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The Fröhlich Polaron at Strong Coupling: Part I—The Quantum Correction to the Classical Energy

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Abstract: We study the Fröhlich polaron model in $\mathbb{R}^3$, and establish the subleading term in the strong coupling asymptotics of its ground state energy, corresponding to the quantum corrections to the classical energy determined by the Pekar approximation.

1. Introduction and Main Results

This is the first part of a study of the asymptotic properties of the Fröhlich polaron, which is a model describing the interaction between an electron and the optical modes of a polar crystal [12]. In the regime of strong coupling between the electron and the optical modes, also called phonons, it is a well known fact [1,7,20] that the ground state energy of the Fröhlich polaron is asymptotically given by the minimal Pekar energy [26], which can be considered as the ground state energy of an electron interacting with a classical phonon field. This result is motivated by using appropriately scaled units, see e.g. [28], which demonstrates that the strong coupling regime is a semi-classical limit in the phonon field variables. In such units the Fröhlich Hamiltonian, acting on the space $L^2(\mathbb{R}^3) \otimes \mathcal{F}\left(L^2(\mathbb{R}^3)\right)$, reads

$$\mathbb{H} := -\Delta_x - a\left(w_x\right) - a^\dagger\left(w_x\right) + \mathcal{N}, \tag{1.1}$$

where the annihilation and creation operators satisfy the rescaled canonical commutation relations $\left[a(f), a^\dagger(g)\right] = \alpha^{-2}\langle f|g\rangle$ for $f, g \in L^2(\mathbb{R}^3)$ with $\alpha > 0$ being the coupling strength, the interaction is given by $w_x(x') := \pi^{-\frac{3}{2}}|x'-x|^{-2}$ and $\mathcal{N}$ is the corresponding (rescaled) particle number operator, i.e. $\mathcal{N} := \sum_{n=1}^{\infty} a^\dagger(\varphi_n)a(\varphi_n)$ where $\{\varphi_n : n \in \mathbb{N}\}$ is an orthonormal basis of $L^2(\mathbb{R}^3)$. The definition of the Fröhlich Hamiltonian in Eq. (1.1) has to be understood in the sense of quadratic forms, see for example [28], due to the ultraviolet singularity in the interaction w_x. By substituting the annihilation and creation operators a and $a^\dagger$ in Eq. (1.1) with a (classical) phonon field $\varphi \in L^2(\mathbb{R}^3)$, i.e. replacing $a(f)$ with $\langle f|\varphi\rangle$ and $a^\dagger(f)$ with $\langle\varphi|f\rangle$, we arrive at the Pekar energy

$$\begin{aligned}\mathcal{E}(\psi,\varphi) &:= \left\langle\psi\right| -\Delta_x - \langle w_x|\varphi\rangle - \langle\varphi|w_x\rangle + \|\varphi\|^2 \left|\psi\right\rangle \\ &= \int |\nabla\psi(x)|^2\,\mathrm{d}x - \iint w_x(x')\left(\varphi(x') + \overline{\varphi(x')}\right)|\psi(x)|^2\,\mathrm{d}x'\mathrm{d}x \\ &\quad + \int |\varphi(x')|^2\mathrm{d}x', \end{aligned} \tag{1.2}$$

where $\psi \in L^2(\mathbb{R}^3)$ is the wave-function of the electron. We further define the Pekar functional $\mathcal{F}^{\mathrm{Pek}}(\varphi) := \inf_{\|\psi\|=1} \mathcal{E}(\psi,\varphi)$ and the minimal Pekar energy $e^{\mathrm{Pek}} := \inf_\varphi \mathcal{F}^{\mathrm{Pek}}(\varphi)$. It is known that the ground state energy $E_\alpha := \inf\sigma(\mathbb{H})$, as a function of the coupling strength α, is asymptotically given by the minimal Pekar energy e^{Pek} in the limit $\alpha\to\infty$ [1,7]. More precisely, one has $e^{\mathrm{Pek}} \geq E_\alpha = e^{\mathrm{Pek}} + O_{\alpha\to\infty}\left(\alpha^{-\frac{1}{5}}\right)$, as shown in [20]. In this work we are going to verify the prediction in the physics literature [2,3,30] that the sub-leading term in this energy asymptotics is actually of order α^{-2} with a rather explicit pre-factor

$$E_\alpha = e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1-\sqrt{H^{\mathrm{Pek}}}\right] + o_{\alpha\to\infty}\left(\alpha^{-2}\right), \tag{1.3}$$

where φ^{Pek} is a minimizer of $\mathcal{F}^{\mathrm{Pek}}$ and H^{Pek} is the Hessian of $\mathcal{F}^{\mathrm{Pek}}$ at φ^{Pek} restricted to real-valued functions $\varphi \in L^2_{\mathbb{R}}(\mathbb{R}^3)$, i.e. H^{Pek} is an operator on $L^2(\mathbb{R}^3)$ defined by

$$\langle\varphi|H^{\mathrm{Pek}}|\varphi\rangle = \lim_{\epsilon\to 0}\frac{1}{\epsilon^2}\left(\mathcal{F}^{\mathrm{Pek}}\left(\varphi^{\mathrm{Pek}} + \epsilon\varphi\right) - e^{\mathrm{Pek}}\right) \tag{1.4}$$

for all $\varphi \in L^2_{\mathbb{R}}(\mathbb{R}^3)$. The prediction in Eq. (1.3) has been verified previously for polaron models either confined to a bounded region of $\mathbb{R}^3$ [11] or to a three-dimensional torus [9]. The methods presented there exhibit substantial problems regarding their extension to the unconfined case, however. In this paper we present a new approach, which is partly based on techniques previously developed in the study of Bose–Einstein condensation and the validity of Bogoliubov's approximation for Bose gases [5,15,16] in the mean-field limit. We employ a localization method for the phonon field, which breaks the translation-invariance and effectively reduces the problem to the confined case, allowing for an application of some of the methods developed in [9,11]. Our main result is the proof of Eq. (1.3) in the following Theorem 1.1.

Theorem 1.1. *Let E_α be the ground state energy of $\mathbb{H}$ in (1.1). For any $s < \frac{1}{29}$*

$$E_\alpha = e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1-\sqrt{H^{\mathrm{Pek}}}\right] + O\left(\alpha^{-(2+s)}\right) \tag{1.5}$$

for all $\alpha \geq \alpha(s)$, where $\alpha(s) > 0$ is a suitable constant.

As an intermediate result, which might be of independent interest, we will establish the existence of a family of approximate ground states, by which we mean states whose energy is given by the right side of (1.3), exhibiting complete Bose–Einstein condensation with respect to a minimizer φ^{Pek} of the Pekar functional $\mathcal{F}^{\mathrm{Pek}}$. We refer to Theorem 3.13 for a precise statement.

In contrast to the lower bound, the proof of the upper bound on E_α in Eq. (1.3) is essentially the same as for confined polarons [9,11] and can be obtained by the same methods. It is also contained as a special case in [22], where it has been verified that the ground state energy $E_\alpha(P)$ as a function of the (conserved) total momentum P can be bounded from above by

$$E_\alpha(P) \leq e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}\left[1 - \sqrt{H^{\mathrm{Pek}}}\right] + \frac{|P|^2}{2\alpha^4 m} + C_\epsilon \alpha^{-\frac{5}{2}+\epsilon}, \tag{1.6}$$

where $m := \frac{2}{3}\|\nabla\varphi^{\mathrm{Pek}}\|^2$ and $\epsilon > 0$, with C_ϵ a suitable constant. Since $E_\alpha = E_\alpha(0)$ [8,13,23], Eq. (1.6) for the specific case $P = 0$ proves (1.5) as an upper bound, hence to establish Theorem 1.1 it suffices to prove (1.5) as a lower bound. Combining (1.6) with Theorem 1.1, one further obtains an upper bound on the increment $E_\alpha(P) - E_\alpha$, a quantity related to the effective mass of the polaron [4,14,18,29].

The proof of Eq. (1.3) for confined systems in [9,11] requires an asymptotically correct local quadratic lower bound on the Pekar functional $\mathcal{F}^{\mathrm{Pek}}(\varphi)$ for configurations close to a minimizer, as well as a sufficiently strong quadratic lower bound valid for all configurations. While our proof of Theorem 1.1 makes use of a local quadratic lower bound as well, we believe that in the translation-invariant setting any globally valid quadratic lower bound cannot be sufficiently strong, and therefore new ideas are necessary. As we explain in the following, we circumvent this problem by constructing an approximate ground state Ψ, which is essentially supported close to a minimizer of the Pekar functional $\mathcal{F}^{\mathrm{Pek}}$, and consequently we only require a locally valid quadratic lower bound.

Proof strategy of Theorem 1.1. Even though we want to verify a lower bound on E_α, let us first discuss how test functions providing an asymptotically correct upper bound are expected to look like. In the following let $(\psi^{\mathrm{Pek}}, \varphi^{\mathrm{Pek}})$ denote a minimizer of the Pekar energy $\mathcal{E}$ defined in Eq. (1.2). It has been established in [17] that all other minimizers are given by translations $\varphi^{\mathrm{Pek}}_x(x') := \varphi^{\mathrm{Pek}}(x' - x)$ and $\psi^{\mathrm{Pek}}_x(x') := e^{i\theta}\psi^{\mathrm{Pek}}(x' - x)$ of φ^{Pek} and $e^{i\theta}\psi^{\mathrm{Pek}}$, where θ is an arbitrary phase. W.l.o.g. let us denote in the following by $(\psi^{\mathrm{Pek}}, \varphi^{\mathrm{Pek}})$ the unique minimizer of $\mathcal{E}$ such that φ^{Pek} is radial and ψ^{Pek} is non-negative. Then all the product states of the form $\psi^{\mathrm{Pek}}_x \otimes \Omega_{\varphi^{\mathrm{Pek}}_x}$ with $x \in \mathbb{R}^3$, where $\Omega_{\varphi^{\mathrm{Pek}}_x}$ is the coherent state corresponding to φ^{Pek}_x (defined by $a(w)\Omega_\varphi = \langle w|\varphi\rangle\Omega_\varphi$ for all $w \in L^2(\mathbb{R}^3)$), have the asymptotically correct leading term in the energy $\langle \psi^{\mathrm{Pek}}_x \otimes \Omega_{\varphi^{\mathrm{Pek}}_x} | \mathbb{H} | \psi^{\mathrm{Pek}}_x \otimes \Omega_{\varphi^{\mathrm{Pek}}_x}\rangle = e^{\mathrm{Pek}}$. By taking convex combinations of these states on the level of density matrices, we can construct a large family of low energy states

$$\Gamma_\mu := \int_{\mathbb{R}^3} |\psi^{\mathrm{Pek}}_x \otimes \Omega_{\varphi^{\mathrm{Pek}}_x}\rangle\langle\psi^{\mathrm{Pek}}_x \otimes \Omega_{\varphi^{\mathrm{Pek}}_x}| \mathrm{d}\mu(x)$$

for any given probability measure μ on $\mathbb{R}^3$. Clearly, Γ_μ exhibits the correct leading energy $\langle \mathbb{H}\rangle_{\Gamma_\mu} = e^{\mathrm{Pek}}$. Our proof of the lower bound given in Eq. (1.5) relies on the observation that asymptotically as $\alpha \to \infty$, any low energy state Ψ is of the form Γ_μ with a suitable probability measure μ on $\mathbb{R}^3$. Since we only need this statement for the phonon part of Ψ, we will verify the weaker statement

$$\mathrm{Tr}_{\mathrm{electron}}\left[|\Psi\rangle\langle\Psi|\right] \approx \int_{\mathbb{R}^3} |\Omega_{\varphi^{\mathrm{Pek}}_x}\rangle\langle\Omega_{\varphi^{\mathrm{Pek}}_x}| \mathrm{d}\mu(x)$$

instead, see Theorem 3.2 for a precise formulation. This statement is analogous to a version of the quantum de Finetti theorem used in [15] in order to verify the Hartree approximation for Bose gases in a general setting. The main technical challenge of this paper will be the construction of approximate ground states Ψ where the corresponding measure is a delta measure, $\mu = \delta_0$, i.e. the construction of states where the phonon part is essentially given by a single coherent state $\Omega_{\varphi^{\mathrm{Pek}}}$. The method presented here is based on a grand-canonical version of the localization techniques previously developed for translation-invariant Bose gases in [5], and in analogy to the concept of Bose–Einstein condensation we say that such states satisfy (complete) condensation with respect to the Pekar minimizer φ^{Pek}. Heuristically this means that only field configurations φ close to the minimizer φ^{Pek} are relevant, hence the translational degree of freedom has been eliminated and the system is effectively confined.

Based on this observation we can adapt the strategy developed for confined polarons in [9,11], which starts by introducing an ultraviolet regularization in the interaction w_x with the aid of a momentum cut-off Λ, leading to the study of the truncated Hamiltonian $\mathbb{H}_\Lambda$. Using a lower bound on the excitation energy $\mathcal{F}^{\mathrm{Pek}}(\varphi)-e^{\mathrm{Pek}}$ that is, up to a canonical transformation, quadratic in the field variables φ and valid for all φ close to the minimizer φ^{Pek}, one can bound the truncated Hamiltonian from below by an operator that is, up to a unitary transformation, quadratic in the creation and annihilation operators. The lower bound is only valid, however, if tested against a state satisfying (complete) condensation in φ^{Pek}. Finally an explicit diagonalization of this quadratic operator yields the desired lower bound in Eq. (1.5).

The canonical transformation on the phase space $L^2(\mathbb{R}^3)$, respectively the corresponding unitary transformation on the Hilbert space $\mathcal{F}\left(L^2(\mathbb{R}^3)\right)$, is one of the key novel ingredients in our proof. It turns out to be necessary due to the presence of the translational symmetry, which makes it impossible to find a non-trivial positive semi-definite quadratic lower bound on $\mathcal{F}^{\mathrm{Pek}}(\varphi) - e^{\mathrm{Pek}}$. This issue has already been addressed in the study of a polaron on the three dimensional torus [9], where a different coordinate transformation is used, however. The canonical/unitary transformation presented in this paper is an adaptation of the one used in the study of translation-invariant Bose gases in [5].

Outline The paper is structured as follows. In Sect. 2 we will introduce an ultraviolet cut-off as well as a discretization in momentum space, and provide estimates on the energy cost associated with such approximations. Section 3 then contains our main technical result Theorem 3.13, in which we verify the existence of approximate ground states satisfying (complete) condensation with respect to a minimizer φ^{Pek} of the Pekar functional $\mathcal{F}^{\mathrm{Pek}}$. Subsequently we will discuss a large deviation estimate for such condensates in Sect. 4, quantifying the heuristic picture that only configurations close to the point of condensation matter. In Sect. 5 we then discuss properties of the Pekar functional $\mathcal{F}^{\mathrm{Pek}}$. In particular, we will discuss quadratic approximations around the minimizer φ^{Pek} as well as lower bounds that are, up to a coordinate transformation, quadratic in φ. Together with the error estimates from Sect. 2 and the large deviation estimate from Sect. 4, applied to the approximate ground state constructed in Sect. 3, this will allow us to verify our main Theorem 1.1 in Sect. 6. The subsequent Sect. 7 contains the proof of Theorem 3.2, which can be interpreted as a version of the quantum de Finetti theorem adapted to our setting. Finally, Appendices A and B contain auxiliary results concerning the Pekar minimizer φ^{Pek} and the projections introduced in Sect. 2, respectively.

Outlook In the second part of this study of the asymptotic properties of the Fröhlich polaron [6], the ground state energy $E_\alpha(P)$ of the operator $\mathbb{H}$ in the presence of a momentum constraint $\mathbb{P} = P$ will be investigated, where the total momentum operator is defined as $\mathbb{P} := \frac{1}{i}\nabla + \alpha^2 \int_{\mathbb{R}^3} k a_k^\dagger a_k \mathrm{d}k$, and the lower bound

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

will be established. Together with the upper bound in Eq. (1.6) derived in [22], one observes that the energy-momentum relation of a polaron agrees asymptotically with the one of a free particle having an effectively increased mass $\alpha^4 m$, where $\alpha^4 m$ is the celebrated Landau–Pekar formula for the mass of a polaron in the regime of strong couplings.

2. Models with Cut-off

In this section we will estimate the effect of the introduction of an ultraviolet cut-off $\Lambda > 0$, as well as a discretization in momentum space with box length $\ell > 0$, on the ground state energy, following similar ideas as in [9,11,20]. We will eventually apply these results for two different levels of coarse graining, a rough scale used in the proof of Theorem 3.2 in Sect. 7, which applies to low energy states with energy $e^{\mathrm{Pek}} + o_{\alpha\to\infty}(1)$, and a fine scale precise enough to yield the correct ground state energy up to errors of order $o_{\alpha\to\infty}\left(\alpha^{-2}\right)$, see the proof of Theorem 1.1 in Sect. 6.

Definition 2.1. Given parameters $0 < \ell < \Lambda$, let us define for $z \in 2\ell\,\mathbb{Z}^3\setminus\{0\}$ the cubes $C_z := [z_1 - \ell, z_1 + \ell) \times [z_2 - \ell, z_2 + \ell) \times [z_3 - \ell, z_3 + \ell)$, and let $z^1, .., z^N$ be an enumeration of the set of all $z = (z_1, z_2, z_3) \in 2\ell\,\mathbb{Z}^3\setminus\{0\}$ such that $C_z \subset B_\Lambda(0)$, where $B_r(0)$ is the (open) ball of radius r around the origin. Then we define the orthonormal system $e_n \in L^2\left(\mathbb{R}^3\right)$ as

$$e_n(x) := \frac{1}{\sqrt{(2\pi)^3 \int_{C_{z^n}} \frac{1}{|k|^2}\mathrm{d}k}} \int_{C_{z^n}} \frac{e^{i\,k\cdot x}}{|k|}\mathrm{d}k,$$

as well as the translated system $e_{y,n}(x) := e_n(x-y)$ and the orthogonal projection $\Pi^y_{\Lambda,\ell}$ onto the space spanned by $\{e_{y,1}, \ldots, e_{y,N}\}$. Furthermore we denote with Π_Λ the projection onto the spectral subspace of momenta $|k| \leq \Lambda$.

Lemma 2.2. *Let $w_x(x') := \pi^{-\frac{3}{2}}|x' - x|^{-2}$. Then we obtain for $0 < \ell < \Lambda$ and $x, y \in \mathbb{R}^3$ the following estimate on the L^2 norm*

$$\left\|\Pi_\Lambda w_x - \Pi^y_{\Lambda,\ell} w_x\right\| \lesssim |x-y|\ell\sqrt{\Lambda} + \sqrt{\ell}.$$

Proof. With $\widehat{\cdot}$ denoting Fourier transformation, we have

$$\sqrt{2\pi^2}\,\widehat{\Pi^y_{\Lambda,\ell} w_x}(k) = \sum_{n=1}^{N} \frac{1}{\int_{C_{z^n}} \frac{1}{|k'|^2}\mathrm{d}k'} \int_{C_{z^n}} \frac{e^{ik'\cdot(y-x)}}{|k'|^2}\mathrm{d}k'\, \frac{1}{|k|}\mathbb{1}_{C_{z^n}}(k),$$

where we have used that $\widehat{\Pi_\Lambda w_x}(k) = \frac{1}{\sqrt{2\pi^2}|k|}\mathbb{1}_{B_\Lambda(0)}(k)$. Defining the function $\sigma_n(k,x,y) := \frac{1}{\int_{C_{z^n}}\frac{1}{|k'|^2}\mathrm{d}k'}\int_{C_{z^n}}\frac{e^{ik'\cdot(y-x)}-e^{ik\cdot(y-x)}}{|k'|^2}\mathrm{d}k'$, we further have

$$\sqrt{2\pi^2}\left(\widehat{\Pi^y_{\Lambda,\ell}w_x}(k) - \widehat{\Pi_\Lambda w_x}(k)\right) = \sum_{n=1}^N \sigma_n(k,x,y)\frac{1}{|k|}\mathbb{1}_{C_{z^n}}(k) - \frac{1}{|k|}\mathbb{1}_A(k)$$

with $A := B_\Lambda(0)\setminus\left(\bigcup_{n=1}^N C_{z^n}\right)$. Making use of the estimate $|\sigma_n(k,x,y)|^2 \leq |y-x|^2\max_{k'\in C_{z^n}}|k'-k|^2 \leq 12|x-y|^2\ell^2$ for $k\in C_{z^n}$, we therefore obtain

$$\sum_{n=1}^N\int_{C_{z^n}}|\sigma_n(k,x,y)|^2\frac{1}{|k|^2}\mathrm{d}k \leq 12|x-y|^2\ell^2\int_{|k|\leq\Lambda}\frac{1}{|k|^2}\mathrm{d}k = 48\pi|x-y|^2\ell^2\Lambda.$$

Since $A\subset B_{2\ell}\cup B_\Lambda\setminus B_{\Lambda-4\ell}$ we consequently have $\int_A\frac{1}{|k|^2}\mathrm{d}k \lesssim \ell$. □

Definition 2.3. For $y\in\mathbb{R}^3$, $0<\ell<\Lambda$, let us define the cut-off Hamiltonians

$$\mathbb{H}^y_{\Lambda,\ell} := -\Delta_x - a\left(\Pi^y_{\Lambda,\ell}w_x\right) - a^\dagger\left(\Pi^y_{\Lambda,\ell}w_x\right) + \mathcal{N}, \tag{2.1}$$

$$\mathbb{H}_\Lambda := -\Delta_x - a\left(\Pi_\Lambda w_x\right) - a^\dagger\left(\Pi_\Lambda w_x\right) + \mathcal{N}. \tag{2.2}$$

These Hamiltonians can be interpreted as the restriction of $\mathbb{H}$ (in the quadratic form sense) to states where only the phonon modes in $\Pi^y_{\Lambda,\ell}L^2(\mathbb{R}^3)$, respectively $\Pi_\Lambda L^2(\mathbb{R}^3)$, are occupied. In particular, this implies that $\inf\sigma(\mathbb{H}^y_{\Lambda,\ell})\geq E_\alpha$ as well as $\inf\sigma(\mathbb{H}_\Lambda)\geq E_\alpha$. In the following we shall quantify the energy increase due to the introduction of the cut-offs.

Note that the α-dependence of the Hamiltonians $\mathbb{H}$, $\mathbb{H}^y_{\Lambda,\ell}$ and $\mathbb{H}_\Lambda$ only enters through the rescaled canonical commutation relations $\left[a(f),a^\dagger(g)\right] = \alpha^{-2}\langle f|g\rangle$ satisfied by the creation and annihilation operators $a^\dagger$ and a, and we will usually suppress the α dependency in our notation for the sake of readability. In the rest of this paper, we will always assume that α is a parameter satisfying $\alpha\geq 1$ and, in case it is not stated otherwise, estimates hold uniformly in this parameter for $\alpha\to\infty$, i.e. we write $X\lesssim Y$ in case there exist constants $C,\alpha_0>0$ such that $X\leq CY$ for all $\alpha\geq\alpha_0$.

The proof of the subsequent Lemma 2.4 closely follows the arguments in [20,21], where it was shown that $\mathbb{H}$ is bounded from below and well approximated by an operator containing only finitely many phonon modes. For the sake of completeness we will illustrate the proof, which is based on the Lieb–Yamazaki commutator method, see [21]. In the following Lemma 2.4, we will use the identification $L^2(\mathbb{R}^3)\otimes\mathcal{F}\left(L^2(\mathbb{R}^3)\right)\cong L^2\left(\mathbb{R}^3,\mathcal{F}\left(L^2(\mathbb{R}^3)\right)\right)$, in order to represent elements $\Psi\in L^2(\mathbb{R}^3)\otimes\mathcal{F}\left(L^2(\mathbb{R}^3)\right)$ as functions $x\mapsto\Psi(x)$ with values in $\mathcal{F}\left(L^2(\mathbb{R}^3)\right)$, allowing us to define the support $\mathrm{supp}\,(\Psi)$ as the closure of $\{x\in\mathbb{R}^3:\Psi(x)\neq 0\}$ and to introduce a space cut-off $L>0$.

Lemma 2.4. *We have for all* $0<\ell<\Lambda\leq K$ *and* $L>0$, *and states* Ψ *with* $\mathrm{supp}\,(\Psi)\subset B_L(y)$ *the estimate*

$$\left|\langle\Psi|\mathbb{H}_K - \mathbb{H}^y_{\Lambda,\ell}|\Psi\rangle\right| \lesssim \left(L\ell\sqrt{\Lambda}+\sqrt{\ell}+\sqrt{\frac{1}{\Lambda}-\frac{1}{K}}\right)\langle\Psi|-\Delta_x+\mathcal{N}+1|\Psi\rangle. \tag{2.3}$$

Furthermore, there exists a constant $d > 0$ such that

$$\mathbb{H}_K \geq -\frac{d}{t^2} - t\left(\mathcal{N} + \alpha^{-2}\right), \tag{2.4}$$

$$\mathbb{H}_K \geq -d + \frac{1}{2}\left(-\Delta_x + \mathcal{N}\right) \tag{2.5}$$

for all $t > 0$, $K \geq 0$ and $\alpha \geq 1$.

