\Lambda$, which includes a wavenumber restriction $|k| \leq \Lambda$, and we are going to state our main technical Theorem

2.1, which provides an analogue of Theorem 1.1 for the truncated model. While the proof of Theorem 2.1 is the content of Sections 3 and 4, we will verify in this Section that Theorem 1.1 is a consequence of Theorem 2.1, i.e. we will explain why it is enough to prove Eq. (1.2) for a model including a wavenumber regularization. The quantum nature of our system, and in particular the discrete spectrum $\sigma(\mathcal{N}) = \{0, \frac{1}{\alpha^2}, \frac{2}{\alpha^2}, \dots\}$ of the number operator $\mathcal{N}$, is essential for this argument to work. In contrast, in the classical case the effective mass is infinite since there nothing prevents a priori the wavenumber from escaping to infinity without an energy penalty, and one has to introduce a suitable regularization in order to observe the expected asymptotics $\mathrm{M}_{\mathrm{eff}} = \alpha^4 m + o_{\alpha\to\infty}(\alpha^4)$, see [3].

Before formulating Theorem 2.1, we shall introduce some useful notation. Following [1], we define for a function $f : \mathrm{X} \longrightarrow \mathbf{R}$, $\epsilon \geq 0$ and $-\infty \leq a \leq b \leq \infty$, the function $\chi^\epsilon(a \leq f \leq b) : \mathrm{X} \longrightarrow [0, 1]$ as

$$\chi^\epsilon\big(a \leq f(x) \leq b\big) := \begin{cases} \alpha\big(\frac{f(x)-b}{\epsilon}\big)\beta\big(\frac{f(x)-a}{\epsilon}\big), & \text{for } \epsilon > 0 \\ \mathbf{1}_{[a,b]}(f(x)), & \text{for } \epsilon = 0, \end{cases} \tag{2.1}$$

where $\alpha, \beta : \mathbf{R} \longrightarrow [0, 1]$ are given C^∞ functions such that $\alpha^2 + \beta^2 = 1$, $\mathrm{supp}(\alpha) \subset (-\infty, 1)$ and $\mathrm{supp}(\beta) \subset (-1, \infty)$. Similarly we define the operator

$$\chi^\epsilon(a \leq \mathrm{T} \leq b) := \int \chi^\epsilon(a \leq t \leq b)\mathrm{dE},$$

where T is a self-adjoint operator and E the corresponding spectral measure. Furthermore let us write $\chi(a \leq f \leq b)$ in case $\epsilon = 0$ and $\chi^\epsilon(\cdot \leq b)$, respectively $\chi^\epsilon(a \leq \cdot)$, in case $a = -\infty$ or $b = \infty$, respectively. With this notation at hand, we define the Hamiltonian $\mathbf{H}_\Lambda$ with wavenumber cut-off $\Lambda \geq 0$ as

$$\mathbf{H}_\Lambda := -\Delta_x - a\big(\chi\big(|\nabla| \leq \Lambda\big)w_x\big) - a^\dagger\big(\chi\big(|\nabla| \leq \Lambda\big)w_x\big) + \mathcal{N}. \tag{2.2}$$

Theorem **2.1.** — *Let* $\mathrm{E}_{\alpha,\Lambda}(\mathrm{P})$ *be the ground state energy of the operator* $\mathbf{H}_\Lambda$ *as a function of the (one-component of the) truncated total momentum*

$$\mathbf{P}_\Lambda := \frac{1}{i}\nabla_{x_1} + \alpha^2 \int \chi^1\big(\Lambda^{-1}|k_1| \leq 2\big)k_1\, a_k^\dagger a_k \mathrm{d}k$$

and let $\Lambda = \alpha^{\frac{4}{5}(1+\sigma)}$ *with* $0 < \sigma < \frac{1}{9}$. *Then there exists a constant* $\epsilon > 0$ *such that for all* $\mathrm{C} > 0$, $|\mathrm{P}| \leq \mathrm{C}\alpha$ *and* $\alpha \geq \alpha_0(\sigma, \mathrm{C})$

$$\mathrm{E}_{\alpha,\Lambda}(\mathrm{P}) \geq e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\Big[1 - \sqrt{\mathrm{H}^{\mathrm{Pek}}}\Big] + \frac{|\mathrm{P}|^2}{2\alpha^4 m} - \alpha^{-(2+\epsilon)}, \tag{2.3}$$

where $\alpha_0(\sigma, \mathrm{C})$ *is a suitable constant.*

For technical reasons we use here the smooth cut-off $\chi^1(\Lambda^{-1}|k_1| \leq 2)$ instead of the sharp cut-off $\chi(\Lambda^{-1}|k_1| \leq 1)$ in the definition of the momentum operator $\mathbf{P}_\Lambda$. Note also that the momentum cut-off appears in (2.2) only in the interaction term, and not in the field energy $\mathcal{N}$. In the following we shall argue that, as a consequence of Theorem 2.1, Eq. (2.3) is also valid with $\mathbf{P}_\Lambda$ replaced by

$$\mathbf{P}'_1 := \frac{1}{i}\nabla_{x_1} + \alpha^2 \int_{|k|\leq\Lambda} k_j\, a_k^\dagger a_k \mathrm{d}k$$

having the sharp cut-off, and with H_Λ replaced by the fully restricted Hamiltonian

$$\mathbf{H}'_\Lambda := \mathbf{H}_\Lambda - \int_{|k|>\Lambda} a_k^\dagger a_k \mathrm{d}k.$$

In order to see this, observe that $\mathbf{P}'_1$ and $\mathbf{H}'_\Lambda$ are the restrictions (in the sense of operators) of $\mathbf{P}_\Lambda$ and $\mathbf{H}_\Lambda$ to states of the form $\Psi' \otimes \Omega$, where Ψ' is an element of the space $\mathrm{L}^2(\mathbf{R}^3, \mathcal{F}(\mathrm{ran}\,\chi(|\nabla| \leq \Lambda)))$ and Ω is the vacuum in $\mathcal{F}(\mathrm{ran}\,\chi(|\nabla| > \Lambda))$. Hence

$$\sigma\left(\mathbf{P}'_1, \mathbf{H}'_\Lambda\right) \subseteq \sigma(\mathbf{P}_\Lambda, \mathbf{H}_\Lambda),$$

and therefore we obtain as an immediate consequence of the previous Theorem 2.1 that

$$\mathrm{E} \geq e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{\mathrm{H}^{\mathrm{Pek}}}\right] + \frac{|\mathrm{P}|^2}{2\alpha^4 m} - \alpha^{-(2+\epsilon)} \tag{2.4}$$

for all $(\mathrm{P}, \mathrm{E}) \in \sigma(\mathbf{P}'_1, \mathbf{H}'_\Lambda)$ with $|\mathrm{P}| \leq \mathrm{C}\alpha$ and $\alpha \geq \alpha_0(\sigma, \mathrm{C})$. In the proof of Theorem 1.1 below it will be useful to have Eq. (2.4) for $\mathbf{P}'_1$ and $\mathbf{H}'_\Lambda$, instead of Eq. (2.3) for $\mathbf{P}_\Lambda$ and $\mathbf{H}_\Lambda$.

In order to verify Theorem 1.1, it is convenient to introduce the ground state energy $\mathrm{E}^*_{\alpha,\Lambda}(\mathrm{P})$ of the operator $\mathbf{H}_\Lambda$ as a function of $\mathbf{P}$. Note that in contrast to $\mathrm{E}_{\alpha,\Lambda}(\mathrm{P})$, we do not use a wavenumber cut-off in the momentum operator here, while we still have the cut-off in the Hamiltonian $\mathbf{H}_\Lambda$. In the following Lemma 2.2 we are going to utilize the results in [4, 13], where the energy cost of introducing a wavenumber cut-off in the Hamiltonian is quantified, in order to compare $\mathrm{E}^*_{\alpha,\Lambda}(\mathrm{P})$ with $\mathrm{E}_\alpha(\mathrm{P})$.

Lemma **2.2.** — *Let* $\Lambda = \alpha^{\frac{4}{5}(1+\sigma)}$ *for* $\sigma > 0$. *Then there exists a constant* $\mathrm{C}' > 0$, *such that for all* $\mathrm{P} \in \mathbf{R}^3$ *and* α *large enough*

$$\mathrm{E}_\alpha(\mathrm{P}) \geq \mathrm{E}^*_{\alpha,\Lambda}(\mathrm{P}) - \mathrm{C}'\alpha^{-2(1+\sigma)}.$$

Proof. — By the results in [4, 13], there exists a $\mathrm{C} > 0$ such that for α large enough

$$\mathbf{H}_\Lambda \leq \mathbf{H} + \mathrm{C}\alpha^{-2(1+\sigma)}\left(\mathbf{H}^2 + 1\right). \tag{2.5}$$

This was first shown in [4] for a confined polaron model on a bounded domain, but the method extends in a straightforward way to the model on $\mathbf{R}^3$, as shown in [13] (see also [2] for the corresponding result for a polaron model on a torus). In the following, let Ψ_ϵ be a state satisfying $\chi(\sum_{j=1}^3(\mathbf{P}_j - \mathrm{P}_j)^2 \leq \epsilon^2)\Psi_\epsilon = \Psi_\epsilon$ and $\langle\Psi_\epsilon|(\mathbf{H} - \mathrm{E}_\alpha(\mathrm{P}))^2|\Psi_\epsilon\rangle \leq \epsilon^2$, where $\epsilon > 0$. By Eq. (2.5) we therefore have

$$\begin{aligned}\langle\Psi_\epsilon|\mathbf{H}_\Lambda|\Psi_\epsilon\rangle &\leq \mathrm{E}_\alpha(\mathrm{P}) + \mathrm{C}\alpha^{-2(1+\sigma)}\big(\langle\Psi_\epsilon\big|\mathbf{H}^2\big|\Psi_\epsilon\rangle + 1\big) + \epsilon\\ &\leq \mathrm{E}_\alpha(\mathrm{P}) + \mathrm{C}\alpha^{-2(1+\sigma)}\big(2\mathrm{E}_\alpha(\mathrm{P})^2 + 2\epsilon^2 + 1\big) + \epsilon\\ &\leq \mathrm{E}_\alpha(\mathrm{P}) + \mathrm{C}'\alpha^{-2(1+\sigma)} + \epsilon\end{aligned}$$

for $0 < \epsilon \leq 1$ and a suitable C', where we used that $\mathrm{E}_\alpha(\mathrm{P})$ is uniformly bounded for $\mathrm{P} \in \mathbf{R}^3$ and $\alpha \geq 1$ in the last inequality. Hence

$$\chi\big(\mathbf{H}_\Lambda \leq \mathrm{E}_\alpha(\mathrm{P}) + \mathrm{C}'\alpha^{-2(1+\sigma)} + \epsilon\big)\Psi_\epsilon \neq 0.$$

Using $\chi(\sum_{j=1}^3(\mathbf{P}_j - \mathrm{P}_j)^2 \leq \epsilon^2)\Psi_\epsilon = \Psi_\epsilon$, we obtain

$$\mathrm{A}_\epsilon := \sigma(\mathbf{P}, \mathbf{H}_\Lambda) \cap (\mathrm{B}_\epsilon(\mathrm{P}) \times \big(-\infty, \mathrm{E}_\alpha(\mathrm{P}) + \mathrm{C}'\alpha^{-2(1+\sigma)} + \epsilon]\big) \neq \emptyset.$$

Since $\mathbf{H}_\Lambda$ is bounded from below, $(\mathrm{A}_\epsilon)_{0<\epsilon\leq 1}$ is a monotone sequence of non-empty compact sets, i.e. $\mathrm{A}_{\epsilon_1} \subseteq \mathrm{A}_{\epsilon_2}$ for $\epsilon_1 \leq \epsilon_2$, and consequently

$$\sigma(\mathbf{P}, \mathbf{H}_\Lambda) \cap (\{\mathrm{P}\} \times \big(-\infty, \mathrm{E}_\alpha(\mathrm{P}) + \mathrm{C}'\alpha^{-2(1+\sigma)}]\big) = \bigcap_{0<\epsilon\leq 1} \mathrm{A}_\epsilon \neq \emptyset,$$

which is equivalent to $\mathrm{E}^*_{\alpha,\Lambda}(\mathrm{P}) \leq \mathrm{E}_\alpha(\mathrm{P}) + \mathrm{C}'\alpha^{-2(1+\sigma)}$. □

Given Theorem 2.1 we can now give a proof of Theorem 1.1.

Proof of Theorem 1.1. — In the first step of the proof, we are going to verify Eq. (1.2) for $|\mathrm{P}| \leq \sqrt{2m\alpha}$. Due to the rotational symmetry, we can assume w.l.o.g. that $\mathrm{P} = (\mathrm{P}_1, 0, 0)$, and by Lemma 2.2 we know that

$$\begin{aligned}\mathrm{E}_\alpha(\mathrm{P}) + \mathrm{C}'\alpha^{-2(1+\sigma)} &\geq \inf\big\{\mathrm{E} : (\mathrm{P}_1, 0, 0, \mathrm{E}) \in \sigma(\mathbf{P}_1, \mathbf{P}_2, \mathbf{P}_3, \mathbf{H}_\Lambda)\big\}\\ &\geq \inf\big\{\mathrm{E} : (\mathrm{P}_1, \mathrm{E}) \in \sigma(\mathbf{P}_1, \mathbf{H}_\Lambda)\big\}.\end{aligned} \tag{2.6}$$

Making use of the fact that the operators $\mathbf{P}_1'$, $\mathbf{H}_\Lambda'$, $\mathbf{P}_1 - \mathbf{P}_1'$ and $\mathbf{H}_\Lambda - \mathbf{H}_\Lambda'$ are pairwise commuting and that $\mathbf{P}_1', \mathbf{H}_\Lambda'$ and $\mathbf{P}_1 - \mathbf{P}_1', \mathbf{H}_\Lambda - \mathbf{H}_\Lambda'$ act on different factors in the tensor product $\mathrm{L}^2(\mathbf{R}^3, \mathcal{F}(\mathrm{ran}\chi(|\nabla| \leq \Lambda))) \otimes \mathcal{F}(\mathrm{ran}\chi(|\nabla| > \Lambda))$, their joint spectrum is well-defined and satisfies

$$\sigma\big(\mathbf{P}_1', \mathbf{H}_\Lambda', \mathbf{P}_1 - \mathbf{P}_1', \mathbf{H}_\Lambda - \mathbf{H}_\Lambda'\big) = \sigma\big(\mathbf{P}_1', \mathbf{H}_\Lambda'\big) \times \sigma\big(\mathbf{P}_1 - \mathbf{P}_1', \mathbf{H}_\Lambda - \mathbf{H}_\Lambda'\big).$$

Hence we can rewrite the right hand side of Eq. (2.6) as

$$\inf_{\mathrm{P}_1'+\widetilde{\mathrm{P}}_1=\mathrm{P}_1}\Big\{\mathrm{E}'+\widetilde{\mathrm{E}}:\big(\mathrm{P}_1',\mathrm{E}'\big)\in\sigma\big(\mathbf{P}_1',\mathbf{H}_\Lambda'\big),\\ (\widetilde{\mathrm{P}}_1,\widetilde{\mathrm{E}})\in\sigma\big(\mathbf{P}_1-\mathbf{P}_1',\mathbf{H}_\Lambda-\mathbf{H}_\Lambda'\big)\Big\}.$$

In order to verify that $\mathrm{E}'+\widetilde{\mathrm{E}}$ is bounded from below by the right hand side of Eq. (1.2) for a suitable $\epsilon>0$ and $|\mathrm{P}_1|\leq\sqrt{2m}\alpha$, let us first consider the case $\widetilde{\mathrm{E}}\geq\alpha^{-2}$. Since $\mathrm{E}'\in\sigma(\mathbf{H}_\Lambda')$, we have $\mathrm{E}'\geq\inf\sigma(\mathbf{H}_\Lambda')\geq\inf\sigma(\mathbf{H})=\mathrm{E}_\alpha$ and therefore

$$\mathrm{E}'+\widetilde{\mathrm{E}}\geq\mathrm{E}_\alpha+\alpha^{-2}\geq e^{\mathrm{Pek}}-\frac{1}{2\alpha^2}\mathrm{Tr}\Big[1-\sqrt{\mathrm{H}^{\mathrm{Pek}}}\Big]+\alpha^{-2}-\alpha^{-(2+\epsilon')}$$

for a suitable $\epsilon'>0$, where we have used [1, Theorem 1.1]. Regarding the other case $\widetilde{\mathrm{E}}<\alpha^{-2}$, note that we have

$$(\widetilde{\mathrm{P}}_1,\widetilde{\mathrm{E}})\in\sigma\big(\mathbf{P}_1-\mathbf{P}_1',\mathbf{H}_\Lambda-\mathbf{H}_\Lambda'\big)=\big\{(0,0)\big\}\cup\bigcup_{\ell=1}^{\infty}\mathbf{R}\times\left\{\frac{\ell}{\alpha^2}\right\},$$

and therefore $\widetilde{\mathrm{E}}=0$ and $\widetilde{\mathrm{P}}_1=0$. Hence $|\mathrm{P}_1'|=|\mathrm{P}_1|\leq\sqrt{2m}\alpha$ and consequently

$$\begin{aligned}\mathrm{E}'+\widetilde{\mathrm{E}}=\mathrm{E}'&\geq e^{\mathrm{Pek}}-\frac{1}{2\alpha^2}\mathrm{Tr}\Big[1-\sqrt{\mathrm{H}^{\mathrm{Pek}}}\Big]+\frac{|\mathrm{P}_1'|^2}{2\alpha^4 m}-\alpha^{-(2+\epsilon)}\\&=e^{\mathrm{Pek}}-\frac{1}{2\alpha^2}\mathrm{Tr}\Big[1-\sqrt{\mathrm{H}^{\mathrm{Pek}}}\Big]+\frac{|\mathrm{P}_1|^2}{2\alpha^4 m}-\alpha^{-(2+\epsilon)},\end{aligned}$$

where we have used $(\mathrm{P}_1',\mathrm{E}')\in\sigma(\mathbf{P}_1',\mathbf{H}_\Lambda')$ together with Eq. (2.4). This concludes the proof of Eq. (1.2) for $|\mathrm{P}|\leq\sqrt{2m}\alpha$.

In order to verify Eq. (1.2) for $|\mathrm{P}|>\sqrt{2m}\alpha$, we are going to use the fact that $\mathrm{P}\mapsto\mathrm{E}_\alpha(\mathrm{P})$ is a monotone radial function, as recently shown in [14], and consequently $\mathrm{E}_\alpha(\mathrm{P})\geq\mathrm{E}_\alpha(\sqrt{2m}\frac{\mathrm{P}}{|\mathrm{P}|})$ for $|\mathrm{P}|\geq\sqrt{2m}\alpha$. This reduces the problem to the previous case, and hence concludes the proof of Theorem 1.1. □

3. Construction of a condensate

This section is devoted to the construction of approximate p ground states Ψ_α satisfying complete condensation in φ^{Pek}, which we will utilize in order to prove Theorem 2.1 in Section 4. In this context, we call Ψ_α an approximate p ground state in case

$$\begin{aligned}&\langle\Psi_\alpha|\mathbf{H}_\Lambda|\Psi_\alpha\rangle=\mathrm{E}_{\alpha,\Lambda}\big(\alpha^2 p\big)+\mathrm{O}_{\alpha\to\infty}\big(\alpha^{-(2+\epsilon)}\big),\\&\big\langle\Psi_\alpha\big|(\Upsilon_\Lambda-p)^2\big|\Psi_\alpha\big\rangle\lesssim\alpha^{-(2+\epsilon)},\end{aligned}$$

with $\epsilon > 0$, where $E_{\alpha,\Lambda}(\alpha^2 p)$ and $\mathbf{H}_\Lambda$ are defined in, respectively above, Theorem 2.1, and we define the (rescaled and truncated) phonon momentum operator

$$\Upsilon_\Lambda := \int \chi^1\left(\Lambda^{-1}|k_1| \leq 2\right) k_1\, a_k^\dagger a_k \mathrm{d}k\,.$$

Similarly to $\mathbf{H}_\Lambda$, it also depends on α due to the rescaled canonical commutation relations $[a(f), a^\dagger(g)] = \alpha^{-2}\langle g|f\rangle$ but we suppress the α dependence for the sake of readability. Here and in the following, we write $X \lesssim Y$ in case there exist constants $C, \alpha_0 > 0$ such that $X \leq CY$ for all $\alpha \geq \alpha_0$. It is clear that there exist states Ψ_α that satisfy both $\langle\Psi_\alpha|\mathbf{H}_\Lambda|\Psi_\alpha\rangle - E_{\alpha,\Lambda}(\alpha^2 p) \lesssim \alpha^{-(2+\epsilon)}$ and $\langle\Psi_\alpha|(\alpha^{-2}\mathbf{P}_\Lambda - p)^2|\Psi_\alpha\rangle \lesssim \alpha^{-(2+\epsilon)}$, since $(p, E_{\alpha,\Lambda}(\alpha^2 p))$ is a point in the joint spectrum of $(\alpha^{-2}\mathbf{P}_\Lambda, \mathbf{H}_\Lambda)$. As part of the subsequent Lemma 3.1 we are going to show that the contribution of $\frac{1}{i\alpha^2}\nabla_{x_1}$ in $\alpha^{-2}\mathbf{P}_\Lambda = \frac{1}{i\alpha^2}\nabla_{x_1} + \Upsilon_\Lambda$ is negligibly small, i.e., we shall show that it does not matter whether one uses Υ_Λ or $\alpha^{-2}\mathbf{P}_\Lambda$ in the definition of approximate ground states. In particular, this will imply the existence of approximate p ground states. We will choose Ψ_α such that $\mathrm{supp}(\Psi_\alpha) \subseteq B_L(0)$ for a suitable L, where we define the support using the identification

$$L^2\left(\mathbf{R}^3\right) \otimes \mathcal{F}\left(L^2\left(\mathbf{R}^3\right)\right) \cong L^2\left(\mathbf{R}^3, \mathcal{F}\left(L^2\left(\mathbf{R}^3\right)\right)\right)$$

in order to represent elements $\Psi \in L^2(\mathbf{R}^3) \otimes \mathcal{F}(L^2(\mathbf{R}^3))$ as functions $x \mapsto \Psi(x)$ with values in $\mathcal{F}(L^2(\mathbf{R}^3))$, i.e. $\mathrm{supp}(\Psi)$ refers to the support of the electron.