Proof. Let us define the functions u_x^n by $\widehat{u_x^n}(k) := \frac{1}{\sqrt{2\pi^2}}\mathbb{1}_{B_K(0)\setminus B_\Lambda(0)}(k)\frac{k_n e^{ik\cdot x}}{|k|^3}$. We have $a\left(\partial_{x_n}u_x^n\right) - a^\dagger\left(\partial_{x_n}u_x^n\right) = \left[\partial_{x_n}, a\left(u_x^n\right) - a^\dagger\left(u_x^n\right)\right]$ and

$$\pm i\left[\partial_{x_n}, a\left(u_x^n\right) - a^\dagger\left(u_x^n\right)\right] \leq -2\epsilon\partial_{x_n}^2 + \frac{1}{\epsilon}\left(a(u_x^n)^\dagger a(u_x^n) + a(u_x^n)a(u_x^n)^\dagger\right)$$
$$\leq -2\epsilon\,\partial_{x_n}^2 + \frac{\|u_x^n\|^2}{\epsilon}\left(2\mathcal{N} + \alpha^{-2}\right) = 2\|u_x^n\|\left(-\partial_{x_n}^2 + \mathcal{N} + \frac{1}{2}\alpha^{-2}\right),$$

where we have applied the Cauchy–Schwarz inequality in the first line and used the specific choice $\epsilon := \|u_x^n\|$ in the last identity. Note that the L^2-norm $\|u_x^n\|$ is independent of x, and furthermore we can express $\pm\left(\mathbb{H}_{\Lambda,\ell}^y - \mathbb{H}_K\right)$ as

$$\pm a\left(\Pi_\Lambda w_x - \Pi_{\Lambda,\ell}^y w_x\right) \pm a^\dagger\left(\Pi_\Lambda w_x - \Pi_{\Lambda,\ell}^y w_x\right) \pm i\sum_{n=1}^3\left(a\left(\partial_{x_n}u_x^n\right) - a^\dagger\left(\partial_{x_n}u_x^n\right)\right)$$
$$\leq 2\left\|\Pi_\Lambda w_x - \Pi_{\Lambda,\ell}^y w_x\right\|(1 + \mathcal{N}) + 2\max_{n\in\{1,2,3\}}\|u_x^n\|\left(-\Delta_x + 3\mathcal{N} + \frac{3}{2}\alpha^{-2}\right).$$

This concludes the proof of Eq. (2.3), since we have $\left\|\Pi_\Lambda w_x - \Pi_{\Lambda,\ell}^y w_x\right\| \lesssim L\ell\sqrt{\Lambda} + \sqrt{\ell}$ for all $x \in \operatorname{supp}(\Psi)$ by Lemma 2.2 and $\|u_x^n\|^2 \lesssim \frac{1}{\Lambda} - \frac{1}{K}$. The other statements in Eqs. (2.4) and (2.5) can be verified similarly, using the decomposition $\Pi_K w_x = \Pi_{K'} w_x + \sum_{n=1}^3 \frac{1}{i}\partial_{x_n} g_x^n$ with $\widehat{g_x^n}(k) := \frac{1}{\sqrt{2\pi^2}}\mathbb{1}_{B_K(0)\setminus B_{K'}(0)}(k)\frac{k_n e^{ik\cdot x}}{|k|^3}$ where $K' \leq K$ is large enough such that $\left\|g_x^n\right\| < \frac{1}{12}$. □

The subsequent Theorem 2.5 is a direct consequence of the results in [11] and [9,25], where multiple Lieb–Yamazaki bounds as well as a suitable Gross transformation are used in order to verify that the energy cost of introducing an ultraviolet cut-off $\Lambda = \alpha^{\frac{4}{5}(1+\sigma)}$ with $\sigma > 0$ is only of order $o_{\alpha\to\infty}\left(\alpha^{-2}\right)$. Combined with an application of the IMS localization formula, as was also done in [20], one can furthermore introduce a space cut-off at length scale $L = \alpha^{1+\sigma}$ with an energy cost of order $o_{\alpha\to\infty}\left(\alpha^{-2}\right)$ as well.

Theorem 2.5. *Given a constant $0 < \sigma \leq \frac{1}{4}$, let us introduce the momentum cut-off $\Lambda := \alpha^{\frac{4}{5}(1+\sigma)}$ as well as the space cut-off $L := \alpha^{1+\sigma}$. Then there exists a sequence of states $\Psi_\alpha^\diamond$ satisfying $\langle\Psi_\alpha^\diamond|\mathbb{H}_\Lambda|\Psi_\alpha^\diamond\rangle - E_\alpha \lesssim \alpha^{-2(1+\sigma)}$ and $\operatorname{supp}\left(\Psi_\alpha^\diamond\right) \subset B_L(0)$, where E_α is the ground state energy of $\mathbb{H}$.*

Proof. We start by arguing that

$$\inf \sigma\left(\mathbb{H}_\Lambda\right) - E_\alpha \lesssim \Lambda^{-\frac{5}{2}} + \alpha^{-1}\Lambda^{-\frac{3}{2}} + \alpha^{-2}\Lambda^{-\frac{1}{2}} \tag{2.6}$$

for large α. An analogous bound was shown in [11, Prop. 7.1] in the confined case, where additional powers of $\ln \Lambda$ appear due to complications coming from the boundary. In the translation-invariant setting on a torus, (2.6) is shown [9, Prop. 4.5], and that proof applies verbatim also in the unconfined case considered here (as has been worked out also in [25]).

By our choice of $\Lambda = \alpha^{\frac{4}{5}(1+\sigma)}$, we immediately obtain $\inf \sigma\left(\mathbb{H}_\Lambda\right) - E_\alpha \lesssim \alpha^{-2(1+\sigma)}$. Hence there exists a state Ψ satisfying $\langle \Psi|\mathbb{H}_\Lambda|\Psi\rangle - E_\alpha \lesssim \alpha^{-2(1+\sigma)}$. In order to construct a state which is furthermore supported on the ball $B_L(0)$, let χ be a non-negative $H^1\big(\mathbb{R}^3\big)$ function with $\int \chi(y)^2 \mathrm{d}y = 1$ and $\operatorname{supp}(\chi) \subset B_1(0)$. We define $\Psi_y(x) := L^{-\frac{3}{2}}\chi\left(L^{-1}(x-y)\right)\Psi(x)$ for $y \in \mathbb{R}^3$ and compute, using the IMS identity,

$$\begin{aligned}\int \langle \Psi_y|\mathbb{H}_\Lambda|\Psi_y\rangle\, \mathrm{d}y &= \langle \Psi|\mathbb{H}_\Lambda|\Psi\rangle + L^{-3}\iint \left|\nabla_x \chi\left(L^{-1}(x-y)\right)\right|^2 \mathrm{d}y\, \|\Psi(x)\|^2 \mathrm{d}x \\ &= \langle \Psi|\mathbb{H}_\Lambda|\Psi\rangle + L^{-2}\|\nabla \chi\|^2 = E_\alpha + O_{\alpha\to\infty}\left(\alpha^{-2(1+\sigma)}\right),\end{aligned}$$

see also [20] where an explicit choice of χ is used. Since $\int \|\Psi_y\|^2 \mathrm{d}y = 1$, there clearly exists a $y \in \mathbb{R}^3$ such that the state $\Psi_\alpha^\diamond := \|\Psi_y\|^{-1}\Psi_y$ satisfies $\langle \Psi_\alpha^\diamond|\mathbb{H}_\Lambda|\Psi_\alpha^\diamond\rangle - E_\alpha \lesssim \alpha^{-2(1+\sigma)}$. By the translation invariance of $\mathbb{H}_\Lambda$ we can assume that $y = 0$. □

3. Construction of a Condensate

The purpose of this section is to construct a sequence of approximate ground states Ψ_α, i.e. states with $\langle \Psi_\alpha|\mathbb{H}_\Lambda|\Psi_\alpha\rangle = E_\alpha + o_{\alpha\to\infty}\left(\alpha^{-2}\right)$ and Λ as in Theorem 2.5, that additionally satisfy complete condensation with respect to a minimizer φ^{Pek} of the Pekar functional $\mathcal{F}^{\mathrm{Pek}}$, i.e. the phonon part of Ψ_α is in a suitable sense close to a coherent state $\Omega_{\varphi^{\mathrm{Pek}}}$ with $\Omega_{\varphi^{\mathrm{Pek}}} := e^{\alpha^2 a^\dagger(\varphi^{\mathrm{Pek}}) - \alpha^2 a(\varphi^{\mathrm{Pek}})}\Omega$, where Ω is the vacuum in $\mathcal{F}\left(L^2\big(\mathbb{R}^3\big)\right)$, see Lemma 3.12 and Theorem 3.13. The construction will be based on various localization procedures of the phonon field with respect to operators of the form $\widehat{F}$ defined in the subsequent Definition 3.1.

3.1. *Properties of the $\widehat{F}$ operators.*

In this subsection we are going to introduce a useful class of operators on $\mathcal{F}\left(L^2\big(\mathbb{R}^3\big)\right)$, which we will refer to as $\widehat{F}$ operators, and provide an asymptotic formula for their expectation value $\langle \Psi_\alpha|\widehat{F}|\Psi_\alpha\rangle$ in Theorem 3.2 as well as an estimate on the energy cost of localizing with respect to such an operator in Lemma 3.3.

Definition 3.1. Given a function $F : \mathcal{M}\left(\mathbb{R}^3\right) \longrightarrow \mathbb{R}$, where $\mathcal{M}\left(\mathbb{R}^3\right)$ is the set of finite (Borel) measures on $\mathbb{R}^3$, let us define the operator $\widehat{F}$ acting on the Fock space $\mathcal{F}\left(L^2\big(\mathbb{R}^3\big)\right) = \bigoplus_{n=0}^{\infty} L^2_{\mathrm{sym}}(\mathbb{R}^{3\times n})$ as $\widehat{F}\bigoplus_{n=0}^{\infty}\Psi_n := \bigoplus_{n=0}^{\infty} F^n\Psi_n$, where

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

and $F_0\Psi_0 = F(0)\Psi_0$, i.e. $\widehat{F}$ acts component-wise on $\bigoplus_{n=0}^{\infty} L^2_{\text{sym}}(\mathbb{R}^{3\times n})$ by multiplication with the real valued function $(x^1, \dots, x^n) \mapsto F\left(\alpha^{-2}\sum_{k=1}^{n}\delta_{x^k}\right)$.

A particularly important example of an $\widehat{F}$ operator is the particle number $\mathcal{N}$, which can be written as $\mathcal{N} = \widehat{F}$ with $F(\rho) := \int \mathrm{d}\rho$. More generally we can write, for any bounded and measurable f, $\int f(x)a_x^\dagger a_x \mathrm{d}x = \widehat{F_f}$ with $F_f(\rho) := \int f \mathrm{d}\rho$. Since the assignment $F \mapsto \widehat{F}$ is linear and multiplicative, we can represent any polynomial in operators of the form $\int f(x)a_x^\dagger a_x \mathrm{d}x$ as an $\widehat{F}$ operator as well.

Note that in order to keep the notation simple, we will allow $F : \mathcal{M}\left(\mathbb{R}^3\right) \longrightarrow \mathbb{R}$ to act on non-negative $L^1\left(\mathbb{R}^3\right)$ functions $q : \mathbb{R}^3 \longrightarrow [0, \infty)$ as well by identifying them with the corresponding measure $\lambda \in \mathcal{M}\left(\mathbb{R}^3\right)$ defined as $\frac{\mathrm{d}\lambda}{\mathrm{d}x} = q(x)$.

Before we discuss the asymptotic formula for the expectation value $\langle\Psi_\alpha|\widehat{F}|\Psi_\alpha\rangle$, let us introduce a family of cut-off functions $\chi^\epsilon\,(a \leq f(\rho) \leq b)$ where $\epsilon \geq 0$ determines the sharpness of the cut-off. In the following let $\alpha, \beta : \mathbb{R} \longrightarrow [0, 1]$ be C^∞ functions such that $\alpha^2 + \beta^2 = 1$, $\operatorname{supp}(\alpha) \subset (-\infty, 1)$ and $\operatorname{supp}(\beta) \subset (-1, \infty)$. For a given function $f : \mathcal{M}\left(\mathbb{R}^3\right) \longrightarrow \mathbb{R}$ and constants $-\infty \leq a < b \leq \infty$, let us define the function $\chi^\epsilon\,(a \leq f \leq b) : \mathcal{M}\left(\mathbb{R}^3\right) \longrightarrow [0, 1]$ as

$$\rho \mapsto \chi^\epsilon\,(a \leq f(\rho) \leq b) := \begin{cases} \alpha\left(\frac{f(\rho)-b}{\epsilon}\right)\beta\left(\frac{f(\rho)-a}{\epsilon}\right), & \text{for } \epsilon > 0 \\ \mathbb{1}_{[a,b]}\left(f(\rho)\right), & \text{for } \epsilon = 0. \end{cases} \tag{3.1}$$

Note that $\sum_{j\in J}\chi^\epsilon\left(a_j \leq f(\rho) \leq b_j\right)^2 = 1$ in case the intervals $[a_j, b_j)$ are a disjoint partition of $\mathbb{R}$ with $-\infty \leq a_j < b_j \leq \infty$. Usually we will use functions f here that are related to an integral over ρ, e.g. $f(\rho) := \int \mathrm{d}\rho$.

Similarly, we define the operator $\chi^\epsilon\,(a \leq T \leq b) := \int \chi^\epsilon\,(a \leq t \leq b)\,\mathrm{d}E(t)$, where T is a self-adjoint operator and E is the spectral measure with respect to T. Furthermore we will write $\chi\,(a \leq f \leq b)$, respectively $\chi\,(a \leq T \leq b)$, in case $\epsilon = 0$ as well as $\chi^\epsilon\,(a \leq f)$, respectively $\chi^\epsilon\,(a \leq T)$, and $\chi^\epsilon\,(f \leq b)$, respectively $\chi^\epsilon\,(T \leq b)$, in case $b = \infty$ or $a = -\infty$, respectively.

The proof of the following Theorem 3.2 will be carried out in Sect. 7. It is reminiscent of the quantum de-Finetti Theorem, and establishes in addition that for low energy states phonon field configurations are necessarily close to the set of Pekar minimizers given by $\{\varphi_x^{\text{Pek}}\}_{x\in\mathbb{R}^3}$.

Theorem 3.2. *Given $m \in \mathbb{N}$, $C > 0$ and $g \in L^2\left(\mathbb{R}^3\right)$, we can find a constant $T > 0$ such that for all $\alpha \geq 1$ and states Ψ satisfying $\chi\,(\mathcal{N} \leq C)\,\Psi = \Psi$ and $\langle\Psi|\mathbb{H}_K|\Psi\rangle \leq e^{\text{Pek}} + \delta e$ with $\delta e \geq 0$ and $K \geq \alpha^{\frac{8}{29}}$, there exists a probability measure μ on $\mathbb{R}^3$, with the property*

$$\left|\left\langle\Psi\middle|\widehat{F}\middle|\Psi\right\rangle - \int_{\mathbb{R}^3} F\left(|\varphi_x^{\text{Pek}}|^2\right)\mathrm{d}\mu(x)\right| \leq T\|f\|_\infty \max\left\{\sqrt{\delta e}, \alpha^{-\frac{2}{29}}\right\} \tag{3.2}$$

for all $F : \mathcal{M}\left(\mathbb{R}^3\right) \longrightarrow \mathbb{R}$ of the form $F(\rho) = \int \dots \int f(x_1, \dots, x_m)\,\mathrm{d}\rho(x_1)\dots\mathrm{d}\rho(x_m)$ with bounded $f : \mathbb{R}^{3\times m} \longrightarrow \mathbb{R}$, and furthermore

$$\left|\left\langle\Psi\middle|W_g^{-1}\mathcal{N}W_g\middle|\Psi\right\rangle - \int_{\mathbb{R}^3}\left\|\varphi_x^{\text{Pek}} - g\right\|^2 \mathrm{d}\mu(x)\right| \leq T\max\left\{\sqrt{\delta e}, \alpha^{-\frac{2}{29}}\right\}, \tag{3.3}$$

where W_g is the Weyl operator characterized by $W_g^{-1}a(h)W_g = a(h) - \langle h|g\rangle$.

In the subsequent Lemma 3.3 we introduce a generalized IMS-type estimate quantifying the energy cost of localizing with respect to an $\widehat{F}$-operator, similar to the generalized IMS results in [19, Theorem A.1] and [16, Proposition 6.1]. In order to formulate the result, let us define for a given subset $\Omega \subset \mathcal{M}\left(\mathbb{R}^3\right)$ and a (quadratic) partition of unity $\mathcal{P} = \{F_j : \mathcal{M}\left(\mathbb{R}^3\right) \longrightarrow \mathbb{R} : j \in J\}$, i.e. $0 \leq F_j \leq 1$ and $\sum_{j\in J} F_j^2 = 1$, the variation of this partition on Ω as

$$V_\Omega\left(\mathcal{P}\right) := \alpha^4 \sup_{\rho\in\Omega,\, y\in\mathbb{R}^3} \sum_{j\in J} \left| F_j\left(\rho + \alpha^{-2}\delta_y\right) - F_j\left(\rho\right)\right|^2 .$$

Lemma 3.3. *There exists a constant $c > 0$, such that for any partition of unity $\mathcal{P} = \{F_j : \mathcal{M}\left(\mathbb{R}^3\right) \longrightarrow \mathbb{R} : j \in J\}$, $\Omega \subset \mathcal{M}\left(\mathbb{R}^3\right)$, $K > 0$, $\alpha \geq 1$ and state Ψ with $\widehat{\mathbb{1}_\Omega}\Psi = \Psi$*

$$\left| \sum_{j\in J} \left\langle \widehat{F_j}\Psi \middle| \mathbb{H}_K \middle| \widehat{F_j}\Psi\right\rangle - \langle \Psi|\mathbb{H}_K|\Psi\rangle \right| \leq c\sqrt{K}\alpha^{-4} V_\Omega\left(\mathcal{P}\right)\left\langle \Psi \middle| \sqrt{\mathcal{N} + \alpha^{-2}} \middle| \Psi\right\rangle. \quad (3.4)$$

Furthermore given $M > 0$, there exists a constant $c' > 0$ such that we have for any $\varphi \in L^2\left(\mathbb{R}^3\right)$ satisfying $\|\varphi\| \leq M$, partition of unity $\{f_j : \mathbb{R} \longrightarrow \mathbb{R} : j \in J\}$, $K \geq 1$, $\alpha \geq 1$ and state Ψ

$$\left| \sum_{j\in J} \langle \Psi_j|\mathbb{H}_K|\Psi_j\rangle - \langle \Psi|\mathbb{H}_K|\Psi\rangle \right| \leq c'\sqrt{K}\alpha^{-4} V_{\mathcal{M}(\mathbb{R}^3)}\left(\mathcal{P}'\right)\left\langle \Psi \middle| \sqrt{\mathcal{N}+1} \middle| \Psi\right\rangle,$$

where we define $\Psi_j := f_j\left(W_\varphi^{-1}\mathcal{N}W_\varphi\right)\Psi$ with W_φ being the corresponding Weyl operator and $\mathcal{P}' := \{F_j' : \mathcal{M}\left(\mathbb{R}^3\right) \longrightarrow \mathbb{R} : j \in J\}$ with $F_j'(\rho) := f_j(\int \mathrm{d}\rho)$.

Proof. By applying the IMS identity, we obtain

$$\sum_{j\in J} \widehat{F_j}\mathbb{H}_K\widehat{F_j} - \mathbb{H}_K = \frac{1}{2}\sum_{j\in J}\left[\left[\widehat{F_j}, \mathbb{H}_K\right], \widehat{F_j}\right] = -\sum_{j\in J}\mathfrak{Re}\left[\left[\widehat{F_j}, a\left(\Pi_K w_x\right)\right], \widehat{F_j}\right],$$

where we have used the fact that F_j commutes with $-\Delta_x$ and $\mathcal{N}$ in the last identity. Since a state Ψ is a function with values in $\mathcal{F}\left(L^2\left(\mathbb{R}^3\right)\right) = \bigoplus_{n=0}^{\infty} L^2_{\mathrm{sym}}(\mathbb{R}^{3\times n})$, we can represent it as $\Psi = \bigoplus_{n=0}^\infty \Psi_n$ where $\Psi_n(y, x^1, \ldots, x^n)$ is a function of the electron variable y and the n phonon coordinates $x^k \in \mathbb{R}^3$. In order to simplify the notation, we will suppress the dependence on the electron variable y in our notation. By an explicit computation, we obtain $\left[\left[\widehat{F}, a\left(v\right)\right], \widehat{F}\right]\bigoplus_{n=0}^\infty \Psi_n = -\bigoplus_{n=0}^\infty \sqrt{\frac{n+1}{\alpha^2}}\Psi_n'$ with

$$\Psi_n'(x^1, \ldots, x^n) = \int\left[F\left(\alpha^{-2}\sum_{k=1}^{n+1}\delta_{x^k}\right) - F\left(\alpha^{-2}\sum_{k=1}^{n}\delta_{x^k}\right)\right]^2 v(x^{n+1})\Psi_{n+1}(x^1, \ldots, x^{n+1})\mathrm{d}x^{n+1},$$

for $v \in L^2\left(\mathbb{R}^3\right)$ and $F : \mathcal{M}\left(\mathbb{R}^3\right) \longrightarrow \mathbb{R}$. By the definition of $V_\Omega\left(\mathcal{P}\right)$ we obtain that

$$\sigma(x^1, \ldots, x^{n+1}) := \sum_{j\in J}\left[F_j\left(\alpha^{-2}\sum_{k=1}^{n+1}\delta_{x^k}\right) - F_j\left(\alpha^{-2}\sum_{k=1}^{n}\delta_{x^k}\right)\right]^2 \leq \alpha^{-4}V_\Omega\left(\mathcal{P}\right)$$

for all $x^{n+1} \in \mathbb{R}^3$ and every $(x^1, \dots, x^n) \in \mathbb{R}^{3n}$ with $\alpha^{-2} \sum_{k=1}^n \delta_{x^k} \in \Omega$. Hence we can estimate $\left|\left\langle \Psi \middle| \sum_{j\in J} \mathfrak{Re}\left[\left[\widehat{F}_j, a(v)\right], \widehat{F}_j\right] \middle| \Psi \right\rangle\right|$, using the notation $X = (x^1, \dots, x^n)$, by

$$\sum_{n=0}^{\infty} \sqrt{\frac{n+1}{\alpha^2}} \int |\Psi_n(X)| \int \sigma(X, x^{n+1}) |v(x_{n+1}) \Psi_{n+1}(X, x_{n+1})| \mathrm{d}x_{n+1} \mathrm{d}X$$
$$\leq \alpha^{-5} V_\Omega(\mathcal{P}) \sum_{n=0}^{\infty} \sqrt{n+1} \int |\Psi_n(X)| \int |v(x_{n+1}) \Psi_{n+1}(X, x_{n+1})| \mathrm{d}x^{n+1} \mathrm{d}X$$
$$\leq \alpha^{-5} V_\Omega(\mathcal{P}) \|v\| \sum_{n=0}^{\infty} \sqrt{n+1} \|\Psi_n\| \, \|\Psi_{n+1}\| \leq \alpha^{-4} V_\Omega(\mathcal{P}) \|v\| \left\langle \Psi \middle| \sqrt{\mathcal{N} + \alpha^{-2}} \middle| \Psi \right\rangle.$$

This concludes the proof of Eq. (3.4), using the concrete choice $v := \Pi_K w_x$, since $\|\Pi_K w_x\|^2 = \frac{1}{2\pi^2} \int_{|k|\leq K} \frac{1}{|k|^2} = \frac{2}{\pi} K$.

In order to verify the second statement we apply the unitary transformation W_φ to the operator $\mathbb{X} := \sum_{j\in J} f_j\left(W_\varphi^{-1} \mathcal{N} W_\varphi\right) \mathbb{H}_K f_j\left(W_\varphi^{-1} \mathcal{N} W_\varphi\right) - \mathbb{H}_K$ and compute

$$W_\varphi \mathbb{X} W_\varphi^{-1} = \frac{1}{2} \sum_{j\in J} \left[\left[f_j(\mathcal{N}), W_\varphi \mathbb{H}_K W_\varphi^{-1}\right], f_j(\mathcal{N})\right]$$
$$= \sum_{j\in J} \mathfrak{Re}\left[\left[f_j(\mathcal{N}), a(\varphi - \Pi_K w_x)\right], f_j(\mathcal{N})\right] = \sum_{j\in J} \mathfrak{Re}\left[\left[\widehat{F}'_j, a(v)\right], \widehat{F}'_j\right],$$

where we defined $v := \varphi - \Pi_K w_x$ and applied the definition $F'_j(\rho) = f_j\left(\int \mathrm{d}\rho\right)$. We know from the previous estimates that

$$\pm \sum_{j\in J} \mathfrak{Re}\left[\left[f_j(\mathcal{N}), a(v)\right], f_j(\mathcal{N})\right] \leq \alpha^{-4} V_{\mathcal{M}(\mathbb{R}^3)}\left(\mathcal{P}'\right) \|v\| \sqrt{\mathcal{N} + \alpha^{-2}}.$$

Clearly $\|v\| \leq \|\varphi\| + \|\Pi_K w_x\| \lesssim \sqrt{K}$ for $K \geq 1$, and consequently

$$\left|\sum_{j\in J} \langle \Psi_j | \mathbb{H}_K | \Psi_j \rangle - \langle \Psi | \mathbb{H}_K | \Psi \rangle\right| \lesssim \sqrt{K} \alpha^{-4} V_{\mathcal{M}(\mathbb{R}^3)}\left(\mathcal{P}'\right) \left\langle \Psi \middle| \sqrt{W_\varphi^{-1} \mathcal{N} W_\varphi + \alpha^{-2}} \middle| \Psi \right\rangle$$
$$\lesssim \sqrt{K} \alpha^{-4} V_{\mathcal{M}(\mathbb{R}^3)}\left(\mathcal{P}'\right) \left\langle \Psi \middle| \sqrt{\mathcal{N} + 1} \middle| \Psi \right\rangle,$$

where we have used that $W_\varphi^{-1} \mathcal{N} W_\varphi \leq 2\left(\mathcal{N} + \|\varphi\|^2\right)$ and the operator-monotonicity of the square root. □

3.2. Auxiliary localization procedures. In the following Eqs. (3.6) and (3.10), we will apply localizations procedures to a given sequence $\Psi_\alpha^\bullet$ in order to construct states having additional useful properties, which we will use in Lemma 3.12 in order to construct a sequence of approximate ground states satisfying complete condensation. Furthermore we will quantify the energy cost of these localizations by $\langle \Psi_\alpha | \mathbb{H}_\Lambda | \Psi_\alpha \rangle - \widetilde{E}_\alpha \lesssim \alpha^{-3}$ in the Lemmas 3.4 and 3.5. In Theorem 3.13 we will then apply a final localization procedure, in order to lift the (weak) condensation from Lemma 3.12 to a strong one, following the argument in [16].

In the following let $L := \alpha^{1+\sigma}$ and $\Lambda := \alpha^{\frac{4}{5}(1+\sigma)}$ with $0 < \sigma \leq \frac{1}{4}$, and let $\Psi_\alpha^\bullet$ be a sequence of states satisfying $\mathrm{supp}\left(\Psi_\alpha^\bullet\right) \subset B_L(0)$ and $\widetilde{E}_\alpha - E_\alpha \lesssim \alpha^{-\frac{4}{29}}$, where

$$\widetilde{E}_\alpha := \langle \Psi_\alpha^\bullet | \mathbb{H}_\Lambda | \Psi_\alpha^\bullet \rangle. \tag{3.5}$$

The exponent $\frac{4}{29}$ is chosen for convenience, as it allows to simplify the right hand side of Eq. (3.2) to $\|f\|_\infty \alpha^{-\frac{2}{29}}$ (using that $E_\alpha \leq e^{\mathrm{Pek}}$). For the proof of Theorem 1.1 we shall use the specific choice $\Psi_\alpha^\diamond$ from Theorem 2.5 for $\Psi_\alpha^\bullet$, but it will be useful in the second part to have the first two localization procedures in Lemma 3.4 and 3.5 formulated for a more general sequence $\Psi_\alpha^\bullet$.

Having Lemma 3.3 at hand, we can verify our first localization result in Lemma 3.4, which allows us to restrict our attention to states Ψ'_α having a (rescaled) particle number $\mathcal{N}$ between some fixed constants c_- and c_+. To be precise, for given c_-, c_+ and ϵ' we use the function $F_*(\rho) := \chi^{\epsilon'}\left(c_- + \epsilon' \leq \int \mathrm{d}\rho \leq c_+ - \epsilon'\right)$ in order to define the states

$$\Psi'_\alpha := Z_\alpha^{-1} \widehat{F}_* \Psi_\alpha^\bullet, \tag{3.6}$$

with the corresponding normalization constants $Z_\alpha := \|\widehat{F}_* \Psi_\alpha^\bullet\|$. By construction we have $\chi\left(c_- \leq \mathcal{N} \leq c_+\right) \Psi'_\alpha = \Psi'_\alpha$ as well as $\mathrm{supp}\left(\Psi'_\alpha\right) \subset B_L(0)$. In the following Lemma 3.4 we derive an upper bound on the energy of Ψ'_α, and in addition we will investigate the large α behavior of Z_α, which will be useful in the second part.

Lemma 3.4. *Let $\Psi_\alpha^\bullet$ be the sequence introduced above Eq. (3.5). Then there exist α-independent constants $c_-, c_+, \epsilon' > 0$ such that the corresponding states Ψ'_α defined in Eq. (3.6) satisfy $\langle \Psi'_\alpha | \mathbb{H}_\Lambda | \Psi'_\alpha \rangle - \widetilde{E}_\alpha \lesssim \alpha^{-\frac{7}{2}}$. Furthermore, $Z_\alpha \underset{\alpha\to\infty}{\longrightarrow} 1$.*

Proof. In the following let F_* be the function defined above Eq. (3.6) and let us complete it to a quadratic partition of unity $\mathcal{P} := \{F_-, F_*, F_+\}$ with the aid of the functions $F_-(\rho) := \chi^{\epsilon'}\left(\int \mathrm{d}\rho \leq c_- + \epsilon'\right)$ and $F_+(\rho) := \chi^{\epsilon'}\left(c_+ - \epsilon' \leq \int \mathrm{d}\rho\right)$. Making use of Lemma 3.3 and $\Lambda = \alpha^{\frac{4}{5}(1+\sigma)} \leq \alpha$, we then obtain

$$\begin{aligned} &Z_{\alpha,-}^2 \langle \Psi_{\alpha,-} | \mathbb{H}_\Lambda | \Psi_{\alpha,-} \rangle + Z_\alpha^2 \langle \Psi'_\alpha | \mathbb{H}_\Lambda | \Psi'_\alpha \rangle + Z_{\alpha,+}^2 \langle \Psi_{\alpha,+} | \mathbb{H}_\Lambda | \Psi_{\alpha,+} \rangle \\ &\quad \leq \langle \Psi_\alpha^\bullet | \mathbb{H}_\Lambda | \Psi_\alpha^\bullet \rangle + c\, \alpha^{-\frac{7}{2}} V_{\mathcal{M}(\mathbb{R}^3)}(\mathcal{P}) \left\langle \Psi_\alpha^\bullet \middle| \sqrt{\mathcal{N} + \alpha^{-2}} \middle| \Psi_\alpha^\bullet \right\rangle, \end{aligned} \tag{3.7}$$

where $\Psi_{\alpha,\pm} := Z_{\alpha,\pm}^{-1} \widehat{F}_{(\pm)} \Psi_\alpha^\bullet$, with corresponding normalization factors $Z_{\alpha,\pm} := \|\widehat{F}_{(\pm)} \Psi_\alpha^\bullet\|$. By Eq. (2.5) there exists a constant d s.t. $\left\langle \Psi_\alpha^\bullet \middle| \mathcal{N} \middle| \Psi_\alpha^\bullet \right\rangle \leq \left\langle \Psi_\alpha^\bullet \middle| 2\mathbb{H}_\Lambda + d \middle| \Psi_\alpha^\bullet \right\rangle \lesssim d + \alpha^{-\frac{4}{29}}$, where we have used the assumption $\left\langle \Psi_\alpha^\bullet \middle| \mathbb{H}_\Lambda \middle| \Psi_\alpha^\bullet \right\rangle = \widetilde{E}_\alpha \leq \widetilde{E}_\alpha - E_\alpha \lesssim \alpha^{-\frac{4}{29}}$. The first derivative of the functions $\chi^{\epsilon'}(\cdot \leq c_- + \epsilon')$, $\chi^{\epsilon'}(c_- + \epsilon' \leq \cdot \leq c_+ - \epsilon')$ and $\chi^{\epsilon'}(\cdot \leq c_+ - \epsilon')$ is uniformly bounded by some ϵ'-dependent constant D, and consequently we have for all finite measures ρ and $\rho' := \rho + \alpha^{-2}\delta_y$ with $y \in \mathbb{R}^3$, and $\diamond \in \{-, *, +\}$,

$$\left|F_\diamond\left(\rho'\right) - F_\diamond\left(\rho\right)\right| \leq D \left| \int \mathrm{d}\rho' - \int \mathrm{d}\rho \right| = D\alpha^{-2}.$$

This implies that $V_{\mathcal{M}(\mathbb{R}^3)}(\mathcal{P}) \lesssim 1$, and therefore the right hand side of Eq. (3.7) is bounded by $\langle \Psi_\alpha^\bullet | \mathbb{H}_\Lambda | \Psi_\alpha^\bullet \rangle + C\alpha^{-\frac{7}{2}}$ for a suitable $C > 0$. Since $Z_{\alpha,-}^2 + Z_\alpha^2 + Z_{\alpha,+}^2 = 1$, this means that at least one of the terms $\langle \Psi_{\alpha,-} | \mathbb{H}_\Lambda | \Psi_{\alpha,-} \rangle$, $\langle \Psi_\alpha' | \mathbb{H}_\Lambda | \Psi_\alpha' \rangle$ or $\langle \Psi_{\alpha,+} | \mathbb{H}_\Lambda | \Psi_{\alpha,+} \rangle$ is bounded from above by $\langle \Psi_\alpha^\bullet | \mathbb{H}_\Lambda | \Psi_\alpha^\bullet \rangle + C\alpha^{-\frac{7}{2}} = \widetilde{E}_\alpha + C\alpha^{-\frac{7}{2}}$. We can however rule out that $\langle \Psi_{\alpha,-} | \mathbb{H}_\Lambda | \Psi_{\alpha,-} \rangle$, respectively $\langle \Psi_{\alpha,+} | \mathbb{H}_\Lambda | \Psi_{\alpha,+} \rangle$, satisfy this upper bound for all small c_-, ϵ' and large α, c_+, since $\widetilde{E}_\alpha \leq E_\alpha + C'\alpha^{-\frac{4}{29}} \leq e^{\text{Pek}} + C'\alpha^{-\frac{4}{29}} < \frac{e^{\text{Pek}}}{2} < 0$ for α large enough and a suitable C', and since we have by Eqs. (2.4) and (2.5) for all $t > 0$

$$\langle \Psi_{\alpha,-} | \mathbb{H}_\Lambda | \Psi_{\alpha,-} \rangle \geq \langle \Psi_{\alpha,-} | -\frac{d}{t^2} - t\left(\mathcal{N} + \alpha^{-2}\right) | \Psi_{\alpha,-} \rangle \geq -\frac{d}{t^2} - t\left(c_- + 2\epsilon' + \alpha^{-2}\right) \geq -\frac{e^{\text{Pek}}}{2}, \tag{3.8}$$

$$\langle \Psi_{\alpha,+} | \mathbb{H}_\Lambda | \Psi_{\alpha,+} \rangle \geq \langle \Psi_{\alpha,+} | -d + \frac{1}{2}\mathcal{N} | \Psi_{\alpha,+} \rangle \geq -d + \frac{1}{2}(c_+ - 2\epsilon') \geq 0, \tag{3.9}$$

where the last inequality in Eq. (3.8), respectively Eq. (3.9), holds for small c_-, ϵ' and large α, c_+ with the concrete choice $t := \left(\frac{d}{c_- + 2\epsilon' + \alpha^{-2}}\right)^{\frac{1}{3}}$. Using again that the right hand side of Eq. (3.7) is bounded by $\langle \Psi_\alpha^\bullet | \mathbb{H}_\Lambda | \Psi_\alpha^\bullet \rangle + C\alpha^{-\frac{7}{2}}$ together with Eqs. (3.8) and (3.9), and the fact that $\mathbb{H}_\Lambda \geq E_\alpha$ and $E_\alpha \leq e^{\text{Pek}}$, yields furthermore

$$(1 - Z_\alpha^2)\left(E_\alpha - \frac{e^{\text{Pek}}}{2}\right) + Z_\alpha^2 E_\alpha \leq (1 - Z_\alpha^2)\frac{e^{\text{Pek}}}{2} + Z_\alpha^2 E_\alpha \leq \widetilde{E}_\alpha + C\alpha^{-\frac{7}{2}},$$

and therefore $-(1 - Z_\alpha^2)\frac{e^{\text{Pek}}}{2} \leq \widetilde{E}_\alpha - E_\alpha + C\alpha^{-\frac{7}{2}} \underset{\alpha\to\infty}{\longrightarrow} 0$. Since $e^{\text{Pek}} < 0$, this immediately implies $Z_\alpha \underset{\alpha\to\infty}{\longrightarrow} 1$. □

Regarding the next localization step in Lemma 3.5, let us introduce for given R and $\epsilon > 0$ satisfying $R > 2\epsilon$ the function $K_R(\rho) := \iint \chi^\epsilon (R - \epsilon \leq |x - y|)\, \mathrm{d}\rho(x)\mathrm{d}\rho(y)$, which measures how sharply the mass of the measure ρ is concentrated. It will be convenient in the second part to have K_R defined for arbitrary $\epsilon \geq 0$ even though we only need it for $\epsilon = 0$ in the following. We also define the function $F_R(\rho) := \chi^{\frac{\delta}{3}}\left(K_R(\rho) \leq \frac{2\delta}{3}\right)$ for $R, \delta > 0$, as well as the states

$$\Psi_\alpha'' := Z_{R,\alpha}^{-1} \widehat{F}_R \Psi_\alpha', \tag{3.10}$$

where Ψ_α' is as in Lemma 3.4 and $Z_{R,\alpha} := \|\widehat{F}_R \Psi_\alpha'\|$. Since Ψ_α' satisfies $\text{supp}\left(\Psi_\alpha'\right) \subset B_L(0)$, we have $\text{supp}\left(\Psi_\alpha''\right) \subset B_L(0)$ as well. Furthermore $\chi\left(\widehat{K}_R \leq \delta\right)\Psi_\alpha'' = \Psi_\alpha''$. Heuristically this means that we can restrict our attention to phonon configurations that concentrate in a ball of fixed radius R.

Lemma 3.5. *Let Ψ_α' be the sequence from Lemma 3.4, and let $\epsilon \geq 0$ and $\delta > 0$ be given constants. Then there exists a α independent $R > 0$, such that the states Ψ_α'' defined in Eq. (3.10) satisfy $\langle \Psi_\alpha'' | \mathbb{H}_\Lambda | \Psi_\alpha'' \rangle - \widetilde{E}_\alpha \lesssim \alpha^{-\frac{7}{2}}$, where $\widetilde{E}_\alpha$ is defined in Eq. (3.5). Furthermore, $Z_{R,\alpha} \underset{\alpha\to\infty}{\longrightarrow} 1$.*

Proof. Since $\mathcal{P} := \{F_R, G_R\}$ with $G_R := \sqrt{1 - F_R^2} = \chi^{\frac{\delta}{3}}\left(\frac{2\delta}{3} \leq K_R(\rho)\right)$ is a partition of unity, we obtain by Lemma 3.3

$$\langle \widehat{F}_R \Psi'_\alpha | \mathbb{H}_\Lambda | \widehat{F}_R \Psi'_\alpha \rangle + \langle \widehat{G}_R \Psi'_\alpha | \mathbb{H}_\Lambda | \widehat{G}_R \Psi'_\alpha \rangle \\ \leq \langle \Psi'_\alpha | \mathbb{H}_\Lambda | \Psi'_\alpha \rangle + c\, \alpha^{-\frac{7}{2}} V_\Omega(\mathcal{P}) \left\langle \Psi'_\alpha \middle| \sqrt{c_+ + \alpha^{-2}} \middle| \Psi'_\alpha \right\rangle \tag{3.11}$$

with $\Omega := \{\rho : \int \mathrm{d}\rho \leq c_+\}$, where we have used $\chi(\mathcal{N} \leq c_+)\Psi'_\alpha = \Psi'_\alpha$ and $\Lambda \leq \alpha$. Since $\frac{\mathrm{d}}{\mathrm{d}x}\chi^{\frac{\delta}{3}}\left(\frac{2\delta}{3} \leq x\right)$ and $\frac{\mathrm{d}}{\mathrm{d}x}\chi^{\frac{\delta}{3}}\left(x \leq \frac{2\delta}{3}\right)$ are bounded by some δ-dependent constant D, we have for all $\rho \in \Omega$ and $\rho' := \rho + \alpha^{-2}\delta_z$ with $z \in \mathbb{R}^3$, and $R > 2\epsilon$, the estimate

$$\left|F_R(\rho') - F_R(\rho)\right| \leq D\left|K_R(\rho') - K_R(\rho)\right| = 2D\alpha^{-2} \int \chi^\epsilon (R - \epsilon \leq |y - z|)\, \mathrm{d}\rho(y) \\ \leq 2D\alpha^{-2} c_+,$$

and the same result holds for G_R. Therefore we have by Eq. (3.11) and Lemma 3.4

$$\langle \widehat{F}_R \Psi'_\alpha | \mathbb{H}_\Lambda | \widehat{F}_R \Psi'_\alpha \rangle + \langle \widehat{G}_R \Psi'_\alpha | \mathbb{H}_\Lambda | \widehat{G}_R \Psi'_\alpha \rangle \leq \langle \Psi'_\alpha | \mathbb{H}_\Lambda | \Psi'_\alpha \rangle + C_1 \alpha^{-\frac{7}{2}} \leq \widetilde{E}_\alpha + C_2 \alpha^{-\frac{7}{2}} \tag{3.12}$$

for suitable constants $C_1, C_2 > 0$. Since $\|\widehat{F}_R \Psi'_\alpha\|^2 + \|\widehat{G}_R \Psi'_\alpha\|^2 = 1$, this means that we either have $\langle \Psi''_\alpha | \mathbb{H}_\Lambda | \Psi''_\alpha \rangle \leq \widetilde{E}_\alpha + C_2 \alpha^{-\frac{7}{2}}$ or $\langle \widetilde{\Psi}_\alpha | \mathbb{H}_\Lambda | \widetilde{\Psi}_\alpha \rangle \leq \widetilde{E}_\alpha + C_2 \alpha^{-\frac{7}{2}}$, where $\widetilde{\Psi}_\alpha := \|\widehat{G}_R \Psi'_\alpha\|^{-1} \widehat{G}_R \Psi'_\alpha$. In the following we are going to rule out the second case for R and α large enough, to be precise we are going to verify $\langle \widetilde{\Psi}_\alpha | \mathbb{H}_\Lambda | \widetilde{\Psi}_\alpha \rangle > \widetilde{E}_\alpha + d\alpha^{-\frac{4}{29}}$ for any $d > 0$ and large enough R and α by contradiction. In order to do this, let us assume $\langle \widetilde{\Psi}_\alpha | \mathbb{H}_\Lambda | \widetilde{\Psi}_\alpha \rangle \leq \widetilde{E}_\alpha + d\alpha^{-\frac{4}{29}}$. Since $\widetilde{E}_\alpha \leq E_\alpha + C\alpha^{-\frac{4}{29}} \leq e^{\mathrm{Pek}} + C\alpha^{-\frac{4}{29}}$ by assumption for a suitable constant C, $\widetilde{\Psi}_\alpha$ satisfies the assumptions of Theorem 3.2 with $\delta e := (d + C)\alpha^{-\frac{4}{29}}$. Hence there exists a measure μ such that Eq. (3.2) holds. By the support properties of G_R we obtain

$$\frac{\delta}{3} \leq \left\langle \widetilde{\Psi}_\alpha \middle| \widehat{K}_R \middle| \widetilde{\Psi}_\alpha \right\rangle = \int K_R\left(\left|\varphi_x^{\mathrm{Pek}}\right|^2\right) \mathrm{d}\mu + O_{\alpha\to\infty}\left(\alpha^{-\frac{2}{29}}\right) \\ = K_R\left(\left|\varphi^{\mathrm{Pek}}\right|^2\right) + O_{\alpha\to\infty}\left(\alpha^{-\frac{2}{29}}\right). \tag{3.13}$$

Since $\lim_{R\to\infty} K_R\left(\left|\varphi^{\mathrm{Pek}}\right|^2\right) = 0$, Eq. (3.13) is a contradiction for large R and α, and consequently we have $\langle \widetilde{\Psi}_\alpha | \mathbb{H}_\Lambda | \widetilde{\Psi}_\alpha \rangle > \widetilde{E}_\alpha + d\alpha^{-\frac{4}{29}}$ for such R and α. In combination with Eq. (3.12) this furthermore yields

$$Z_{R,\alpha}^2 E_\alpha + (1 - Z_{R,\alpha}^2)\left(E_\alpha + d\alpha^{-\frac{4}{29}}\right) \leq Z_{R,\alpha}^2 E_\alpha + (1 - Z_{R,\alpha}^2)\left(\widetilde{E}_\alpha + d\alpha^{-\frac{4}{29}}\right) \leq \widetilde{E}_\alpha + C_2 \alpha^{-\frac{7}{2}},$$

and therefore $1 - Z_{R,\alpha}^2 \leq \frac{\alpha^{\frac{4}{29}}}{d}\left(\widetilde{E}_\alpha - E_\alpha + C_2 \alpha^{-\frac{7}{2}}\right) \leq \frac{1}{d} + \frac{C_2}{d}\alpha^{\frac{4}{29} - \frac{7}{2}}$. Since this holds for any $d > 0$ and α large enough, we conclude that $Z_{R,\alpha} \underset{\alpha\to\infty}{\longrightarrow} 1$. □

3.3. Localization of the median. The previous localizations in the Lemmas 3.4 and 3.5 will allow us to control the energy error in the proof of Lemma 3.12, where we carry out the main localization procedure with respect to the (regularized) median m_q defined in Definition 3.8. Before we come to the proof of Lemma 3.12, we are going to derive Lemma 3.10, which provides an upper bound on the variation $V_\Omega(\mathcal{P})$ for partitions $\mathcal{P} = \{F_j : j \in J\}$ of the form $F_j(\rho) = f_j\left(m_q(\rho)\right)$. The following auxiliary Lemmas 3.6, 3.7 and 3.9 will be useful in proving Lemma 3.10.

Lemma 3.6. *Let us define the set Ω_{reg} as the set of all $\rho \in \mathcal{M}\left(\mathbb{R}^3\right)$ satisfying*

$$\rho_i(\{t\}) \leq \alpha^{-2}$$

for all $t \in \mathbb{R}$ and $i \in \{1,2,3\}$, where ρ_1, ρ_2 and ρ_3 are the marginal measures of ρ defined by $\rho_i(A) := \rho([x_i \in A])$. Then $\widehat{\mathbb{1}_{\Omega_{\mathrm{reg}}}}\Psi = \Psi$ for all $\Psi \in \mathcal{F}\left(L^2(\mathbb{R}^3)\right)$.

Proof. For given $x = (x^1, \ldots, x^n) \in \mathbb{R}^{3\times n}$, define the measure $\rho_x := \alpha^{-2}\sum_{k=1}^n \delta_{x^k}$. Note that $\rho_x \notin \Omega_{\mathrm{reg}}$ if and only if there exists an $i \in \{1,2,3\}$ such that $x_i^k = x_i^{k'}$ for indices $k \neq k'$. Clearly the set of all such $x \in \mathbb{R}^{3\times n}$ has Lebesgue measure zero. Hence the multiplication operator by the function $(x^1, \ldots, x^n) \mapsto \mathbb{1}_{\Omega_{\mathrm{reg}}}(\rho_x)$ is equal to the identity on $L^2_{\mathrm{sym}}\left(\mathbb{R}^{3\times n}\right)$, which concludes the proof according to Definition 3.1. □

Lemma 3.7. *Let ν, ν' be finite measures on $\mathbb{R}$ such that $\nu(\{t\}) \leq \epsilon$ and $\nu'(\{t\}) \leq \epsilon$ for all $t \in \mathbb{R}$, and let $x^\kappa(\nu)$ be the κ-quantile of the measure ν with $0 \leq \kappa \leq 1$, to be precise $x^\kappa(\nu)$ is the supremum over all numbers $t \in \mathbb{R}$ satisfying $\int_{-\infty}^t \mathrm{d}\nu \leq \kappa \int \mathrm{d}\nu$, where we use the convention that the boundaries are included in the domain of integration $\int_a^b f\,\mathrm{d}\nu := \int_{[a,b]} f\,\mathrm{d}\nu$. Then*

$$\left|\int_{-\infty}^{x^\kappa(\nu')} \mathrm{d}\nu - \int_{-\infty}^{x^\kappa(\nu)} \mathrm{d}\nu\right| \leq 2\|\nu' - \nu\|_{\mathrm{TV}} + \epsilon,$$

where $\|\nu' - \nu\|_{\mathrm{TV}} := \sup_{\|f\|_\infty = 1} \left|\int f\,\mathrm{d}\nu' - \int f\,\mathrm{d}\nu\right|$.

Proof. We estimate

$$\begin{aligned}
\int_{-\infty}^{x^\kappa(\nu')} \mathrm{d}\nu - \int_{-\infty}^{x^\kappa(\nu)} \mathrm{d}\nu &\leq \int_{-\infty}^{x^\kappa(\nu')} \mathrm{d}\nu - \kappa \int \mathrm{d}\nu \\
&\leq \int_{-\infty}^{x^\kappa(\nu')} \mathrm{d}\nu' + \|\nu' - \nu\|_{\mathrm{TV}} - \kappa \int \mathrm{d}\nu \\
&\leq \kappa \int \mathrm{d}\nu' + \epsilon + \|\nu' - \nu\|_{\mathrm{TV}} - \kappa \int \mathrm{d}\nu \leq 2\|\nu' - \nu\|_{\mathrm{TV}} + \epsilon,
\end{aligned}$$

where we have used $\int_{-\infty}^{x^\kappa(\nu)} \mathrm{d}\nu \geq \kappa \int \mathrm{d}\nu$ and $\int_{-\infty}^{x^\kappa(\nu')} \mathrm{d}\nu' \leq \kappa \int \mathrm{d}\nu' + \epsilon$. The bound from below can be obtained by interchanging the role of ν and ν'. □

Definition 3.8. Let $x^\kappa(\nu)$ be the κ-quantile of a measure ν on $\mathbb{R}$ defined in Lemma 3.7 and let us denote $K_q(\nu) := [x^{\frac{1}{2}-q}(\nu), x^{\frac{1}{2}+q}(\nu)]$ for $0 < q < \frac{1}{2}$. Then we define

$$m_q(\nu) := \frac{1}{\int_{K_q(\nu)} \mathrm{d}\nu} \int_{K_q(\nu)} t\,\mathrm{d}\nu(t) \in \mathbb{R} \tag{3.14}$$

for $\nu \neq 0$ and $m_q(0) := 0$. Furthermore we define for a measure ρ on $\mathbb{R}^3$ the regularized median as $m_q(\rho) := \Big(m_q(\rho_1), m_q(\rho_2), m_q(\rho_3)\Big) \in \mathbb{R}^3$, where ρ_1, ρ_2 and ρ_3 are the marginal measures of ρ.

Note that $x^\kappa(\nu)$ is the largest value, such that both $\int_{-\infty}^{x^\kappa(\nu)} \mathrm{d}\nu \geq \kappa \int \mathrm{d}\nu$ and $\int_{x^\kappa(\nu)}^{\infty} \mathrm{d}\nu \geq (1-\kappa)\int \mathrm{d}\nu$ hold. As an immediate consequence, we obtain that the expression in Eq. (3.14) is well-defined for $\nu \neq 0$ and $0 < q < \frac{1}{2}$, since

$$\int_{K_q(\nu)} \mathrm{d}\nu = \int_{-\infty}^{x^{\frac{1}{2}+q}(\nu)} \mathrm{d}\nu + \int_{x^{\frac{1}{2}-q}(\nu)}^{\infty} \mathrm{d}\nu - \int \mathrm{d}\nu \geq 2q \int \mathrm{d}\nu > 0. \tag{3.15}$$

In the following Lemma 3.9 we are going to show that the quantiles $x^{\frac{1}{2}\pm q}$ are positioned in a ball of radius R around the median $x^{\frac{1}{2}}$ for all measures ρ that concentrate in a ball of radius R around the median, in the sense that $\underset{|x-y|\geq R}{\int\int} \mathrm{d}\rho(x)\mathrm{d}\rho(y) \leq \delta$, see also the definition of F_R above Eq. (3.10), where δ is a small enough constant depending on q and the total mass $\int \mathrm{d}\rho$.

Lemma 3.9. *Given constants $R, c > 0$ and $0 < \delta < \frac{c^2}{2}$, let ρ satisfy $c \leq \int \mathrm{d}\rho$ and $\underset{|x-y|\geq R}{\int\int} \mathrm{d}\rho(x)\mathrm{d}\rho(y) \leq \delta$ and let q be a constant satisfying $0 < q \leq \frac{1}{2} - \frac{\delta}{c^2}$. Then we have for all $i \in \{1,2,3\}$ that $x^{\frac{1}{2}}(\rho_i) - R \leq x^{\frac{1}{2}-q}(\rho_i) \leq x^{\frac{1}{2}+q}(\rho_i) \leq x^{\frac{1}{2}}(\rho_i) + R$.*

Proof. Since x^κ is translation covariant, i.e. $x^\kappa(\nu(\cdot - t)) = x^\kappa(\nu) + t$, we can assume w.l.o.g. that $x^{\frac{1}{2}}(\rho_i) = 0$ for $i \in \{1,2,3\}$. Then

$$\begin{aligned}\delta &\geq \underset{|x-y|\geq R}{\int\int} \mathrm{d}\rho(x)\mathrm{d}\rho(y) \geq 2\int_{x_i\geq 0} \mathrm{d}\rho(x) \int_{y_i \leq -R} \mathrm{d}\rho(y) \geq \int \mathrm{d}\rho \int_{y_i\leq -R} \mathrm{d}\rho(y)\\ &\geq c\int_{y_i\leq -R} \mathrm{d}\rho(y),\end{aligned}$$

where we have used that $x^{\frac{1}{2}}(\rho_i) = 0$ and $\int \mathrm{d}\rho \geq c$ in the last two inequalities. Hence

$$\int_{y_i\leq -R} \mathrm{d}\rho(y) \leq \frac{\delta}{c} \leq \frac{\delta}{c^2}\int \mathrm{d}\rho \leq \kappa \int \mathrm{d}\rho$$

for all $\kappa \geq \frac{\delta}{c^2}$ and consequently we have $-R \leq x^\kappa(\rho_i)$ for all such κ by the definition of $x^\kappa(\rho_i)$. Similarly we obtain $x^\kappa(\rho_i) \leq R$ for all κ satisfying $\kappa \leq 1 - \frac{\delta}{c^2}$. Therefore $|x^{\frac{1}{2}\pm q}(\rho_i)| \leq R$ for $q \leq \frac{1}{2} - \frac{\delta}{c^2}$. □

Lemma 3.10. *Given constants $R, c > 0$ and $0 < \delta < \frac{c^2}{2}$, let Ω be the set of $\rho \in \Omega_{\mathrm{reg}}$ satisfying $c \leq \int \mathrm{d}\rho$ and $\underset{|x-y|\geq R}{\int\int} \mathrm{d}\rho(x)\mathrm{d}\rho(y) \leq \delta$. Then*

$$\left| m_q\left(\rho + \alpha^{-2}\delta_x\right) - m_q(\rho)\right| \lesssim \frac{R}{c\alpha^2 q}$$

for all $\rho \in \Omega$, $x \in \mathbb{R}^3$ and $0 < q < \frac{1}{2} - \frac{\delta}{c^2}$, where m_q is defined in Definition 3.8.