In the rest of this paper, we will always assume that $\alpha \geq 1$. Most of the results in this Section include $E_{\alpha,\Lambda}(\alpha^2 p) \leq E_\alpha + C|p|^2$ as an assumption for an arbitrary, but fixed, constant $C > 0$, where E_α denotes the ground state energy of $\mathbf{H}$. For the purpose of proving Theorem 2.1 this is not a restriction, since we can always pick $C \geq \frac{1}{2m}$ and therefore $E_{\alpha,\Lambda}(\alpha^2 p) > E_\alpha + C|p|^2$ immediately implies the statement of Theorem 2.1

$$E_{\alpha,\Lambda}\left(\alpha^2 p\right) > E_\alpha + C|p|^2 \geq e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + \frac{|p|^2}{2m} - \alpha^{-(2+\epsilon)},$$

where we used $E_\alpha \geq e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}[1 - \sqrt{H^{\mathrm{Pek}}}] - \alpha^{-(2+\epsilon)}$ by [1, Theorem 1.1].

Lemma **3.1.** — *Given* $0 < \sigma < \frac{1}{4}$, *let* $\Lambda = \alpha^{\frac{4}{5}(1+\sigma)}$ *and* $L = \alpha^{1+\sigma}$, *and assume* p *satisfies* $|p| \leq \frac{C}{\alpha}$ *and* $E_{\alpha,\Lambda}(\alpha^2 p) \leq E_\alpha + C|p|^2$ *for a given* $C > 0$, *where* E_α *is the ground state energy of* $\mathbf{H}$. *Then there exist states* $\Psi_\alpha^\bullet$ *satisfying*

$$\begin{aligned}
&\langle\Psi_\alpha^\bullet|\mathbf{H}_\Lambda|\Psi_\alpha^\bullet\rangle - E_{\alpha,\Lambda}\left(\alpha^2 p\right) \lesssim \alpha^{-2(1+\sigma)},\\
&\left\langle\Psi_\alpha^\bullet\middle|(\Upsilon_\Lambda - p)^2\middle|\Psi_\alpha^\bullet\right\rangle \lesssim \alpha^{2\sigma-4},
\end{aligned}$$

as well as $\mathrm{supp}(\Psi_\alpha^\bullet) \subseteq B_L(0)$.

Proof. — Since $(p, \mathrm{E}_{\alpha,\Lambda}(\alpha^2 p))$ is an element of the joint spectrum $\sigma(\frac{1}{i\alpha^2}\nabla_{x_1} + \Upsilon_\Lambda, \mathbf{H}_\Lambda)$, there exist states Ψ_α^0 satisfying $\langle \Psi_\alpha^0 | (\frac{1}{i\alpha^2}\nabla_{x_1} + \Upsilon_\Lambda - p)^2 | \Psi_\alpha^0 \rangle \leq \alpha^{-4}$ and

$$\langle \Psi_\alpha^0 | \mathbf{H}_\Lambda | \Psi_\alpha^0 \rangle \leq \mathrm{E}_{\alpha,\Lambda}\big(\alpha^2 p\big) + \frac{1}{2}\alpha^{-2(1+\sigma)}. \tag{3.1}$$

From [1, Lemma 2.4] we know that $\langle \Psi_\alpha^0 | -\Delta_x | \Psi_\alpha^0 \rangle \leq 2\,\langle \Psi_\alpha^0 | \mathbf{H}_\Lambda | \Psi_\alpha^0 \rangle + d$ for a suitable constant $d > 0$, which implies that $\langle \Psi_\alpha^0 | -\Delta_x | \Psi_\alpha^0 \rangle \lesssim 1$ due to Eq. (3.1) and our assumption $\mathrm{E}_{\alpha,\Lambda}(\alpha^2 p) \leq \mathrm{E}_\alpha + \mathrm{C}|p|^2 \leq \mathrm{C}|p|^2 \leq \frac{\mathrm{C}^3}{\alpha^2}$, and hence

$$\begin{aligned}\big\langle \Psi_\alpha^0 \big| (\Upsilon_\Lambda - p)^2 \big| \Psi_\alpha^0 \big\rangle &\leq 2\Big\langle \Psi_\alpha^0 \Big| \Big(\frac{1}{i\alpha^2}\nabla_{x_1} + \Upsilon_\Lambda - p\Big)^2 \Big| \Psi_\alpha^0 \Big\rangle \\ &\quad - 2\alpha^{-4}\big\langle \Psi_\alpha^0 | \Delta_x | \Psi_\alpha^0 \big\rangle \\ &\leq c\alpha^{-4}\end{aligned} \tag{3.2}$$

for a suitable $c > 0$.

Let $\eta : \mathbf{R}^3 \longrightarrow [0,\infty)$ be a smooth function that is supported on $\mathrm{B}_1(0)$ and satisfies $\int \eta^2 = 1$. With this at hand we define $\Psi_y(x) := \mathrm{L}^{-\frac{3}{2}}\eta(\mathrm{L}^{-1}(x-y))\Psi_\alpha^0(x)$ and $\mathrm{Z}_y := \|\Psi_y\|$, as well as the set $\mathrm{S} \subseteq \mathbf{R}^3$ containing all y satisfying

$$\langle \Psi_y | \mathbf{H}_\Lambda | \Psi_y \rangle > \mathrm{Z}_y^2\Big(\mathrm{E}_{\alpha,\Lambda}\big(\alpha^2 p\big) + \big(1 + \|\nabla\eta\|^2\big)\alpha^{-2(1+\sigma)}\Big).$$

Making use of the IMS identity we obtain

$$\begin{aligned}\langle \Psi_\alpha^0 | \mathbf{H}_\Lambda | \Psi_\alpha^0 \rangle &= \int \langle \Psi_y | \mathbf{H}_\Lambda | \Psi_y \rangle \, \mathrm{d}y - \mathrm{L}^{-2}\|\nabla\eta\|^2 \\ &\geq \int_\mathrm{S} \mathrm{Z}_y^2 \mathrm{d}y\Big(\mathrm{E}_{\alpha,\Lambda}\big(\alpha^2 p\big) + \big(1 + \|\nabla\eta\|^2\big)\alpha^{-2(1+\sigma)}\Big) \\ &\quad + \Big(1 - \int_\mathrm{S} \mathrm{Z}_y^2 \, \mathrm{d}y\Big)\mathrm{E}_\alpha - \mathrm{L}^{-2}\|\nabla\eta\|^2,\end{aligned}$$

where we have used $\langle \Psi_y | \mathbf{H}_\Lambda | \Psi_y \rangle \geq \mathrm{E}_\alpha$ for $y \notin \mathrm{S}$ and $\int \mathrm{Z}_y^2 \, \mathrm{d}y = 1$. Using Eq. (3.1) and $\mathrm{L}^{-2} = \alpha^{-2(1+\sigma)}$ therefore yields

$$\begin{aligned}&\Big(\mathrm{E}_{\alpha,\Lambda}\big(\alpha^2 p\big) - \mathrm{E}_\alpha + \big(1 + \|\nabla\eta\|^2\big)\alpha^{-2(1+\sigma)}\Big) \int_\mathrm{S} \mathrm{Z}_y^2 \, \mathrm{d}y \\ &\qquad \leq \mathrm{E}_{\alpha,\Lambda}\big(\alpha^2 p\big) - \mathrm{E}_\alpha + \Big(\frac{1}{2} + \|\nabla\eta\|^2\Big)\alpha^{-2(1+\sigma)},\end{aligned}$$

and consequently $\int_{\mathrm{S}} \mathrm{Z}_y^2 \, \mathrm{d}y \leq 1-\gamma_\alpha$ with $\gamma_\alpha := \frac{1}{2}\frac{\alpha^{-2(1+\sigma)}}{\mathrm{E}_{\alpha,\Lambda}(\alpha^2 p)-\mathrm{E}_\alpha+(1+\|\nabla\eta\|^2)\alpha^{-2(1+\sigma)}}$. Let us further define $\mathrm{S}' \subseteq \mathbf{R}^3$ as the set of all y satisfying

$$\left\langle \Psi_y \middle| (\Upsilon_\Lambda - p)^2 \middle| \Psi_y \right\rangle > \mathrm{Z}_y^2 \frac{2c}{\gamma_\alpha}\alpha^{-4}.$$

Clearly we have, using Eq. (3.2),

$$\frac{2c}{\gamma_\alpha}\alpha^{-4}\int_{\mathrm{S}'} \mathrm{Z}_y^2 \, \mathrm{d}y \leq \int \left\langle \Psi_y \middle| (\Upsilon_\Lambda - p)^2 \middle| \Psi_y \right\rangle \mathrm{d}y = \left\langle \Psi_\alpha^0 \middle| (\Upsilon_\Lambda - p)^2 \middle| \Psi_\alpha^0 \right\rangle \leq c\alpha^{-4},$$

and hence $\int_{\mathrm{S}'} \mathrm{Z}_y^2 \, \mathrm{d}y \leq \frac{\gamma_\alpha}{2}$. Consequently

$$\int_{\mathrm{S}\cup\mathrm{S}'} \mathrm{Z}_y^2 \, \mathrm{d}y \leq \int_{\mathrm{S}} \mathrm{Z}_y^2 \, \mathrm{d}y + \int_{\mathrm{S}'} \mathrm{Z}_y^2 \, \mathrm{d}y \leq 1 - \frac{\gamma_\alpha}{2} < 1.$$

Since $\int \mathrm{Z}_y^2 \, \mathrm{d}y = 1$, this means in particular that there exists a $y \notin \mathrm{S} \cup \mathrm{S}'$ with $\mathrm{Z}_y > 0$, i.e. $\Psi_\alpha^\bullet := \mathrm{Z}_y^{-1}\Psi_y$ satisfies

$$\langle \Psi_\alpha^\bullet | \mathbf{H}_\Lambda | \Psi_\alpha^\bullet \rangle \leq \mathrm{E}_{\alpha,\Lambda}\left(\alpha^2 p\right) + \left(1 + \|\nabla\eta\|^2\right)\alpha^{-2(1+\sigma)},$$

$$\left\langle \Psi_\alpha^\bullet \middle| (\Upsilon_\Lambda - p)^2 \middle| \Psi_\alpha^\bullet \right\rangle \leq \frac{2c}{\gamma_\alpha}\alpha^{-4} \lesssim \alpha^{2\sigma-4},$$

where we have used $\mathrm{E}_{\alpha,\Lambda}(\alpha^2 p) - \mathrm{E}_\alpha \lesssim |p|^2 \lesssim \alpha^{-2}$ in the last estimate. Moreover, we clearly have $\mathrm{supp}(\Psi_\alpha^\bullet) \subseteq \mathrm{B_L}(y)$. By the translation invariance of $\mathbf{H}_\Lambda$ and Υ_Λ, we can assume w.l.o.g. that $y = 0$, which concludes the proof. □

In the following Lemmas 3.2 and 3.4, we will use localization methods in order to construct approximate p ground states with useful additional properties, which we will use in Lemma 3.6, together with an additional localization procedure, in order to show the existence of approximate p ground states satisfying complete condensation. In Theorem 3.7 we will then apply a final localization step in order to obtain complete condensation in a stronger sense, following the argument in [8].

In order to formulate our various localization results, we follow [1] and define for a function $\mathrm{F} : \mathcal{M}(\mathbf{R}^3) \longrightarrow \mathbf{R}$, where $\mathcal{M}(\mathbf{R}^3)$ is the set of all finite (Borel) measures on $\mathbf{R}^3$, the operator $\widehat{\mathrm{F}}$ on $\mathcal{F}(\mathrm{L}^2(\mathbf{R}^3)) = \bigoplus_{n=0}^\infty \mathrm{L}^2_{\mathrm{sym}}(\mathbf{R}^{3\times n})$ as

$$\widehat{\mathrm{F}} \bigoplus_{n=0}^{\infty} \Psi_n := \bigoplus_{n=0}^{\infty} \Psi_n^* \tag{3.3}$$

with $\Psi_n^*(x^1,\ldots,x^n) := \mathrm{F}^n(x^1,\ldots,x^n)\Psi_n(x^1,\ldots,x^n)$, where

$$\mathrm{F}^n\left(x^1,\ldots,x^n\right) := \mathrm{F}\left(\alpha^{-2}\sum_{k=1}^n \delta_{x^k}\right), \tag{3.4}$$

and $\widehat{\mathrm{F}}_0 := \mathrm{F}(0)$, i.e. $\widehat{\mathrm{F}}$ acts component-wise on $\bigoplus_{n=0}^{\infty} \mathrm{L}^2_{\mathrm{sym}}(\mathbf{R}^{3\times n})$ by multiplication with the real-valued function $(x^1, \dots, x^n) \mapsto \mathrm{F}(\alpha^{-2} \sum_{k=1}^{n} \delta_{x^k})$.

With this notation at hand, we define for given positive c_-, c_+ and ϵ' the function $\mathrm{F}_*(\rho) := \chi^{\epsilon'}(c_- + \epsilon' \leq \int \mathrm{d}\rho \leq c_+ - \epsilon')$ and the states

$$\Psi'_\alpha := \mathrm{Z}_\alpha^{-1} \widehat{\mathrm{F}}_* \Psi^\bullet_\alpha, \tag{3.5}$$

with normalization constants $\mathrm{Z}_\alpha := \|\widehat{\mathrm{F}}_* \Psi^\bullet_\alpha\|$, where $\Psi^\bullet_\alpha$ is the sequence constructed in Lemma 3.1. Since $\mathcal{N} = \widehat{\mathrm{G}}$ with $\mathrm{G}(\rho) := \int \mathrm{d}\rho$, it is clear that the states Ψ'_α are localized to a region where the (scaled) number operator $\mathcal{N}$ is between c_- and c_+, i.e. $\chi(c_- \leq \mathcal{N} \leq c_+)\Psi'_\alpha = \Psi'_\alpha$. The following Lemma 3.2 quantifies the energy and momentum error of this localization procedure. The subsequent results in Lemmas 3.2, 3.4 and 3.6 as well as Theorem 3.7, which quantify the energy and momentum error of specific localization procedures, are generalizations of the corresponding results in [1], where only the energy cost of such localization procedures is discussed. In the following we will usually refer to the respective results in [1] when it comes to quantifying the energy error, and only discuss the localization error of the momentum operator Υ_Λ.

Lemma **3.2.** — *Given* $0 < \sigma < \frac{1}{4}$, *let* $\Lambda = \alpha^{\frac{4}{5}(1+\sigma)}$ *and* $\mathrm{L} = \alpha^{1+\sigma}$, *and assume* p *satisfies* $|p| \leq \frac{\mathrm{C}}{\alpha}$ *and* $\mathrm{E}_{\alpha,\Lambda}(\alpha^2 p) \leq \mathrm{E}_\alpha + \mathrm{C}|p|^2$ *for a given* $\mathrm{C} > 0$. *Then there exist constants* c_-, c_+ *and* ϵ', *such that the states* Ψ'_α *defined in Eq. (3.5) satisfy*

$$\langle \Psi'_\alpha | \mathbf{H}_\Lambda | \Psi'_\alpha \rangle - \mathrm{E}_{\alpha,\Lambda}\big(\alpha^2 p\big) \lesssim \alpha^{-2(1+\sigma)},$$
$$\big\langle \Psi'_\alpha \big| (\Upsilon_\Lambda - p)^2 \big| \Psi'_\alpha \big\rangle \lesssim \alpha^{2\sigma - 4}.$$

Proof. — By our assumptions we clearly have $\widetilde{\mathrm{E}}_\alpha - \mathrm{E}_\alpha \lesssim \alpha^{-\frac{4}{29}}$ with $\widetilde{\mathrm{E}}_\alpha := \langle \Psi^\bullet_\alpha | \mathbf{H}_\Lambda | \Psi^\bullet_\alpha \rangle$, and therefore we can apply [1, Lemma 3.4], which tells us that we can choose c_-, c_+ and ϵ', such that $\langle \Psi'_\alpha | \mathbf{H}_\Lambda | \Psi'_\alpha \rangle - \mathrm{E}_{\alpha,\Lambda}(\alpha^2 p) \lesssim \alpha^{-2(1+\sigma)}$, and furthermore $\mathrm{Z}_\alpha \underset{\alpha\to\infty}{\longrightarrow} 1$. Since $\widehat{\mathrm{F}}_*$ commutes with Υ_Λ, we obtain with $\widetilde{\Psi}_\alpha := \sqrt{\frac{1-\widehat{\mathrm{F}}_*^2}{1-\mathrm{Z}_\alpha^2}} \Psi^\bullet_\alpha$

$$\begin{aligned} &\mathrm{Z}_\alpha^2 \big\langle \Psi'_\alpha \big| (\Upsilon_\Lambda - p)^2 \big| \Psi'_\alpha \big\rangle + \big(1 - \mathrm{Z}_\alpha^2\big) \big\langle \widetilde{\Psi}_\alpha \big| (\Upsilon_\Lambda - p)^2 \big| \widetilde{\Psi}_\alpha \big\rangle \\ &\quad = \big\langle \Psi^\bullet_\alpha \big| (\Upsilon_\Lambda - p)^2 \big| \Psi^\bullet_\alpha \big\rangle \end{aligned}$$

Hence $\langle \Psi'_\alpha | (\Upsilon_\Lambda - p)^2 | \Psi'_\alpha \rangle \leq \mathrm{Z}_\alpha^{-2} \langle \Psi^\bullet_\alpha | (\Upsilon_\Lambda - p)^2 | \Psi^\bullet_\alpha \rangle \lesssim \alpha^{2\sigma-4}$. □

When it comes to localizations with respect to more complicated functions F compared to the one used in Eq. (3.5), we first need to introduce some tools in order to quantify the localization error of the momentum operator. Given a function $\mathrm{F} : \mathcal{M}(\mathbf{R}^3) \longrightarrow \mathbf{R}$, $\Omega \subseteq \mathcal{M}(\mathbf{R}^3)$ and $\lambda > 0$, let us define

$$\|\mathrm{F}\|^2_{\Omega,\lambda} := \sup_{1 \leq n \leq \lambda\alpha^2} \sup_{x \in \Omega_n} \Big\| \big(\mathrm{F}^{n,\bar{x}}\big)' \Big\|^2 = \sup_{1 \leq n \leq \lambda\alpha^2} \sup_{x \in \Omega_n} \int_{\mathbf{R}} \left| \frac{\mathrm{d}}{\mathrm{d}t} \mathrm{F}^n(t, \bar{x}) \right|^2 \mathrm{d}t, \tag{3.6}$$

where $x=(x^1,\dots,x^n)\in\mathbf{R}^{3\times n}$ with $x^k=(x^k_1,x^k_2,x^k_3)$ and $\bar{x}:=(x^1_2,x^1_3,x^2,\dots,x^n)\in\mathbf{R}^{3\times n-1}$, i.e. we define $\bar{x}$ such that $x=(x^1_1,\bar{x})$, Ω_n is the set of all x such that $\alpha^{-2}\sum_{j=1}^n\delta_{x^j}\in\Omega$ and $\mathrm{F}^{n,y}:\mathbf{R}\longrightarrow\mathbf{R}$ is defined as $\mathrm{F}^{n,y}(t):=\mathrm{F}^n(t,y)$ for $y\in\mathbf{R}^{3\times n-1}$, where F^n is as in Eq. (3.4).