Proof. Since m_q acts translation covariant on any $\rho \neq 0$, i.e. $m_q(\rho(\cdot - y)) = m_q(\rho) + y$, we can assume w.l.o.g. that $x^{\frac{1}{2}}(\rho_i) = 0$ for $i \in \{1, 2, 3\}$. By Lemma 3.9 we therefore obtain $|x^{\frac{1}{2}\pm q}(\rho_i)| \leq R$ for $\rho \in \Omega$ and $0 < q \leq \frac{1}{2} - \frac{\delta}{c^2}$. Note that the marginal measures ρ_i and ρ_i', where $\rho' := \rho + \alpha^{-2}\delta_x$, satisfy $\rho_i(\{y\}) \leq \alpha^{-2}$ and $\rho_i'(\{y\}) \leq 2\alpha^{-2}$ by our assumption $\rho \in \Omega_{\text{reg}}$. Therefore $x^{\kappa_*}(\rho_i) \leq x^{\kappa}(\rho_i') \leq x^{\kappa^*}(\rho_i)$ for $\rho \in \Omega$ and $\kappa > 0$, with $\kappa_* := \kappa - 2\frac{1}{c}\alpha^{-2}$ and $\kappa^* := \kappa + 3\frac{1}{c}\alpha^{-2}$. In particular, this implies $|x^{\frac{1}{2}\pm q}(\rho_i')| \leq R$ for $0 < q < 1/2 - \delta/c^2$ and α large enough. In the following it will be convenient to write the difference $m_q(\rho_i') - m_q(\rho_i)$ as

$$\left(\frac{1}{\int_{K_q(\rho_i')} \mathrm{d}\rho_i'} - \frac{1}{\int_{K_q(\rho_i)} \mathrm{d}\rho_i}\right) \int_{K_q(\rho_i')} t \, \mathrm{d}\rho_i'(t) + \frac{1}{\int_{K_q(\rho_i)} \mathrm{d}\rho_i} \left(\int_{K_q(\rho_i')} t \, \mathrm{d}\rho_i'(t) - \int_{K_q(\rho_i)} t \, \mathrm{d}\rho_i(t)\right). \tag{3.16}$$

Making use of $\int_{K_q(\rho_i)} \mathrm{d}\rho_i \geq 2qc$, see Eq. (3.15), and $K_q(\rho_i') \subset [-R, R]$ for all $\rho \in \Omega$, we can estimate the individual terms in Eq. (3.16) by

$$\left|\left(\frac{1}{\int_{K_q(\rho_i')} \mathrm{d}\rho_i'} - \frac{1}{\int_{K_q(\rho_i)} \mathrm{d}\rho_i}\right) \int_{K_q(\rho_i')} t \, \mathrm{d}\rho_i'(t)\right| \leq R \frac{\left|\int_{K_q(\rho_i')} \mathrm{d}\rho_i' - \int_{K_q(\rho_i)} \mathrm{d}\rho_i\right|}{2qc},$$

$$\left|\frac{1}{\int_{K_q(\rho_i)} \mathrm{d}\rho_i} \left(\int_{K_q(\rho_i')} t \, \mathrm{d}\rho_i'(t) - \int_{K_q(\rho_i)} t \, \mathrm{d}\rho_i(t)\right)\right| \leq \frac{\left|\int_{K_q(\rho_i')} t \, \mathrm{d}\rho_i'(t) - \int_{K_q(\rho_i)} t \, \mathrm{d}\rho_i(t)\right|}{2qc}.$$

Note that $K_q(\rho_i)$ is contained in $[-R, R]$ as well and consequently t is bounded by R on the subset $K_q(\rho_i) \cup K_q(\rho_i')$. In order to verify the statement of the Lemma, it is therefore sufficient to prove that $\left|\int_{K_q(\rho_i')} f(t) \, \mathrm{d}\rho_i'(t) - \int_{K_q(\rho_i)} f(t) \, \mathrm{d}\rho_i(t)\right| \lesssim \alpha^{-2} \|f\|_\infty$ for an arbitrary measurable and bounded $f : \mathbb{R} \to \mathbb{R}$. We estimate

$$\begin{aligned} \left|\int_{K_q(\rho_i')} f(t) \, \mathrm{d}\rho_i'(t) - \int_{K_q(\rho_i)} f(t) \, \mathrm{d}\rho_i(t)\right| &\leq \left|\int_{K_q(\rho_i')} f(t) \, \mathrm{d}\rho_i'(t) - \int_{K_q(\rho_i')} f(t) \, \mathrm{d}\rho_i(t)\right| \\ &\quad + \left|\int_{K_q(\rho_i')} f(t) \, \mathrm{d}\rho_i(t) - \int_{K_q(\rho_i)} f(t) \, \mathrm{d}\rho_i(t)\right| \\ &\leq \|f\|_\infty \left(\|\rho_i' - \rho_i\|_{\mathrm{TV}} + \int_{K_q(\rho_i') \Delta K_q(\rho_i)} \mathrm{d}\rho_i\right), \end{aligned}$$

where $A \Delta B := (A \cup B) \setminus (A \cap B)$ is the symmetric difference. Note that $\|\rho_i' - \rho_i\|_{\mathrm{TV}} = \alpha^{-2}$. Furthermore we can estimate the expression $\int_{K_q(\rho_i') \Delta K_q(\rho_i)} \mathrm{d}\rho_i$ by

$$\left|\int_{-\infty}^{x^{\frac{1}{2}-q}(\rho_i')} \mathrm{d}\rho_i - \int_{-\infty}^{x^{\frac{1}{2}-q}(\rho_i)} \mathrm{d}\rho_i\right| + \left|\int_{-\infty}^{x^{\frac{1}{2}+q}(\rho_i')} \mathrm{d}\rho_i - \int_{-\infty}^{x^{\frac{1}{2}+q}(\rho_i)} \mathrm{d}\rho_i\right|.$$

Since the distributions ρ_i and ρ_i' satisfy the assumptions of Lemma 3.7 with $\epsilon := 2\alpha^{-2}$, we conclude that every term in the sum above is bounded by $2\|\rho' - \rho\|_{\mathrm{TV}} + \epsilon = 4\alpha^{-2}$. □

Before we state the central Lemma 3.12, let us verify in the subsequent Lemma 3.11 that low energy states with a localized median necessarily satisfy (complete) condensation with respect to a minimizer of the Pekar functional.

Lemma 3.11. *Given a constant $C > 0$, there exists a constant $T > 0$, such that*

$$\left\langle \Psi \middle| W^{-1}_{\varphi^{\mathrm{Pek}}} \mathcal{N} W_{\varphi^{\mathrm{Pek}}} \middle| \Psi \right\rangle \leq T \left(\alpha^{-\frac{2}{29}} + q + \epsilon \right)$$

for all states Ψ satisfying $\langle \Psi | \mathbb{H}_K | \Psi \rangle \leq e^{\mathrm{Pek}} + \alpha^{-\frac{4}{29}}$ with $K \geq \alpha^{\frac{8}{29}}$ and $\widehat{\mathbb{1}_{\Omega^*}} \Psi = \Psi$, where Ω^* is the set of all ρ satisfying $\int \mathrm{d}\rho \leq C$ and $|m_q(\rho)| \leq \epsilon$ with $q, \epsilon > 0$.

Proof. Let us begin by defining the functions

$$P_i^\epsilon(\rho) := \left(\frac{1}{2} \int \mathrm{d}\rho \right)^2 - \int_{x_i \leq \epsilon} \mathrm{d}\rho(x) \int_{y_i \geq -\epsilon} \mathrm{d}\rho(y). \tag{3.17}$$

Observe that $|m_q(\rho)| \leq \epsilon$ implies $-\epsilon \leq x^{\frac{1}{2}+q}(\rho_i)$ and $x^{\frac{1}{2}-q}(\rho_i) \leq \epsilon$ for all such ρ which additionally satisfy $\rho \neq 0$, see Definition 3.8. Therefore $P_i^\epsilon(\rho) \leq \left(\int \mathrm{d}\rho \right)^2 \left(\frac{1}{4} - \left(\frac{1}{2} - q \right)^2 \right) \lesssim q$ for all $\rho \in \Omega^*$, and consequently the measure μ from Theorem 3.2 corresponding to the state Ψ satisfies $\int P_i^\epsilon \left(\left| \varphi_x^{\mathrm{Pek}} \right|^2 \right) \mathrm{d}\mu(x) \leq \left\langle \Psi \middle| \widehat{P_i^\epsilon} \middle| \Psi \right\rangle + D\alpha^{-\frac{2}{29}} \lesssim q + \alpha^{-\frac{2}{29}}$ for a suitable $D > 0$, where we have used Eq. (3.2) in the first inequality. Furthermore we know that $\| \varphi_x^{\mathrm{Pek}} - \varphi^{\mathrm{Pek}} \|^2 \lesssim \sum_{i=1}^3 P_i^\epsilon \left(\left| \varphi_x^{\mathrm{Pek}} \right|^2 \right) + \epsilon$ by Lemma A.3, hence

$$\int \| \varphi_x^{\mathrm{Pek}} - \varphi^{\mathrm{Pek}} \|^2 \, \mathrm{d}\mu(x) \lesssim \sum_{i=1}^3 \int P_i^\epsilon \left(\left| \varphi_x^{\mathrm{Pek}} \right|^2 \right) \mathrm{d}\mu(x) + \epsilon \lesssim q + \alpha^{-\frac{2}{29}} + \epsilon.$$

Therefore Eq. (3.3) immediately concludes the proof of Eq. (3.18). □

Lemma 3.12. *Given $0 < \sigma \leq \frac{1}{4}$, let Λ and L be as in Theorem 2.5. Then there exist states Ψ'''_α satisfying $\langle \Psi'''_\alpha | \mathbb{H}_\Lambda | \Psi'''_\alpha \rangle - E_\alpha \lesssim \alpha^{-2(1+\sigma)}$, $\mathrm{supp}\left(\Psi'''_\alpha \right) \subset B_{4L}(0)$ and*

$$\left\langle \Psi'''_\alpha \middle| W^{-1}_{\varphi^{\mathrm{Pek}}} \mathcal{N} W_{\varphi^{\mathrm{Pek}}} \middle| \Psi'''_\alpha \right\rangle \lesssim \alpha^{-\frac{2}{29}}, \tag{3.18}$$

where $W_{\varphi^{\mathrm{Pek}}}$ is the Weyl operator corresponding to the Pekar minimizer φ^{Pek}.

Proof. It is clearly sufficient to consider only the case $\alpha \geq \alpha_0$ for a suitable (large) α_0, since we can always re-define $\Psi'''_\alpha := \Psi$ for $\alpha < \alpha_0$ where Ψ is an arbitrary state satisfying $\mathrm{supp}\,(\Psi) \subset B_{4L}(0)$. In the following let us use the concrete choice $\Psi^\bullet_\alpha := \Psi^\diamond_\alpha$ for the sequence in Eq. (3.5), where $\Psi^\diamond_\alpha$ is defined in in Theorem 2.5, which is a valid choice since it satisfies the assumptions $\mathrm{supp}\left(\Psi^\diamond_\alpha \right) \subset B_L(0)$ and $\widetilde{E}_\alpha - E_\alpha \lesssim \alpha^{-2(1+\sigma)} \leq \alpha^{-\frac{4}{29}}$. Furthermore let $\{\chi_z : z \in \mathbb{Z}^3\}$ be a smooth (quadratic) partition of unity on $\mathbb{R}^3$, i.e. $0 \leq \chi_z \leq 1$ and $\sum_{z \in \mathbb{Z}^3} \chi_z^2 = 1$, with $\chi_z(x) = \chi_0(x - z)$ and $\mathrm{supp}\,(\chi_0) \subset B_1(0)$. Then we define for $z \in \mathbb{Z}^3$ and $u, v \geq \frac{2}{29}$ with $u + v \leq \frac{1}{4}$ the function $F_z(\rho) := \chi_z\big(\alpha^u \, m_{\alpha^{-v}}(\rho)\big)$, as well as the states

$$\Psi_{\alpha,z} := Z_{\alpha,z}^{-1} \widehat{F}_z \Psi''_\alpha \tag{3.19}$$

with $Z_{\alpha,z} := \|\widehat{F_z}\Psi''_\alpha\|$ and Ψ''_α as in Lemma 3.5 for $\epsilon = 0$ and $0 < \delta < \frac{c^2}{2}$, where $c := c_-$ is as in Lemma 3.4. Applying Lemma 3.3 with respect to $\mathcal{P} := \{F_z : z \in \mathbb{Z}^3\}$, where the functions F_z are defined above Eq. (3.19) and Ω is defined as the set of all $\rho \in \Omega_{\mathrm{reg}}$ satisfying $c_- \leq \int \mathrm{d}\rho \leq c_+$ and $\int\int_{|x-y|\geq R} \mathrm{d}\rho(x)\mathrm{d}\rho(y) \leq \delta$, yields

$$\sum_{z\in\mathbb{Z}^3} Z^2_{\alpha,z}\langle\Psi_{\alpha,z}|\mathbb{H}_\Lambda|\Psi_{\alpha,z}\rangle \leq \langle\Psi''_\alpha|\mathbb{H}_\Lambda|\Psi''_\alpha\rangle + c\alpha^{-\frac{7}{2}} V_\Omega(\mathcal{P})\sqrt{c_+ + \alpha^{-2}}, \tag{3.20}$$

where we used Lemma 3.6, $\Lambda \leq \alpha$ and $\widehat{\mathbb{1}_\Omega}\Psi''_\alpha = \Psi''_\alpha$ by the definition of Ψ''_α in Eq. (3.10). Since the support of χ_z only overlaps with the support of finitely many other $\chi_{z'}$, we obtain for $v > 0$ and α large enough

$$\begin{aligned} V_\Omega(\mathcal{P}) &\lesssim \alpha^4 \sup_{\rho\in\Omega, y\in\mathbb{R}^3} \sup_{z\in\mathbb{Z}^3} \left|\chi_z\left(\alpha^u m_{\alpha^{-v}}(\rho + \alpha^{-2}\delta_y)\right) - \chi_z\left(\alpha^u m_{\alpha^{-v}}(\rho)\right)\right|^2 \\ &\lesssim \alpha^{2u+4} \sup_{\rho\in\Omega, y\in\mathbb{R}^3} \left|m_{\alpha^{-v}}(\rho + \alpha^{-2}\delta_y) - m_{\alpha^{-v}}(\rho)\right|^2 \lesssim \alpha^{2(u+v)}, \end{aligned}$$

where we have used $\sup_{z\in\mathbb{Z}^3} |\chi_z(y) - \chi_z(x)| \leq \|\nabla\chi_0\|_\infty |y - x|$ in the first inequality and Lemma 3.10 in the second one. Combining this with Eq. (3.20) and the fact that $u + v \leq \frac{1}{4}$ yields

$$\sum_{z\in\mathbb{Z}^3} Z^2_{\alpha,z}\langle\Psi_{\alpha,z}|\mathbb{H}_\Lambda|\Psi_{\alpha,z}\rangle - \langle\Psi''_\alpha|\mathbb{H}_\Lambda|\Psi''_\alpha\rangle \lesssim \alpha^{-3}. \tag{3.21}$$

Since $\sum_{z\in\mathbb{Z}^3} Z^2_{\alpha,z} = 1$, this in particular means that there exists a $z_\alpha \in \mathbb{Z}^3$ such that $\langle\Psi_{\alpha,z_\alpha}|\mathbb{H}_\Lambda|\Psi_{\alpha,z_\alpha}\rangle - E_\alpha \lesssim \alpha^{-2(1+\sigma)}$, and by the translation invariance of $\mathbb{H}_\Lambda$ we obtain $\langle\Psi'''_\alpha|\mathbb{H}_\Lambda|\Psi'''_\alpha\rangle - E_\alpha \lesssim \alpha^{-2(1+\sigma)}$ where $\Psi'''_\alpha = \mathcal{T}_{-\alpha^{-u}z_\alpha}\Psi_{\alpha,z_\alpha}$. Using the fact that $\mathbb{1}_{\Omega^*}\Psi'''_\alpha = \Psi'''_\alpha$, where Ω^* is the set of all ρ satisfying $\int \mathrm{d}\rho \leq c_+$ and $|m_{\alpha^{-v}}(\rho)| \leq \alpha^{-u}$, together with Lemma 3.11, immediately concludes the proof of Eq. (3.18).

Finally let us verify that $\mathrm{supp}\left(\Psi'''_\alpha\right) \subset B_{4L}(0)$. By definition of $\Psi'''_\alpha = \mathcal{T}_{-\alpha^{-u}z_\alpha}\Psi_{\alpha,z_\alpha}$, and the fact that $\mathrm{supp}\left(\Psi_{\alpha,z_\alpha}\right) \subset B_L(0)$, it is clear that $\mathrm{supp}\left(\Psi'''_\alpha\right) \subset B_L(-w_\alpha)$ with $w_\alpha := \alpha^{-u}z_\alpha$. In the following we show that $|w_\alpha| \leq 3L$ by contradiction for α large enough, and therefore $\mathrm{supp}\left(\Psi'''_\alpha\right) \subset B_{L+|w_\alpha|}(0) \subset B_{4L}(0)$. Assuming $|w_\alpha| > 3L$, we obtain $\mathrm{supp}\left(\Psi'''_\alpha\right) \subset \mathbb{R}^3 \setminus B_{2L}(0)$ and Corollary B.7 consequently yields $\langle\Psi'''_\alpha|\mathbb{H}_\Lambda|\Psi'''_\alpha\rangle \geq E_\alpha + \langle\Psi'''_\alpha|\mathcal{N}_{B_L(0)}|\Psi'''_\alpha\rangle - \sqrt{\frac{D}{L}}$, where $\mathcal{N}_{B_L(0)}$ denotes the number operator in the ball $B_L(0)$ (as defined in Cor. B.7). Defining $\varphi_L(x) := \chi(|x| \leq L)\varphi^{\mathrm{Pek}}(x)$, we further have

$$\begin{aligned} \langle\Psi'''_\alpha|\mathcal{N}_{B_L(0)}|\Psi'''_\alpha\rangle &= \left\langle\Psi'''_\alpha\middle|W^{-1}_{\varphi^{\mathrm{Pek}}}\left(\mathcal{N}_{B_L(0)} + a(\varphi_L) + a^\dagger(\varphi_L) + \|\varphi_L\|^2\right)W_{\varphi^{\mathrm{Pek}}}\middle|\Psi'''_\alpha\right\rangle \\ &\geq -\left\langle\Psi'''_\alpha\middle|W^{-1}_{\varphi^{\mathrm{Pek}}}\mathcal{N}W_{\varphi^{\mathrm{Pek}}}\middle|\Psi'''_\alpha\right\rangle + \frac{1}{2}\|\varphi_L\|^2 \geq -D'\alpha^{-\frac{2}{29}} + \frac{1}{2}\|\varphi_L\|^2 \end{aligned}$$

for a suitable constant D', where we have used the operator inequality $\mathcal{N}_{B_L(0)} + a(\varphi_L) + a^\dagger(\varphi_L) + \|\varphi_L\|^2 \geq -\mathcal{N} + \frac{1}{2}\|\varphi_L\|^2$ as well as Eq. (3.18). Therefore we obtain

$$\langle\Psi'''_\alpha|\mathbb{H}_\Lambda|\Psi'''_\alpha\rangle - E_\alpha \geq \frac{1}{2}\|\varphi_L\|^2 - D'\alpha^{-\frac{2}{29}} - \sqrt{\frac{D}{L}} \underset{\alpha\to\infty}{\longrightarrow} \frac{1}{2}\|\varphi^{\mathrm{Pek}}\|^2 > 0,$$

where we have used that $L = \alpha^{1+\sigma} \underset{\alpha\to\infty}{\longrightarrow} \infty$. This, however, is a contradiction to $\langle \Psi'''_\alpha | \mathbb{H}_\Lambda | \Psi'''_\alpha \rangle - E_\alpha \lesssim \alpha^{-2(1+\sigma)}$. □

Following the method in [16], we are going to lift the weak condensation derived in Lemma 3.12 to a strong one in the subsequent Theorem 3.13, which represents the main result of this section.

Theorem 3.13. *Given* $0 < \sigma \leq \frac{1}{4}$ *and* $h < \frac{2}{29}$, *let* Λ *and* L *be as in Theorem 2.5. Then there exist states* Ψ_α *with* $\langle \Psi_\alpha | \mathbb{H}_\Lambda | \Psi_\alpha \rangle - E_\alpha \lesssim \alpha^{-2(1+\sigma)}$ *and* $\operatorname{supp}(\Psi_\alpha) \subset B_{4L}(0)$, *satisfying*

$$\chi\left(W_{\varphi^{\mathrm{Pek}}}^{-1} \mathcal{N} W_{\varphi^{\mathrm{Pek}}} \leq \alpha^{-h}\right) \Psi_\alpha = \Psi_\alpha \tag{3.22}$$

for large enough α.

Proof. Using the states Ψ'''_α from Lemma 3.12, we define for $0 < \epsilon < \frac{1}{2}$

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

where Z_α is a normalizing constant. Clearly the states Ψ_α satisfy the strong condensation property $\chi\left(W_{\varphi^{\mathrm{Pek}}}^{-1} \mathcal{N} W_{\varphi^{\mathrm{Pek}}} \leq \alpha^{-h}\right) \Psi_\alpha = \Psi_\alpha$. In order to control the energy cost of the localization with respect to the operator $W_{\varphi^{\mathrm{Pek}}}^{-1} \mathcal{N} W_{\varphi^{\mathrm{Pek}}}$, note that the partition $\mathcal{P}' := \{F', G'\}$ with $F'(\rho) := \chi^\epsilon\left(\alpha^h \int \mathrm{d}\rho \leq \frac{1}{2}\right)$ and $G'(\rho) := \chi^\epsilon\left(\frac{1}{2} \leq \alpha^h \int \mathrm{d}\rho\right)$ satisfies

$$\kappa := V_{\mathcal{M}(\mathbb{R}^3)}\left(\mathcal{P}'\right) \lesssim \alpha^4 \sup_{\rho, x \in \mathbb{R}^3} \left| \alpha^h \int \mathrm{d}\left(\rho + \alpha^{-2}\delta_x\right) - \alpha^h \int \mathrm{d}\rho \right|^2 = \alpha^{2h},$$

where we used $\left|\chi^\epsilon\left(y \leq \frac{1}{2}\right) - \chi^\epsilon\left(x \leq \frac{1}{2}\right)\right| \leq \left\| \frac{\mathrm{d}}{\mathrm{d}x} \chi^\epsilon\left(\cdot \leq \frac{1}{2}\right) \right\|_\infty |y - x|$ and the corresponding estimate for $\chi^\epsilon\left(\frac{1}{2} \leq \cdot\right)$. Therefore we obtain by Lemma 3.3, using $\Lambda \leq \alpha$,

$$\begin{aligned} Z_\alpha^2 \langle \Psi_\alpha | \mathbb{H}_\Lambda | \Psi_\alpha \rangle + (1 - Z_\alpha^2) \langle \widetilde{\Psi}_\alpha | \mathbb{H}_\Lambda | \widetilde{\Psi}_\alpha \rangle &\leq \langle \Psi'''_\alpha | \mathbb{H}_\Lambda | \Psi'''_\alpha \rangle + c' \alpha^{-\frac{7}{2}} \kappa \left\langle \Psi''' \middle| \sqrt{\mathcal{N}+1} \middle| \Psi''' \right\rangle \\ &\leq E_\alpha + O_{\alpha\to\infty}\left(\alpha^{-2(1+\sigma)}\right) + O_{\alpha\to\infty}\left(\alpha^{2h - \frac{7}{2}}\right) = E_\alpha + O_{\alpha\to\infty}\left(\alpha^{-2(1+\sigma)}\right), \end{aligned} \tag{3.23}$$

with $\widetilde{\Psi}_\alpha := \sqrt{1 - Z_\alpha^2}^{-1} \chi^\epsilon\left(\frac{1}{2} \leq \alpha^h W_{\varphi^{\mathrm{Pek}}}^{-1} \mathcal{N} W_{\varphi^{\mathrm{Pek}}}\right) \Psi'''_\alpha$. Making use of the trivial lower bound $E_\alpha \leq \langle \widetilde{\Psi}_\alpha | \mathbb{H}_\Lambda | \widetilde{\Psi}_\alpha \rangle$, Eq. (3.23) implies $\langle \Psi_\alpha | \mathbb{H}_\Lambda | \Psi_\alpha \rangle \leq E_\alpha + Z_\alpha^{-2} O_{\alpha\to\infty}\left(\alpha^{-2(1+\sigma)}\right)$, which concludes the proof since

$$\begin{aligned} 1 - Z_\alpha^2 &= \left\langle \Psi'''_\alpha \middle| \chi^\epsilon \left(\frac{1}{2} \leq \alpha^h W_{\varphi^{\mathrm{Pek}}}^{-1} \mathcal{N} W_{\varphi^{\mathrm{Pek}}}\right)^2 \middle| \Psi'''_\alpha \right\rangle \\ &\leq \frac{1}{\frac{1}{2} - \epsilon} \alpha^h \left\langle \Psi'''_\alpha \middle| W_{\varphi^{\mathrm{Pek}}}^{-1} \mathcal{N} W_{\varphi^{\mathrm{Pek}}} \middle| \Psi'''_\alpha \right\rangle \lesssim \frac{1}{\frac{1}{2} - \epsilon} \alpha^h \alpha^{-\frac{2}{29}} \underset{\alpha\to\infty}{\longrightarrow} 0. \end{aligned}$$

□

4. Large Deviation Estimates for Strong Condensates

In this Section we will derive a large deviation principle for states with suitably small particle number (compared to α^2), which can be interpreted as complete condensation with respect to the vacuum. We will show that such states are, up to an error which is exponentially small in α^2, contained in the spectral subspace $\left|a(f)+a^\dagger(f)\right| \leq \epsilon$, see Eq. (4.6). Note that taking the point of condensation to be the vacuum is not a real restriction, since this is the case after applying a suitable Weyl transformation. Before we can formulate the main result of this section in Proposition 4.2, we need to introduce some notation.