Lemma **3.3.** — *Given* $\lambda>0$, *there exists a constant* $\mathrm{T}>0$ *such that we have for all quadratic partitions of unity* $\mathcal{P}=\{\mathrm{F}_j:\mathcal{M}(\mathbf{R}^3)\longrightarrow\mathbf{R}:j\in\mathrm{J}\}$, *i.e. families of functions satisfying* $0\leq\mathrm{F}_j\leq 1$ *and* $\sum_{j\in\mathrm{J}}\mathrm{F}_j^2=1$, $\Lambda>0$, $|p|\leq\Lambda$, $\Omega\subseteq\mathcal{M}(\mathbf{R}^3)$ *and states* Ψ *satisfying* $\chi(\mathcal{N}\leq\lambda)\Psi=\Psi$ *and* $\widehat{\mathbf{1}_\Omega}\Psi=\Psi$

$$\left|\sum_{j\in\mathrm{J}}\langle\Psi_j|(\Upsilon_\Lambda-p)^2|\Psi_j\rangle-\langle\Psi|(\Upsilon_\Lambda-p)^2|\Psi\rangle\right|\leq\mathrm{T}\Lambda\sum_{j\in\mathrm{J}}\|\mathrm{F}_j\|^2_{\Omega,\lambda},$$

where we define $\Psi_j:=\widehat{\mathrm{F}}_j\Psi$ *with* $\widehat{\mathrm{F}}_j$ *being introduced in Eq. (3.3).*

Proof. — Using the IMS identity we can write

$$\begin{aligned}\sum_{j\in\mathrm{J}}&\langle\Psi_j|(\Upsilon_\Lambda-p)^2|\Psi_j\rangle-\langle\Psi|(\Upsilon_\Lambda-p)^2|\Psi\rangle\\&=-\frac{1}{2}\sum_{j\in\mathrm{J}}\Big\langle\Psi\Big|\Big[\big[(\Upsilon_\Lambda-p)^2,\widehat{\mathrm{F}}_j\big],\widehat{\mathrm{F}}_j\Big]\Big|\Psi\Big\rangle.\end{aligned}$$

Hence it suffices to show that

$$\pm\Big\langle\Psi\Big|\Big[\big[(\Upsilon_\Lambda-p)^2,\widehat{\mathrm{F}}\big],\widehat{\mathrm{F}}\Big]\Big|\Psi\Big\rangle\lesssim\Lambda\|\mathrm{F}\|^2_{\Omega,\lambda}$$

for any bounded $\mathrm{F}:\mathcal{M}(\mathbf{R}^3)\longrightarrow\mathbf{R}$ and state satisfying $\chi(\mathcal{N}\leq\lambda)\Psi=\Psi$ and $\widehat{\mathbf{1}_\Omega}\Psi=\Psi$. Let us start by estimating

$$\begin{aligned}\pm\Big[\big[(\Upsilon_\Lambda-p)^2,\widehat{\mathrm{F}}\big],\widehat{\mathrm{F}}\Big]&=\pm2[\Upsilon_\Lambda,\widehat{\mathrm{F}}]^2\pm\Big\{\Upsilon_\Lambda-p,\big[[\Upsilon_\Lambda,\widehat{\mathrm{F}}],\widehat{\mathrm{F}}\big]\Big\}\\&\leq-2[\Upsilon_\Lambda,\widehat{\mathrm{F}}]^2+\frac{\|\mathrm{F}\|^2_{\Omega,\lambda}}{\Lambda}(\Upsilon_\Lambda-p)^2\\&\quad+\frac{\Lambda}{\|\mathrm{F}\|^2_{\Omega,\lambda}}\big[[\Upsilon_\Lambda,\widehat{\mathrm{F}}],\widehat{\mathrm{F}}\big]^2,\end{aligned}$$

where $\{\mathrm{A},\mathrm{B}\}:=\mathrm{AB}+\mathrm{BA}$. By the definition of Υ_Λ it is clear that

$$\frac{\|\mathrm{F}\|^2_{\Omega,\lambda}}{\Lambda}(\Upsilon_\Lambda-p)^2\lesssim\Lambda\|\mathrm{F}\|^2_{\Omega,\lambda}(\mathcal{N}+1)^2$$

for $|p|\leq\Lambda$, and consequently $\pm\langle\Psi|\frac{\|\mathrm{F}\|^2_{\Omega,\lambda}}{\Lambda}(\Upsilon_\Lambda-p)^2|\Psi\rangle\lesssim\Lambda\|\mathrm{F}\|^2_{\Omega,\lambda}$. Using that Ψ is a function with values in $\mathcal{F}_{\leq\lambda\alpha^2}(\mathrm{L}^2(\mathbf{R}^3)):=\bigoplus_{n\leq\lambda\alpha^2}\mathrm{L}^2_{\mathrm{sym}}(\mathbf{R}^{3\times n})$, we are going to represent it as $\Psi = \bigoplus_{n\leq\lambda\alpha^2}\Psi_n$ where $\Psi_n(z, x^1, \dots, x^n)$ is a function of the electron variable z and the n phonon coordinates $x^j \in \mathbf{R}^3$ satisfying $\Psi_n(z, x^1, \dots, x^n) = 0$ for all $(x^1, \dots, x^n) \notin \Omega_n$. In order to simplify the notation, we will suppress the dependence on the electron variable z. We have

$$[\Upsilon_\Lambda, \widehat{\mathrm{F}}]\Psi = \bigoplus_{1\leq n\leq\lambda\alpha^2} \alpha^{-2} n \Psi_n^*$$

with $\Psi_n^* := \frac{1}{n}\sum_{j=1}^n [g(\frac{1}{i}\nabla_{x_1^j}), \mathrm{F}^n]\Psi_n$, where $g(k) := \chi^1(\Lambda^{-1}|k| \leq 2)k$ for $k \in \mathbf{R}$. Hence

$$\begin{aligned}\left\langle \Psi \middle| -[\Upsilon_\Lambda, \widehat{\mathrm{F}}]^2 \middle| \Psi \right\rangle &= \left\| [\Upsilon_\Lambda, \widehat{\mathrm{F}}]\Psi \right\|^2 \\ &= \sum_{1\leq n\leq\lambda\alpha^2} \alpha^{-4} n^2 \left\| \Psi_n^* \right\|^2 \leq \lambda^2 \sum_{1\leq n\leq\lambda\alpha^2} \left\| \Psi_n^* \right\|^2,\end{aligned}$$

and $\|\Psi_n^*\| \leq \frac{1}{n}\sum_{j=1}^n \|[g(\frac{1}{i}\nabla_{x_1^j}), \mathrm{F}^n]\Psi_n\| = \|[g(\frac{1}{i}\nabla_{x_1^1}), \mathrm{F}^n]\Psi_n\|$, where we have used the permutation symmetry of Ψ_n. By Lemma A.1 we know that

$$\begin{aligned}\left\| \left[g\left(\frac{1}{i}\nabla_{x_1^1}\right), \mathrm{F}^n \right]\Psi_n \right\| &\leq \sup_{x\in\mathrm{supp}(\Psi_n)} \left\| \left[g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t}\right), \mathrm{F}^{n,\bar{x}} \right] \right\|_{\mathrm{op}} \|\Psi_n\| \\ &\lesssim \sqrt{\Lambda} \sup_{x\in\Omega_n} \left\| \left(\mathrm{F}^{n,\bar{x}}\right)' \right\| \|\Psi_n\|,\end{aligned}$$

and therefore

$$\left\langle \Psi \middle| -[\Upsilon_\Lambda, \widehat{\mathrm{F}}]^2 \middle| \Psi \right\rangle \leq \lambda^2 \Lambda \sup_{1\leq n\leq\lambda\alpha^2, x\in\Omega_n} \left\| \left(\mathrm{F}^{n,\bar{x}}\right)' \right\|^2 \sum_{n\leq\lambda\alpha^2} \|\Psi_n\|^2 = \lambda^2 \Lambda \|\mathrm{F}\|^2_{\Omega,\lambda}.$$

In order to estimate the expectation value of $[[\Upsilon_\Lambda, \widehat{\mathrm{F}}], \widehat{\mathrm{F}}]^2$ we proceed similarly, by writing

$$\left[[\Upsilon_\Lambda, \widehat{\mathrm{F}}], \widehat{\mathrm{F}}\right]\Psi = \bigoplus_{n\leq\lambda\alpha^2} \alpha^{-2} n \widetilde{\Psi}_n$$

with $\widetilde{\Psi}_n = \frac{1}{n}\sum_{j=1}^n [[g(\frac{1}{i}\nabla_{x_1^j}), \mathrm{F}^n], \mathrm{F}^n]\Psi_n$, and estimating

$$\left\langle \Psi \middle| \left[[\Upsilon_\Lambda, \widehat{\mathrm{F}}], \widehat{\mathrm{F}}\right]^2 \middle| \Psi \right\rangle \leq \lambda^2 \sum_{n\leq\lambda\alpha^2} \|\widetilde{\Psi}_n\|^2$$

as well as

$$\|\widetilde{\Psi}_n\| \leq \sup_{x\in\mathrm{supp}(\Psi_n)} \left\| \left[\left[g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t}\right), \mathrm{F}^{n,\bar{x}} \right], \mathrm{F}^{n,\bar{x}} \right] \right\|_{\mathrm{op}} \|\Psi_n\| \leq \sup_{x\in\Omega_n} \left\| \left(\mathrm{F}^{n,\bar{x}}\right)' \right\|^2 \|\Psi_n\|,$$

where we have again applied Lemma A.1. This concludes the proof. □

With the subsequent localization step in Eq. (3.7), we want to restrict the state Ψ'_α to phonon density configurations ρ which have a sharp concentration of their mass. To be precise, for given R and $\epsilon, \delta > 0$, let us define

$$\begin{aligned} \mathrm{K_R}(\rho) &:= \iint \chi^\epsilon\big(\mathrm{R}-\epsilon \leq |x-y|\big)\mathrm{d}\rho(x)\mathrm{d}\rho(y), \\ \mathrm{F_R}(\rho) &:= \chi^{\frac{\delta}{3}}\left(\mathrm{K_R}(\rho) \leq \frac{2\delta}{3}\right), \qquad (3.7) \\ \Psi''_\alpha &:= \mathrm{Z}^{-1}_{\mathrm{R},\alpha}\widehat{\mathrm{F}}_\mathrm{R}\Psi'_\alpha, \end{aligned}$$

where Ψ'_α is as in Lemma 3.2 and $\mathrm{Z}_{\mathrm{R},\alpha} := \|\widehat{\mathrm{F}}_\mathrm{R}\Psi'_\alpha\|$. Clearly $\widehat{\mathbf{1}_\Omega}\Psi''_\alpha = \Psi''_\alpha$ where Ω is the set of all ρ satisfying $\iint_{|x-y|\geq \mathrm{R}} \mathrm{d}\rho(x)\mathrm{d}\rho(y) \leq \delta$. In the following Lemma 3.4 we are going to quantify the energy and momentum cost of this localization procedure.

Lemma **3.4.** — *Given* $0 < \sigma < \frac{1}{4}$, *let* $\Lambda = \alpha^{\frac{4}{5}(1+\sigma)}$ *and* $\mathrm{L} := \alpha^{1+\sigma}$, *and assume* p *satisfies* $|p| \leq \frac{\mathrm{C}}{\alpha}$ *and* $\mathrm{E}_{\alpha,\Lambda}(\alpha^2 p) \leq \mathrm{E}_\alpha + \mathrm{C}|p|^2$ *for a given* $\mathrm{C} > 0$. *Then for any* $\epsilon, \delta > 0$, *there exists a constant* $\mathrm{R} > 0$, *such that the states* Ψ''_α *defined in Eq. (3.7) satisfy*

$$\begin{aligned} \langle \Psi''_\alpha|\mathbf{H}_\Lambda|\Psi''_\alpha\rangle - \mathrm{E}_{\alpha,\Lambda}\big(\alpha^2 p\big) &\lesssim \alpha^{-2(1+\sigma)}, \\ \big\langle \Psi''_\alpha\big|(\Upsilon_\Lambda - p)^2\big|\Psi''_\alpha\big\rangle &\lesssim \alpha^{\frac{4}{5}\sigma - \frac{16}{5}}. \end{aligned}$$

Proof. — By the results in [1, Lemma 3.5], there exists a constant $\mathrm{R} > 0$ such that $\langle \Psi''_\alpha|\mathbf{H}_\Lambda|\Psi''_\alpha\rangle - \mathrm{E}_{\alpha,\Lambda}(\alpha^2 p) \lesssim \alpha^{-2(1+\sigma)}$ and $\mathrm{Z}_{\mathrm{R},\alpha} \underset{\alpha\to\infty}{\longrightarrow} 1$. Applying Lemma 3.3 yields

$$\begin{aligned} &\langle \widehat{\mathrm{F}}_\mathrm{R}\Psi'_\alpha\big|(\Upsilon_\Lambda - p)^2\big|\widehat{\mathrm{F}}_\mathrm{R}\Psi'_\alpha\rangle + \langle \widehat{\mathrm{G}}_\mathrm{R}\Psi'_\alpha\big|(\Upsilon_\Lambda - p)^2\big|\widehat{\mathrm{G}}_\mathrm{R}\Psi'_\alpha\rangle \qquad (3.8) \\ &\qquad \lesssim \alpha^{2\sigma-4} + \alpha^{\frac{4}{5}(1+\sigma)}\big(\|\mathrm{F_R}\|^2_{\mathcal{M}(\mathbf{R}^3),c_+} + \|\mathrm{G_R}\|^2_{\mathcal{M}(\mathbf{R}^3),c_+}\big) \end{aligned}$$

with $\mathrm{G_R} := \sqrt{1-\mathrm{F_R^2}}$, where we used $\langle \Psi'_\alpha|(\Upsilon_\Lambda - p)^2|\Psi'_\alpha\rangle \lesssim \alpha^{2\sigma-4}$ and $\chi(\mathcal{N} \leq c_+)\Psi'_\alpha = \Psi'_\alpha$. In order to estimate $\|\mathrm{F_R}\|_{\mathcal{M}(\mathbf{R}^3),c_+}$, let us define the functions $g(s) := \chi^{\frac{\delta}{3}}(s \leq \frac{2\delta}{3})$ and $h(s) := \chi^\epsilon(\mathrm{R}-\epsilon \leq \sqrt{s})$. Then $\mathrm{F}^n_\mathrm{R}(x) = g(\alpha^{-4}\sum_{i,j=1}^n h(|x^i - x^j|^2))$ and therefore

$$\mathrm{F}^{n,y}_\mathrm{R}(t) = g\left(\alpha^{-4}\sum_{i=2}^n h\Big(\big(t - y^i_1\big)^2 + \delta^i_y\Big) + \mu_y\right)$$

with $\delta^i_y := (y^1_2 - y^i_2)^2 + (y^1_3 - y^i_3)^2$ and $\mu_y := \alpha^{-4}\sum_{i,j=2}^n h(|y^i - y^j|^2)$. Hence

$$\begin{aligned} \big\|\big(\mathrm{F}^{n,y}_\mathrm{R}\big)'\big\| &\leq 4\alpha^{-4}\big\|g'\big\|_\infty \sum_{i=2}^n \sqrt{\int_\mathbf{R} |t|^2\big|h'\big(t^2 + \delta^i_y\big)\big|^2 \mathrm{d}t} \\ &\leq 4\alpha^{-4}\big\|g'\big\|_\infty (n-1)\big\|h'\big\|_\infty \sqrt{\frac{2\mathrm{R}^3}{3}}, \end{aligned}$$

where we have used $\mathrm{supp}(h') \subseteq [0, \mathrm{R}^2)$ in the second inequality. Consequently

$$\|\mathrm{F}_\mathrm{R}\|_{\mathcal{M}(\mathbf{R}^3),c_+} = \sup_{1\leq n\leq c_+\alpha^2} \sup_{x\in\mathbf{R}^{3\times n}} \left\| \left(\mathrm{F}_\mathrm{R}^{n,\bar{x}}\right)' \right\| \lesssim \alpha^{-2}.$$

Similarly we have $\|\mathrm{G}_\mathrm{R}\|_{\mathcal{M}(\mathbf{R}^3),c_+} \lesssim \alpha^{-2}$. In combination with Eq. (3.8) we obtain

$$\begin{aligned}&\left\langle \Psi''_\alpha \middle| (\Upsilon_\Lambda - p)^2 \middle| \Psi''_\alpha \right\rangle \\ &\quad \lesssim \mathrm{Z}_{\mathrm{R},\alpha}^{-2}\left(\alpha^{2\sigma-4} + \alpha^{\frac{4}{5}(1+\sigma)}\left(\|\mathrm{F}_\mathrm{R}\|^2_{\mathcal{M}(\mathbf{R}^3),c_+} + \|\mathrm{G}_\mathrm{R}\|^2_{\mathcal{M}(\mathbf{R}^3),c_+}\right)\right) \\ &\quad \lesssim \alpha^{\frac{4}{5}\sigma - \frac{16}{5}}.\end{aligned}$$ □

Before we come to our next localization step in Lemma 3.6, we need to define the regularized median of a measure $\nu \in \mathcal{M}(\mathbf{R})$, see also [1, Definition 3.8], and derive a useful estimate for it in the subsequent Lemma 3.5. In the following let $x^\kappa(\nu) := \sup\{t : \int_{-\infty}^t \mathrm{d}\nu \leq \kappa \int \mathrm{d}\nu\}$ denote the κ-quantile, where we use the convention that boundaries are included in the domain of integration $\int_a^b f\,\mathrm{d}\nu := \int_{[a,b]} f\,\mathrm{d}\nu$, and let us define for $0 < q < \frac{1}{2}$ and $\nu \neq 0$

$$(\mathbf{3.9}) \qquad m_q(\nu) := \frac{1}{\int_{\mathrm{K}_q(\nu)} \mathrm{d}\nu} \int_{\mathrm{K}_q(\nu)} h\,\mathrm{d}\nu(h),$$

where $\mathrm{K}_q(\nu) := [x^{\frac{1}{2}-q}(\nu), x^{\frac{1}{2}+q}(\nu)]$, and $m_q(0) := 0$. Furthermore we will denote the marginal measures of $\rho \in \mathcal{M}(\mathbf{R}^3)$ as ρ_i, i.e. $\rho_i(\mathrm{A}) := \rho([x_i \in \mathrm{A}])$, where $\mathrm{A} \subseteq \mathbf{R}$ is measurable and $i \in \{1, 2, 3\}$.