For $0 < \sigma < \frac{1}{4}$ let us define the momentum cut-off $\Lambda := \alpha^{\frac{4}{5}(1+\sigma)}$ and the discretization parameter of the momentum space $\ell := \alpha^{-4(1+\sigma)}$, and the associated projection

$$\Pi := \Pi^0_{\Lambda,\ell}, \tag{4.1}$$

see Definition 2.1, and let us identify $\mathcal{F}\left(\Pi L^2(\mathbb{R}^3)\right)$ with $L^2(\mathbb{R}^N)$ using the representation of real functions $\varphi = \sum_{n=1}^N \lambda_n \varphi_n \in \Pi L^2(\mathbb{R}^3)$ by points $\lambda = (\lambda_1, \ldots, \lambda_N) \in \mathbb{R}^N$, where $N := \dim \Pi L^2(\mathbb{R}^3)$ and $\{\varphi_1, \ldots, \varphi_N\}$ is a real orthonormal basis of $\Pi L^2(\mathbb{R}^3)$. We choose this identification such that the annihilation operators $a_n := a(\varphi_n)$ read

$$a_n = \lambda_n + \frac{1}{2\alpha^2}\partial_{\lambda_n}, \tag{4.2}$$

where λ_n is the multiplication operator by the function $\lambda \mapsto \lambda_n$ on $L^2(\mathbb{R}^N)$. From the construction one readily checks that $N \lesssim (\Lambda/\ell)^3 \leq \alpha^p$ for suitable $p > 0$.

In the following we will verify a large deviation principle for the density function $\rho(\lambda) := \gamma(\lambda, \lambda)$ corresponding to a density matrix γ on $\mathcal{F}\left(\Pi L^2(\mathbb{R}^3)\right)$ that satisfies the strong condensation condition

$$\chi\left(\sum_{n=1}^N a_n^\dagger a_n \leq \alpha^{-h}\right)\gamma = \gamma \tag{4.3}$$

for some condensation rate $h > 0$. This result is comparable to [5, Lemma C.2]. For this purpose, we define a convenient norm $|\cdot|_\diamond$ on $\mathbb{R}^N$ in the subsequent Definition.

Definition 4.1. Let $|\lambda| := \sqrt{\sum_{n=1}^N \lambda_n^2}$ denote the standard norm on $\mathbb{R}^N$ and let us define the norm $|\cdot|_\diamond$ on $\mathbb{R}^N$, using the identification $\varphi = \sum_{n=1}^N \lambda_n \varphi_n$, as

$$|\lambda|_\diamond := 2 \sup_{x\in\mathbb{R}^3} \sqrt{\int_{B_1(x)} \left|\left((-\Delta)^{-\frac{1}{2}}\varphi\right)(y)\right|^2 \mathrm{d}y}. \tag{4.4}$$

The norm $|\cdot|_\diamond$ will again appear naturally in Sect. 5 where we investigate properties of the Pekar functional $\mathcal{F}^{\mathrm{Pek}}$ (see Eq. (5.2) and the subsequent comment). In the following Proposition 4.2 we establish a large deviation like estimate on the ϵ-tail of the probability distribution ρ in the limit of $\alpha \to \infty$, where ϵ is even allowed to go to zero simultaneously as α goes to infinity, as long as $\epsilon \geq D\alpha^{-s}$ for a h and σ dependent constant s.

Proposition 4.2. *Let* $0 < s < \min\left\{\frac{h}{2}, \frac{1}{5}(1-4\sigma)\right\}$ *and* $D > 0$. *Then there exist constants* $\beta, \alpha_0 > 0$, *such that we have for all* $\alpha \geq \alpha_0$, $\epsilon \geq D\alpha^{-s}$ *and* γ *satisfying Eq.* (4.3)

$$\int_{|\lambda|_\diamond \geq \epsilon} \left(1 + |\lambda|^2\right) \rho(\lambda) \mathrm{d}\lambda \leq e^{-\beta\epsilon^2\alpha^2}, \tag{4.5}$$

where $\rho(\lambda) := \gamma(\lambda, \lambda)$ *is the density function corresponding to the state* γ. *Furthermore for all* $\zeta \in \mathbb{R}^N$ *and* $\beta < \frac{1}{|\zeta|^2}$, *there exists a constant* $\alpha(\beta, |\zeta|)$ *such that*

$$\int_{|\langle\zeta|\lambda\rangle| \geq \epsilon} \left(1 + |\lambda|^2\right) \rho(\lambda) \mathrm{d}\lambda \leq e^{-\beta\epsilon^2\alpha^2} \tag{4.6}$$

for all $\alpha \geq \alpha(\beta, |\zeta|)$ *and* $\epsilon \geq D\alpha^{-s}$.

The restriction to the finite dimensional space $\Pi L^2\left(\mathbb{R}^3\right)$ will be essential in the proof of Proposition 4.2, to be precise we will make use of the fact that $N \lesssim \alpha^p$ for a suitable $p > 0$, which in particular implies that $N \lesssim e^{\alpha^t}$, uniformly in α, for any $t > 0$. Before we prove Proposition 4.2, we first need auxiliary results concerning the $|\cdot|_\diamond$ norm.

Definition 4.3. For $x \in \mathbb{R}^3$ and $r > 0$, let us define $T_x\lambda := -2\chi\left(|\cdot - x| \leq 1\right)(-\Delta)^{-\frac{1}{2}}\varphi$ and $T_{\geq r}\lambda := -2\chi\left(|\cdot| \geq r\right)(-\Delta)^{-\frac{1}{2}}\varphi$ with the above identification $\varphi = \sum_{n=1}^N \lambda_n\varphi_n$. Furthermore let us define the operators $A_x := \sqrt{T_x^\dagger T_x}$ and $A_{\geq r} := \sqrt{T_{\geq r}^\dagger T_{\geq r}}$, as well as the constant $\beta_0 := \inf_{x\in\mathbb{R}^3} \|A_x\|^{-2}$.

Using the operators A_x we can write $|\lambda|_\diamond = \sup_{x\in\mathbb{R}^3} |A_x\lambda|$, which is bounded by

$$|\lambda|_\diamond \leq 65 \max\left\{\sup_{z\in\mathbb{Z}^3:|z|\leq r+1} |A_z\lambda|,\ |A_{\geq r}\lambda|\right\} \tag{4.7}$$

for any $r > 0$. In order to see this, note that for any $y \in \mathbb{R}^3$ there exists a $z \in \mathbb{Z}^3$ with $|y - z| < 1$. In case $y \in B_r(0) \cap B_1(x)$, where $x \in \mathbb{R}^3$, we see that z satisfies $|z| \leq r + 1$ and $|x - z| < 2$. Denoting the set of such z by $M(x, r) \subset \mathbb{Z}^3$, we obtain $B_1(x) \subset \bigcup_{z\in M(x,r)} B_1(z) \cup \left(\mathbb{R}^3 \setminus B_r(0)\right)$. Consequently

$$\begin{aligned} |\lambda|_\diamond &\leq \sup_x \sum_{z\in M(x,r)} |A_z\lambda| + |A_{\geq r}\lambda| \\ &\leq \sup_x \left(|M(x,r)| + 1\right) \max_x \left\{\sup_{z\in M(x,r)} |A_z\lambda|,\ |A_{\geq r}\lambda|\right\}. \end{aligned}$$

This concludes the proof of Eq. (4.7), since there are at most 64 elements $z \in \mathbb{Z}^3$ satisfying $|x - z| < 2$.

Lemma 4.4. *The constant* β_0 *from Definition* 4.3 *is positive, uniformly in* α, *and* $\|A_x\|_{\mathrm{HS}} \lesssim \Lambda$ *uniformly in* $x \in \mathbb{R}^3$, *where* Λ *is defined above Eq.* (4.1). *Furthermore there exists a constant* $\upsilon > 0$ *such that* $\|A_{\geq r}\|_{\mathrm{HS}} \lesssim \frac{\alpha^\upsilon}{\sqrt{r}}$ *for all* $\alpha \geq 1$ *and* $r > 0$.

Proof. Note that the space $\Pi L^2(\mathbb{R}^3)$ is contained in the spectral subspace $-\Delta \leq \Lambda^2$, hence $\Pi \leq \left(1+\Lambda^2\right)(1-\Delta)^{-1}$, and therefore

$$\begin{aligned}\|A_x\|_{\mathrm{HS}}^2 &= 4\left\|\chi\left(|\cdot - x| \leq 1\right)(-\Delta)^{-\frac{1}{2}}\,\Pi\right\|_{\mathrm{HS}}^2\\ &\leq 4\left(1+\Lambda^2\right)\left\|\chi\left(|\cdot - x| \leq 1\right)(-\Delta)^{-\frac{1}{2}}(1-\Delta)^{-\frac{1}{2}}\right\|_{\mathrm{HS}}^2\\ &= 4\left(1+\Lambda^2\right)\left\|\chi\left(|\cdot| \leq 1\right)(-\Delta)^{-\frac{1}{2}}(1-\Delta)^{-\frac{1}{2}}\right\|_{\mathrm{HS}}^2.\end{aligned}$$

Applying Eq. (B.5) with $\psi = \chi\left(|.| \leq 1\right)$ yields that $\chi\left(|\cdot| \leq 1\right)(-\Delta)^{-\frac{1}{2}}(1-\Delta)^{-\frac{1}{2}}$ is Hilbert-Schmidt, hence $\|A_x\|_{\mathrm{HS}} \lesssim \Lambda$. In order to prove the uniform lower bound $\beta_0 > 0$, it is enough to verify the boundedness of $\chi\left(|.| \leq 1\right) f(-\Delta)$, where $f(t) := \frac{\chi(|t| \leq 1)}{\sqrt{t}}$. An explicit computation in Fourier space yields for $\varphi \in L^2(\mathbb{R}^3)$

$$\begin{aligned}&\langle\varphi| f(-\Delta)\chi\left(|.| \leq 1\right) f(-\Delta)|\varphi\rangle = \int_{|k|\leq 1}\int_{|k|\leq 1} \frac{\widehat{\chi\left(|\cdot| \leq 1\right)}(k-k')\overline{\widehat{\varphi}(k)}\widehat{\varphi}(k')}{|k|\,|k'|}\,\mathrm{dkdk}\\ &\leq \left\|\widehat{\chi\left(|\cdot| \leq 1\right)}\right\|_\infty \left|\int_{|k|\leq 1}\frac{|\widehat{\varphi}(k)|}{|k|}\,\mathrm{dk}\right|^2 \lesssim \|\varphi\|^2.\end{aligned}$$

Finally we are going to verify $\|A_{\geq r}\|_{\mathrm{HS}} \lesssim \frac{\alpha^v}{\sqrt{r}}$, using that

$$\|A_{\geq r}\|_{\mathrm{HS}} = 2\sqrt{\sum_{n=1}^N \left\|\chi\left(|\cdot| \geq r\right)(-\Delta)^{-\frac{1}{2}}\varphi_n\right\|^2} \lesssim \sqrt{N}\frac{\alpha^v}{\sqrt{r}}$$

for a suitable constant $v > 0$ by Corollary B.2, where N is the dimension of $\Pi L^2(\mathbb{R}^3)$. This concludes the proof, since $N \lesssim \alpha^p$ for some $p > 0$. □

Proof of Proposition 4.2. Making use of Eq. (4.7) and defining $\epsilon_* := \frac{\epsilon}{65}$, we obtain

$$\int_{|\lambda|_\diamond \geq \epsilon}\left(1+|\lambda|^2\right)\rho(\lambda)\mathrm{d}\lambda \leq \sum_{|z|\leq r+1}\int_{|A_z\lambda|\geq\epsilon_*}\left(1+|\lambda|^2\right)\rho(\lambda)\mathrm{d}\lambda + \int_{|A_{\geq r}\lambda|\geq\epsilon_*}\left(1+|\lambda|^2\right)\rho(\lambda)\mathrm{d}\lambda,$$

where the sum runs over $z \in \mathbb{Z}^3$ with $|z| \leq r+1$. In the following we are going to verify that every contribution of the form $\int_{|A_x\lambda|\geq\epsilon_*}\left(1+|\lambda|^2\right)\rho(\lambda)\mathrm{d}\lambda$ is exponentially small uniformly in $x \in \mathbb{R}^3$. As a consequence of Eq. (4.3), we have for $t \geq 0$ the estimate

$$\gamma \leq \chi\left(\sum_{n=1}^N a_n^\dagger a_n \leq \alpha^{-h}\right) \leq e^{t\left(\alpha^{-h} - \sum_{n=1}^N a_n^\dagger a_n\right)}.$$

By our assumption on s, there exists a h' such that $2s < h' < h$. Consequently we obtain for $t := \alpha^{2+(h-h')}$, using Mehler's kernel,

$$\rho(\lambda) = \gamma(\lambda,\lambda) \leq e^{\alpha^{2-h'}} e^{-t\sum_{n=1}^N a_n^\dagger a_n}(\lambda,\lambda) = e^{\alpha^{2-h'}}\left(\frac{1}{1-e^{-\alpha^{h-h'}}}\right)^N\left(\frac{\alpha^2 w_\alpha}{\pi}\right)^{\frac{N}{2}} e^{-\alpha^2 w_\alpha|\lambda|^2}, \tag{4.8}$$

with $w_\alpha := \coth\left(\alpha^{h-h'}\right) - \operatorname{cosech}\left(\alpha^{h-h'}\right)$. Since $Ne^{-\alpha^{h-h'}} \underset{\alpha\to\infty}{\longrightarrow} 0$, it is clear that $\left(\frac{1}{1-e^{-\alpha^{h-h'}}}\right)^N$ is bounded uniformly in α. Since $w_\alpha \geq 0$ is strictly increasing in α, we can choose $0 < \beta' < \beta_0 \inf_{\alpha\geq 1} w_\alpha$, where β_0 is the constant from Definition 4.3. Consequently $\|\frac{\beta'}{w_\alpha}|A_x|^2\| < 1$ uniformly in $x \in \mathbb{R}^3$ and $\alpha \geq 1$, and in particular $\left(1 - \frac{\beta'}{w_\alpha}|A_x|^2\right)^{-1}$ is a bounded operator. Hence we obtain for $x \in \mathbb{R}^3$

$$\int_{|A_x\lambda|\geq\epsilon_*}\left(1+|\lambda|^2\right)\rho(\lambda)\mathrm{d}\lambda \lesssim e^{\alpha^{2-h'}}\left(\frac{\alpha^2 w_\alpha}{\pi}\right)^{\frac{N}{2}}\int_{|A_x\lambda|\geq\epsilon_*}\left(1+|\lambda|^2\right)e^{-\alpha^2 w_\alpha|\lambda|^2}\mathrm{d}\lambda$$
$$\leq e^{\alpha^{2-h'}}\left(\frac{\alpha^2 w_\alpha}{\pi}\right)^{\frac{N}{2}}\int_{\mathbb{R}^N}\left(1+|\lambda|^2\right)e^{-\alpha^2\left(w_\alpha|\lambda|^2+\beta'\epsilon_*^2-\beta'|A_x\lambda|^2\right)}\mathrm{d}\lambda$$
$$= e^{\alpha^{2-h'}}\frac{w_\alpha+\alpha^{-2}\mathrm{Tr}\left(1-\frac{\beta'}{w_\alpha}|A_x|^2\right)^{-1}}{w_\alpha\det\sqrt{1-\frac{\beta'}{w_\alpha}|A_x|^2}}e^{-\beta'\epsilon_*^2\alpha^2}.$$

Furthermore, for a suitable, x-independent, constant μ

$$e^{\alpha^{2-h'}}\frac{w_\alpha+\alpha^{-2}\mathrm{Tr}\left(1-\frac{\beta'}{w_\alpha}|A_x|^2\right)^{-1}}{w_\alpha\det\sqrt{1-\frac{\beta'}{w_\alpha}|A_x|^2}} \lesssim e^{\alpha^{2-h'}}\frac{\alpha^p}{\det\sqrt{1-\frac{\beta'}{w_\alpha}|A_x|^2}}$$
$$= e^{\alpha^{2-h'}+p\ln\alpha-\frac{1}{2}\mathrm{Tr}\ln\left(1-\frac{\beta'}{w_\alpha}|A_x|^2\right)} \leq e^{\alpha^{2-h'}+p\ln\alpha+\mu\|A_x\|_{\mathrm{HS}}^2} \leq e^{\alpha^{2-h'}+p\ln\alpha+\mu C\Lambda^2}, \tag{4.9}$$

where we have used the rough estimate $w_\alpha + \alpha^{-2}\mathrm{Tr}\left(1-\frac{\beta'}{w_\alpha}|A_x|^2\right)^{-1} \lesssim 1+\alpha^{-2}N \lesssim \alpha^p$ for a suitable exponent $p > 0$ in the first inequality and Lemma 4.4 in the last inequality. Note that the exponent in Eq. (4.9) is of order $\alpha^{\max\left\{2-h',\frac{8}{5}(1+\sigma)\right\}} \ll \epsilon_*^2\alpha^2$ since $\Lambda^2 = \alpha^{\frac{8}{5}(1+\sigma)}$ and $\epsilon \geq D\alpha^{-s}$ with $s < \min\left\{\frac{h'}{2}, \frac{1}{5}(1-4\sigma)\right\}$.

Defining $r := \alpha^{2q}$ with $q > v$, where v is the constant from Lemma 4.4 and making use of the fact that the number of $z \in \mathbb{Z}^3$ with $|z| \leq r+1$ is of order $r^3 = \alpha^{6q}$, we obtain

$$\sum_{|z|\leq r+1}\int_{|A_z\lambda|\geq\epsilon_*}\left(1+|\lambda|^2\right)\rho(\lambda)\mathrm{d}\lambda\,\mathrm{d}x \lesssim \alpha^{6q}e^{\alpha^{2-h'}+p\ln\alpha+\mu C\Lambda^2-\beta'\epsilon_*^2\alpha^2} \leq e^{-\beta\epsilon_*^2\alpha^2}$$

for $\beta < \beta'$ and α large enough. We have $\|A_{\geq r}\|_{\mathrm{HS}} \underset{\alpha\to\infty}{\longrightarrow} 0$ by Lemma 4.4 and our choice $r = \alpha^{2q}$ with $q > v$. Using Eq. (4.8), and an argument similar to the one in Eq. (4.9), we can therefore estimate $\int_{|A_{\geq r}\lambda|\geq\epsilon_*}\left(1+|\lambda|^2\right)\rho(\lambda)\mathrm{d}\lambda$ by

$$\int_{|A_{\geq r}\lambda|\geq\epsilon_*}\left(1+|\lambda|^2\right)\rho(\lambda)\mathrm{d}\lambda \lesssim e^{\alpha^{2-h'}}\left(\frac{\alpha^2 w_\alpha}{\pi}\right)^{\frac{N}{2}}\int_{|A_{\geq r}\lambda|\geq\epsilon_*}\left(1+|\lambda|^2\right)e^{-\alpha^2 w_\alpha|\lambda|^2}\mathrm{d}\lambda$$
$$\lesssim e^{\alpha^{2-h'}}\frac{\alpha^p}{\det\sqrt{1-\frac{\beta'}{w_\alpha}|A_{\geq r}|^2}}e^{-\beta'\epsilon_*^2\alpha^2} \lesssim e^{\alpha^{2-h'}+p\ln\alpha+\mu\|A_{\geq r}\|_{\mathrm{HS}}^2-\beta'\epsilon_*^2\alpha^2}.$$

Again we observe that the exponent $\alpha^{2-h'} + p \ln \alpha + \mu \|A_{\geq r}\|_{\text{HS}}^2$ is small compared to $\epsilon_*^2 \alpha^2$, which concludes the proof of Eq. (4.5).

The proof of Eq. (4.6) can be carried out analogously with the help of the operator $A_\zeta \lambda := \langle \zeta | \lambda \rangle \frac{\zeta}{\|\zeta\|}$ using the fact that $\|A_\zeta\|_{\text{HS}} = \|A_\zeta\| = |\zeta|$ and the assumption $\beta < \frac{1}{|\zeta|^2}$. More precisely we obtain for $\beta < \beta' < \frac{1}{|\zeta|^2}$

$$\int_{|\langle \zeta|\lambda\rangle| \geq \epsilon} \left(1 + |\lambda|^2\right) \rho(\lambda) \mathrm{d}\lambda \lesssim e^{\alpha^{2-h'}} \left(\frac{\alpha^2 w_\alpha}{\pi}\right)^{\frac{N}{2}} \int_{|A_\zeta \lambda| \geq \epsilon} \left(1 + |\lambda|^2\right) e^{-\alpha^2 w_\alpha |\lambda|^2} \mathrm{d}\lambda$$

$$\lesssim e^{\alpha^{2-h'}} \frac{\alpha^p}{\det \sqrt{1 - \frac{\beta'}{w_\alpha} |A_\zeta|^2}} e^{-\beta' \epsilon^2 \alpha^2} \lesssim e^{\alpha^{2-h'} + p \ln \alpha + \mu \|A_\zeta\|_{\text{HS}}^2 - \beta' \epsilon^2 \alpha^2} \leq e^{-\beta \epsilon^2 \alpha^2}.$$

□

5. Properties of the Pekar Functional

In this section we are going to discuss essential properties of the Pekar functional $\mathcal{F}^{\text{Pek}}$, and we are going to verify an asymptomatically sharp quadratic approximation for $\mathcal{F}^{\text{Pek}}(\varphi)$, which is valid for all field configurations φ close to a minimizer φ^{Pek}. It has been proven in [11] that a suitable quadratic approximation of $\mathcal{F}^{\text{Pek}}$ holds for all configurations φ satisfying $\|V_{\varphi - \varphi^{\text{Pek}}}\| \ll 1$, where

$$V_\varphi := -2\,(-\Delta)^{-\frac{1}{2}}\, \mathfrak{Re}\, \varphi. \tag{5.1}$$

In the following we are showing that this result is still valid, in case we substitute the L^2-norm with the weaker $\|\cdot\|_\diamond$ norm, which is a hybrid between the L^2 and the L^∞ norm defined as

$$\|V\|_\diamond := \sup_{x \in \mathbb{R}^3} \sqrt{\int_{B_1(x)} |V(y)|^2 \, \mathrm{d}y}, \tag{5.2}$$

where $B_1(x)$ is the unit ball centered at $x \in \mathbb{R}^3$. This will be the content of Lemma 5.2 and Theorem 5.4, respectively. We have $\|V_\varphi\|_\diamond = |\lambda|_\diamond$ for $\varphi = \sum_{n=1}^N \lambda_n \varphi_n$, where $|\cdot|_\diamond$ is the norm defined in Eq. (4.4). Before we come to the proof of Lemma 5.2, we first need the subsequent auxiliary Lemma 5.1.

Lemma 5.1. *There exists a constant $C > 0$ such that the operator inequality*

$$V^2 \leq C \|V\|_\diamond^2 \,(1 - \Delta)^2 \tag{5.3}$$

holds for all (measurable) $V : \mathbb{R}^3 \longrightarrow \mathbb{R}$, where V^2 is interpreted as a multiplication operator.

Proof. As a first step, we are going to verify that Eq. (5.3) holds in case we use the L^2 norm $\|V\|$ instead of $\|V\|_\diamond$. This follows from $V^2 \leq \left\|V(1 - \Delta)^{-1}\right\|_{\text{HS}}^2 (1 - \Delta)^2$, where $\|\cdot\|_{\text{HS}}$ is the Hilbert-Schmidt norm, and

$$\left\|V(1 - \Delta)^{-1}\right\|_{\text{HS}}^2 = \int \int V(x)^2 K(y - x)^2 \, \mathrm{d}x \mathrm{d}y = \int K(y)^2 \mathrm{d}y \, \|V\|^2$$

with $K(y-x)$ being the kernel of the operator $(1-\Delta)^{-1}$. Note that $C' := \int K(y)^2 \mathrm{d}y$ is finite, which concludes the first step. In order to obtain the analogue statement for $\|V\|_\diamond$, let χ be a smooth, non-negative, function with $\operatorname{supp}(\chi) \subset B_1(0)$ and $\int_{\mathbb{R}^3} \chi(y)^2 \, \mathrm{d}y = 1$. Defining $\chi_y(x) := \chi(x-y)$ for $y \in \mathbb{R}^3$ and using the previously derived inequality $V^2 \leq C'\|V\|^2 (1-\Delta)^2$, which holds for any $V \in L^2(\mathbb{R}^3)$, we obtain

$$V^2 = \int \chi_y V^2 \chi_y \, \mathrm{d}y = \int \chi_y \left(\mathbb{1}_{B_1(y)} V\right)^2 \chi_y \, \mathrm{d}y \leq C' \int \|\mathbb{1}_{B_1(y)} V\|^2 \chi_y \, (1-\Delta)^2 \, \chi_y \, \mathrm{d}y$$

$$\leq C'\|V\|_\diamond^2 \int \chi_y \, (1-\Delta)^2 \, \chi_y \, \mathrm{d}y = C'\|V\|_\diamond^2 \int \left|(1-\Delta)\chi_y\right|^2 \mathrm{d}y,$$

where $|A|^2 = A^\dagger A$. Furthermore $(1-\Delta)\chi_y = \chi_y(1-\Delta) - 2\left(\nabla \chi_y\right)\nabla - \left(\Delta \chi_y\right)$, which yields together with a Cauchy–Schwarz inequality the estimate

$$\int \left|(1-\Delta)\chi_y\right|^2 \mathrm{d}y \leq 3 \int \left((1-\Delta)\chi_y^2(1-\Delta) - 4\nabla \left|\nabla \chi_y\right|^2 \nabla + |\Delta \chi_y|^2\right) \mathrm{d}y$$

$$= 3(1-\Delta)^2 - 12\,\nabla\left(\int \left|\nabla \chi_y^2\right| \mathrm{d}y\right)\nabla + 3\int |\Delta \chi_y|^2 \mathrm{d}y \lesssim (1-\Delta)^2,$$

where we have used that $\int |\nabla \chi(y)|^2 \, \mathrm{d}y$ and $\int |\Delta \chi(y)|^2 \, \mathrm{d}y$ are finite. □

In the following we are going to use that we can write the Pekar energy as

$$\mathcal{F}^{\text{Pek}}(\varphi) = \|\varphi\|^2 + \inf \sigma\left(-\Delta + V_\varphi\right), \tag{5.4}$$

where V_φ is defined in Eq. (5.1). As an immediate consequence of Eq. (5.3) we have $\pm V \leq \sqrt{C}\|V\|_\diamond (1-\Delta)$ and consequently there exists a $\delta_0 > 0$ and a contour $\mathcal{C} \subset \mathbb{C}$, such that $\mathcal{C}$ separates the ground state energy $\inf \sigma(-\Delta + V)$ from the excitation spectrum of $H_V := -\Delta + V$ for all V with $\|V - V_{\varphi^{\text{Pek}}}\|_\diamond < \delta_0$, see also the proof of Proposition 3.1 in [11]. This allows us to further identify $\mathcal{F}^{\text{Pek}}(\varphi)$ as

$$\mathcal{F}^{\text{Pek}}(\varphi) = \|\varphi\|^2 + \operatorname{Tr} \int_{\mathcal{C}} \frac{z}{z - H_{V_\varphi}} \frac{\mathrm{d}z}{2\pi i} \tag{5.5}$$

for all φ satisfying $\|V_{\varphi-\varphi^{\text{Pek}}}\|_\diamond < \delta_0$. Following the strategy in [11], we will use Eq. (5.5) to compare $\mathcal{F}^{\text{Pek}}(\varphi)$ with $e^{\text{Pek}} = \mathcal{F}^{\text{Pek}}\left(\varphi^{\text{Pek}}\right)$. Before we do this let us introduce the operators

$$K^{\text{Pek}} := 1 - H^{\text{Pek}} = 4\,(-\Delta)^{-\frac{1}{2}}\, \psi^{\text{Pek}} \frac{1 - |\psi^{\text{Pek}}\rangle\langle\psi^{\text{Pek}}|}{H_{V^{\text{Pek}}} - \mu^{\text{Pek}}} \psi^{\text{Pek}}\, (-\Delta)^{-\frac{1}{2}}, \tag{5.6}$$

$$L^{\text{Pek}} := 4\,(-\Delta)^{-\frac{1}{2}}\, \psi^{\text{Pek}}\, (1-\Delta)^{-1}\, \psi^{\text{Pek}}\, (-\Delta)^{-\frac{1}{2}}, \tag{5.7}$$

where H^{Pek} is defined in Eq. (1.4), $\mu^{\text{Pek}} := e^{\text{Pek}} - \|\varphi^{\text{Pek}}\|^2$ and ψ^{Pek} is the, non-negative, ground state of the operator $H_{V^{\text{Pek}}}$ with $V^{\text{Pek}} := V_{\varphi^{\text{Pek}}}$, which we interpret as a multiplication operator in Eqs. (5.6) and (5.7). The following Lemma 5.2 can be proved in the same way as [11, Proposition 3.3], using Lemma 5.1.

Lemma 5.2. *There exist constants* $c, \delta_0 > 0$ *such that for all* φ *with* $\|V_{\varphi-\varphi^{\text{Pek}}}\|_\diamond < \delta_0$

$$\left|\mathcal{F}^{\text{Pek}}(\varphi) - e^{\text{Pek}} - \langle \varphi - \varphi^{\text{Pek}} | 1 - K^{\text{Pek}} | \varphi - \varphi^{\text{Pek}}\rangle\right|$$

$$\leq c\|V_{\varphi-\varphi^{\text{Pek}}}\|_\diamond \langle \varphi - \varphi^{\text{Pek}} | L^{\text{Pek}} | \varphi - \varphi^{\text{Pek}}\rangle. \tag{5.8}$$

Proof. By taking δ_0 small enough, we can assume for all V with $\|V_{\varphi-\varphi^{\text{Pek}}}\|_\diamond < \delta_0$ that

$$\sup_{z\in\mathcal{C}}\left\|V_{\varphi-\varphi^{\text{Pek}}}\frac{1}{z-H_{V^{\text{Pek}}}}\right\|_{\text{op}} < 1, \tag{5.9}$$

where $\|\cdot\|_{\text{op}}$ denotes the operator norm. This immediately follows from

$$\left\|V_{\varphi-\varphi^{\text{Pek}}}\frac{1}{H_{V^{\text{Pek}}}-z}\right\|_{\text{op}}^2 \lesssim \left\|\left(V_\varphi - V^{\text{Pek}}\right)(1-\Delta)^{-1}\right\|_{\text{op}}^2 \leq C\|V_{\varphi-\varphi^{\text{Pek}}}\|_\diamond^2,$$

where we used Eq. (5.3) and the fact that the spectrum of $H_{V^{\text{Pek}}}$ has a positive distance to the contour $\mathcal{C}$, allowing us to bound the operator norm of $(1-\Delta)\frac{1}{H_{V^{\text{Pek}}}-z}$ uniformly in $z\in\mathcal{C}$. Given Eq. (5.9), it has been verified in the proof of [11, Proposition 3.3] that

$$\begin{aligned}&\left|\|\varphi\|^2 + \text{Tr}\int_{\mathcal{C}}\frac{z}{z-H_{V_\varphi}}\frac{\mathrm{d}z}{2\pi i} - e^{\text{Pek}} - \langle\varphi-\varphi^{\text{Pek}}|1-K^{\text{Pek}}|\varphi-\varphi^{\text{Pek}}\rangle\right|\\ &\quad\lesssim \epsilon\langle\varphi-\varphi^{\text{Pek}}|L^{\text{Pek}}|\varphi-\varphi^{\text{Pek}}\rangle\end{aligned}$$

for $\epsilon := \sup_{z\in\mathcal{C}}\left\{\left\|\frac{A}{1-A}\right\|_{\text{op}} + \left\|\frac{B}{1-B}\right\|_{\text{op}} + \left\|(1-\Delta)^{\frac12}\frac{1}{z-H_{V^{\text{Pek}}}}\frac{A}{1-A}(1-\Delta)^{\frac12}\right\|_{\text{op}}\right\}$, where we denote $A := \left(V_{\varphi-\varphi^{\text{Pek}}}\right)\frac{1}{z-H_{V^{\text{Pek}}}}$ and $B := \left(1-|\psi^{\text{Pek}}\rangle\langle\psi^{\text{Pek}}|\right)A^\dagger$. In the following we want to verify that $\epsilon \lesssim \|V_{\varphi-\varphi^{\text{Pek}}}\|_\diamond$, which concludes the proof by Eq. (5.5). Since $(1-\Delta)\frac{1}{z-H_{V^{\text{Pek}}}}$ is uniformly bounded in z, $\left\|\frac{A}{1-A}\right\|_{\text{op}} \leq \frac{\|A\|_{\text{op}}}{1-\|A\|_{\text{op}}} \lesssim \|\left(V_{\varphi-\varphi^{\text{Pek}}}\right)(1-\Delta)^{-1}\|_{\text{op}} \lesssim \|V_{\varphi-\varphi^{\text{Pek}}}\|_\diamond$ by Eq. (5.3). Similarly $\left\|\frac{B}{1-B}\right\|_{\text{op}} \lesssim \|V_{\varphi-\varphi^{\text{Pek}}}\|_\diamond$. Regarding the final term in the definition of ϵ, note that $(1-\Delta)^{\frac12}\frac{1}{z-H_{V^{\text{Pek}}}}(1-\Delta)^{\frac12}$ is uniformly bounded in z, and therefore

$$\left\|(1-\Delta)^{\frac12}\frac{1}{z-H_{V^{\text{Pek}}}}\frac{A}{1-A}(1-\Delta)^{\frac12}\right\|_{\text{op}} \lesssim \left\|(1-\Delta)^{-\frac12}\frac{A}{1-A}(1-\Delta)^{\frac12}\right\|_{\text{op}} = \left\|\frac{A'}{1-A'}\right\|_{\text{op}},$$

with $A' := (1-\Delta)^{-\frac12}A(1-\Delta)^{\frac12}$. Furthermore $\left\|\frac{A'}{1-A'}\right\|_{\text{op}} \leq \frac{\|A'\|_{\text{op}}}{1-\|A'\|_{\text{op}}}$ and

$$\begin{aligned}\|A'\|_{\text{op}} &\lesssim \left\|(1-\Delta)^{-\frac12}\left(V_{\varphi-\varphi^{\text{Pek}}}\right)(1-\Delta)^{-\frac12}\right\|_{\text{op}} \leq \|\left(V_{\varphi-\varphi^{\text{Pek}}}\right)(1-\Delta)^{-1}\|_{\text{op}}\\ &\lesssim \|V_{\varphi-\varphi^{\text{Pek}}}\|_\diamond.\end{aligned}$$

□

Lemma 5.2 gives a lower bound on $\mathcal{F}^{\text{Pek}}\left(\varphi^{\text{Pek}}+\xi\right) - e^{\text{Pek}}$ in terms of a quadratic function $\xi \mapsto \langle\xi|1-\left(K^{\text{Pek}}+\epsilon L^{\text{Pek}}\right)|\xi\rangle$ for ξ satisfying $\|V_\xi\|_\diamond < \min\{\frac{\epsilon}{c},\delta_0\}$. Due to the translation invariance of $\mathcal{F}^{\text{Pek}}$, this lower bound is however insufficient, since we have for all $\xi \in \text{span}\{\partial_{y_1}\varphi^{\text{Pek}}, \partial_{y_2}\varphi^{\text{Pek}}, \partial_{y_3}\varphi^{\text{Pek}}\}\setminus\{0\}$

$$\langle\xi|1-\left(K^{\text{Pek}}+\epsilon L^{\text{Pek}}\right)|\xi\rangle = \text{Hess}|_{\varphi^{\text{Pek}}}\mathcal{F}^{\text{Pek}}[\xi] - \epsilon\langle\xi|L^{\text{Pek}}|\xi\rangle = -\epsilon\langle\xi|L^{\text{Pek}}|\xi\rangle < 0, \tag{5.10}$$

i.e. the quadratic lower bound is not even non-negative. In order to improve this lower bound, we will introduce a suitable coordinate transformation τ in Definition 5.3. Before we can formulate Definition 5.3 we need some auxiliary preparations.

In the following let Π be the projection defined in Eq. (4.1) and let us define the real orthonormal system

$$\varphi_n := \frac{\Pi \partial_{y_n} \varphi^{\mathrm{Pek}}}{\|\Pi \partial_{y_n} \varphi^{\mathrm{Pek}}\|} \tag{5.11}$$

for $n \in \{1, 2, 3\}$, which we complete to a real orthonormal basis $\{\varphi_1, .., \varphi_N\}$ of $\Pi L^2(\mathbb{R}^3)$. Furthermore let us write $\varphi_x^{\mathrm{Pek}}(y) := \varphi^{\mathrm{Pek}}(y - x)$ for the translations of φ^{Pek} and let us define the map $\omega : \mathbb{R}^3 \longrightarrow \mathbb{R}^3$ as

$$\omega(x) := \left(\langle \varphi_n | \varphi_x^{\mathrm{Pek}} \rangle\right)_{n=1}^{3} \in \mathbb{R}^3. \tag{5.12}$$

Since $\varphi^{\mathrm{Pek}} \in H^1(\mathbb{R}^3)$, ω is differentiable. Moreover, since φ^{Pek} is invariant under the action of $O(3)$ and since the operator Π commutes with the reflections $y_i \to -y_i$ and permutations $y_i \leftrightarrow y_j$, it is clear that $\omega(0) = 0$. By the same argument we see that $D|_0\omega$ has full rank and therefore there exists a local inverse $t \mapsto x_t$ for $|t| < \delta_*$ and a suitable constant $\delta_* > 0$.

Definition 5.3. We define the map $\tau : \Pi L^2(\mathbb{R}^3) \longrightarrow \Pi L^2(\mathbb{R}^3)$ as

$$\tau(\varphi) := \varphi - f(t^{\varphi}),$$

where $t^{\varphi} := \left(\langle \varphi_1 | \varphi \rangle, \langle \varphi_2 | \varphi \rangle, \langle \varphi_3 | \varphi \rangle\right) \in \mathbb{R}^3$ and $f(t)$ is defined as

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

The map τ is constructed in a way such that it "flattens" the manifold of Pekar minimizers $\{\varphi_x^{\mathrm{Pek}} : x \in \mathbb{R}^3\}$. More precisely, we have that $\tau\left(\Pi \varphi_x^{\mathrm{Pek}}\right)$ is for all small enough $x \in \mathbb{R}^3$ an element of the linear space spanned by $\{\varphi_1, \varphi_2, \varphi_3\}$. A similar construction appears in [5] and, in a somewhat different way, in [9].

Recall the operators K^{Pek} and L^{Pek} from Eqs. (5.6) and (5.7), and let T_x be the translation operator defined by $(T_x\varphi)(y) := \varphi(y - x)$. Then we define the operators $K_x^{\mathrm{Pek}} := T_x K^{\mathrm{Pek}} T_{-x}$ and $L_x^{\mathrm{Pek}} := T_x L^{\mathrm{Pek}} T_{-x}$, as well as for $|t| < \epsilon$ with $\epsilon < \delta_*$

$$J_{t,\epsilon} := \pi\left(1 - (1+\epsilon)\left(K_{x_t}^{\mathrm{Pek}} + \epsilon L_{x_t}^{\mathrm{Pek}}\right)\right)\pi, \tag{5.13}$$

where $\pi : L^2(\mathbb{R}^3) \longrightarrow L^2(\mathbb{R}^3)$ is the orthogonal projection onto the subspace spanned by $\{\varphi_4, \ldots, \varphi_N\}$. Furthermore we define $J_{t,\epsilon} := \pi$ for $|t| \geq \epsilon$. In contrast to the operator $1 - \left(K^{\mathrm{Pek}} + \epsilon L^{\mathrm{Pek}}\right)$ from Eq. (5.10), the operator $J_{t,\epsilon}$ is non-negative for ϵ small enough, as will be shown in Lemma B.5. With the operator $J_{t,\epsilon}$ and the transformation τ at hand we can formulate a strong lower bound for $\mathcal{F}^{\mathrm{Pek}}(\varphi) - e^{\mathrm{Pek}}$ in the subsequent Theorem 5.4, where we use the shorthand notation $J_{t,\epsilon}[\varphi] := \langle \varphi | J_{t,\epsilon} | \varphi \rangle$.

Theorem 5.4. *There exist constants $C > 0$, $0 < \epsilon_0 \le \delta_*$ and $0 < D \le 1$ such that*

$$\mathcal{F}^{\text{Pek}}(\varphi) \ge e^{\text{Pek}} + J_{t^\varphi,\epsilon}\big[\tau(\varphi)\big] - \frac{C}{\epsilon}\left\|(1-\Pi)\,\varphi^{\text{Pek}}_{x_{t^\varphi}}\right\|^2 \tag{5.14}$$

for all $0 < \epsilon < \epsilon_0$ and $\varphi \in \Pi L^2(\mathbb{R}^3)$ satisfying $\left\|V_{\varphi-\varphi^{\text{Pek}}}\right\|_\diamond < \epsilon D$ and $|t^\varphi| < \epsilon D$, where $J_{t,\epsilon}$ is defined in Eq. (5.13).

Proof. In the following we use the abbreviation $t := t^\varphi$. Since $\left\|V_{\varphi^{\text{Pek}}-\varphi^{\text{Pek}}_x}\right\|_\diamond \lesssim |x|$ and $|x_t| \lesssim |t|$ for $|t| \le \frac{\delta_*}{2}$, we have for all φ satisfying $\left\|V_{\varphi-\varphi^{\text{Pek}}}\right\|_\diamond < D\epsilon$ and $|t| < \min\{D\epsilon, \frac{\delta_*}{2}\}$

$$\begin{aligned}\left\|V_{T_{-x_t}\varphi-\varphi^{\text{Pek}}}\right\|_\diamond &= \left\|V_{\varphi-\varphi^{\text{Pek}}_{x_t}}\right\|_\diamond \le \left\|V_{\varphi-\varphi^{\text{Pek}}}\right\|_\diamond + \left\|V_{\varphi^{\text{Pek}}-\varphi^{\text{Pek}}_{x_t}}\right\|_\diamond \\ &\lesssim \left\|V_{\varphi-\varphi^{\text{Pek}}}\right\|_\diamond + |t| \lesssim D\epsilon.\end{aligned}$$

By taking D small enough we obtain $\left\|V_{T_{-x_t}\varphi-\varphi^{\text{Pek}}}\right\|_\diamond \le \frac{\epsilon}{c}$ where c is the constant from Lemma 5.2. Let us define $\epsilon_0 := \min\left\{c\delta_0, \frac{\delta_*}{2D}, \delta_*\right\}$. Using the translation-invariance of $\mathcal{F}^{\text{Pek}}$ and applying Lemma 5.2 yields

$$\begin{aligned}\mathcal{F}^{\text{Pek}}(\varphi)-e^{\text{Pek}} &= \mathcal{F}^{\text{Pek}}\big(T_{-x_t}\varphi\big)-e^{\text{Pek}} \ge \langle T_{-x_t}\varphi-\varphi^{\text{Pek}}|1-\Big(K^{\text{Pek}}+\epsilon L^{\text{Pek}}\Big)|T_{-x_t}\varphi-\varphi^{\text{Pek}}\rangle \\ &= \langle\varphi-\varphi^{\text{Pek}}_{x_t}|1-\Big(K^{\text{Pek}}_{x_t}+\epsilon L^{\text{Pek}}_{x_t}\Big)|\varphi-\varphi^{\text{Pek}}_{x_t}\rangle \\ &\ge \|\varphi-\Pi\varphi^{\text{Pek}}_{x_t}\|^2 - \langle\varphi-\varphi^{\text{Pek}}_{x_t}|K^{\text{Pek}}_{x_t}+\epsilon L^{\text{Pek}}_{x_t}|\varphi-\varphi^{\text{Pek}}_{x_t}\rangle \\ &\ge \|\varphi-\Pi\varphi^{\text{Pek}}_{x_t}\|^2 - (1+\epsilon)\,\langle\varphi-\Pi\varphi^{\text{Pek}}_{x_t}|K^{\text{Pek}}_{x_t}+\epsilon L^{\text{Pek}}_{x_t}|\varphi-\Pi\varphi^{\text{Pek}}_{x_t}\rangle \\ &\quad - \Big(1+\epsilon^{-1}\Big)\,\langle(1-\Pi)\,\varphi^{\text{Pek}}_{x_t}|K^{\text{Pek}}_{x_t}+\epsilon L^{\text{Pek}}_{x_t}|\,(1-\Pi)\,\varphi^{\text{Pek}}_{x_t}\rangle,\end{aligned} \tag{5.15}$$

where we have used the positivity of K^{Pek}_x and L^{Pek}_x, and the Cauchy–Schwarz inequality in the last estimate. Note that by construction of x_t as the local inverse of the function ω from Eq. (5.12), we have $\langle\varphi_n|\varphi-\Pi\varphi^{\text{Pek}}_{x_t}\rangle = 0$ for $n \in \{1, 2, 3\}$ and therefore

$$\varphi - \Pi\varphi^{\text{Pek}}_{x_t} = \pi\left(\varphi - \Pi\varphi^{\text{Pek}}_{x_t}\right) = \pi\,(\varphi - f(t)) = \pi\,(\tau\,(\varphi))$$

with π being defined below Eq. (5.13), where we used $|t| < \delta_*$. This concludes the proof with $C := (1+\epsilon_0)\left(\|K\|_{\text{op}} + \epsilon_0\|L\|_{\text{op}}\right)$. □

6. Proof of Theorem 1.1

In the following we will combine the results of the previous sections in order to prove the lower bound on the ground state energy E_α in Theorem 1.1. We start by verifying the subsequent Lemma 6.1, which provides a lower bound on E_α in terms of an operator that is, up to a coordinate transformation τ and a non-negative term, a harmonic oscillator.

Let us again use the identification $\mathcal{F}\left(\Pi L^2(\mathbb{R}^3)\right) \cong L^2\left(\mathbb{R}^N\right)$ utilizing the representation of real functions $\varphi = \sum_{n=1}^N \lambda_n\varphi_n \in \Pi L^2\left(\mathbb{R}^3\right)$ by points $\lambda = (\lambda_1, \ldots, \lambda_N) \in \mathbb{R}^N$, such that the annihilation operators $a_n := a\,(\varphi_n)$ are given by $a_n = \lambda_n + \frac{1}{2\alpha^2}\partial_{\lambda_n}$, where λ_n is the multiplication operator by the function $\lambda \mapsto \lambda_n$ on $L^2\left(\mathbb{R}^N\right)$, see also Eq. (4.2), where Π is the projection from Eq. (4.1) and $\{\varphi_1, \ldots, \varphi_N\}$ is the orthonormal basis of $\Pi L^2(\mathbb{R}^3)$ constructed around Eq. (5.11). Let us also use for functions $\varphi \mapsto g(\varphi)$ depending on elements $\varphi \in \Pi L^2(\mathbb{R}^3)$ the convenient notation $g(\lambda) := g\left(\sum_{n=1}^N \lambda_n \varphi_n\right)$, where $\lambda \in \mathbb{R}^N$.

Lemma 6.1. *Let $C > 0$ and $0 < \sigma \leq \frac{1}{4}$, and assume s, h and σ satisfy $2s < h$ and $\sigma < \frac{1-5s}{4}$. Furthermore let us define $\Lambda := \alpha^{\frac{4}{5}(1+\sigma)}$ and $L := \alpha^{1+\sigma}$. Then we obtain for any state Ψ satisfying $\langle \Psi | \mathbb{H}_\Lambda | \Psi \rangle \leq C$, $\mathrm{supp}\,(\Psi) \subset B_{4L}(0)$ and*

$$\chi\left(W_{\varphi^{\mathrm{Pek}}}^{-1} \mathcal{N} W_{\varphi^{\mathrm{Pek}}} \leq \alpha^{-h}\right)\Psi = \Psi, \tag{6.1}$$

that

$$\langle \Psi | \mathbb{H}_\Lambda | \Psi \rangle \geq e^{\mathrm{Pek}} + \left\langle \Psi \middle| -\frac{1}{4\alpha^4}\sum_{n=1}^N \partial_{\lambda_n}^2 + J_{t^\lambda, \alpha^{-s}}\big[\tau(\lambda)\big] + \mathcal{N} - \sum_{n=1}^N a_n^\dagger a_n \middle| \Psi \right\rangle - \frac{N}{2\alpha^2}$$
$$+ O\left(\alpha^{s - \frac{12}{5}(1+\sigma)} + \alpha^{-2(1+\sigma)}\right), \tag{6.2}$$

where t^φ and $\tau(\varphi)$ are defined in Lemma 5.3 and $J_{t,\epsilon}$ is defined in Eq. (5.13). Furthermore, there exists a $\beta > 0$, such that $\langle \Psi | 1 - \mathbb{B} | \Psi \rangle \leq e^{-\beta \alpha^{2(1-s)}}$, where $\mathbb{B}$ is the multiplication operator by the function $\lambda \mapsto \chi\left(|t^\lambda| < \alpha^{-s}\right)$.

Proof. Applying Eq. (2.3) with Λ and ℓ as in the definition of Π, see Eq. (4.1), and $K := \Lambda$, and utilizing Eq. (2.5), we obtain for a suitable C'

$$\langle \Psi | \mathbb{H}_\Lambda | \Psi \rangle \geq \langle \Psi | \mathbb{H}_{\Lambda,\ell}^0 | \Psi \rangle - C' \alpha^{-2(1+\sigma)}. \tag{6.3}$$

Making use of $\sum_{n=1}^N a_n^\dagger a_n = \sum_{n=1}^N \left(-\frac{1}{4\alpha^4}\partial_{\lambda_n}^2 + \lambda_n^2\right) - \frac{N}{2\alpha^2}$ and $a_n + a_n^\dagger = 2\lambda_n$, we further have the identity

$$\mathbb{H}_{\Lambda,\ell}^0 = -\Delta_x - 2\sum_{n=1}^N \langle \varphi_n | w_x \rangle \lambda_n + \sum_{n=1}^N \left(-\frac{1}{4\alpha^4}\partial_{\lambda_n}^2 + \lambda_n^2\right) - \frac{N}{2\alpha^2} + \mathcal{N} - \sum_{n=1}^N a_n^\dagger a_n$$
$$= -\Delta_x + V_\lambda(x) + \sum_{n=1}^N \left(-\frac{1}{4\alpha^4}\partial_{\lambda_n}^2 + \lambda_n^2\right) - \frac{N}{2\alpha^2} + \mathcal{N} - \sum_{n=1}^N a_n^\dagger a_n,$$

with V_φ defined in Eq. (5.1). Clearly $-\Delta_x + V_\lambda \geq \inf \sigma\,(-\Delta_x + V_\lambda) = \mathcal{F}^{\mathrm{Pek}}(\lambda) - \sum_{n=1}^N \lambda_n^2$, which yields the inequality $\mathbb{H}_{\Lambda,\ell}^0 \geq \mathbb{K} + \mathcal{N} - \sum_{n=1}^N a_n^\dagger a_n$ with

$$\mathbb{K} := -\frac{1}{4\alpha^4}\sum_{n=1}^N \partial_{\lambda_n}^2 + \mathcal{F}^{\mathrm{Pek}}(\lambda) - \frac{N}{2\alpha^2}. \tag{6.4}$$

Combining Eqs. (6.3) and (6.4), we obtain

$$\left\langle \Psi \middle| \mathbb{H}_\Lambda - \mathcal{N} + \sum_{n=1}^N a_n^\dagger a_n \middle| \Psi \right\rangle + C'\alpha^{-2(1+\sigma)} \geq \langle \Psi | \mathbb{K} | \Psi \rangle = \langle \mathbb{K} \rangle_\gamma, \tag{6.5}$$

where γ is the reduced density matrix on the Hilbert space $\mathcal{F}\left(\Pi L^2(\mathbb{R}^3)\right) \cong L^2(\mathbb{R}^N)$ corresponding to the state Ψ, i.e. we trace out the electron component as well as all the modes in the orthogonal complement of $\Pi L^2(\mathbb{R}^3)$,

$$\gamma := \mathrm{Tr}_{L^2(\mathbb{R}^3)\otimes\mathcal{F}(L^2(\mathbb{R}^3))\to\mathcal{F}(\Pi L^2(\mathbb{R}^3))}\left[\,|\Psi\rangle\langle\Psi|\,\right].$$

Note that we have the inequality $W^{-1}_{\Pi\varphi^{\mathrm{Pek}}}\left(\sum_{n=1}^N a_n^\dagger a_n\right) W_{\Pi\varphi^{\mathrm{Pek}}} \leq W^{-1}_{\varphi^{\mathrm{Pek}}}\mathcal{N} W_{\varphi^{\mathrm{Pek}}}$. The operators on the left and right hand side commute, and consequently (6.1) implies that $\chi\left(W^{-1}_{\Pi\varphi^{\mathrm{Pek}}}\left(\sum_{n=1}^N a_n^\dagger a_n\right) W_{\Pi\varphi^{\mathrm{Pek}}} \leq \alpha^{-h}\right)\Psi = \Psi$. This in particular means that the transformed reduced density matrix $\widetilde{\gamma} := W_{\Pi\varphi^{\mathrm{Pek}}}\gamma W^{-1}_{\Pi\varphi^{\mathrm{Pek}}}$ satisfies

$$\chi\left(\sum_{n=1}^N a_n^\dagger a_n \leq \alpha^{-h}\right)\widetilde{\gamma} = \widetilde{\gamma}. \tag{6.6}$$

Using the identification $\varphi = \sum_{n=1}^N \lambda_n\varphi_n$ as before, the Weyl operator $W_{\Pi\varphi^{\mathrm{Pek}}}$ acts as $\left(W_{\Pi\varphi^{\mathrm{Pek}}}\Psi\right)(\lambda) = \Psi\left(\lambda + \lambda^{\mathrm{Pek}}\right)$ with $\lambda^{\mathrm{Pek}} := \left(\langle\varphi_1|\varphi^{\mathrm{Pek}}\rangle, \ldots, \langle\varphi_N|\varphi^{\mathrm{Pek}}\rangle\right)$. Due to Eq. (6.6), and the fact that $2s < h$ and $\sigma < \frac{1-5s}{4}$, the assumptions of Proposition 4.2 are satisfied, and therefore we obtain for any $D > 0$ the existence of a constant $\beta > 0$ such that for α large enough

$$\int_{|\lambda-\lambda^{\mathrm{Pek}}|_\diamond \geq \alpha^{-s}D}\left(1+|\lambda-\lambda^{\mathrm{Pek}}|^2\right)\rho(\lambda)\mathrm{d}\lambda = \int_{|\lambda|_\diamond\geq\alpha^{-s}D}\left(1+|\lambda|^2\right)\widetilde{\rho}(\lambda)\mathrm{d}\lambda \leq e^{-\beta\alpha^{2(1-s)}}, \tag{6.7}$$

$$\begin{aligned}\int_{|t^\lambda|\geq\alpha^{-s}D}\left(1+|\lambda-\lambda^{\mathrm{Pek}}|^2\right)\rho(\lambda)\mathrm{d}\lambda &\leq \sum_{n=1}^3\int_{|\lambda_n|\geq\frac{\alpha^{-s}}{\sqrt{3}}D}\left(1+|\lambda-\lambda^{\mathrm{Pek}}|^2\right)\rho(\lambda)\mathrm{d}\lambda \\ &= \sum_{n=1}^3\int_{|\lambda_n|\geq\frac{\alpha^{-s}}{\sqrt{3}}D}\left(1+|\lambda|^2\right)\widetilde{\rho}(\lambda)\mathrm{d}\lambda \leq e^{-\beta\alpha^{2(1-s)}},\end{aligned} \tag{6.8}$$

where ρ and $\widetilde{\rho}$ are the density functions corresponding to γ and $\widetilde{\gamma}$, respectively, and where we have used $t^\lambda = (\lambda_1, \lambda_2, \lambda_3) \in \mathbb{R}^3$. For the concrete choice $D := 1$, Eq. (6.8) immediately yields the claim $\langle\Psi|1-\mathbb{B}|\Psi\rangle = \int_{|t^\lambda|\geq\alpha^{-s}}\rho(\lambda)\mathrm{d}\lambda \leq e^{-\beta\alpha^{2(1-s)}}$.