Lemma **3.5.** — *Let us define* Ω_{reg} *as the set of all* $\rho \in \mathcal{M}(\mathbf{R}^3)$ *satisfying* $\int_{x_i=t} \mathrm{d}\rho(x) \leq \alpha^{-2}$ *for* $t \in \mathbf{R}$ *and* $i \in \{1, 2, 3\}$, *and* Ω *as the set of all* $\rho \in \Omega_{\mathrm{reg}}$ *satisfying* $c \leq \int \mathrm{d}\rho$ *and* $\iint_{|x-y|\geq \mathrm{R}} \mathrm{d}\rho(x)\mathrm{d}\rho(y) \leq \delta$ *for given* $\mathrm{R}, c, \delta > 0$. *Furthermore let* q *be a constant satisfying* $q + \frac{\alpha^{-2}}{c} \leq \frac{1}{2} - \frac{\delta}{c^2}$. *Then we have for any* $n \geq 1$ *and function of the form* $\mathrm{F}(\rho) = f(m_q(\rho_1))$ *the estimate*

$$(\mathbf{3.10}) \qquad \sup_{x\in\Omega_n} \left\| \left(\mathrm{F}^{n,\bar{x}}\right)' \right\| \leq \alpha^{-2} \frac{\|f'\|_\infty}{2qc} \sqrt{2\mathrm{R}},$$

where m_q *is defined in Eq. (3.9) and* Ω_n *below Eq. (3.6).*

Proof. — Given $x \in \Omega_n$, let us define $\nu_t := \alpha^{-2}(\delta_t + \sum_{j=2}^n \delta_{x_1^j})$, which allows us to rewrite $\mathrm{F}^{n,\bar{x}}(t) = f(m_q(\nu_t))$. Let us first compute the derivative $\frac{\mathrm{d}}{\mathrm{d}t} m_q(\nu_t)$ for $t \in \mathbf{R} \setminus \{x_1^2, \ldots, x_1^n\}$. For such t, there clearly exists an $\epsilon > 0$ such that $(t - \epsilon, t + \epsilon) \subset \mathbf{R} \setminus \{x_1^2, \ldots, x_1^n\}$. It will be useful in the following that the set $\mathrm{Y} := \{x_1^2, \ldots, x_1^n\} \cap \mathrm{K}_q(\nu_s)$ is independent of $s \in (t - \epsilon, t + \epsilon)$, with $\mathrm{K}_q(\nu)$ being defined below Eq. (3.9). Furthermore we have for $s \in (t - \epsilon, t + \epsilon)$ that $s \in \mathrm{K}_q(s)$ if and only if $t \in \mathrm{K}_q(t)$. Therefore $\alpha^2 \int_{\mathrm{K}_q(\nu_s)} h\,\mathrm{d}\nu_s(h) = \sum_{h\in\mathrm{Y}} h + s\mathbf{1}_{\mathrm{K}_q(s)}(s) = \sum_{h\in\mathrm{Y}} h + s\mathbf{1}_{\mathrm{K}_q(t)}(t)$ and $\alpha^2 \int_{\mathrm{K}_q(\nu_s)} \mathrm{d}\nu_s =$

$|\mathrm{Y}| + \mathbf{1}_{\mathrm{K}_q(s)}(s) = \alpha^2 \int_{\mathrm{K}_q(\nu_t)} \mathrm{d}\nu_t$ for $s \in (t-\epsilon, t+\epsilon)$, and consequently we obtain for $t \in \mathbf{R} \setminus \{x_1^2, \ldots, x_1^n\}$

$$\frac{\mathrm{d}}{\mathrm{d}t} m_q(\nu_t) = \alpha^{-2} \frac{\mathrm{d}}{\mathrm{d}s}\Big|_{s=t} \frac{\sum_{h \in \mathrm{Y}} h + s\mathbf{1}_{\mathrm{K}_q(t)}(t)}{\int_{\mathrm{K}_q(\nu_t)} \mathrm{d}\nu_t} = \alpha^{-2} \frac{\mathbf{1}_{\mathrm{K}_q(t)}(t)}{\int_{\mathrm{K}_q(\nu_t)} \mathrm{d}\nu_t}.$$

Note that due to our assumption $\rho \in \Omega_{\mathrm{reg}}$, $m_q(\nu_t)$ can be continuously extended from $\mathbf{R} \setminus \{x_1^2, \ldots, x_1^n\}$ to all of $\mathbf{R}$, and therefore $\frac{\mathrm{d}}{\mathrm{d}t} m_q(\nu_t) = \alpha^{-2} \frac{\mathbf{1}_{\mathrm{K}_q(t)}(t)}{\int_{\mathrm{K}_q(\nu_t)} \mathrm{d}\nu_t}$ in the sense of distributions. Since $\int_{\mathrm{K}_q(\nu_t)} \mathrm{d}\nu_t \geq 2qc$ we conclude $|(\mathrm{F}^{n,\tilde{x}})'(t)| \leq \alpha^{-2} \frac{\|f'\|_\infty}{2qc} \mathbf{1}_{\mathrm{K}_q(t)}(t)$ for almost every t. In order to obtain from this the upper bound on the $\mathrm{L}^2(\mathbf{R})$-norm in Eq. (3.10), we are going to verify that the support of $t \mapsto \mathbf{1}_{\mathrm{K}_q(t)}(t)$ is contained in an interval of the form $(\xi - \mathrm{R}, \xi + \mathrm{R})$ for a suitable $\xi \in \mathbf{R}$. Let us start by verifying that

$$x^\kappa(\nu_{t_1}) \geq x^{\kappa - \frac{\alpha^{-2}}{c}}(\nu_{t_2}) \tag{3.11}$$

for $0 < \kappa < 1$ and $t_1, t_2 \in \mathbf{R}$. Note that any $y \in \mathbf{R}$ satisfying the inequality $\int_{-\infty}^{y} \mathrm{d}\nu_{t_2} \leq (\kappa - \frac{\alpha^{-2}}{c}) \int \mathrm{d}\nu_{t_2}$, also satisfies

$$\begin{aligned} \int_{-\infty}^{y} \mathrm{d}\nu_{t_1} &\leq \alpha^{-2} + \int_{-\infty}^{y} \mathrm{d}\nu_{t_2} \leq \alpha^{-2} + \left(\kappa - \frac{\alpha^{-2}}{c}\right) \int \mathrm{d}\nu_{t_2} \\ &\leq \kappa \int \mathrm{d}\nu_{t_2} = \kappa \int \mathrm{d}\nu_{t_1}, \end{aligned}$$

where we have used $\alpha^{-2} \leq \frac{\alpha^{-2}}{c} \int \mathrm{d}\nu_{t_2}$, and therefore $y \leq x^\kappa(\nu_{t_1})$. Using that $x^{\kappa - \frac{\alpha^{-2}}{c}}(\nu_{t_2})$ is the supremum over all such y, we conclude with the desired Eq. (3.11). Furthermore observe that $\nu_{t_0} = \rho_1$ with $t_0 := x_1^1$ and $\rho := \alpha^{-2} \sum_{j=1}^{n} \delta_{x^j} \in \Omega$, and therefore we know by [1, Lemma 3.9] that there exists a $\xi \in \mathbf{R}$ such that $\xi - \mathrm{R} \leq x^{\frac{1}{2} - q'}(\nu_{t_0}) \leq x^{\frac{1}{2} + q'}(\nu_{t_0}) \leq \xi + \mathrm{R}$ for $q' \leq \frac{1}{2} - \frac{\delta}{c^2}$. By our assumptions, $q' := q + \frac{\alpha^{-2}}{c}$ satisfies this condition, and therefore we obtain using Eq. (3.11) with $t_1 := t$, $t_2 := t_0$ and $\kappa := \frac{1}{2} - q$, respectively $t_1 := t_0$, $t_2 := t$ and $\kappa := \frac{1}{2} + q + \frac{\alpha^{-2}}{c}$, that

$$\xi - \mathrm{R} \leq x^{\frac{1}{2} - q}(\nu_t) \leq x^{\frac{1}{2} + q}(\nu_t) \leq \xi + \mathrm{R}$$

for all $t \in \mathbf{R}$, and consequently $\mathbf{1}_{\mathrm{K}_q(t)}(t) = 0$ for $|t - \xi| > \mathrm{R}$. □

Lemma **3.6.** — *Given* $0 < \sigma < \frac{1}{9}$ *and* $\mathrm{C} > 0$, *let* $\Lambda = \alpha^{\frac{4}{5}(1+\sigma)}$ *and* $\mathrm{L} = \alpha^{1+\sigma}$, *and assume* p *satisfies* $|p| \leq \frac{\mathrm{C}}{\alpha}$ *and* $\mathrm{E}_{\alpha,\Lambda}(\alpha^2 p) \leq \mathrm{E}_\alpha + \mathrm{C}|p|^2$ *for a given* $\mathrm{C} > 0$. *Then there exist* $r', c_+ > 0$ *and states* Ψ'''_α *with*

$$\langle \Psi'''_\alpha | \mathbf{H}_\Lambda | \Psi'''_\alpha \rangle - \mathrm{E}_{\alpha,\Lambda}\left(\alpha^2 p\right) \lesssim \alpha^{-(2+r')},$$

$$\left\langle \Psi'''_\alpha \middle| (\Upsilon_\Lambda - p)^2 \middle| \Psi'''_\alpha \right\rangle \lesssim \alpha^{-(2+r')},$$

as well as $\mathrm{supp}(\Psi'''_\alpha) \subseteq \mathrm{B}_{4\mathrm{L}}(0)$ *and* $\chi(\mathcal{N} \leq c_+)\Psi'''_\alpha = \Psi'''_\alpha$, *such that*

$$\left\langle \Psi'''_\alpha \middle| \mathrm{W}^{-1}_{\varphi^{\mathrm{Pek}}} \mathcal{N} \mathrm{W}_{\varphi^{\mathrm{Pek}}} \middle| \Psi'''_\alpha \right\rangle \lesssim \alpha^{-r'}, \tag{3.12}$$

where $\mathrm{W}_{\varphi^{\mathrm{Pek}}}$ *is the Weyl operator corresponding to the Pekar minimizer* φ^{Pek}, *characterized by* $\mathrm{W}^{-1}_{\varphi^{\mathrm{Pek}}} a(f) \mathrm{W}_{\varphi^{\mathrm{Pek}}} = a(f) - \langle f|\varphi^{\mathrm{Pek}}\rangle$ *for all* $f \in \mathrm{L}^2(\mathbf{R}^3)$.

Proof. — For $u > 0$, let us define the functions $f_\ell(y) := \chi^{\frac{1}{2}}(\ell - \frac{1}{2} < \alpha^u y \leq \ell + \frac{1}{2})$ for $\ell \in \mathbf{Z}$ satisfying $|\ell| \leq \frac{3}{2}\alpha^u \mathrm{L}$, as well as $f_{-\infty}(y) := \chi^{\frac{1}{2}}(\alpha^u y \leq -\lfloor \frac{3}{2}\alpha^u \mathrm{L} \rfloor - \frac{1}{2})$ and $f_\infty(\rho) := \chi^{\frac{1}{2}}(\lfloor \frac{3}{2}\alpha^u \mathrm{L}\rfloor + \frac{1}{2} < \alpha^u y)$. With these functions at hand we define for $i \in \{1, 2, 3\}$ and $v > 0$ the partitions $\mathcal{P}_i := \{\mathrm{F}_{\ell,i} : \ell \in \mathrm{A}\}$, where

$$\begin{aligned} \mathrm{F}_{\ell,i}(\rho) &:= f_\ell\big(m_{\alpha^{-v}}(\rho_i)\big), \\ \mathrm{A} &:= \left\{-\infty, -\left\lfloor \frac{3}{2}\alpha^u \mathrm{L}\right\rfloor, -\left\lfloor \frac{3}{2}\alpha^u \mathrm{L}\right\rfloor + 1, \dots, \left\lfloor \frac{3}{2}\alpha^u \mathrm{L}\right\rfloor, \infty\right\} \\ &\subseteq \mathbf{Z} \cup \{-\infty, \infty\}, \end{aligned}$$

as well as $\mathcal{P} := \{\mathrm{F}_z : z \in \mathrm{A}^3\}$ with $\mathrm{F}_z := \mathrm{F}_{z_3,3}\mathrm{F}_{z_2,2}\mathrm{F}_{z_1,1}$. In the following let Ψ''_α be as in Lemma 3.4 with $\delta < \frac{c_-^2}{2}$ and let Ω_{reg} and Ω be the sets from Lemma 3.5 with δ and R as in Lemma 3.4, $q := \alpha^{-v}$ and $c := c_-$. Due to the straightforward result [1, Lemma 3.6] we have $\widehat{\mathbf{1}_{\Omega_{\mathrm{reg}}}}\Psi''_\alpha = \Psi''_\alpha$, and by the definition of Ψ''_α in Eq. (3.7) it is clear that we furthermore have $\widehat{\mathbf{1}_\Omega}\Psi''_\alpha = \Psi''_\alpha$. Therefore we can apply Lemma 3.3 together with Eq. (3.10) in order to obtain

$$\begin{aligned} &\sum_{z_1 \in \mathrm{A}} \left\langle \widehat{\mathrm{F}}_{z_1,1}\Psi''_\alpha \middle| (\Upsilon_\Lambda - p)^2 \middle| \widehat{\mathrm{F}}_{z_1,1}\Psi''_\alpha \right\rangle \\ &\quad \leq \langle \Psi''_\alpha | (\Upsilon_\Lambda - p)^2 | \Psi''_\alpha \rangle + \mathrm{T}\alpha^{\frac{4}{5}(1+\sigma)} \sum_{z_1 \in \mathrm{A}} \alpha^{-4} \frac{\|f'_{z_1}\|^2_\infty}{2\alpha^{-2v} c_-^2} \mathrm{R} \\ &\quad \lesssim \alpha^{\frac{4}{5}\sigma - \frac{16}{5}} + \alpha^{\frac{4}{5}\sigma - \frac{16}{5} + 2v} \sup_{z_1 \in \mathrm{A}} \|f'_{z_1}\|^2_\infty \sum_{z_1 \in \mathrm{A}} 1 \lesssim \alpha^{\frac{9}{5}\sigma + 2v + 3u - \frac{1}{5}} \alpha^{-2} \end{aligned}$$

for all α large enough such that $\alpha^{-v} + \frac{\alpha^{-2}}{c_-} < \frac{1}{2} - \frac{\delta}{c_-^2}$, where we have used $\sup_{z_1 \in \mathrm{A}} \|f'_{z_1}\| \lesssim \alpha^u$, as well as $\sum_{z_1 \in \mathrm{A}} 1 \leq 3(\alpha^u \mathrm{L} + 1) \lesssim \alpha^{u+1+\sigma}$. Since the functions $\mathrm{F}^n_{\ell,i}$ are independent of x^1_1 for $i \in \{2, 3\}$, we furthermore obtain

$$\begin{aligned} &\left\langle \widehat{\mathrm{F}}_{z_1,1}\Psi''_\alpha \middle| (\Upsilon_\Lambda - p)^2 \middle| \widehat{\mathrm{F}}_{z_1,1}\Psi''_\alpha \right\rangle \\ &\quad = \sum_{z_2, z_3 \in \mathrm{A}} \left\langle \widehat{\mathrm{F}}_{z_3,3}\widehat{\mathrm{F}}_{z_2,2}\widehat{\mathrm{F}}_{z_1,1}\Psi''_\alpha \middle| (\Upsilon_\Lambda - p)^2 \middle| \widehat{\mathrm{F}}_{z_3,3}\widehat{\mathrm{F}}_{z_2,2}\widehat{\mathrm{F}}_{z_1,1}\Psi''_\alpha \right\rangle \end{aligned}$$

and therefore

$$\sum_{z\in A^3} Z_z^2 \langle \Psi_z | (\Upsilon_\Lambda - p)^2 | \Psi_z \rangle \lesssim \alpha^{\frac{9}{5}\sigma+2v+3u-\frac{1}{5}} \alpha^{-2} \tag{3.13}$$

with $\Psi_z := Z_z^{-1} \widehat{F}_z \Psi_\alpha''$ and $Z_z := \|\widehat{F}_z \Psi_\alpha''\|$.

Regarding the localization error of the energy, we obtain by [1, Lemma 3.3] and [1, Lemma 3.10] (see also the proof of [1, Eq. (3.22)]) that

$$\begin{aligned}\sum_{z\in A^3} Z_z^2 \langle \Psi_z | \mathbf{H}_\Lambda | \Psi_z \rangle &\leq \langle \Psi_\alpha'' | \mathbf{H}_\Lambda | \Psi_\alpha'' \rangle + O_{\alpha\to\infty}\left(\alpha^{-3}\right) \\ &\leq E_{\alpha,\Lambda}\left(\alpha^2 p\right) + C\alpha^{-2(1+\sigma)}\end{aligned} \tag{3.14}$$

for a suitable constant $C > 0$, as long as $u + v \leq \frac{1}{2}$. In the following, let S be the set of all $z \in A^3$ such that

$$\langle \Psi_z | \mathbf{H}_\Lambda | \Psi_z \rangle > E_{\alpha,\Lambda}\left(\alpha^2 p\right) + \alpha^{-(2+\epsilon)}$$

for a given $\epsilon > 0$, and define $M := \sum_{z\in S} Z_z^2$. By Eq. (3.14), we have

$$M\left(E_{\alpha,\Lambda}\left(\alpha^2 p\right) + \alpha^{-(2+\epsilon)}\right) + (1-M)E_\alpha \leq E_{\alpha,\Lambda}\left(\alpha^2 p\right) + C\alpha^{-2(1+\sigma)},$$

and therefore $1 - M \geq \frac{\alpha^{-(2+\epsilon)} - C\alpha^{-2(1+\sigma)}}{E_{\alpha,\Lambda}(\alpha^2 p) - E_\alpha + \alpha^{-(2+\epsilon)}} \geq C_1 \alpha^{-\epsilon}$ for $\epsilon < 2\sigma$, α large enough and a suitable constant C_1, where we have used the assumption $E_{\alpha,\Lambda}(\alpha^2 p) - E_\alpha \lesssim |p|^2 \lesssim \alpha^{-2}$. Moreover, let us define S' as the set containing all $z \in A^3$, such that

$$\langle \Psi_z | (\Upsilon_\Lambda - p)^2 | \Psi_z \rangle > \alpha^{\frac{1}{2}(\frac{9}{5}\sigma+2v+3u-\frac{1}{5})} \alpha^{-2}$$

and $M' := \sum_{z\in S'} Z_z^2$. By Eq. (3.13) we see that $M' \leq C_2 \alpha^{\frac{1}{2}(\frac{9}{5}\sigma+2v+3u-\frac{1}{5})}$ for a suitable constant C_2. Consequently

$$\sum_{z\notin S\cup S'} Z_z^2 \geq 1 - M - M' \geq C_1\alpha^{-\epsilon} - C_2 \alpha^{\frac{1}{2}(\frac{9}{5}\sigma+2v+3u-\frac{1}{5})}$$

for α large enough. Since $\sigma < \frac{1}{9}$, we can take u, v and ϵ small enough, such that $2\epsilon + \frac{9}{5}\sigma + 2v + 3u < \frac{1}{5}$, and consequently $\sum_{z\notin S\cup S'} Z_z^2 > 0$ for α large enough, which implies the existence of a $z^* \notin S \cup S'$ with $Z_{z_*} > 0$, i.e.

$$\begin{aligned}\langle \Psi_{z^*} | \mathbf{H}_\Lambda | \Psi_{z^*} \rangle &\leq E_{\alpha,\Lambda}\left(\alpha^2 p\right) + \alpha^{-(2+\epsilon)}, \\ \langle \Psi_{z^*} | (\Upsilon_\Lambda - p)^2 | \Psi_{z^*} \rangle &\leq \alpha^{\frac{1}{2}(\frac{9}{5}\sigma+2v+3u-\frac{1}{5})-2}.\end{aligned}$$

In order to rule out that one of the components z_i^* is infinite, let us verify that $\langle \Psi_z | \mathbf{H}_\Lambda | \Psi_z \rangle > E_{\alpha,\Lambda}(\alpha^2 p) + \alpha^{-(2+\epsilon)}$ for α large enough in case there exists an

$i \in \{1,2,3\}$ with $z_i = \pm\infty$. Note that $\rho \in \mathrm{supp}(\mathrm{F}_{-\infty,i})$ implies $m_{\alpha^{-v}}(\rho_i) < -\frac{3}{2}\mathrm{L}$ and therefore $\int_{|x|>\frac{3}{2}\mathrm{L}} \mathrm{d}\rho \geq \int_{-\infty}^{-\frac{3}{2}\mathrm{L}} \mathrm{d}\rho_i \geq \int_{-\infty}^{m_{\alpha^{-v}}(\rho_i)} \mathrm{d}\rho_i \geq (\frac{1}{2} - \alpha^{-v}) \int \mathrm{d}\rho$. Similarly $\int_{|x|>\frac{3}{2}\mathrm{L}} \mathrm{d}\rho \geq (\frac{1}{2} - \alpha^{-v}) \int \mathrm{d}\rho$ for $\rho \in \mathrm{supp}(\mathrm{F}_{\infty,i})$. Consequently we have for any z with $z_i = \pm\infty$ for some $i \in \{1,2,3\}$

$$\langle \Psi_z | \mathcal{N}_{\mathbf{R}^3 \setminus \mathrm{B}_{\frac{3}{2}\mathrm{L}}(0)} | \Psi_z \rangle \geq \left(\frac{1}{2} - \alpha^{-v} \right) \langle \Psi_z | \mathcal{N} | \Psi_z \rangle ,$$

where $\mathcal{N}_{\mathbf{R}^3 \setminus \mathrm{B}_{\frac{3}{2}\mathrm{L}}(0)} := \widehat{\mathrm{G}}$ with $\mathrm{G}(\rho) := \int_{|x|>\frac{3}{2}\mathrm{L}} \mathrm{d}\rho$. Therefore [1, Corollary B.7] together with the fact that $\mathrm{supp}(\Psi_z) \subset \mathrm{supp}(\Psi''_\alpha) \subset \mathrm{B}_\mathrm{L}(0)$, yields

$$\begin{aligned}
\langle \Psi_z | \mathbf{H}_\Lambda | \Psi_z \rangle &\geq \mathrm{E}_\alpha + \left(\frac{1}{2} - \alpha^{-v} \right) \langle \Psi_z | \mathcal{N} | \Psi_z \rangle - \sqrt{\frac{\mathrm{D}}{\frac{3}{2}\mathrm{L} - \mathrm{L}}} \\
&\geq \mathrm{E}_\alpha + \left(\frac{1}{2} - \alpha^{-v} \right) c_- - \sqrt{2\mathrm{D}\alpha^{-(1+\sigma)}} \\
&= \mathrm{E}_{\alpha,\Lambda}\left(\alpha^2 p\right) + \frac{1}{2} + \mathrm{O}_{\alpha\to\infty}\left(\alpha^{-v}\right) \\
&> \mathrm{E}_{\alpha,\Lambda}\left(\alpha^2 p\right) + \alpha^{-(2+\epsilon)}
\end{aligned}$$

for a suitable constant $\mathrm{D} > 0$ and α large enough. Hence we obtain that all components z_i^* are finite, i.e. $m_{\alpha^{-v}}(\rho) \in \mathrm{B}_{\sqrt{3}\alpha^{-u}}(\alpha^{-u} z^*) \subseteq \mathbf{R}^3$ for $\rho \in \mathrm{supp}(\mathrm{F}_{z_3^*,3}\mathrm{F}_{z_2^*,2}\mathrm{F}_{z_1^*,1})$.