In order to verify Eq. (6.2), we need to find a sufficient lower bound for the expectation value $\langle\mathbb{K}\rangle_\gamma$, where $\mathbb{K}$ is the operator from Eq. (6.4). Recall the definition of the transformation $\tau : \Pi L^2(\mathbb{R}^3) \longrightarrow \Pi L^2(\mathbb{R}^3)$ from Definition 5.3 and the operator $J_{t,\epsilon}$ from Eq. (5.13). As a first step we will provide a lower bound on $\langle\mathcal{F}^{\mathrm{Pek}}(\lambda)\rangle_\gamma$, using Eq. (5.14) and the fact that $\sup_{|t|\leq t_0}\left\|(1-\Pi)\,\varphi^{\mathrm{Pek}}_{x_t}\right\|^2 \lesssim \alpha^{-\frac{12}{5}(1+\sigma)}$ for t_0 small enough, which follows from Lemma A.1 together with $x_t \underset{t\to 0}{\longrightarrow} 0$. We define the operator $\mathbb{A} := \chi\left(|\lambda-\lambda^{\mathrm{Pek}}|_\diamond < \alpha^{-s}D\right)\chi\left(\left|t^\lambda\right| < \alpha^{-s}D\right)$, where D is as in Theorem 5.4, and estimate

$$\begin{aligned}\langle \mathcal{F}^{\text{Pek}}(\lambda)\rangle_\gamma &= \langle \mathcal{F}^{\text{Pek}}(\lambda)\,\mathbb{A}\rangle_\gamma + \langle \mathcal{F}^{\text{Pek}}(\lambda)\,(1-\mathbb{A})\rangle_\gamma\\ &\geq \left\langle \left(e^{\text{Pek}} + J_{t^\lambda,\alpha^{-s}}\left[\tau(\lambda)\right]\right)\mathbb{A}\right\rangle_\gamma + \langle \mathcal{F}^{\text{Pek}}(\lambda)\,(1-\mathbb{A})\rangle_\gamma + O\left(\alpha^{s-\frac{12}{5}(1+\sigma)}\right)\\ &= \left\langle e^{\text{Pek}} + J_{t^\lambda,\alpha^{-s}}\left[\tau(\lambda)\right]\right\rangle_\gamma + \left\langle X\right\rangle_\gamma + O\left(\alpha^{s-\frac{12}{5}(1+\sigma)}\right)\end{aligned} \tag{6.9}$$

with $X := \left(\mathcal{F}^{\text{Pek}}(\lambda) - e^{\text{Pek}} - J_{t^\lambda,\alpha^{-s}}\left[\tau(\lambda)\right]\right)(1-\mathbb{A})$. Using Eqs. (6.7) and (6.8) as well as the fact that $1-\mathbb{A} \leq \chi\left(|\lambda - \lambda^{\text{Pek}}|_\diamond \geq D\alpha^{-s}\right) + \chi\left(\left|t^\lambda\right| \geq D\alpha^{-s}\right)$, we obtain $\left\langle X\right\rangle_\gamma \lesssim e^{-\beta\alpha^{2(1-s)}}$, where we have used that $\mathcal{F}^{\text{Pek}}(\lambda)$ and $J_{t^\lambda,\alpha^{-s}}\left[\tau(\lambda)\right]$ are bounded by $C(1+|\lambda|^2)$ for suitable $C > 0$. By Eq. (6.9) we therefore have the estimate $\langle \mathcal{F}^{\text{Pek}}(\lambda)\rangle_\gamma \geq \left\langle e^{\text{Pek}} + J_{t^\lambda,\alpha^{-s}}\left[\tau(\lambda)\right]\right\rangle_\gamma + O\left(\alpha^{s-\frac{12}{5}(1+\sigma)}\right)$, and consequently

$$\langle \mathbb{K}\rangle_\gamma \geq e^{\text{Pek}} + \left\langle -\frac{1}{4\alpha^4}\sum_{n=1}^N \partial^2_{\lambda_n} + J_{t^\lambda,\alpha^{-s}}\left[\tau(\lambda)\right]\right\rangle_\gamma - \frac{N}{2\alpha^2} + O\left(\alpha^{s-\frac{12}{5}(1+\sigma)}\right). \tag{6.10}$$

Since $\left\langle -\frac{1}{4\alpha^4}\sum_{n=4}^N \partial^2_{\lambda_n} + J_{t^\lambda,\alpha^{-s}}\left[\tau(\lambda)\right]\right\rangle_\gamma = \left\langle \Psi\middle| -\frac{1}{4\alpha^4}\sum_{n=4}^N \partial^2_{\lambda_n} + J_{t^\lambda,\alpha^{-s}}\left[\tau(\lambda)\right]\middle|\Psi\right\rangle$, this concludes the proof together with Eq. (6.5). □

In the following, let Ψ_α be the sequence of states constructed in Theorem 3.13, satisfying $\langle \Psi_\alpha|\mathbb{H}_\Lambda|\Psi_\alpha\rangle - E_\alpha \lesssim \alpha^{-2(1+\sigma)}$, $\text{supp}\,(\Psi_\alpha) \subset B_{4L}(0)$ with $L = \alpha^{1+\sigma}$ and strong condensation with respect to φ^{Pek}, i.e. $\chi\left(W^{-1}_{\varphi^{\text{Pek}}}\mathcal{N}W_{\varphi^{\text{Pek}}} \leq \alpha^{-h}\right)\Psi_\alpha = \Psi_\alpha$, and furthermore let $s < \frac{1}{29}$ be a given constant and let us choose σ and h such that $2s < h < \frac{2}{29}$ and $\frac{s}{2} \leq \sigma < \frac{1-5s}{4}$. Note that $h < \frac{2}{29}$ makes sure that the assumption of Theorem 3.13 is satisfied, while $2s < h$ and $\sigma < \frac{1-5s}{4}$ are necessary in order to apply Lemma 6.1. The final assumption $\frac{s}{2} \leq \sigma$ will be useful later in Eq. (6.15) in order to make sure that $\alpha^{-2(1+\sigma)} \leq \alpha^{-(2+s)}$. Making use of $-\frac{1}{4\alpha^4}\sum_{n=1}^3 \partial^2_{\lambda_n} \geq 0$ and $\mathcal{N} \geq \sum_{n=1}^N a_n^\dagger a_n$, we obtain by Lemma 6.1 that

$$E_\alpha \geq e^{\text{Pek}} + \left\langle \Psi_\alpha\middle| -\frac{1}{4\alpha^4}\sum_{n=4}^N \partial^2_{\lambda_n} + J_{t^\lambda,\alpha^{-s}}\left[\tau(\lambda)\right]\middle|\Psi_\alpha\right\rangle - \frac{N}{2\alpha^2} + O\left(\alpha^{-2(1+\sigma)}\right) \tag{6.11}$$

for a suitable C', where we have used $\alpha^{s-\frac{12}{5}(1+\sigma)} \leq \alpha^{-2(1+\sigma)}$ and $E_\alpha - \langle \Psi_\alpha|\mathbb{H}_\Lambda|\Psi_\alpha\rangle \gtrsim -\alpha^{-2(1+\sigma)}$. In order to further estimate the expectation value in Eq. (6.11), let us define the unitary transformation $(\mathcal{U}\Psi)(\lambda) := \Psi\left(\tau'(\lambda)\right)$ with $\tau'(\lambda) := \left(\left\langle \varphi_n|\tau(\lambda)\right\rangle\right)_{n=1}^N \in \mathbb{R}^N$. Since τ' acts as a shift operator on each of the planes $X_t := \{\lambda : (\lambda_1, \lambda_2, \lambda_3) = t\}$ for $t \in \mathbb{R}^3$, it is clear that $\det \mathrm{D}|_\lambda \tau' = 1$, which in particular means that the operator $\mathcal{U}$ is indeed unitary, and we have $\partial_{\lambda_n} = \mathcal{U}^{-1}\partial_{\lambda_n}\mathcal{U}$ for $n \geq 4$. Furthermore we define the operator

$$\mathbb{Q}_{t,\epsilon} := -\frac{1}{4\alpha^4}\sum_{n=4}^N \partial^2_{\lambda_n} + \sum_{n,m=1}^N \left(J_{t,\epsilon}\right)_{n,m}\lambda_n\lambda_m$$

with $\left(J_{t,\epsilon}\right)_{n,m} := \langle\varphi_n|J_{t,\epsilon}|\varphi_m\rangle$. Note that $\left(J_{t,\epsilon}\right)_{n,m} = \left(J_{t,\epsilon}\right)_{m,n} = 0$ in case $n \in \{1, 2, 3\}$, i.e. the operator $\mathbb{Q}_{t,\epsilon}$ depends only on the variables λ_n for $n \geq 4$ and not on $t^\lambda = (\lambda_1, \lambda_2, \lambda_3)$, hence it acts on the Fock space $\mathcal{F}\left(\text{span}\{\varphi_4, \ldots, \varphi_N\}\right) \cong L^2\left(\mathbb{R}^{N-3}\right)$ only. Utilizing the fact that $\mathcal{U}^{-1} J_{t^\lambda,\alpha^{-s}}\left[\tau(\lambda)\right]\mathcal{U} = J_{t^\lambda,\alpha^{-s}}\left[\lambda\right] = \sum_{n,m=1}^N \left(J_{t^\lambda,\alpha^{-s}}\right)_{n,m} \lambda_n\lambda_m$, where we used that $\mathcal{U}^{-1}t^\lambda\mathcal{U} = t^\lambda$, we obtain

$$\mathcal{U}^{-1}\left(-\frac{1}{4\alpha^4}\sum_{n=4}^N \partial_{\lambda_n}^2 + J_{t^\lambda,\alpha^{-s}}\left[\tau(\lambda)\right]\right)\mathcal{U} = \mathbb{Q}_{t^\lambda,\alpha^{-s}} \geq \mathbb{Q}_{t^\lambda,\alpha^{-s}}\mathbb{B} \geq \inf_{|t|<\alpha^{-s}} \inf\sigma\left(\mathbb{Q}_{t,\alpha^{-s}}\right)\mathbb{B},$$

where $\mathbb{B}$ is as in Lemma 6.1. Here we have used $\mathbb{Q}_{t^\lambda,\alpha^{-s}} \geq 0$, which follows from Lemma B.5, as well as the fact that $1 - \mathbb{B}$ is non-negative and commutes with $\mathbb{Q}_{t^\lambda,\alpha^{-s}}$. Applying this inequality with respect to the state $\widetilde{\Psi}_\alpha := \mathcal{U}^{-1}\Psi_\alpha$ yields

$$\begin{aligned}\left\langle\Psi_\alpha\right| -\frac{1}{4\alpha^4}\sum_{n=4}^N \partial_{\lambda_n}^2 + J_{t^\lambda,\alpha^{-s}}\left[\tau(\lambda)\right]\left|\Psi_\alpha\right\rangle &\geq \inf_{|t|<\alpha^{-s}} \inf\sigma\left(\mathbb{Q}_{t,\alpha^{-s}}\right)\left\langle\widetilde{\Psi}_\alpha\middle|\mathbb{B}\middle|\widetilde{\Psi}_\alpha\right\rangle \\ &\geq \inf_{|t|<\alpha^{-s}} \inf\sigma\left(\mathbb{Q}_{t,\alpha^{-s}}\right) - \frac{N}{2\alpha^2}\left\langle\widetilde{\Psi}_\alpha\middle|1-\mathbb{B}\middle|\widetilde{\Psi}_\alpha\right\rangle \end{aligned} \tag{6.12}$$

where we have used $J_{t,\epsilon} \leq 1$, and therefore $\inf\sigma\left(\mathbb{Q}_{t,\epsilon}\right) \leq \frac{N}{2\alpha^2}$. By Lemma 6.1, we know that $\left\langle\widetilde{\Psi}_\alpha\middle|1-\mathbb{B}\middle|\widetilde{\Psi}_\alpha\right\rangle = \left\langle\Psi_\alpha\middle|1-\mathbb{B}\middle|\Psi_\alpha\right\rangle \leq e^{-\beta\alpha^{2-2s}}$. Combining Eqs. (6.11) and (6.12), and making use of the fact that $N \lesssim \alpha^p$ for some $p > 0$, yields

$$E_\alpha \geq e^{\text{Pek}} + \inf_{|t|<\alpha^{-s}} \inf\sigma\left(\mathbb{Q}_{t,\alpha^{-s}}\right) - \frac{N}{2\alpha^2} + O\left(\alpha^{-2(1+\sigma)}\right). \tag{6.13}$$

Since the operator $\mathbb{Q}_{t,\alpha^{-s}}$ is quadratic in ∂_{λ_n} and λ_n, we have an explicit formula for its ground state energy, given by

$$\inf\sigma\left(\mathbb{Q}_{t,\alpha^{-s}}\right) - \frac{N}{2\alpha^2} = -\frac{\text{Tr}_{\Pi L^2(\mathbb{R}^3)}\left[1-\sqrt{J_{t,\alpha^{-s}}}\right]}{2\alpha^2}, \tag{6.14}$$

where we used the fact that $J_{t,\alpha^{-s}} \geq 0$ for α large enough, as shown in Lemma B.5. Using Eq. (B.7), we can approximate this quantity by

$$\sup_{|t|<\alpha^{-s}}\left|\text{Tr}_{\Pi L^2(\mathbb{R}^3)}\left[1-\sqrt{J_{t,\alpha^{-s}}}\right] - \text{Tr}\left[1-\sqrt{H^{\text{Pek}}}\right]\right| \lesssim \alpha^{-s} + \alpha^{-\frac{1}{5}},$$

where H^{Pek} is defined in Eq. (1.4). Consequently Eq. (6.13) yields

$$E_\alpha - e^{\text{Pek}} + \frac{1}{2\alpha^2}\text{Tr}\left[1-\sqrt{H^{\text{Pek}}}\right] \gtrsim -\alpha^{-2(1+\sigma)} - \alpha^{-(2+s)} - \alpha^{-\left(2+\frac{1}{5}\right)}, \tag{6.15}$$

which concludes the proof, since all the terms on the right side are of order $\alpha^{-(2+s)}$.

7. Approximation by Coherent States

This section is devoted to the proof of Theorem 3.2, which states that asymptotically the phonon part of any low energy state is a convex combination of the coherent states $\Omega_{\varphi_x^{\mathrm{Pek}}}$ with $x \in \mathbb{R}^3$, where the convex combination is taken on the level of density matrices. As a central tool we will verify in Lemma 7.2 an asymptotic formula for the expectation value $\langle \Psi | \widehat{F} | \Psi \rangle$ in terms of the lower symbol $\mathbb{P}_y$ corresponding to the state Ψ, see Eq. (7.6). Furthermore we will make use of the inequality

$$\inf_{x\in\mathbb{R}^3} \|\varphi - \varphi_x^{\mathrm{Pek}}\|^2 \lesssim \mathcal{F}^{\mathrm{Pek}}(\varphi) - e^{\mathrm{Pek}} \tag{7.1}$$

derived in [10, Lemma 7], which implies that the only coherent states Ω_φ with a low energy have their point of condensation φ close to the manifold of Pekar minimizers $\{\varphi_x^{\mathrm{Pek}} : x \in \mathbb{R}^3\}$. We start with the subsequent Lemma 7.1, which provides an asymptotic formula for $\widehat{F}$ operators in terms of creation and annihilation operators.

Lemma 7.1. *Let $m \in \mathbb{N}$ and $C > 0$ be given constants, $\{g_n : n \in \mathbb{N}\}$ an orthonormal basis of $L^2(\mathbb{R}^3)$ and let us denote $a_n := a(g_n)$. Then there exists a constant $T > 0$ such that for all functions F of the form*

$$F(\rho) = \int \dots \int f(x_1, \dots, x_m)\, \mathrm{d}\rho(x_1) \dots \mathrm{d}\rho(x_m), \tag{7.2}$$

with $f : \mathbb{R}^{3\times m} \longrightarrow \mathbb{R}$ bounded, and states Ψ satisfying $\chi(\mathcal{N} \le C)\Psi = \Psi$, we can approximate the operator $\widehat{F}$ from Definition 3.1 by

$$\left| \langle \Psi | \widehat{F} | \Psi \rangle - \sum_{I,J\in\mathbb{N}^m} f_{I,J} \langle \Psi | a_{I_1}^\dagger \dots a_{I_m}^\dagger a_{J_1} \dots a_{J_m} | \Psi \rangle \right| \le T \|f\|_\infty \alpha^{-2}, \tag{7.3}$$

where we interpret f as a multiplication operator on $L^2(\mathbb{R}^3)^{\otimes m} \cong L^2(\mathbb{R}^{3\times m})$ and denote the matrix elements $f_{I,J} := \langle g_{I_1} \otimes \dots \otimes g_{I_m} | f | g_{J_1} \otimes \dots \otimes g_{J_m} \rangle$.

Proof. By the assumption $\chi(\mathcal{N} \le C)\Psi = \Psi$, we can represent the state Ψ as $\Psi = \bigoplus_{n\le C\alpha^2} \Psi_n$ where $\Psi_n(y, x^1, \dots, x^n)$ is a function of the electron variable y and the n phonon coordinates $x^k \in \mathbb{R}^3$. As in the proof of Lemma 3.3, we will suppress the dependence on the electron variable y in our notation. Using the definition of $\widehat{F}$ in Definition 3.1, as well as the notation $X = (x^1, \dots, x^n)$, we can write

$$\begin{aligned}\langle \Psi | \widehat{F} | \Psi \rangle &= \sum_{n\le C\alpha^2} \int_{\mathbb{R}^{3n}} F\left(\alpha^{-2} \sum_{k=1}^n \delta_{x^k}\right) |\Psi_n(X)|^2 \mathrm{d}X \\ &= \alpha^{-2m} \sum_{n\le C\alpha^2} \sum_{k\in\{1,\dots,n\}^m} \int_{\mathbb{R}^{3n}} f(x^{k_1}, \dots, x^{k_m}) |\Psi_n(X)|^2 \mathrm{d}X.\end{aligned}$$

Defining $\mathcal{K}$ as the set of all $k \in \{1, \dots, n\}^m$ satisfying $k_i \ne k_j$ for all $i \ne j$, we can further express the operator $\sum_{I,J\in\mathbb{N}^m} f_{I,J}\, a_{I_1}^\dagger \dots a_{I_m}^\dagger a_{J_1} \dots a_{J_m}$ as

$$\sum_{I,J\in\mathbb{N}^m} f_{I,J} \langle \Psi | a_{I_1}^\dagger \dots a_{I_m}^\dagger a_{J_1} \dots a_{J_m} | \Psi \rangle = \alpha^{-2m} \sum_{n\le C\alpha^2} \sum_{k\in\mathcal{K}} \int_{\mathbb{R}^{3n}} f(x^{k_1}, \dots, x^{k_m}) |\Psi_n(X)|^2 \mathrm{d}X.$$

Consequently we can identify the left hand side of Eq. (7.3) as

$$\left|\alpha^{-2m}\sum_{n\leq C\alpha^2}\sum_{k\in\{1,\dots,n\}^m\setminus\mathcal{K}}\int_{\mathbb{R}^{3n}} f(x^{k_1},\dots,x^{k_m})|\Psi_n(X)|^2\mathrm{d}X\right|$$
$$\leq \|f\|_\infty \sum_{n\leq C\alpha^2}\left(\sum_{k\in\{1,\dots,n\}^m\setminus\mathcal{K}}\alpha^{-2m}\right)\int_{\mathbb{R}^{3n}}|\Psi_n(X)|^2\mathrm{d}X.$$

Since $\sum_{k\in\{1,\dots,n\}^m\setminus\mathcal{K}}\alpha^{-2m} = \left(n^m - \frac{n!}{(n-m)!}\right)\alpha^{-2m} \leq m2^m n^{m-1}\alpha^{-2m} \lesssim \alpha^{-2}$ for $n \leq C\alpha^2$ and since $\sum_{n\leq C\alpha^2}\int_{\mathbb{R}^{3n}}|\Psi_n(X)|^2\mathrm{d}X = \|\Psi\|^2 = 1$, this concludes the proof. □

In the following we are going to define the lower symbol $\mathbb{P}_y$ corresponding to a state $\Psi \in L^2\big(\mathbb{R}^3, \mathcal{F}\big(L^2(\mathbb{R}^3)\big)\big)$. Since we consider the Fock space over the infinite dimensional Hilbert space $L^2(\mathbb{R}^3)$, we need to modify the usual definition of the lower symbol by introducing suitable localizations. For $0 < s \leq \frac{4}{27}$ and $y \in \mathbb{R}^3$, let us define $\ell_* := \alpha^{-\frac{5}{2}s}$ and $\Lambda_* := \alpha^{2s}$, and the projection

$$\Pi_y := \Pi^y_{\Lambda_*,\ell_*}, \tag{7.4}$$

see Definition 2.1. We have $N_* := \dim \Pi_y L^2(\mathbb{R}^3) \lesssim (\Lambda_*/\ell_*)^3 \leq \alpha^2$ by our assumption $s \leq \frac{4}{27}$. Using the notation $\{e_{y,1},\dots,e_{y,N_*}\}$ for the orthonormal basis of $\Pi_y L^2(\mathbb{R}^3)$ from Definition 2.1, we introduce for $\xi \in \mathbb{C}^{N_*}$ the coherent states $\Omega_{y,\xi} := e^{\alpha^2 a^\dagger(\varphi_{y,\xi})-\alpha^2 a(\varphi_{y,\xi})}\Omega$, where Ω is the vacuum in $\mathcal{F}\left(\Pi_y L^2(\mathbb{R}^3)\right)$ and $\varphi_{y,\xi} := \sum_{n=1}^{N_*}\xi_n e_{y,n} \in \Pi_y L^2(\mathbb{R}^3)$. Furthermore we define wave-functions Ψ_y localized in the electron coordinates x as

$$\Psi_y(x) := L_*^{-\frac{3}{2}}\chi\left(\frac{x-y}{L_*}\right)\Psi(x), \tag{7.5}$$

where $y \in \mathbb{R}^3$ and $L_* := \alpha^{\frac{s}{2}}$, and χ is a smooth non-negative function with $\operatorname{supp}(\chi) \subset B_1(0)$ and $\int \chi(y)^2\,\mathrm{d}y = 1$. For the following construction, note that we can identify $L^2\big(\mathbb{R}^3, \mathcal{F}\big(L^2(\mathbb{R}^3)\big)\big) \cong \mathcal{F}\left(\Pi_y L^2(\mathbb{R}^3)\right) \otimes L^2\Big(\mathbb{R}^3, \mathcal{F}\Big(\Pi_y L^2(\mathbb{R}^3)^\perp\Big)\Big)$. Let us now define measures $\mathbb{P}_y$ on $\mathbb{C}^{N_*} \cong \mathbb{R}^{2N_*}$ corresponding to the state Ψ_y as

$$\frac{\mathrm{d}\mathbb{P}_y}{\mathrm{d}\xi} := \frac{1}{\pi^{N_*}}\left\|\Theta_{y,\xi}\Psi_y\right\|^2, \tag{7.6}$$

where $\Theta_{y,\xi}$ is the orthogonal projection onto the set spanned by elements of the form $\Omega_{y,\xi} \otimes \widetilde{\Psi}$ with $\widetilde{\Psi} \in L^2\Big(\mathbb{R}^3, \mathcal{F}\Big(\Pi_y L^2(\mathbb{R}^3)^\perp\Big)\Big)$. Note that the coherent states $\Omega_{y,\xi}$ provide a resolution of the identity $\frac{1}{\pi^{N_*}}\int_{\mathbb{C}^{N_*}}|\Omega_{y,\xi}\rangle\langle\Omega_{y,\xi}|\mathrm{d}\xi = 1_{\mathcal{F}(\Pi_y L^2(\mathbb{R}^3))}$, see for example [20], and consequently the projections $\Theta_{y,\xi}$ satisfy $\frac{1}{\pi^{N_*}}\int_{\mathbb{C}^{N_*}}\Theta_{y,\xi}\,\mathrm{d}\xi = 1$. In particular we see that the total mass of the measure $\mathbb{P}_y$ is $\int \mathrm{d}\mathbb{P}_y = \|\Psi_y\|^2$ and therefore

$$\iint \mathrm{d}\mathbb{P}_y\mathrm{d}y = \int \|\Psi_y\|^2\mathrm{d}y = \|\Psi\|^2 = 1.$$

In the following Lemma 7.2 and Corollary 7.3 we will provide an asymptotic formula for the expectation value $\langle\Psi_y|\widehat{F}|\Psi_y\rangle$, respectively $\langle\Psi|\widehat{F}|\Psi\rangle$, in terms of the measures $\mathbb{P}_y$.