Let $\Psi'''_\alpha := \mathcal{T}_{-\alpha^{-u}z^*} \Psi_{z^*}$, where $\mathcal{T}_z$ is a joint translation in the electron and phonon component, i.e. $(\mathcal{T}_z \Psi)(x) := \mathrm{U}_z \Psi(x - z)$ with U_z being defined by $\mathrm{U}_z^{-1} a(f) \mathrm{U}_z = a(f_z)$ and $f_z(y) := f(y - z)$. Using the fact that

$$\langle \Psi_{z^*} | \mathbf{H}_\Lambda | \Psi_{z^*} \rangle \leq \mathrm{E}_{\alpha,\Lambda}\left(\alpha^2 p\right) + \alpha^{-(2+\epsilon)} \lesssim \mathrm{E}_\alpha + \alpha^{-\frac{2}{29}}$$

as well as $\mathbf{1}_{\Omega^*} \Psi'''_\alpha = \Psi'''_\alpha$, where Ω^* is the set of all ρ satisfying $\int \mathrm{d}\rho \leq c_+$ and $m_{\alpha^{-v}}(\rho) \in \mathrm{B}_{\sqrt{3}\alpha^{-u}}(0)$, we can apply [1, Lemma 3.11], which yields

$$\left\langle \Psi'''_\alpha \middle| \mathrm{W}^{-1}_{\varphi^{\mathrm{Pek}}} \mathcal{N} \mathrm{W}_{\varphi^{\mathrm{Pek}}} \middle| \Psi'''_\alpha \right\rangle \lesssim \alpha^{-\frac{2}{29}} + \alpha^{-u} + \alpha^{-v}.$$

By taking $r' > 0$ small enough such that $r' \leq \frac{1}{2}(\frac{1}{5} - \frac{9}{5}\sigma - 2v - 3u)$, $r' \leq \epsilon$ and $r' \leq \min\{\frac{2}{29}, u, v\}$, we conclude that $\langle \Psi'''_\alpha | \mathrm{W}^{-1}_{\varphi^{\mathrm{Pek}}} \mathcal{N} \mathrm{W}_{\varphi^{\mathrm{Pek}}} | \Psi'''_\alpha \rangle \lesssim \alpha^{-r'}$. Since $\mathrm{supp}(\Psi'''_\alpha) \subset \mathrm{B}_\mathrm{L}(-\alpha^{-u} z^*) \subset \mathrm{B}_{\mathrm{L}+\alpha^{-u}|z^*|}(0) \subset \mathrm{B}_{4\mathrm{L}}(0)$, this concludes the proof. □

In the following Theorem 3.7, which is the main result of this section, we will lift the (weak) condensation from Eq. (3.12) to a strong one without introducing a large energy penalty, using an argument in [8]. We will verify that the momentum error due to the localization is negligibly small as well.

Theorem **3.7.** — *Given* $0 < \sigma < \frac{1}{9}$ *and* $C > 0$, *let* $\Lambda = \alpha^{\frac{4}{5}(1+\sigma)}$ *and* $L = \alpha^{1+\sigma}$, *and assume* p *satisfies* $|p| \leq \frac{C}{\alpha}$ *and* $E_{\alpha,\Lambda}(\alpha^2 p) \leq E_\alpha + C|p|^2$ *for a given* $C > 0$. *Then there exists a* $r > 0$ *and states* Ψ_α *with*

$$\langle \Psi_\alpha | \mathbf{H}_\Lambda | \Psi_\alpha \rangle - E_{\alpha,\Lambda}\left(\alpha^2 p\right) \lesssim \alpha^{-(2+r)},$$
$$\left\langle \Psi_\alpha \middle| (\Upsilon_\Lambda - p)^2 \middle| \Psi_\alpha \right\rangle \lesssim \alpha^{-(2+r)}$$

and $\mathrm{supp}(\Psi_\alpha) \subseteq B_{4L}(0)$, *such that*

$$\chi\left(W^{-1}_{\varphi^{\mathrm{Pek}}-i\xi} \mathcal{N} W_{\varphi^{\mathrm{Pek}}-i\xi} \leq \alpha^{-r}\right)\Psi_\alpha = \Psi_\alpha, \tag{3.15}$$

where $\xi := \frac{p}{m}\widetilde{\nabla}_{x_1}\varphi^{\mathrm{Pek}}$ *with* $\widetilde{\nabla}_{x_1} := \chi^1(\Lambda^{-1}|\nabla_{x_1}| \leq 2)\nabla_{x_1}$.

Note that ξ is small in magnitude, $\|\xi\| \lesssim |p| \lesssim \alpha^{-1}$. The statement of Theorem 3.7 is also valid for $\xi = 0$, i.e., in case we conjugate by the Weyl transformation $W_{\varphi^{\mathrm{Pek}}}$ instead of $W_{\varphi^{\mathrm{Pek}}-i\xi}$. For technical reasons, it will however be useful in the proof of Theorem 2.1 to use $\varphi^{\mathrm{Pek}} - i\xi \approx \varphi^{\mathrm{Pek}} - i\frac{p}{m}\nabla_{x_1}\varphi^{\mathrm{Pek}}$ as a reference state, since the latter satisfies the momentum constraint

$$\left\langle \varphi^{\mathrm{Pek}} - i\frac{p}{m}\nabla_{x_1}\varphi^{\mathrm{Pek}} \middle| \frac{1}{i}\nabla \middle| \varphi^{\mathrm{Pek}} - i\frac{p}{m}\nabla_{x_1}\varphi^{\mathrm{Pek}} \right\rangle = p.$$

Proof. — Let Ψ'''_α be as in Lemma 3.6 and let us define for $0 < \epsilon < \frac{1}{2}$ and $0 < h < \min\{r', \frac{1}{4}\}$

$$\Psi_\alpha := Z_\alpha^{-1}\chi^\epsilon\left(\alpha^h W^{-1}_{\varphi^{\mathrm{Pek}}-i\xi}\mathcal{N}W_{\varphi^{\mathrm{Pek}}-i\xi} \leq \frac{1}{2}\right)\Psi'''_\alpha,$$

where $Z_\alpha := \|\chi^\epsilon(\alpha^h W^{-1}_{\varphi^{\mathrm{Pek}}-i\xi}\mathcal{N}W_{\varphi^{\mathrm{Pek}}-i\xi} \leq \frac{1}{2})\Psi'''_\alpha\|$ is a normalization constant. Clearly the states Ψ_α satisfy Eq. (3.15) for $r \leq h$. Let us furthermore define

$$\widetilde{\Psi}_\alpha := \frac{1}{\sqrt{1 - Z_\alpha^2}}\chi^\epsilon\left(\frac{1}{2} \leq \alpha^h W^{-1}_{\varphi^{\mathrm{Pek}}-i\xi}\mathcal{N}W_{\varphi^{\mathrm{Pek}}-i\xi}\right)\Psi'''_\alpha$$

An application of [1, Lemma 3.3] yields

$$\begin{aligned}
&Z_\alpha^2\langle\Psi_\alpha|\mathbf{H}_\Lambda|\Psi_\alpha\rangle + \left(1 - Z_\alpha^2\right)\langle\widetilde{\Psi}_\alpha|\mathbf{H}_\Lambda|\widetilde{\Psi}_\alpha\rangle \\
&\quad\leq \langle\Psi'''_\alpha|\mathbf{H}_\Lambda|\Psi'''_\alpha\rangle + C_0\alpha^{2h-\frac{7}{2}}\langle\Psi'''_\alpha|\sqrt{\mathcal{N}+1}|\Psi'''_\alpha\rangle \\
&\quad\leq E_{\alpha,\Lambda}\left(\alpha^2 p\right) + C_1\alpha^{-(2+r'')}
\end{aligned}$$

for suitable constants $C_0, C_1 > 0$ and $r'' := \min\{r', \frac{3}{2} - 2h\} > 0$. We have

$$\begin{aligned} 1 - Z_\alpha^2 &= \left\langle \Psi_\alpha''' \middle| \chi^\epsilon \left(\frac{1}{2} \leq \alpha^h W^{-1}_{\varphi^{\text{Pek}} - i\xi} \mathcal{N} W_{\varphi^{\text{Pek}} - i\xi} \right)^2 \middle| \Psi_\alpha''' \right\rangle \\ &\leq \frac{2\alpha^h}{1 - 2\epsilon} \langle \Psi_\alpha''' | W^{-1}_{\varphi^{\text{Pek}} - i\xi} \mathcal{N} W_{\varphi^{\text{Pek}} - i\xi} | \Psi_\alpha''' \rangle \\ &\leq \frac{4\alpha^h}{1 - 2\epsilon} \langle \Psi_\alpha''' | W^{-1}_{\varphi^{\text{Pek}}} \mathcal{N} W_{\varphi^{\text{Pek}}} | \Psi_\alpha''' \rangle + \frac{4\alpha^h \|\xi\|^2}{1 - 2\epsilon} \\ &\lesssim \frac{1}{1 - 2\epsilon} \left(\alpha^{h - r'} + \alpha^{h-2} \right) \underset{\alpha \to \infty}{\longrightarrow} 0, \end{aligned}$$

where we used Eq. (3.12) and the inequalities

$$\begin{aligned} &W^{-1}_{\varphi^{\text{Pek}} - i\xi} \mathcal{N} W_{\varphi^{\text{Pek}} - i\xi} \leq 2 \left(W^{-1}_{\varphi^{\text{Pek}}} \mathcal{N} W_{\varphi^{\text{Pek}}} + \|\xi\|^2 \right), \\ &\|\xi\|^2 \leq |p|^2 \left\| \nabla \varphi^{\text{Pek}} \right\|^2 \lesssim \alpha^{-2}. \end{aligned}$$

Making use of $\langle \widetilde{\Psi}_\alpha | \mathbf{H}_\Lambda | \widetilde{\Psi}_\alpha \rangle \geq E_\alpha$ and $E_{\alpha,\Lambda}(\alpha^2 p) - E_\alpha \lesssim |p|^2 \lesssim \alpha^{-2}$, we therefore obtain

$$\begin{aligned} &\langle \Psi_\alpha | \mathbf{H}_\Lambda | \Psi_\alpha \rangle - E_{\alpha,\Lambda}\left(\alpha^2 p\right) \\ &\quad \leq Z_\alpha^{-2} \left(C_1 \alpha^{-(2 + r'')} + \left(1 - Z_\alpha^2\right) \left(E_{\alpha,\Lambda}\left(\alpha^2 p\right) - E_\alpha \right) \right) \\ &\quad \lesssim \alpha^{-(2 + r'')} + \left(\alpha^{h - r'} + \alpha^{h-2} \right) \left(E_{\alpha,\Lambda}\left(\alpha^2 p\right) - E_\alpha \right) \lesssim \alpha^{-(2 + r''')} \end{aligned}$$

with $r''' := \min\{r'', r' - h, 2 - h\} > 0$.

In order to estimate $\langle \Psi_\alpha | (\Upsilon_\Lambda - p)^2 | \Psi_\alpha \rangle$, let us apply the IMS identity

$$\begin{aligned} &Z_\alpha^2 \langle \Psi_\alpha | (\Upsilon_\Lambda - p)^2 | \Psi_\alpha \rangle + \left(1 - Z_\alpha^2\right) \langle \widetilde{\Psi}_\alpha | (\Upsilon_\Lambda - p)^2 | \widetilde{\Psi}_\alpha \rangle \\ &\quad = \langle \Psi_\alpha''' | (\Upsilon_\Lambda - p)^2 | \Psi_\alpha''' \rangle - \langle \Psi_\alpha''' | X | \Psi_\alpha''' \rangle, \end{aligned} \tag{3.16}$$

where we define $X := \frac{1}{2}[[(\Upsilon_\Lambda - p)^2, A_1], A_1] + \frac{1}{2}[[(\Upsilon_\Lambda - p)^2, A_2], A_2]$ using the operators $A_1 := f_1(W^{-1}_{\varphi^{\text{Pek}} - i\xi} \mathcal{N} W_{\varphi^{\text{Pek}} - i\xi})$ and $A_2 := f_2(W^{-1}_{\varphi^{\text{Pek}} - i\xi} \mathcal{N} W_{\varphi^{\text{Pek}} - i\xi})$ with $f_1(x) := \chi^\epsilon(\alpha^h x \leq \frac{1}{2})$ and $f_2 := \chi^\epsilon(\frac{1}{2} \leq \alpha^h x)$. In the following let us compute

$$\begin{aligned} &\left[\left[(\Upsilon_\Lambda - p)^2, A_j\right], A_j\right] \\ &\quad = W^{-1}_{\varphi^{\text{Pek}} - i\xi} \left[\left[\left(W_{\varphi^{\text{Pek}} - i\xi} \Upsilon_\Lambda W^{-1}_{\varphi^{\text{Pek}} - i\xi} - p\right)^2, f_j(\mathcal{N})\right], f_j(\mathcal{N})\right] W_{\varphi^{\text{Pek}} - i\xi} \\ &\quad = W^{-1}_{\varphi^{\text{Pek}} - i\xi} \left[\left[\left(\Upsilon_\Lambda - \widetilde{p} + 2\mathfrak{Re}\, a^\dagger(\varphi)\right)^2, f_j(\mathcal{N})\right], f_j(\mathcal{N})\right] W_{\varphi^{\text{Pek}} - i\xi} \end{aligned}$$

where $\varphi := \frac{1}{i} \widetilde{\nabla}_{x_1} (\varphi^{\text{Pek}} - i\xi)$ and

$$\widetilde{p} := p - \left\langle \varphi^{\text{Pek}} - i\xi \middle| \frac{1}{i} \widetilde{\nabla}_{x_1} \middle| \varphi^{\text{Pek}} - i\xi \right\rangle = p \left(1 - \frac{2}{m} \left\| \widetilde{\nabla}_{x_1} \varphi^{\text{Pek}} \right\|^2 \right).$$

We have $|\widetilde{p}| \leq |p| \leq \frac{C}{\alpha}$ since $m = \frac{2}{3}\|\nabla\varphi^{\mathrm{Pek}}\|^2 = 2\|\nabla_{x_1}\varphi^{\mathrm{Pek}}\|^2 \geq 2\|\widetilde{\nabla}_{x_1}\varphi^{\mathrm{Pek}}\|^2$. Defining the discrete derivative $\delta f_j(x) := \alpha^2(f_j(x+\alpha^{-2}) - f_j(x))$, we can further write

$$\begin{aligned}
&\Big[\Big[\big(\Upsilon_\Lambda - \widetilde{p} + 2\mathfrak{Re}\, a^\dagger(\varphi)\big)^2, f_j(\mathcal{N})\Big], f_j(\mathcal{N})\Big] \\
&\quad = 8\big[\mathfrak{Re}\, a^\dagger(\varphi), f(\mathcal{N})\big]^2 \\
&\qquad + 2\big\{\Upsilon_\Lambda - \widetilde{p} + 2\mathfrak{Re}\, a^\dagger(\varphi), \big[\big[\mathfrak{Re}\, a^\dagger(\varphi), f_j(\mathcal{N})\big], f_j(\mathcal{N})\big]\big\} \\
&\quad = -8\alpha^{-4}\big(\mathfrak{Im}\big(a^\dagger(\varphi)\delta f_j(\mathcal{N})\big)\big)^2 \\
&\qquad + 2\alpha^{-4}\big\{\Upsilon_\Lambda - \widetilde{p} + 2\mathfrak{Re} a^\dagger(\varphi), \mathfrak{Re}\big(a^\dagger(\varphi)(\delta f_j)^2(\mathcal{N})\big)\big\}
\end{aligned}$$

where we used

$$\begin{aligned}
&\big[\Upsilon_\Lambda - \widetilde{p} + 2\mathfrak{Re}\, a^\dagger(\varphi), f_j(\mathcal{N})\big] = 2\big[\mathfrak{Re}\, a^\dagger(\varphi), f_j(\mathcal{N})\big], \\
&\big[\mathfrak{Re}\, a^\dagger(\varphi), f_j(\mathcal{N})\big] = \alpha^{-2} i\mathfrak{Im}\big(a^\dagger(\varphi)\delta f_j(\mathcal{N})\big), \\
&\big[\big[\mathfrak{Re}\, a^\dagger(\varphi), f_j(\mathcal{N})\big], f_j(\mathcal{N})\big] = \alpha^{-4}\mathfrak{Re}\big(a^\dagger(\varphi)(\delta f_j)^2(\mathcal{N})\big).
\end{aligned}$$

Hence

$$\begin{aligned}
&-\Big[\Big[\big(\Upsilon_\Lambda - \widetilde{p} + 2\mathfrak{Re}\, a^\dagger(\varphi)\big)^2, f_j(\mathcal{N})\Big], f_j(\mathcal{N})\Big] \\
&\quad \leq 8\alpha^{-4}\mathfrak{Im}\big(a^\dagger(\varphi)\delta f_j(\mathcal{N})\big)^2 \\
&\qquad + 4\alpha^{-3}\,\mathfrak{Re}\big(a^\dagger(\varphi)(\delta f_j)^2(\mathcal{N})\big)^2 + \alpha^{-5}\big(\Upsilon_\Lambda - \widetilde{p} + 2\mathfrak{Re}\, a^\dagger(\varphi)\big)^2 \\
&\quad \leq 2\|\varphi\|^2\big(2\alpha^{-4}\|\delta f_j\|_\infty^2 + 2\alpha^{-3}\|\delta f_j\|_\infty^4 + 3\alpha^{-5}\big)\big(2\mathcal{N} + \alpha^{-2}\big) \\
&\qquad + 27\alpha^{-3}\mathcal{N}^2 + 3\alpha^{-5}|\widetilde{p}|^2,
\end{aligned} \tag{3.17}$$

where we have applied multiple Cauchy–Schwarz estimates and used $\Upsilon_\Lambda^2 \leq 9\alpha^2\mathcal{N}^2$. Note that the expression in the last line of Eq. (3.17) is of order $\alpha^{4h-3}(\mathcal{N}+1)^2$, since $\|\delta f_j\|_\infty \lesssim \alpha^h$ and $\|\varphi\| \lesssim 1$. Using $W^{-1}_{\varphi^{\mathrm{Pek}}-i\xi}(\mathcal{N}+1)^2 W_{\varphi^{\mathrm{Pek}}-i\xi} \lesssim (\mathcal{N}+1)^2$ we therefore obtain

$$-X = -\frac{1}{2}\sum_{j=1}^{2}\big[\big[(\Upsilon_\Lambda - p)^2, A_j\big], A_j\big] \lesssim \alpha^{4h-3}(\mathcal{N}+1)^2.$$

Using this together with Eq. (3.16) and $\langle\widetilde{\Psi}_\alpha|(\Upsilon_\Lambda - p)^2|\widetilde{\Psi}_\alpha\rangle \geq 0$, yields

$$\begin{aligned}
\big\langle\Psi_\alpha\big|(\Upsilon_\Lambda - p)^2\big|\Psi_\alpha\big\rangle &\leq Z_\alpha^{-2}\big(\big\langle\Psi_\alpha'''\big|(\Upsilon_\Lambda - p)^2\big|\Psi_\alpha'''\big\rangle - \big\langle\Psi_\alpha'''|X|\Psi_\alpha'''\big\rangle\big) \\
&\lesssim \alpha^{-(2+r')} + \alpha^{4h-3}\big\langle\Psi_\alpha'''\big|(\mathcal{N}+1)^2\big|\Psi_\alpha'''\big\rangle \\
&\lesssim \alpha^{-(2+r')} + \alpha^{4h-3}.
\end{aligned}$$

Since $h < \frac{1}{4}$ we have $\min\{r', 1 - 4h\} > 0$, and therefore we can choose $r > 0$ small enough such that $r \leq \min\{r', 1 - 4h\}$, $r \leq r'''$ and $r \leq h$, which concludes the proof. □

4. Proof of Theorem 2.1

In this section we shall prove the main technical Theorem 2.1, using the results of the previous sections as well as the results in the previous part of this paper series [1]. Before we do this let us recall some definitions from [1].

Definition **4.1** *(Finite dimensional Projection* Π*). — Given* $\sigma > 0$*, let* $\Lambda := \alpha^{\frac{4}{5}(1+\sigma)}$ *and* $\ell := \alpha^{-4(1+\sigma)}$*, and let us introduce the cubes*

$$C_z := [z_1 - \ell, z_1 + \ell) \times [z_2 - \ell, z_2 + \ell) \times [z_3 - \ell, z_3 + \ell)$$

for $z = (z_1, z_2, z_3) \in 2\ell\,\mathbf{Z}^3$*. Then we define* Π *as the orthogonal projection onto the subspace spanned by the functions* $x \mapsto \int_{C_z} \frac{e^{ik\cdot x}}{|k|}\,\mathrm{d}k$ *for* $z \in 2\ell\,\mathbf{Z}^3 \setminus \{0\}$ *satisfying* $C_z \subset B_\Lambda(0)$*. Furthermore, let* $\varphi_1, \ldots, \varphi_N$ *be a real orthonormal basis of* $\Pi L^2(\mathbf{R}^3)$*, such that* $\varphi_n = \frac{\Pi\nabla_{x_n}\varphi^{\mathrm{Pek}}}{\|\Pi\nabla_{x_n}\varphi^{\mathrm{Pek}}\|}$ *for* $n \in \{1, 2, 3\}$*.*

Definition **4.2** *(Coordinate Transformation* τ*). — Let* $\varphi_x^{\mathrm{Pek}}(y) := \varphi^{\mathrm{Pek}}(y - x)$ *and let* $t \mapsto x_t$ *be the local inverse of the function* $x \mapsto (\langle\varphi_n|\varphi_x^{\mathrm{Pek}}\rangle)_{n=1}^3 \in \mathbf{R}^3$ *defined for* $t \in B_{\delta_*}(0)$ *with a suitable* $\delta_* > 0$*. Note that we can take* $B_{\delta_*}(0)$ *as the domain of the local inverse, since* $\langle\varphi_n|\varphi_0^{\mathrm{Pek}}\rangle = 0$ *for all* $n \in \{1, 2, 3\}$ *due to the fact that* φ^{Pek} *and* Π *respect the reflection symmetry* $y_n \mapsto -y_n$*. Then we define* $f : \mathbf{R}^3 \longrightarrow \Pi L^2(\mathbf{R}^3)$ *as*

$$f(t) := \chi\big(|t| < \delta_*\big)\left(\Pi\varphi_{x_t}^{\mathrm{Pek}} - \sum_{n=1}^{3} t_n\varphi_n\right)$$

and the transformation $\tau : \Pi L^2(\mathbf{R}^3) \longrightarrow \Pi L^2(\mathbf{R}^3)$ *as*

$$\tau(\varphi) := \varphi - f\big(t^\varphi\big)$$

with $t^\varphi := (\langle\varphi_1|\varphi\rangle, \langle\varphi_2|\varphi\rangle, \langle\varphi_3|\varphi\rangle) \in \mathbf{R}^3$*.*

Definition **4.3** *(Quadratic Approximation* $J_{t,\gamma}$*). — Let us first define the operators*

$$K^{\mathrm{Pek}} := 1 - H^{\mathrm{Pek}} = 4(-\Delta)^{-\frac{1}{2}}\psi^{\mathrm{Pek}}\frac{1 - |\psi^{\mathrm{Pek}}\rangle\langle\psi^{\mathrm{Pek}}|}{-\Delta + V^{\mathrm{Pek}} - \mu^{\mathrm{Pek}}}\psi^{\mathrm{Pek}}(-\Delta)^{-\frac{1}{2}}, \tag{4.1}$$

$$L^{\mathrm{Pek}} := 4(-\Delta)^{-\frac{1}{2}}\psi^{\mathrm{Pek}}(1 - \Delta)^{-1}\psi^{\mathrm{Pek}}(-\Delta)^{-\frac{1}{2}}, \tag{4.2}$$

where $V^{\mathrm{Pek}} := -2(-\Delta)^{-\frac{1}{2}}\varphi^{\mathrm{Pek}}$*,* $\mu^{\mathrm{Pek}} := e^{\mathrm{Pek}} - \|\varphi^{\mathrm{Pek}}\|^2$ *and* ψ^{Pek} *is the, non-negative, ground state of the operator* $-\Delta + V^{\mathrm{Pek}}$*. Furthermore let* T_x *be the translation operator, i.e.* $(T_x\varphi)(y) := \varphi(y - x)$*,* *and let* $\mathrm{K}_x^{\mathrm{Pek}} := \mathrm{T}_x \mathrm{K}^{\mathrm{Pek}} \mathrm{T}_{-x}$ *and* $\mathrm{L}_x^{\mathrm{Pek}} := \mathrm{T}_x \mathrm{L}^{\mathrm{Pek}} \mathrm{T}_{-x}$. *Then we define*

$$\mathrm{J}_{t,\gamma} := \pi\left(1-(1+\gamma)\left(\mathrm{K}_{x_t}^{\mathrm{Pek}}+\gamma \mathrm{L}_{x_t}^{\mathrm{Pek}}\right)\right)\pi$$

for $|t|<\gamma$ *and* $\gamma<\delta_*$, *where* δ_* *and* x_t *are as in Definition 4.2 and* $\pi : \mathrm{L}^2(\mathbf{R}^3) \longrightarrow \mathrm{L}^2(\mathbf{R}^3)$ *is the orthogonal projection on the space spanned by* $\{\varphi_4, \dots, \varphi_{\mathrm{N}}\}$ *with* φ_n *as in Definition 4.1. Furthermore we define* $\mathrm{J}_{t,\gamma} := \pi$ *for* $|t| \geq \gamma$ *and we will use the shorthand notation* $\mathrm{J}_{t,\gamma}[\varphi] := \langle \varphi | \mathrm{J}_{t,\gamma} | \varphi \rangle$.

Recall the definition of $\mathrm{E}_{\alpha,\Lambda}$ in Theorem 2.1. In the following we will assume that p satisfies the assumption $\mathrm{E}_{\alpha,\Lambda}(\alpha^2 p) \leq \mathrm{E}_\alpha + \mathrm{C}|p|^2$ of Theorem 3.7 with $\mathrm{C} \geq \frac{1}{2m}$, which we can do w.l.o.g., since $\mathrm{E}_{\alpha,\Lambda}(\alpha^2 p) > \mathrm{E}_\alpha + \mathrm{C}|p|^2$ immediately implies the statement of Theorem 2.1 (compare with the comment above Lemma 3.1). We shall also assume in the following that $|p| \leq \frac{\mathrm{C}}{\alpha}$. Due to these assumptions we can apply Theorem 3.7, which yields the existence of a sequence Ψ_α with

$$\langle \Psi_\alpha | \mathbf{H}_\Lambda | \Psi_\alpha \rangle - \mathrm{E}_{\alpha,\Lambda}\left(\alpha^2 p\right) \lesssim \alpha^{-(2+r)},$$
$$\left\langle \Psi_\alpha \middle| (\Upsilon_\Lambda - p)^2 \middle| \Psi_\alpha \right\rangle \lesssim \alpha^{-(2+r)},$$

and $\mathrm{supp}(\Psi_\alpha) \subseteq \mathrm{B}_{4\mathrm{L}}(0)$ with $\mathrm{L} = \alpha^{1+\sigma}$, such that $\widetilde{\Psi}_\alpha := \mathrm{W}_{-i\xi} \Psi_\alpha$ with $\xi = \frac{p}{m} \widetilde{\nabla}_{x_1} \varphi^{\mathrm{Pek}}$ satisfies condensation with respect to φ^{Pek}, i.e.

$$\chi\left(\mathrm{W}_{\varphi^{\mathrm{Pek}}}^{-1} \mathcal{N} \mathrm{W}_{\varphi^{\mathrm{Pek}}} \leq \alpha^{-r}\right) \widetilde{\Psi}_\alpha = \widetilde{\Psi}_\alpha. \tag{4.3}$$

Using $\frac{p}{m}(p - \Upsilon_\Lambda) \leq \alpha^{-\frac{r}{2}} \frac{|p|^2}{4m^2} + \alpha^{\frac{r}{2}} (p - \Upsilon_\Lambda)^2$ and $|p| \leq \frac{\mathrm{C}}{\alpha}$, we therefore have

$$\mathrm{E}_{\alpha,\Lambda}\left(\alpha^2 p\right) \geq \left\langle \Psi_\alpha \middle| \mathbf{H}_\Lambda + \frac{p}{m}(p - \Upsilon_\Lambda) \middle| \Psi_\alpha \right\rangle + \mathrm{O}_{\alpha \to \infty}\left(\alpha^{-(2+\frac{r}{2})}\right), \tag{4.4}$$

where $\frac{p}{m}$ formally acts as a Lagrange multiplier for the minimization of $\mathbf{H}_\Lambda$ subject to the constraint $\Upsilon_\Lambda = p$. In the rest of this Section we will verify that

$$\mathbf{H}_\Lambda + \frac{p}{m}(p - \Upsilon_\Lambda)$$

is bounded from below by the right hand side of Eq. (2.3) when tested against a state Ψ satisfying $\mathrm{supp}(\Psi) \subseteq \mathrm{B}_{4\mathrm{L}}(0)$ and complete condensation with respect to $\varphi^{\mathrm{Pek}} - i\xi$ (where we find it convenient to use $\varphi^{\mathrm{Pek}} - i\xi$ instead of φ^{Pek} for technical reasons). The momentum constraint on Ψ will not be needed for this; i.e., we have transformed our original constrained minimization problem into a global one, which we handle similarly as in the previous part [1] concerning a lower bound on the global minimum $\mathrm{E}_\alpha = \inf \sigma(\mathbf{H})$. As already stressed in the Section 1, it is essential to work with the truncated Hamiltonian $\mathbf{H}_\Lambda$ and the truncated momentum Υ_Λ here, since in contrast to $\mathbf{H}_\Lambda + \frac{p}{m}(p - \Upsilon_\Lambda)$ the operator $\mathbf{H} + \frac{p}{m}(p - \mathbf{P})$ is not bounded from below for $p \neq 0$.

Following [1], we will identify $\mathcal{F}(\Pi L^2(\mathbf{R}^3))$ with $L^2(\mathbf{R}^N)$ using the representation of real-valued functions $\varphi = \sum_{n=1}^N \lambda_n \varphi_n$ by points

$$\lambda = (\lambda_1, \ldots, \lambda_N) \in \mathbf{R}^N.$$

With this identification, we can represent the annihilation operators $a_n := a(\varphi_n)$ as $a_n = \lambda_n + \frac{1}{2\alpha^2}\partial_{\lambda_n}$, where λ_n is the multiplication operator by the function $\lambda \mapsto \lambda_n$ on $L^2(\mathbf{R}^N)$. Let us also use for functions $\varphi \mapsto g(\varphi)$ depending on elements $\varphi \in \Pi L^2(\mathbf{R}^3)$ the convenient notation $g(\lambda) := g(\sum_{n=1}^N \lambda_n \varphi_n)$, where $\lambda \in \mathbf{R}^N$.

It is essential for our proof that $\widetilde{\Psi}_\alpha$ satisfies complete condensation in φ^{Pek}, see Eq. (4.3), since it allows us to apply [1, Lemma 6.1] which states that in terms of the quadratic operator $J_{t,\gamma}$ and the transformation τ on $\Pi L^2(\mathbf{R}^3)$ in Definitions 4.3 and 4.2 we have

$$\langle \widetilde{\Psi}_\alpha | \mathbf{H}_\Lambda | \widetilde{\Psi}_\alpha \rangle \geq e^{\mathrm{Pek}} + \left\langle \widetilde{\Psi}_\alpha \middle| -\frac{1}{4\alpha^4} \sum_{n=1}^N \partial_{\lambda_n}^2 + J_{t^\lambda, \alpha^{-s}}\big[\tau(\lambda)\big] + \mathcal{N}_{>N} \middle| \widetilde{\Psi}_\alpha \right\rangle - \frac{N}{2\alpha^2} + O_{\alpha\to\infty}\big(\alpha^{-(2+\epsilon)}\big) \tag{4.5}$$

for suitable $\epsilon, s_0 > 0$ and any $0 < s < s_0$, where we define

$$\mathcal{N}_{>N} := \mathcal{N} - \sum_{k=1}^N a_k^\dagger a_k$$

and t^φ is defined as in Definition 4.2 such that $t^\lambda = (\lambda_1, \lambda_2, \lambda_3) \in \mathbf{R}^3$. Furthermore it is shown in [1, Lemma 6.1], that there exists a $\beta > 0$, such that

$$\langle \widetilde{\Psi}_\alpha | 1 - \mathbf{B} | \widetilde{\Psi}_\alpha \rangle \leq e^{-\beta \alpha^{2-2s}} \tag{4.6}$$

for all $0 < s < s_0$, where $\mathbf{B}$ is the multiplication operator by the function $\lambda \mapsto \chi(|t^\lambda| < \alpha^{-s})$. In the following we will always choose $s < 1$. We will use the symbol w for a generic, positive constant, which is allowed to vary from line to line.

4.1. *Quasi-quadratic lower bound.* — In order to find a good lower bound on

$$\left\langle \Psi_\alpha \middle| \mathbf{H}_\Lambda + \frac{p}{m}(p - \Upsilon_\Lambda) \middle| \Psi_\alpha \right\rangle,$$

and therefore on $E_{\alpha,\Lambda}(\alpha^2 p)$, it is natural to conjugate $\mathbf{H}_\Lambda + \frac{p}{m}(p - \Upsilon_\Lambda)$ with the Weyl transformation $W_{\varphi^{\mathrm{Pek}} - i\xi} = W_{\varphi^{\mathrm{Pek}}} W_{-i\xi}$, since $\varphi^{\mathrm{Pek}} - i\xi$ is close to the minimizer $\varphi^{\mathrm{Pek}} - i\frac{p}{m}\nabla_{x_1}\varphi^{\mathrm{Pek}}$ of the corresponding classical problem, see [3]. Since $i\xi$ is purely imaginary, the interaction term in $\mathbf{H}_\Lambda$ is invariant under the transformation $W_{-i\xi}$, i.e. $W_{-i\xi}\mathfrak{Re}[a(\chi(|\nabla| \leq$

$\Lambda)w_x)]\mathrm{W}_{-i\xi}^{-1} = \mathfrak{Re}[a(\chi(|\nabla| \leq \Lambda)w_x)]$, and furthermore

$$\mathrm{W}_{-i\xi}\Upsilon_\Lambda \mathrm{W}_{-i\xi}^{-1} = \Upsilon_\Lambda - 2\mathfrak{Re}\left[a\left(\frac{1}{i}\widetilde{\nabla}_{x_1} i\xi\right)\right] + \left\langle i\xi\left|\frac{1}{i}\widetilde{\nabla}_{x_1}\right|i\xi\right\rangle = \Upsilon_\Lambda - 2\mathfrak{Re}\left[a(\widetilde{\nabla}_{x_1}\xi)\right], \tag{4.7}$$

where we have used $\langle i\xi|\frac{1}{i}\widetilde{\nabla}_{x_1}|i\xi\rangle = 0$ (since $\langle h|\frac{1}{i}\widetilde{\nabla}_{x_1}|h\rangle = 0$ for any real-valued or imaginary-valued function $h \in \mathrm{L}^2(\mathbf{R}^3)$). Therefore conjugating $\mathbf{H}_\Lambda + \frac{p}{m}(p - \Upsilon_\Lambda)$ with $\mathrm{W}_{-i\xi}$ yields

$$\begin{aligned}
&\left\langle \Psi_\alpha \left| \mathbf{H}_\Lambda + \frac{p}{m}(p - \Upsilon_\Lambda)\right| \Psi_\alpha\right\rangle \\
&= \left\langle \widetilde{\Psi}_\alpha \left| \mathbf{H}_\Lambda - \frac{p}{m}\Upsilon_\Lambda + 2\mathfrak{Re}\left[a\left(\frac{p}{m}\widetilde{\nabla}_{x_1}\xi - i\xi\right)\right]\right| \widetilde{\Psi}_\alpha\right\rangle + \frac{|p|^2}{m} + \|\xi\|^2 \\
&\geq e^{\mathrm{Pek}} + \left\langle \widetilde{\Psi}_\alpha \left| -\frac{1}{4\alpha^4}\sum_{n=1}^{\mathrm{N}} \partial_{\lambda_n}^2 + \mathrm{J}_{t^\lambda,\alpha^{-s}}\left[\tau(\lambda)\right] + \mathcal{N}_{>\mathrm{N}} - \frac{p}{m}\Upsilon_\Lambda\right| \widetilde{\Psi}_\alpha\right\rangle \\
&\quad - \frac{\mathrm{N}}{2\alpha^2} + 2\mathfrak{Re}\left\langle \widetilde{\Psi}_\alpha \left| a\left(\frac{p}{m}\widetilde{\nabla}_{x_1}\xi - i\xi\right)\right| \widetilde{\Psi}_\alpha\right\rangle \\
&\quad + \frac{|p|^2}{m} + \|\xi\|^2 + \mathrm{O}_{\alpha\to\infty}\left(\alpha^{-(2+\epsilon)}\right),
\end{aligned}$$

where we have used Eq. (4.5). In the next step we apply the Weyl transformation $\mathrm{W}_{\varphi^{\mathrm{Pek}}}$, which satisfies $\mathrm{W}_{\varphi^{\mathrm{Pek}}}\lambda \mathrm{W}_{\varphi^{\mathrm{Pek}}}^{-1} = \lambda + \lambda^{\mathrm{Pek}}$ and hence

$$\begin{aligned}
&\mathrm{W}_{\varphi^{\mathrm{Pek}}}\frac{p}{m}\Upsilon_\Lambda \mathrm{W}_{\varphi^{\mathrm{Pek}}}^{-1} = \frac{p}{m}\Upsilon_\Lambda + 2\mathfrak{Re}\left[a\left(\frac{p}{im}\widetilde{\nabla}_{x_1}\varphi^{\mathrm{Pek}}\right)\right] = \frac{p}{m}\Upsilon_\Lambda - 2\mathfrak{Re}\left[a(i\xi)\right], \\
&\mathrm{W}_{\varphi^{\mathrm{Pek}}}\mathfrak{Re}\left[a\left(\frac{p}{m}\widetilde{\nabla}_{x_1}\xi - i\xi\right)\right]\mathrm{W}_{\varphi^{\mathrm{Pek}}}^{-1} = \mathfrak{Re}\left[a\left(\frac{p}{m}\widetilde{\nabla}_{x_1}\xi - i\xi\right)\right] - \|\xi\|^2,
\end{aligned}$$

where we have used $\mathfrak{Re}\,\langle\varphi^{\mathrm{Pek}}|\frac{p}{m}\widetilde{\nabla}_{x_1}\xi - i\xi\rangle = \langle\varphi^{\mathrm{Pek}}|\frac{p}{m}\widetilde{\nabla}_{x_1}\xi\rangle = -\|\xi\|^2$. Furthermore

$$\mathrm{W}_{\varphi^{\mathrm{Pek}}}t^\lambda \mathrm{W}_{\varphi^{\mathrm{Pek}}}^{-1} = \left(\lambda_1 + \lambda_1^{\mathrm{Pek}}, \lambda_2 + \lambda_2^{\mathrm{Pek}}, \lambda_3 + \lambda_3^{\mathrm{Pek}}\right) = (\lambda_1, \lambda_2, \lambda_3) = t^\lambda$$

with $\lambda^{\mathrm{Pek}} := (\langle\varphi_n|\Pi\varphi^{\mathrm{Pek}}\rangle)_{n=1}^{\mathrm{N}}$. Therefore defining

$$\Psi_\alpha^* := \mathrm{W}_{\varphi^{\mathrm{Pek}}}\widetilde{\Psi}_\alpha = \mathrm{W}_{\varphi^{\mathrm{Pek}} - i\xi}\Psi_\alpha$$

and conjugating with $W_{\varphi^{\mathrm{Pek}}}$ yields the lower bound

$$\begin{aligned}\left\langle \Psi_\alpha \middle| \mathbf{H}_\Lambda + \frac{p}{m}(p - \Upsilon_\Lambda) \middle| \Psi_\alpha \right\rangle & \\ \geq e^{\mathrm{Pek}} + \Big\langle \Psi_\alpha^* \Big| & -\frac{1}{4\alpha^4}\sum_{n=1}^{N} \partial_{\lambda_n}^2 + J_{t^\lambda, \alpha^{-s}}\left[\tau\left(\lambda + \lambda^{\mathrm{Pek}}\right)\right] \\ & + W_{\varphi^{\mathrm{Pek}}} \mathcal{N}_{>N} W_{\varphi^{\mathrm{Pek}}}^{-1} - \frac{p}{m}\Upsilon_\Lambda \Big| \Psi_\alpha^* \Big\rangle \\ & - \frac{N}{2\alpha^2} + 2\mathfrak{Re}\left\langle \Psi_\alpha^* \middle| a\left(\frac{p}{m}\widetilde{\nabla}_{x_1}\xi\right) \middle| \Psi_\alpha^* \right\rangle \\ & + \frac{|p|^2}{m} - \|\xi\|^2 + O_{\alpha\to\infty}\left(\alpha^{-(2+\epsilon)}\right).\end{aligned} \tag{4.8}$$

The advantage of conjugating with the Weyl transformation $W_{\varphi^{\mathrm{Pek}} - i\xi} = W_{\varphi^{\mathrm{Pek}}} W_{-i\xi}$ stems from the observation that we have an almost complete cancellation of linear terms, i.e., as we will verify below, the term linear in creation and annihilation operators $\mathfrak{Re}\langle \Psi_\alpha^* | a(\frac{p}{m}\widetilde{\nabla}_{x_1}\xi) | \Psi_\alpha^* \rangle$ in Eq. (4.8) is of negligible order, and the function $\lambda \mapsto J_{t^\lambda,\alpha^{-s}}[\tau(\lambda + \lambda^{\mathrm{Pek}})]$ vanishes quadratically at $\lambda = 0$. The latter follows from the fact that $\tau(\lambda^{\mathrm{Pek}}) = 0$. Utilizing the inequalities $\langle \Psi_\alpha^* | \mathcal{N} | \Psi_\alpha^* \rangle = \langle \Psi_\alpha | W_{\varphi^{\mathrm{Pek}} - i\xi}^{-1} \mathcal{N} W_{\varphi^{\mathrm{Pek}} - i\xi} | \Psi_\alpha \rangle \leq \alpha^{-r}$, see Eq. (3.15), and $\| \frac{p}{m} \widetilde{\nabla}_{x_1} \xi \| \lesssim |p|^2$, where we have used that $\varphi^{\mathrm{Pek}} \in H^2(\mathbf{R}^3)$, see [9, 12], we obtain that

$$2\mathfrak{Re}\left\langle \Psi_\alpha^* \middle| a\left(\frac{p}{m}\widetilde{\nabla}_{x_1}\xi\right) \middle| \Psi_\alpha^* \right\rangle \lesssim \alpha^{-\frac{r}{2}} |p|^2 \lesssim \alpha^{-(2+\frac{r}{2})} \tag{4.9}$$

is indeed negligible small. Furthermore we can estimate, up to a term of order $\alpha^{-(2+\frac{2}{5})}$, $W_{\varphi^{\mathrm{Pek}}} \mathcal{N}_{>N} W_{\varphi^{\mathrm{Pek}}}^{-1}$ from below by a proper quadratic expression

$$\begin{aligned} W_{\varphi^{\mathrm{Pek}}} \mathcal{N}_{>N} W_{\varphi^{\mathrm{Pek}}}^{-1} &= \mathcal{N}_{>N} + a\left((1-\Pi)\varphi^{\mathrm{Pek}}\right) \\ &\quad + a^\dagger\left((1-\Pi)\varphi^{\mathrm{Pek}}\right) + \left\|(1-\Pi)\varphi^{\mathrm{Pek}}\right\|^2 \\ &\geq \frac{1}{2}\mathcal{N}_{>N} - 2\left\|(1-\Pi)\varphi^{\mathrm{Pek}}\right\|^2 \\ &= \frac{1}{2}\mathcal{N}_{>N} + O_{\alpha\to\infty}\left(\alpha^{-(2+\frac{2}{5})}\right), \end{aligned} \tag{4.10}$$

where we have used $\|(1-\Pi)\varphi^{\mathrm{Pek}}\|^2 \lesssim \alpha^{-(2+\frac{2}{5})}$, see [1, Lemma A.1]. In the following let us use the convenient notation $e_p^{\mathrm{Pek}} := e^{\mathrm{Pek}} + \frac{|p|^2}{2m}$. Combining Eq. (4.8) with Eq. (4.9), Eq. (4.10) and the observation that $\frac{|p|^2}{m} - \|\xi\|^2 \geq \frac{|p|^2}{2m}$, and using the fact that

$$\mathrm{E}_{\alpha,\Lambda}\left(\alpha^2 p\right) \geq \left\langle \Psi_\alpha \middle| \mathbf{H}_\Lambda + \frac{p}{m}(p - \Upsilon_\Lambda) \middle| \Psi_\alpha \right\rangle + \mathrm{O}_{\alpha\to\infty}\left(\alpha^{-(2+\frac{r}{2})}\right),$$

see Eq. (4.4), we obtain

$$\textbf{(4.11)}\quad \mathrm{E}_{\alpha,\Lambda}\left(\alpha^2 p\right) \geq e_p^{\mathrm{Pek}} + \left\langle \Psi_\alpha^* \middle| -\frac{1}{4\alpha^4}\sum_{n=1}^{\mathrm{N}} \partial_{\lambda_n}^2 + \mathrm{J}_{t^\lambda,\alpha^{-s}}\left[\tau\left(\lambda + \lambda^{\mathrm{Pek}}\right)\right] + \frac{1}{2}\mathcal{N}_{>\mathrm{N}} - \frac{p}{m}\Upsilon_\Lambda \middle| \Psi_\alpha^* \right\rangle - \frac{\mathrm{N}}{2\alpha^2} + \mathrm{O}_{\alpha\to\infty}\left(\alpha^{-(2+\epsilon)}\right).$$

The right hand side of Eq. (4.11) is up to a coordinate transformation in the argument of $\mathrm{J}_{t^\lambda,\alpha^{-s}}$ quadratic in creation and annihilation operators. In the next subsection we will apply a unitary transformation in order to arrive at a proper quadratic expression.

4.2. *Conjugation with the unitary* $\mathcal{U}$. — In order to get rid of the coordinate transformation τ in the argument of $\mathrm{J}_{t^\lambda,\alpha^{-s}}$, let us define the unitary operator $\mathcal{U}$ on $\mathcal{F}(\Pi \mathrm{L}^2(\mathbf{R}^3)) \cong \mathrm{L}^2(\mathbf{R}^{\mathrm{N}})$ as

$$\mathcal{U}(\Psi)(\lambda) := \Psi\left(\Xi(\lambda)\right),$$

where $\Xi : \mathbf{R}^{\mathrm{N}} \longrightarrow \mathbf{R}^{\mathrm{N}}$ is defined as

$$\Xi(\lambda) := \tau\left(\lambda + \lambda^{\mathrm{Pek}}\right) \in \Pi \mathrm{L}^2\left(\mathbf{R}^3\right) \cong \mathbf{R}^{\mathrm{N}}.$$

Note that the inverse of τ is simply given by $\tau^{-1}(\varphi) = \varphi + f(t^\varphi)$ where $f : \mathbf{R}^3 \longrightarrow \Pi \mathrm{L}^2(\mathbf{R}^3)$ is defined in Definition 4.2, which can be checked easily using the fact that $\langle \varphi_n | f(t) \rangle = 0$ for $n \in \{1, 2, 3\}$ and consequently $t^{\tau(\varphi)} = t^\varphi$. Hence

$$\textbf{(4.12)}\quad \mathcal{U}^{-1}\lambda_n \mathcal{U} = \langle \varphi_n | \tau^{-1}(\lambda) \rangle - \lambda_n^{\mathrm{Pek}} = \lambda_n + \langle \varphi_n | f\left(t^\lambda\right) \rangle - \lambda_n^{\mathrm{Pek}}$$

and therefore

$$\begin{aligned} \mathcal{U}^{-1} t^\lambda \mathcal{U} &= \left(\langle \varphi_1 | \tau^{-1}(\lambda) \rangle - \lambda_1^{\mathrm{Pek}}, \ldots, \langle \varphi_3 | \tau^{-1}(\lambda) \rangle - \lambda_3^{\mathrm{Pek}}\right) \\ &= (\lambda_1, \ldots, \lambda_3) = t^\lambda. \end{aligned}$$

Defining the matrix $(\mathrm{J}_{t,\gamma})_{n,m} := \langle \varphi_n | \mathrm{J}_{t,\gamma} | \varphi_m \rangle$ we furthermore have

$$\mathcal{U}^{-1}\mathrm{J}_{t^\lambda,\alpha^{-s}}\left[\tau\left(\lambda + \lambda^{\mathrm{Pek}}\right)\right]\mathcal{U} = \mathrm{J}_{t^\lambda,\alpha^{-s}}[\lambda] = \sum_{n,m=4}^{\mathrm{N}} (\mathrm{J}_{t^\lambda,\alpha^{-s}})_{n,m}\lambda_n\lambda_m$$

as well as $\mathcal{U}^{-1} i\partial_{\lambda_n} \mathcal{U} = i\partial_{\lambda_n}$ for $3 < n \leq \mathrm{N}$, which immediately follows from the observation that Ξ is a $t^\lambda = (\lambda_1, \lambda_2, \lambda_3)$-dependent shift. In the following let us extend $\{\varphi_1, \dots, \varphi_{\mathrm{N}}\}$ to an orthonormal basis $\{\varphi_n : n \in \mathbf{N}\}$ of $\mathrm{L}^2(\mathbf{R}^3)$ and introduce $a_n := a(\varphi_n)$ for all $n \in \mathbf{N}$, and let us extend the action of $\mathcal{U}$ to all of $\mathcal{F}(\mathrm{L}^2(\mathbf{R}^3))$ such that $\mathcal{U}^{-1} a_n \mathcal{U} = a_n$ for $n > \mathrm{N}$. Defining

$$\Psi'_\alpha := \mathcal{U}^{-1} \Psi^*_\alpha,$$

we obtain by Eq. (4.11)

$$\begin{aligned}(\mathbf{4.13}) \qquad \mathrm{E}_{\alpha,\Lambda}\left(\alpha^2 p\right) \geq e_p^{\mathrm{Pek}} + \Bigg\langle \Psi'_\alpha \Bigg| &-\frac{1}{4\alpha^4} \sum_{n=1}^{3} \mathcal{U}^{-1} \partial_{\lambda_n}^2 \mathcal{U} - \frac{1}{4\alpha^4} \sum_{n=4}^{\mathrm{N}} \partial_{\lambda_n}^2 \\ &+ \sum_{n,m=4}^{\mathrm{N}} (\mathrm{J}_{t^\lambda,\alpha^{-s}})_{n,m} \lambda_n \lambda_m + \frac{1}{2}\mathcal{N}_{>\mathrm{N}} - \mathcal{U}^{-1} \frac{p}{m} \Upsilon_\Lambda \mathcal{U} \Bigg| \Psi'_\alpha \Bigg\rangle \\ &- \frac{\mathrm{N}}{2\alpha^2} + \mathrm{O}_{\alpha\to\infty}\left(\alpha^{-(2+\epsilon)}\right).\end{aligned}$$

Using Eq. (4.12) and $\mathcal{U}^{-1} i\partial_{\lambda_n} \mathcal{U} = i\partial_{\lambda_n}$ for $3 < n \leq \mathrm{N}$, we further obtain the transformation law $\mathcal{U}^{-1} a_n \mathcal{U} = a_n + \langle \varphi_n | f(t^\lambda) - \Pi\varphi^{\mathrm{Pek}} \rangle$ for all $n > 3$.

In order to express $\mathcal{U}^{-1} \frac{p}{m} \Upsilon_\Lambda \mathcal{U}$, let us introduce the operators c_n defined as

$$c_n := \frac{1}{2\alpha^2} \mathcal{U}^{-1} \partial_{\lambda_n} \mathcal{U}$$

for $n \in \{1, 2, 3\}$ and $c_n := a_n$ for $n > 3$, as well as

$$g(t) := f(t) - \Pi\varphi^{\mathrm{Pek}} + \sum_{n=1}^{3} t_n \varphi_n \in \Pi\mathrm{L}^2\left(\mathbf{R}^3\right)$$

and $g_n(t) := \langle \varphi_n | g(t) \rangle$. With these definitions at hand we obtain

$$\begin{aligned}\mathcal{U}^{-1} a_n \mathcal{U} &= \mathcal{U}^{-1} \left(\frac{1}{2\alpha^2} \partial_{\lambda_n} + \lambda_n \right) \mathcal{U} = \frac{1}{2\alpha^2} \mathcal{U}^{-1} \partial_{\lambda_n} \mathcal{U} + \lambda_n \\ &= c_n + g_n\left(t^\lambda\right), \quad \text{for } 1 \leq n \leq 3, \\ \mathcal{U}^{-1} a_n \mathcal{U} &= a_n + \langle \varphi_n | f\left(t^\lambda\right) - \Pi\varphi^{\mathrm{Pek}} \rangle = c_n + g_n\left(t^\lambda\right), \quad \text{for } 4 \leq n \leq \mathrm{N}\end{aligned}$$

and $\mathcal{U}^{-1} a_n \mathcal{U} = c_n = c_n + g_n(t^\lambda)$ for $n > \mathrm{N}$, and therefore

$$\mathcal{U}^{-1} a_n \mathcal{U} = c_n + g_n\left(t^\lambda\right)$$

for all $n \in \mathbf{N}$. In the following we want to think of c_n as being a variable of magnitude α^{-1} and t^λ as being of order α^{-r} for some $r > 0$, and consequently we think of $g_n(t^\lambda)$ as being of order α^{-r} as well, since $g(0)=0$. While the former will be a consequence of the proof presented below, the control on t^λ follows from our assumption that we have condensation with respect to the state φ^{Pek}.

In the following we want to show that for suitable $\epsilon'>0$, $\frac{p}{m}\Upsilon_\Lambda$ is bounded by $\beta(-\frac{1}{4\alpha^4}\sum_{n=1}^{3}\mathcal{U}^{-1}\partial_{\lambda_n}^2\mathcal{U}+\sum_{n=4}^{\mathrm{N}}a_n^\dagger a_n+\mathcal{N}_{>\mathrm{N}})$ with $\beta=\alpha^{-\epsilon'}$, up to a term of negligible magnitude, see Eq. (4.16). Since $-\frac{1}{4\alpha^4}\sum_{n=1}^{3}\mathcal{U}^{-1}\partial_{\lambda_n}^2\mathcal{U}$ and $\mathcal{N}_{>\mathrm{N}}$ appear in the expression on the right hand side of Eq. (4.13) as well, and since they are non-negative, this will leave us with the study of

$$-\frac{1}{4\alpha^4}\sum_{n=4}^{\mathrm{N}}\partial_{\lambda_n}^2+\sum_{n,m=4}^{\mathrm{N}}(\mathrm{J}_{t^\lambda,\alpha^{-s}})_{n,m}\lambda_n\lambda_m-\beta\sum_{n=4}^{\mathrm{N}}a_n^\dagger a_n$$

for a lower bound on the expression on the right hand side of Eq. (4.13). Using the representation

$$\frac{p}{m}\Upsilon_\Lambda=\sum_{n,m=1}^{\infty}\left\langle\varphi_n\middle|\frac{p}{i\,m}\widetilde{\nabla}_{x_1}\middle|\varphi_m\right\rangle a_n^\dagger a_m,$$

we obtain

$$\begin{aligned}(\mathbf{4.14})\qquad \mathcal{U}^{-1}\frac{p}{m}\Upsilon_\Lambda\mathcal{U}&=\sum_{n,m=1}^{\infty}\left\langle\varphi_n\middle|\frac{p}{i\,m}\widetilde{\nabla}_{x_1}\middle|\varphi_m\right\rangle\big(c_n+g_n(t^\lambda)\big)^\dagger\big(c_m+g_m(t^\lambda)\big)\\&=\sum_{n,m=1}^{\infty}\left\langle\varphi_n\middle|\frac{p}{i\,m}\widetilde{\nabla}_{x_1}\middle|\varphi_m\right\rangle c_n^\dagger c_m\\&\quad+\sum_{n,m=1}^{\infty}\left\langle\varphi_n\middle|\frac{p}{i\,m}\widetilde{\nabla}_{x_1}\middle|\varphi_m\right\rangle\big(c_n^\dagger g_m(t^\lambda)+g_n(t^\lambda)\,c_m\big),\end{aligned}$$

where we have used

$$\sum_{n,m=1}^{\infty}\left\langle\varphi_n\middle|\frac{p}{i\,m}\widetilde{\nabla}_{x_1}\middle|\varphi_m\right\rangle g_n(t^\lambda)g_m(t^\lambda)=\left\langle g(t^\lambda)\middle|\frac{p}{i\,m}\widetilde{\nabla}_{x_1}\middle|g(t^\lambda)\right\rangle=0,$$

see the comment below Eq. (4.7). Using the bound on the operator norm

$$\left\|\frac{p}{m}\widetilde{\nabla}_{x_1}\right\|_{\mathrm{op}}\leq\frac{|p|}{m}3\Lambda=\frac{|p|}{m}3\alpha^{\frac{4}{5}(1+\sigma)}\lesssim\alpha^{\frac{4}{5}(1+\sigma)-1}$$

yields

$$(\mathbf{4.15})\qquad \pm\sum_{n,m=1}^{\infty}\left\langle\varphi_n\middle|\frac{p}{i\,m}\widetilde{\nabla}_{x_1}\middle|\varphi_m\right\rangle c_n^\dagger c_m\lesssim\alpha^{\frac{4}{5}(1+\sigma)-1}\sum_{n=1}^{\infty}c_n^\dagger c_n.$$

For the bound in Eq. (4.15) it is essential that we are using the truncated momentum Υ_Λ defined in terms of the bounded operator $\widetilde{\nabla}_{x_1}$ instead of the unbounded operator ∇_{x_1}. Defining the coefficients

$$h_n(t) := \sum_{m=1}^{\infty} \left\langle \varphi_n \middle| \frac{p}{i\,m} \widetilde{\nabla}_{x_1} \middle| \varphi_m \right\rangle g_m(t)$$

and applying Cauchy–Schwarz furthermore yields for all $\beta > 0$

$$\begin{aligned} &\pm \sum_{n,m=1}^{\infty} \left\langle \varphi_n \middle| \frac{p}{i\,m} \widetilde{\nabla}_{x_1} \middle| \varphi_m \right\rangle \left(c_n^\dagger g_m\left(t^\lambda\right) + g_n\left(t^\lambda\right) c_m\right) \\ &= \pm \sum_{n=1}^{\infty} \left(c_n^\dagger h_n\left(t^\lambda\right) + \overline{h_n\left(t^\lambda\right)} c_n\right) \\ &\leq \beta \sum_{n=1}^{\infty} c_n^\dagger c_n + \beta^{-1} \sum_{n=1}^{\infty} \left|h_n\left(t^\lambda\right)\right|^2 = \beta \sum_{n=1}^{\infty} c_n^\dagger c_n + \beta^{-1} \left\| \frac{p}{m} \widetilde{\nabla}_{x_1} g\left(t^\lambda\right) \right\|^2 . \end{aligned}$$

Note that $\|\frac{p}{m}\widetilde{\nabla}_{x_1} g(t)\| \leq \frac{|p|}{m}\|\nabla g(t)\|$. Making use of $\nabla g(t) = \nabla \Pi \eta(t)$ with

$$\begin{aligned} \eta(t) := {}& \chi\left(|t| < \delta_*\right)\left(\varphi_{x_t}^{\mathrm{Pek}} - \varphi^{\mathrm{Pek}}\right) \\ &+ \chi\left(\delta_* \leq |t|\right)\left(\sum_{n=1}^{3} t_n \frac{\nabla_{x_n}\varphi^{\mathrm{Pek}}}{\|\Pi \nabla_{x_n}\varphi^{\mathrm{Pek}}\|} - \varphi^{\mathrm{Pek}}\right), \end{aligned}$$

we obtain $\|\nabla g(t)\| \lesssim \|\nabla \eta(t)\| + \alpha^{-4(1+\sigma)}\|\eta(t)\|$ by Lemma A.3. Using again $\varphi^{\mathrm{Pek}} \in \mathrm{H}^2(\mathbf{R}^3)$, we have $\|\eta(t)\| + \|\nabla \eta(t)\| \lesssim 1 + |t|$, as well as

$$\left\|\nabla \eta(t)\right\| = \left\|\nabla \varphi_{x_t}^{\mathrm{Pek}} - \nabla \varphi^{\mathrm{Pek}}\right\| \leq |x_t| \left\|\Delta \varphi^{\mathrm{Pek}}\right\| \lesssim |t|$$

for $|t| < \delta_*$. Consequently, $\|\frac{p}{m}\widetilde{\nabla}_{x_1} g(t)\| \leq \mathrm{C}_0|p|(|t| + \alpha^{-4(1+\sigma)}(1+|t|))$ for a suitable constant C_0. The choice $\beta := \alpha^{-\min\{\frac{r}{2},1\}}$ yields for α large enough

$$\begin{aligned} \pm \mathcal{U}^{-1} \frac{p}{m} \Upsilon_\Lambda \mathcal{U} \leq {}& \alpha^{-\epsilon'} \sum_{n=1}^{\infty} c_n^\dagger c_n \\ &+ \mathrm{C}_0 \mathrm{C}^2 \left(\alpha^{-2} \alpha^{\min\{\frac{r}{2},1\}} \left|t^\lambda\right|^2 + \alpha^{-5-4\sigma}\left(1 + \left|t^\lambda\right|\right)^2\right) \end{aligned} \tag{4.16}$$

with $\epsilon' < \min\{\frac{r}{2}, 1 - \frac{4}{5}(1+\sigma)\}$. In the following let α be large enough such that $\epsilon' \leq \frac{1}{2}$. Then we have

$$\alpha^{-\epsilon'} \sum_{n \notin \{4,\ldots,N\}} c_n^\dagger c_n = \alpha^{-\epsilon'} \left(\sum_{n>N} a_n^\dagger a_n - \frac{1}{4\alpha^4} \sum_{n=1}^{3} \mathcal{U}^{-1} \partial_{\lambda_n}^2 \mathcal{U} \right)$$
$$\leq \frac{1}{2} \mathcal{N}_{>N} - \frac{1}{4\alpha^4} \sum_{n=1}^{3} \mathcal{U}^{-1} \partial_{\lambda_n}^2 \mathcal{U}.$$

Using Eq. (4.13), Eq. (4.16) and

$$\langle \Psi'_\alpha | \left| t^\lambda \right|^2 | \Psi'_\alpha \rangle = \langle \widetilde{\Psi}_\alpha | \left| t^\lambda \right|^2 | \widetilde{\Psi}_\alpha \rangle \leq \langle \widetilde{\Psi}_\alpha | \mathcal{N} | \widetilde{\Psi}_\alpha \rangle + \frac{3}{2\alpha^2} \leq \alpha^{-r} + \frac{3}{2\alpha^2},$$

see Theorem 3.7 for the last estimate, we obtain for a suitable $\epsilon > 0$

$$\mathrm{E}_{\alpha,\Lambda}\left(\alpha^2 p\right) \geq e_p^{\mathrm{Pek}} + \left\langle \Psi'_\alpha \middle| - \frac{1}{4\alpha^4} \sum_{n=4}^{N} \partial_{\lambda_n}^2 + \sum_{n,m=4}^{N} (\mathrm{J}_{t^\lambda,\alpha^{-s}})_{n,m} \lambda_n \lambda_m \right.$$
$$\left. - \alpha^{-\epsilon'} \sum_{n=4}^{N} a_n^\dagger a_n \middle| \Psi'_\alpha \right\rangle - \frac{N}{2\alpha^2} + O_{\alpha\to\infty}\left(\alpha^{-(2+\epsilon)}\right)$$
$$= e_p^{\mathrm{Pek}} + \left(1 - \alpha^{-\epsilon'}\right) \left\langle \Psi'_\alpha \middle| \mathbf{Q}_{t^\lambda,\alpha^{-s}}^{\alpha^{-\epsilon'}} - \frac{N}{2\alpha^2} \middle| \Psi'_\alpha \right\rangle + O_{\alpha\to\infty}\left(\alpha^{-(2+\epsilon)}\right)$$

with

$$\mathbf{Q}_{t,\gamma}^{\kappa} := -\frac{1}{4\alpha^4} \sum_{n=4}^{N} \partial_{\lambda_n}^2 + \frac{1}{1-\kappa} \sum_{n,m=4}^{N} \left((\mathrm{J}_{t,\gamma})_{n,m} - \kappa \delta_{n,m} \right) \lambda_n \lambda_m,$$

where we used the fact that $\sum_{n=4}^{N} a_n^\dagger a_n = -\frac{1}{4\alpha^4} \sum_{n=4}^{N} \partial_{\lambda_n}^2 + \sum_{n=4}^{N} \lambda_n^2 - \frac{N-3}{2\alpha^2}$.

4.3. *Properties of the harmonic oscillators* $\mathbf{Q}_{t,\gamma}^{\kappa}$. — Let π be the projection from Definition 4.3 and note that $\mathrm{J}_{t,\gamma} \geq c\pi$ for suitable $c > 0$, γ small enough and α large enough by [1, Lemma B.5]. Therefore $\mathbf{Q}_{t,\alpha^{-s}}^{\alpha^{-\epsilon'}} \geq 0$ for α large enough. Since $\mathrm{J}_{t,\gamma} \leq 1$, we furthermore have

$$(1-\kappa) \inf \sigma\left(\mathbf{Q}_{t,\gamma}^{\kappa}\right) \leq \frac{N}{2\alpha^2} \lesssim \alpha^{-2} \left(\frac{\Lambda}{\ell}\right)^3 \leq \alpha^q$$

for a suitable exponent q, see Definition 4.1. Combining this with the estimate

$$\langle \Psi'_\alpha | 1 - \mathbf{B} | \Psi'_\alpha \rangle = \langle \widetilde{\Psi}_\alpha | 1 - \mathbf{B} | \widetilde{\Psi}_\alpha \rangle \leq e^{-\beta \alpha^{2-2s}}$$

for a suitable $\beta > 0$, where $\mathbf{B} := \chi(|t^\lambda| < \alpha^{-s})$, see Eq. (4.6), yields

$$\inf_{|t|<\alpha^{-s}} \inf\sigma\left(\mathbf{Q}^{\alpha^{-\epsilon'}}_{t,\alpha^{-s}}\right)\langle\Psi_\alpha|\mathbf{B}|\Psi_\alpha\rangle \geq \inf_{|t|<\alpha^{-s}} \inf\sigma\left(\mathbf{Q}^{\alpha^{-\epsilon'}}_{t,\alpha^{-s}}\right) + \mathrm{O}_{\alpha\to\infty}\left(\alpha^q e^{-\beta\alpha^{2-2s}}\right).$$

Therefore we obtain for a suitable $\epsilon > 0$

$$\begin{aligned}
(\mathbf{4.17}) \qquad & \mathrm{E}_{\alpha,\Lambda}\left(\alpha^2 p\right) \\
&\geq e^{\mathrm{Pek}}_p + \left(1-\alpha^{-\epsilon'}\right)\left\langle\Psi'_\alpha\middle|\mathbf{Q}^{\alpha^{-\epsilon'}}_{t^\lambda,\alpha^{-s}}\mathbf{B} - \frac{\mathrm{N}}{2\alpha^2}\middle|\Psi'_\alpha\right\rangle + \mathrm{O}_{\alpha\to\infty}\left(\alpha^{-(2+\epsilon)}\right) \\
&\geq e^{\mathrm{Pek}}_p + \left(1-\alpha^{-\epsilon'}\right)\left(\inf_{|t|<\alpha^{-s}} \inf\sigma\left(\mathbf{Q}^{\alpha^{-\epsilon'}}_{t,\alpha^{-s}}\right)\langle\Psi_\alpha|\mathbf{B}|\Psi_\alpha\rangle - \frac{\mathrm{N}}{2\alpha^2}\right) \\
&\quad + \mathrm{O}_{\alpha\to\infty}\left(\alpha^{-(2+\epsilon)}\right) \\
&\geq e^{\mathrm{Pek}}_p + \left(1-\alpha^{-\epsilon'}\right)\left(\inf_{|t|<\alpha^{-s}} \inf\sigma\left(\mathbf{Q}^{\alpha^{-\epsilon'}}_{t,\alpha^{-s}}\right) - \frac{\mathrm{N}}{2\alpha^2}\right) + \mathrm{O}_{\alpha\to\infty}\left(\alpha^{-(2+\epsilon)}\right).
\end{aligned}$$

Since $\mathbf{Q}^\kappa_{t,\gamma}$ is a harmonic oscillator, we can write its ground state energy explicitly as

$$\begin{aligned}
\inf\sigma\left(\mathbf{Q}^\kappa_{t,\gamma}\right) &= \frac{1}{2\alpha^2}\mathrm{Tr}_{\Pi L^2(\mathbf{R}^3)}\sqrt{\frac{\mathrm{J}_{t,\gamma} - \kappa\pi}{1-\kappa}} \\
&= \inf\sigma\left(\mathbf{Q}^0_{t,\gamma}\right) + \frac{1}{2\alpha^2}\mathrm{Tr}_{\Pi L^2(\mathbf{R}^3)}\left[\sqrt{\frac{\mathrm{J}_{t,\gamma} - \kappa\pi}{1-\kappa}} - \sqrt{\mathrm{J}_{t,\gamma}}\right].
\end{aligned}$$

Using $\mathrm{J}_{t,\gamma}\pi = \mathrm{J}_{t,\gamma}$, and therefore $[\mathrm{J}_{t,\gamma}, \pi] = 0$, and again the fact that $\mathrm{J}_{t,\gamma} \geq c\pi$ for γ small enough and α large enough, as well as $|\sqrt{x} - \sqrt{y}| \leq \frac{1}{\sqrt{c}}|x-y|$ for $x \geq 0$ and $y \geq c$, we obtain for such γ, α, and $\kappa \leq c$

$$\begin{aligned}
&\pm \mathrm{Tr}_{\Pi L^2(\mathbf{R}^3)}\left[\sqrt{\frac{\mathrm{J}_{t,\gamma} - \kappa\pi}{1-\kappa}} - \sqrt{\mathrm{J}_{t,\gamma}}\right] \\
&\quad\leq \frac{1}{\sqrt{c}}\mathrm{Tr}_{\Pi L^2(\mathbf{R}^3)}\left|\frac{\mathrm{J}_{t,\gamma} - \kappa\pi}{1-\kappa} - \mathrm{J}_{t,\gamma}\right| \\
&\quad= \frac{\kappa}{\sqrt{c}(1-\kappa)}\mathrm{Tr}|\mathrm{J}_{t,\gamma} - \pi| \\
&\quad= \frac{\kappa(1+\gamma)}{\sqrt{c}(1-\kappa)}\mathrm{Tr}\left[\mathrm{K}^{\mathrm{Pek}} + \gamma \mathrm{L}^{\mathrm{Pek}}\right] \lesssim \frac{\kappa}{1-\kappa},
\end{aligned}$$

where we have used that $\mathrm{K}^{\mathrm{Pek}}$ and $\mathrm{L}^{\mathrm{Pek}}$ defined in Definition 4.3 are trace-class. Combining what we have so far with the bound

$$\inf\sigma\left(\mathbf{Q}^0_{t,\gamma}\right) \geq \frac{\mathrm{N}}{2\alpha^2} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{\mathrm{H}^{\mathrm{Pek}}}\right] - \mathrm{D}\left(\alpha^{-2}\gamma + \alpha^{-(2+\frac{1}{5})}\right)$$

for small γ, $|t| < \gamma$ and large α, and a suitable $\mathrm{D} > 0$, see [1, Lemma B.5], yields

$$\inf_{|t|<\alpha^{-s}} \inf \sigma\left(\mathbf{Q}^{\alpha^{-\epsilon'}}_{t,\alpha^{-s}}\right) - \frac{\mathrm{N}}{2\alpha^2} + \frac{1}{2\alpha^2}\mathrm{Tr}\left[1-\sqrt{\mathrm{H}^{\mathrm{Pek}}}\right]$$
$$\gtrsim -\left(\alpha^{-(2+s)} + \alpha^{-(2+\frac{1}{5})} + \alpha^{-(2+\epsilon')}\right).$$

In combination with Eq. (4.17) we therefore obtain for a suitable $\epsilon > 0$

$$\mathrm{E}_{\alpha,\Lambda}\left(\alpha^2 p\right) \geq e^{\mathrm{Pek}}_p - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1-\sqrt{\mathrm{H}^{\mathrm{Pek}}}\right] + \mathrm{O}_{\alpha\to\infty}\left(\alpha^{-(2+\epsilon)}\right),$$

which concludes the proof of Eq. (2.3).

Appendix A: Auxiliary results

Lemma **A.1.** — *Let* $g(k) := \chi^1(\mathrm{K}^{-1}|k| \leq 2)k$ *for* $k \in \mathbf{R}$. *Then there exists a constant* $\mathrm{C} > 0$ *such that for any bounded function* $f : \mathbf{R} \to \mathbf{R}$ *with* $f' \in \mathrm{L}^2(\mathbf{R})$ *and* $\mathrm{K} > 0$, *the double commutator is bounded by*

$$\left\|\left[\left[g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t}\right), f(t)\right], f(t)\right]\right\|_{\mathrm{op}} \leq \mathrm{C}\left\|f'\right\|^2, \tag{A.1}$$

where we write $f(t)$ *for the multiplication operator with respect to the function* $t \mapsto f(t)$. *Furthermore we can choose the constant* $\mathrm{C} > 0$ *such that*

$$\left\|\left[g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t}\right), f(t)\right]\right\|_{\mathrm{op}} \leq \mathrm{C}\sqrt{\mathrm{K}}\left\|f'\right\|. \tag{A.2}$$

Proof. — Let us denote with $\mathrm{T}_z\phi(y) := \phi(y+z)$ the translation operator on $\mathrm{L}^2(\mathbf{R})$ and let us write $\mathcal{F}(\cdot)$ for the Fourier transformation. Then

$$\left[\left[g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t}\right), f(t)\right], f(t)\right] = \int_{\mathbf{R}} \mathcal{F}^{-1}(g)(z)\,\mathrm{T}_z\left[f(t+z)-f(t)\right]^2 \mathrm{d}z.$$

Using the Sobolev inequality

$$\left|f(t+z)-f(t)\right|^2 \leq \left\|f'\right\|^2 |z|$$

and the fact that $\mathcal{F}^{-1}(g)(z) = \mathrm{K}^2\mathcal{F}^{-1}(g_*)(\mathrm{K}z)$, where $g_*(k) := \chi^1(|k| \leq 2)k$ is a K-independent smooth function with compact support, therefore yields

$$\left\| \left[\left[g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t}\right), f(t)\right], f(t)\right] \right\|_{\mathrm{op}} \leq \int_{\mathbf{R}} \left|\mathcal{F}^{-1}(g)(z)\right| \sup_{t\in\mathbf{R}} \left|f(t+z) - f(t)\right|^2 \mathrm{d}z$$
$$\leq \mathrm{K}^2 \|f'\|^2 \int_{\mathbf{R}} \left|\mathcal{F}^{-1}(g_*)(\mathrm{K}z)\right| |z| \mathrm{d}z$$
$$= \|f'\|^2 \int_{\mathbf{R}} \left|\mathcal{F}^{-1}(g_*)(z)\right| |z| \mathrm{d}z.$$

Since $\int_{\mathbf{R}} |\mathcal{F}^{-1}(g_*)(z)||z|\mathrm{d}z < \infty$, this concludes the proof of Eq. (A.1). Regarding Eq. (A.2), we obtain in a similar fashion

$$\left\| \left[g\left(\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}t}\right), f(t)\right] \right\|_{\mathrm{op}} \leq \mathrm{K}^2 \|f'\| \int_{\mathbf{R}} \left|\mathcal{F}^{-1}(g_*)(\mathrm{K}z)\right| \sqrt{|z|} \mathrm{d}z$$
$$\leq \sqrt{\mathrm{K}} \|f'\| \int_{\mathbf{R}} \left|\mathcal{F}^{-1}(g_*)(z)\right| \sqrt{|z|} \mathrm{d}z. \qquad \square$$

Lemma **A.2.** — *For* $\mathrm{K} > 0$ *we have the estimate* $\|\chi(|\nabla| > \mathrm{K})\nabla\varphi^{\mathrm{Pek}}\| \lesssim \frac{1}{\sqrt{\mathrm{K}}}$.

Proof. — We can write $\varphi^{\mathrm{Pek}} = 4\sqrt{\pi}(-\Delta)^{-\frac{1}{2}}|\psi^{\mathrm{Pek}}|^2$, where ψ^{Pek} is as in Definition 4.3. Hence the Fourier transform of $\nabla\varphi^{\mathrm{Pek}}$ reads

$$\mathcal{F}\left(\nabla\varphi^{\mathrm{Pek}}\right)(k) = \frac{ik}{|k|}\mathcal{F}\left(\left|\psi^{\mathrm{Pek}}\right|^2\right)(k),$$

and therefore

$$\left\|\chi\left(|\nabla| > \mathrm{K}\right)\nabla\varphi^{\mathrm{Pek}}\right\|^2 = \int_{|k|>\mathrm{K}} \left|\mathcal{F}\left(\left|\psi^{\mathrm{Pek}}\right|^2\right)(k)\right|^2 \mathrm{d}k$$
$$\leq \left\||k|^2\mathcal{F}\left(\left|\psi^{\mathrm{Pek}}\right|^2\right)(k)\right\|_\infty^2 \int_{|k|>\mathrm{K}} \frac{1}{|k|^4}\mathrm{d}k \lesssim \frac{1}{\mathrm{K}},$$

where we used $\psi^{\mathrm{Pek}} \in \mathrm{H}^2(\mathbf{R}^3)$ and consequently $\||k|^2\mathcal{F}(|\psi^{\mathrm{Pek}}|^2)(k)\|_\infty < \infty$. $\square$

Lemma **A.3.** — *With* Π *the projection defined in Definition 4.1, we have*

$$\left\|\left[|\nabla|, \Pi\right]\right\|_{\mathrm{op}} \lesssim \alpha^{-4(1+\sigma)}.$$

Proof. — Using the Fourier transformation, we can write

$$\mathcal{F}(\Pi\varphi)(k) = \sum_{n=1}^{\mathrm{N}} \langle f_n|\mathcal{F}(\varphi)\rangle f_n(k),$$

with the help of non-negative functions f_n having pairwise disjoint support, which additionally satisfy $\|f_n\| = 1$ and $\mathrm{supp}(f_n) \subset B_{\sqrt{3}\alpha^{-4(1+\sigma)}}(z^n)$ for some $z^n \in \mathbf{R}^3$. Therefore

$$\mathcal{F}\big([|\nabla|, \Pi]\varphi\big)(k) = \sum_{n=1}^{N} \big(\langle f_n|\mathcal{F}(\varphi)\rangle\, |k| - \langle f_n|\mathcal{F}\big(|\nabla|\varphi\big)\rangle\big) f_n(k)$$
$$= \sum_{n=1}^{N} \int f_n(k')\mathcal{F}(\varphi)(k')\big(|k| - |k'|\big)\mathrm{d}k' f_n(k).$$

Using that the functions f_n have disjoint support, as well as the fact that $||k| - |k'|| \leq 2\sqrt{3}\alpha^{-4(1+\sigma)}$ for $k, k' \in \mathrm{supp}(f_n)$, we obtain furthermore

$$\big\|[|\nabla|, \Pi]\varphi\big\|^2 = \sum_{n=1}^{N} \int \left| \int f_n(k')\mathcal{F}(\varphi)(k')\big(|k| - |k'|\big)\mathrm{d}k' \right|^2 |f_n(k)|^2 \mathrm{d}k$$
$$\leq 12\alpha^{-8(1+\sigma)} \sum_{n=1}^{N} \left| \int f_n(k') \left|\mathcal{F}(\varphi)(k')\right| \mathrm{d}k' \right|^2$$
$$\leq 12\alpha^{-8(1+\sigma)} \big\| |\mathcal{F}(\varphi)| \big\|^2 = 12\alpha^{-8(1+\sigma)} \|\varphi\|^2,$$

where we have used that f_n is an orthonormal system. □

Declarations:

Competing Interests

The authors declare no competing interests.

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