Lemma 7.2. *Given $m\in\mathbb{N}$, $C>0$ and $g\in L^2(\mathbb{R}^3)$, there exists a $T>0$ such that for all F of the form (7.2), $y\in\mathbb{R}^3$ and $\epsilon>0$, and states Ψ satisfying $\chi(\mathcal{N}\leq C)\Psi=\Psi$*

$$\frac{1}{T\|f\|_\infty}\left|\langle\Psi_y|\widehat{F}|\Psi_y\rangle-\int F\left(|\varphi_{y,\xi}|^2\right)\mathrm{d}\mathbb{P}_y(\xi)\right|\leq\left(\frac{N_*}{\alpha^2}+\epsilon\right)\|\Psi_y\|^2+\epsilon^{-1}\langle\Psi_y|\mathcal{N}^y_{>N_*}|\Psi_y\rangle, \tag{7.7}$$

with $\mathcal{N}^y_{>N_*}:=\mathcal{N}-\sum_{n=1}^{N_*}a^\dagger_{y,n}a_{y,n}$ and $a_{y,n}:=a\left(e_{y,n}\right)$, and furthermore

$$\frac{1}{T}\left|\langle\Psi_y|W_g^{-1}\mathcal{N}W_g|\Psi_y\rangle-\int\|\varphi_{y,\xi}-g\|^2\mathrm{d}\mathbb{P}_y(\xi)\right|\leq\left(\frac{N_*}{\alpha^2}+\epsilon\right)\|\Psi_y\|^2+\epsilon^{-1}\langle\Psi_y|\mathcal{N}^y_{>N_*}|\Psi_y\rangle, \tag{7.8}$$

where W_g is the corresponding Weyl transformation.

Proof. Let $\{g_n:n\in\mathbb{N}\}$ be a completion of $\{e_{y,1},\dots,e_{y,N_*}\}$ to an orthonormal basis of $L^2(\mathbb{R}^3)$ and let us define $a_n:=a(g_n)$. We further introduce an operator $\widetilde{F}$ as

$$\widetilde{F}:=\sum_{I,J\in\{1,\dots,N_*\}^m}f_{I,J}\,a^\dagger_{I_1}\dots a^\dagger_{I_m}a_{J_1}\dots a_{J_m}=\sum_{I,J\in\mathbb{N}^m}\left(\Pi_y^{\otimes^m}f\,\Pi_y^{\otimes^m}\right)_{I,J}a^\dagger_{I_1}\dots a^\dagger_{I_m}a_{J_1}\dots a_{J_m}. \tag{7.9}$$

In the following we want to verify that both $\|f\|_\infty^{-1}\left|\langle\Psi_y|\widehat{F}|\Psi_y\rangle-\langle\Psi_y|\widetilde{F}|\Psi_y\rangle\right|$ and $\|f\|_\infty^{-1}\left|\langle\Psi_y|\widetilde{F}|\Psi_y\rangle-\int F\left(|\varphi_{y,\xi}|^2\right)\mathrm{d}\mathbb{P}_y(\xi)\right|$ are, up to a multiplicative constant, bounded by the right hand side of Eq. (7.7). Applying the Cauchy–Schwarz inequality, we obtain for all $\epsilon>0$

$$\begin{aligned}\pm\left(f-\Pi_y^{\otimes^m}f\,\Pi_y^{\otimes^m}\right)&=\pm f\left(1-\Pi_y^{\otimes^m}\right)\pm\left(1-\Pi_y^{\otimes^m}\right)f\,\Pi_y^{\otimes^m}\\&\leq\epsilon\|f\|_\infty+\epsilon^{-1}\|f\|_\infty\left(1-\Pi_y^{\otimes^m}\right)\\&\leq\epsilon\|f\|_\infty+\epsilon^{-1}\|f\|_\infty\left((1-\Pi_y)_1+\dots+(1-\Pi_y)_m\right),\end{aligned}$$

where $(1-\Pi_y)_j$ means that the operator $1-\Pi_y$ acts on the j-th factor in the tensor product. Consequently we have the operator inequality

$$\pm\left(\sum_{I,J\in\mathbb{N}^m}f_{I,J}\,a^\dagger_{I_1}\dots a^\dagger_{I_m}a_{J_1}\dots a_{J_m}-\widetilde{F}\right)\leq\epsilon\|f\|_\infty\mathcal{N}^m+\epsilon^{-1}\|f\|_\infty m\,\mathcal{N}^y_{>N_*}\mathcal{N}^{m-1}.$$

Making use of Eq. (7.3) and the fact that $\chi(\mathcal{N}\leq C)\Psi_y=\Psi_y$ further yields

$$\left|\langle\Psi_y|\widehat{F}|\Psi_y\rangle-\sum_{I,J\in\mathbb{N}^m}f_{I,J}\,\langle\Psi_y|a^\dagger_{I_1}\dots a^\dagger_{I_m}a_{J_1}\dots a_{J_m}|\Psi_y\rangle\right|\leq d\alpha^{-2}\|f\|_\infty\|\Psi_y\|^2$$

for a suitable constant $d > 0$. We have thus shown the bound

$$\frac{1}{\|f\|_\infty}\left|\langle\Psi_y|\widehat{F}|\Psi_y\rangle-\langle\Psi_y|\widetilde{F}|\Psi_y\rangle\right|\leq\left(d\alpha^{-2}+\epsilon C^m\right)\|\Psi_y\|^2+\epsilon^{-1}mC^{m-1}\left\langle\Psi_y\middle|\mathcal{N}^y_{>N_*}\middle|\Psi_y\right\rangle \tag{7.10}$$

which is of the desired form.

In order to verify that $\frac{1}{\|f\|_\infty}\left|\left\langle\Psi_y\middle|\widetilde{F}\middle|\Psi_y\right\rangle-\int F\left(|\varphi_{y,\xi}|^2\right)\mathrm{d}\mathbb{P}_y(\xi)\right|$ is of the same order as the right hand side of Eq. (7.7) as well, we will first compute $\widetilde{F}$ with reversed operator ordering, i.e. we compute

$$\sum_{I,J\in\{1,\dots,N_*\}^m} f_{I,J}\, a_{J_1}\dots a_{J_m}a^\dagger_{I_1}\dots a^\dagger_{I_m}=\sum_{I,J\in\{1,\dots,N_*\}^m} f_{I,J}\, a^\dagger_{I_1}\dots a^\dagger_{I_m}a_{J_1}\dots a_{J_m}$$
$$+\sum_{n=1}^m\frac{1}{\alpha^{2n}n!}\sum_{\sigma,\tau\in\mathcal{S}^{m,n}}\left(\sum_{I',J'}f^{\sigma,\tau}_{I',J'}\prod_{k\notin\{\sigma_1,\dots,\sigma_n\}}a^\dagger_{I'_k}\prod_{\ell\notin\{\tau_1,\dots,\tau_n\}}a_{J'_\ell}\right) \tag{7.11}$$

where $\mathcal{S}^{m,n}$ is the set of all sequences $\sigma=(\sigma_1,\dots,\sigma_n)$ without repetitions having values $\sigma_k\in\{1,\dots,m\}$ and the coordinate matrices $f^{\sigma,\tau}$ are defined as

$$f^{\sigma,\tau}_{I',J'}:=\sum_{I,J\in\{1,\dots,N_*\}^m}f_{I,J}\,\delta_{I_{\sigma_1},J_{\tau_1}}\dots\delta_{I_{\sigma_n},J_{\tau_n}}\prod_{k\notin\{\sigma_1,\dots,\sigma_n\}}\delta_{I_k,I'_k}\prod_{\ell\notin\{\tau_1,\dots,\tau_n\}}\delta_{J_\ell,J'_\ell}$$

for $I'\in\{1,\dots,N_*\}^{\{1,\dots,m\}\setminus\{\sigma_1,\dots,\sigma_n\}}$ and $J'\in\{1,\dots,N_*\}^{\{1,\dots,m\}\setminus\{\tau_1,\dots,\tau_n\}}$. One can verify Eq. (7.11) either by iteratively applying the (rescaled) canonical commutation relations $[a_i,a^\dagger_j]=\alpha^{-2}\delta_{i,j}$, or by using the fact that the operator $e^{\alpha^{-2}\nabla_{\bar{\xi}}\nabla_\xi}$, which is well defined on polynomials in ξ and $\bar{\xi}$, transforms the upper symbol into the lower symbol (see e.g. [27]), and computing its action on $P(\xi):=\sum_{I,J\in\{1,\dots,N_*\}^m}f_{I,J}\overline{\xi_{I_1}\dots\xi_{I_m}}\xi_{J_1}\dots\xi_{J_m}$ as

$$e^{\alpha^{-2}\nabla_{\bar{\xi}}\nabla_\xi}(P)(\xi)=P(\xi)+\sum_{n=1}^m\frac{1}{\alpha^{2n}n!}\sum_{\sigma,\tau\in\mathcal{S}^{m,n}}\left(\sum_{I',J'}f^{\sigma,\tau}_{I',J'}\prod_{k\notin\{\sigma_1,\dots,\sigma_n\}}\overline{\xi_{I'_k}}\prod_{\ell\notin\{\tau_1,\dots,\tau_n\}}\xi_{J'_\ell}\right).$$

In order to identify the left hand side of Eq. (7.11), we will make use of the resolution of identity $\frac{1}{\pi^{N_*}}\int_{\mathbb{C}^{N_*}}\Theta_{y,\xi}\,\mathrm{d}\xi=1$, where $\Theta_{y,\xi}$ is defined below Eq. (7.6), which allows us to rewrite the anti-wick ordered term $a_{J_1}\dots a_{J_m}a^\dagger_{I_1}\dots a^\dagger_{I_m}$ as

$$\frac{1}{\pi^{N_*}}\int_{\mathbb{C}^{N_*}}a_{J_1}\dots a_{J_m}\Theta_{y,\xi}a^\dagger_{I_1}\dots a^\dagger_{I_m}\,\mathrm{d}\xi=\frac{1}{\pi^{N_*}}\int_{\mathbb{C}^{N_*}}\xi_{J_1}\dots\xi_{J_m}\overline{\xi_{I_1}\dots\xi_{I_m}}\Theta_{y,\xi}\,\mathrm{d}\xi.$$

Here we have used that $a_i\Theta_{y,\xi}=\xi_i\Theta_{y,\xi}$ for all $i\in\{1,\dots,N_*\}$. By the definition of $\mathbb{P}_y$ in Eq. (7.6) we can therefore rewrite the expectation value of the first term on the left hand side of Eq. (7.11) with respect to the state Ψ_y as

$$\sum_{I,J\in\{1,\dots,N_*\}^m}f_{I,J}\left\langle\Psi_y\middle|a_{J_1}\dots a_{J_m}a^\dagger_{I_1}\dots a^\dagger_{I_m}\middle|\Psi_y\right\rangle=\sum_{I,J\in\{1,\dots,N_*\}^m}f_{I,J}\int\xi_{J_1}\dots\xi_{J_m}\overline{\xi_{I_1}\dots\xi_{I_m}}\mathrm{d}\mathbb{P}_y(\xi)$$
$$=\int\left\langle\varphi^{\otimes m}_{y,\xi}\middle|f\middle|\varphi^{\otimes m}_{y,\xi}\right\rangle\mathrm{d}\mathbb{P}_y(\xi)=\int F\left(\left|\varphi_{y,\xi}\right|^2\right)\mathrm{d}\mathbb{P}_y(\xi). \tag{7.12}$$

In order to control the terms in the second line of Eq. (7.11), we can estimate the norm $\|f^{\sigma,\tau}\|_{\mathrm{op}} \leq \|f\|_\infty N_*^n$ for all $\sigma, \tau \in \mathcal{S}^{m,n}$, which follow from

$$\langle v|f^{\sigma,\tau}|w\rangle = \sum_{I,J\in\{1,\dots,N_*\}^m} f_{I,J}\delta_{I_{\sigma_1},J_{\tau_1}}\dots\delta_{I_{\sigma_n},J_{\tau_n}}\overline{v_{I'}}w_{J'} = \sum_{k\in\{1,\dots,N_*\}^n}\left\langle v^k\middle|f\middle|w^k\right\rangle$$
$$\leq \|f\|_\infty \sum_{k\in\{1,\dots,N_*\}^n}\|v^k\|\|w^k\| \leq \|f\|_\infty N_*^n\|v\|\|w\|,$$

where I' denotes the restriction of I to $\{1,\dots,m\}\backslash\{\sigma_1,\dots,\sigma_n\}$ and v^k is defined as $\left(v^k\right)_I := \delta_{I_{\sigma_1},k_1}\dots\delta_{I_{\sigma_n},k_n}v_{I'}$, and J' and w^k are defined analogue. Hence we obtain

$$\left|\frac{1}{\alpha^{2n}}\sum_{I',J'} f^{\sigma,\tau}_{I',J'}\langle\Psi_y|\prod_{k\notin\{\sigma_1,\dots,\sigma_n\}}a^\dagger_{I'_k}\prod_{\ell\notin\{\tau_1,\dots,\tau_n\}}a_{J'_\ell}|\Psi_y\rangle\right| \leq \|f\|_\infty\left(\frac{N_*}{\alpha^2}\right)^n\langle\Psi_y|\mathcal{N}^{m-n}|\Psi_y\rangle$$

for $n \geq 1$. Since $\chi(\mathcal{N}\leq C)\Psi_y = \Psi_y$ and $N_* \lesssim \alpha^2$, see the comment below Eq. (7.4), this is a quantity of order $\|f\|_\infty\frac{N_*}{\alpha^2}\|\Psi_y\|^2$. Combing this estimate with Eq. (7.11) and Eq. (7.12) yields that $\frac{1}{\|f\|_\infty}\left|\left\langle\Psi_y\middle|\widetilde{F}\middle|\Psi_y\right\rangle - \int F\left(|\varphi_{y,\xi}|^2\right)\,\mathrm{d}\mathbb{P}_y(\xi)\right|$ is, up to a multiplicative factor, bounded by the right hand side of Eq. (7.7). Together with Eq. (7.10), this concludes the proof of Eq. (7.7).

In order to verify Eq. (7.8), let us define $G(\rho) := \int \mathrm{d}\rho$. Note that $W_g^{-1}\mathcal{N}W_g = \mathcal{N} - a(g) - a^\dagger(g) + \|g\|^2 = \widehat{G} - a(g) - a^\dagger(g) + \|g\|^2$. Furthermore we have $\left\langle\Psi_y\middle|a(\Pi_y g) + a^\dagger(\Pi_y g)\middle|\Psi_y\right\rangle = \int\left(\langle g|\varphi_{y,\xi}\rangle + \langle\varphi_{y,\xi}|g\rangle\right)\mathrm{d}\mathbb{P}_y(\xi)$, where we used that $a(g) + a^\dagger(g)$ is anti-Wick ordered, and

$$\left|\left\langle\Psi_y\middle|a(g) + a^\dagger(g) - a(\Pi_y g) - a^\dagger(\Pi_y g)\middle|\Psi_y\right\rangle\right| \leq \epsilon^{-1}\langle\Psi_y|\mathcal{N}^y_{>N_*}|\Psi_y\rangle + \epsilon\|g\|^2\|\Psi_y\|^2.$$

Hence, applying Eq. (7.7) with respect to the function G and using that $\int\|\varphi_{y,\xi} - g\|^2\mathrm{d}\mathbb{P}_y = \int\left(G\left(|\varphi_{y,\xi}|^2\right) + \langle g|\varphi_{y,\xi}\rangle + \langle\varphi_{y,\xi}|g\rangle\right)\mathrm{d}\mathbb{P}_y(\xi) + \|g\|^2\|\Psi_y\|^2$ concludes the proof of Eq. (7.8). □

Corollary 7.3. *Given constants $m \in \mathbb{N}$, $C > 0$ and $g \in L^2\left(\mathbb{R}^3\right)$, there exists a constant $T > 0$ such that for all F of the form (7.2) and states Ψ satisfying $\chi(\mathcal{N}\leq C)\Psi = \Psi$ and $\langle\Psi|\mathbb{H}_K|\Psi\rangle \leq e^{\mathrm{Pek}} + \delta e$, with $\delta e \geq 0$ and $K \geq \Lambda_* = \alpha^{2s}$,*

$$\frac{1}{T\|f\|_\infty}\left|\left\langle\Psi\middle|\widehat{F}\middle|\Psi\right\rangle - \iint F\left(\left|\varphi_{y,\xi}\right|^2\right)\mathrm{d}\mathbb{P}_y(\xi)\,\mathrm{d}y\right| \leq \sqrt{\delta e} + \alpha^{-\frac{s}{2}} + \alpha^{\frac{27}{2}s-2}, \quad (7.13)$$

and furthermore

$$\frac{1}{T}\left|\left\langle\Psi\middle|W_g^{-1}\mathcal{N}W_g\middle|\Psi\right\rangle - \iint\|\varphi_{y,\xi} - g\|^2\mathrm{d}\mathbb{P}_y(\xi)\,\mathrm{d}y\right| \leq \sqrt{\delta e} + \alpha^{-\frac{s}{2}} + \alpha^{\frac{27}{2}s-2}. \quad (7.14)$$

Proof. Using the fact that we have $\left\langle\Psi\middle|\widehat{F}\middle|\Psi\right\rangle = \int\left\langle\Psi_y\middle|\widehat{F}\middle|\Psi_y\right\rangle\mathrm{d}y$ and $\left\langle\Psi\middle|W_g^{-1}\mathcal{N}W_g\middle|\Psi\right\rangle = \int\left\langle\Psi_y\middle|W_g^{-1}\mathcal{N}W_g\middle|\Psi_y\right\rangle\mathrm{d}y$, and applying Eq. (7.7), respectively Eq. (7.8), immediately yields that the left hand sides of Eqs. (7.13) and (7.14) are bounded by

$$\frac{N_*}{\alpha^2} + \epsilon + \epsilon^{-1}\int\langle\Psi_y|\mathcal{N}^y_{>N_*}|\Psi_y\rangle\mathrm{d}y \quad (7.15)$$

for any $\epsilon > 0$. In order to bound $\int \langle \Psi_y | \mathcal{N}^y_{>N_*} | \Psi_y \rangle \mathrm{d}y$ from above, let us first apply Eq. (2.3) together with Eq. (2.5), which provides the auxiliary estimate

$$\int |\langle \Psi_y | \mathbb{H}^y_{\Lambda_*,\ell_*} | \Psi_y \rangle - \langle \Psi_y | \mathbb{H}_K | \Psi_y \rangle | \mathrm{d}y \lesssim \alpha^{-s} \int \langle \Psi_y | -\Delta_x + \mathcal{N} + 1 | \Psi_y \rangle \mathrm{d}y$$
$$\leq \alpha^{-s} \int \langle \Psi_y | 2\mathbb{H}_K + d + 1 | \Psi_y \rangle \mathrm{d}y.$$

Note that the assumptions of Eq. (2.3) are indeed satisfied, since $K \geq \Lambda_*$ and $\operatorname{supp}(\Psi_y) \subset B_{L_*}(y)$. In combination with the IMS identity $\int \langle \Psi_y | \mathbb{H}_K | \Psi_y \rangle \mathrm{d}y = \langle \Psi | \mathbb{H}_K | \Psi \rangle + L_*^{-2} \|\nabla \chi\|^2$, where χ is the function from Eq. (7.5), this furthermore yields

$$\left| \int \langle \Psi_y | \mathbb{H}^y_{\Lambda_*,\ell_*} | \Psi_y \rangle \mathrm{d}y - \langle \Psi | \mathbb{H}_K | \Psi \rangle \right| \lesssim \alpha^{-s} \left(\langle \Psi | \mathbb{H}_K | \Psi \rangle + d + 1 \right), \tag{7.16}$$

where we have used $L_*^{-2} = \alpha^{-s}$. Furthermore $\langle \Psi | \mathbb{H}_K | \Psi \rangle \leq e^{\mathrm{Pek}} + \delta e$ by assumption, and consequently $| \int \langle \Psi_y | \mathbb{H}^y_{\Lambda_*,\ell_*} | \Psi_y \rangle \mathrm{d}y - \langle \Psi | \mathbb{H}_K | \Psi \rangle | \leq D\alpha^{-s}(\delta e + 1)$ for a suitable D. Consequently

$$\langle \Psi | \mathbb{H}_K | \Psi \rangle \geq \int \langle \Psi_y | \mathbb{H}^y_{\Lambda_*,\ell_*} | \Psi_y \rangle \mathrm{d}y - D\alpha^{-s}(\delta e + 1)$$
$$\geq E_\alpha + \int \langle \Psi_y | \mathcal{N}^y_{>N_*} | \Psi_y \rangle \mathrm{d}y - D\alpha^{-s}(\delta e + 1). \tag{7.17}$$

where we have used that $\mathbb{H}^y_{\Lambda_*,\ell_*} \geq E_\alpha + \mathcal{N}^y_{>N_*}$ in the second inequality. Using Eq. (7.17) as well as the fact that $E_\alpha - e^{\mathrm{Pek}} \gtrsim -\alpha^{-\frac{1}{5}} \geq -\alpha^{-s}$, see [20], we obtain the upper bound

$$\int \langle \Psi_y | \mathcal{N}^y_{>N_*} | \Psi_y \rangle \mathrm{d}y \lesssim \langle \Psi | \mathbb{H}_K | \Psi \rangle - e^{\mathrm{Pek}} + \alpha^{-s}(\delta e + 1) \lesssim \delta e + \alpha^{-s}. \tag{7.18}$$

Choosing $\epsilon := \sqrt{\delta e + \alpha^{-s}}$ in Eq. (7.15) therefore concludes the proof together with the observation that $\frac{N_*}{\alpha^2} \lesssim \alpha^{\frac{27}{2}s - 2}$. □

In the following Lemma 7.4 we are investigating the support properties of the lower symbol $\mathbb{P}_y$. In particular we derive bounds on the associated moments and verify that $\varphi_{y,\xi}$ is typically close to the manifold of minimizers $\{\varphi^{\mathrm{Pek}}_x : x \in \mathbb{R}^3\}$.

Lemma 7.4. *Given constants $m \in \mathbb{N}$ and $C > 0$, there exists a $T > 0$, such that $\iint |\xi|^{2m} \mathrm{d}\mathbb{P}_y(\xi)\, \mathrm{d}y \leq T$ for all Ψ satisfying $\chi(\mathcal{N} \leq C)\Psi = \Psi$, and furthermore we have for all $K \geq \Lambda_*$, where Λ_* is as in the definition of Π^y in Eq. (7.4),*

$$\frac{1}{T} \iint \inf_{x \in \mathbb{R}^3} \|\varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_x\|^2 \mathrm{d}\mathbb{P}_y(\xi)\, \mathrm{d}y \leq \langle \Psi | \mathbb{H}_K | \Psi \rangle - e^{\mathrm{Pek}} + \alpha^{-s} + \alpha^{\frac{27}{2}s - 2}. \tag{7.19}$$

Proof. For $m \in \mathbb{N}$, let us define the function $G(\rho) := \left(\int \mathrm{d}\rho(x)\right)^m = \int \ldots \int \mathrm{d}\rho(x_1)\ldots \mathrm{d}\rho(x_m)$, which is clearly of the form given in Eq. (7.2). Consequently by Lemma 7.2

$$\begin{aligned}\int |\xi|^{2m} \mathrm{d}\mathbb{P}_y(\xi) &= \int G\left(|\varphi_{y,\xi}|^2\right) \mathrm{d}\mathbb{P}_y(\xi)\\ &\lesssim \left\langle \Psi_y \middle| \widehat{G} \middle| \Psi_y \right\rangle + \left(\frac{N_*}{\alpha^2}+1\right) \|\Psi_y\|^2 + \langle \Psi_y | \mathcal{N}^y_{>N_*} | \Psi_y\rangle\\ &= \left\langle \Psi_y \middle| \mathcal{N}^{2m} \middle| \Psi_y \right\rangle + \left(\frac{N_*}{\alpha^2}+1\right) \|\Psi_y\|^2 + \langle \Psi_y | \mathcal{N}^y_{>N_*} | \Psi_y\rangle\\ &\le \left(C^{2m} + \frac{N_*}{\alpha^2} + 1 + C\right) \|\Psi_y\|^2,\end{aligned}$$

which concludes the proof of the first part, since $N_* \lesssim \alpha^2$ and $\int \|\Psi_y\|^2 \mathrm{d}y = \|\Psi\|^2 = 1$.

Regarding the proof of Eq. (7.19), we have the simple bound

$$\begin{aligned}\mathbb{H}^y_{\Lambda_*,\ell_*} &= -\Delta_x - a\left(\Pi_y w_x\right) - a^\dagger\left(\Pi_y w_x\right) + \mathcal{N}\\ &\ge -\Delta_x - a\left(\Pi_y w_x\right) - a^\dagger\left(\Pi_y w_x\right) + \sum_{n=1}^{N_*} a^\dagger_{y,n} a_{y,n}\\ &= -\Delta_x - a\left(\Pi_y w_x\right) - a^\dagger\left(\Pi_y w_x\right) + \sum_{n=1}^{N_*} a_{y,n} a^\dagger_{y,n} - \frac{N_*}{\alpha^2}.\end{aligned} \tag{7.20}$$

Since all terms in Eq. (7.20) are represented in anti-Wick ordering, we can follow [20] and express, similar as in the proof of Lemma 7.2, their expectation value as

$$\begin{aligned}&\left\langle \Psi_y \middle| -\Delta_x - a\left(\Pi_y w_x\right) - a^\dagger\left(\Pi_y w_x\right) + \sum_{n=1}^{N_*} a_{y,n} a^\dagger_{y,n} \middle| \Psi_y \right\rangle\\ &= \int \left(\langle \psi^\xi_y | -\Delta_x + V_{\varphi_{y,\xi}} | \psi^\xi_y \rangle + \|\varphi_{y,\xi}\|^2 \right) \mathrm{d}\mathbb{P}_y(\xi)\\ &\ge \int \left(\inf \sigma\left(-\Delta_x + V_{\varphi_{y,\xi}}\right) + \|\varphi_{y,\xi}\|^2 \right) \mathrm{d}\mathbb{P}_y(\xi) = \int \mathcal{F}^{\mathrm{Pek}}\left(\varphi_{y,\xi}\right) \mathrm{d}\mathbb{P}_y(\xi),\end{aligned} \tag{7.21}$$

with $\psi^\xi_y := \frac{\Theta_{y,\xi}\Psi_y}{\|\Theta_{y,\xi}\Psi_y\|}$ where $\Theta_{y,\xi}$ is defined below Eq. (7.6), $\mathcal{F}^{\mathrm{Pek}}$ is the Pekar functional and V_φ is defined in Eq. (5.1). Making use of Eq. (7.1) we obtain together with Eqs. (7.16), (7.20) and (7.21)

$$\begin{aligned}\int\int \inf_{x\in\mathbb{R}^3} \|\varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_x\|^2 \mathrm{d}\mathbb{P}_y(\xi)\,\mathrm{d}y &\lesssim \int \langle \Psi_y | \mathbb{H}^y_{\Lambda_*,\ell_*} | \Psi_y \rangle \mathrm{d}y - e^{\mathrm{Pek}} + \frac{N_*}{\alpha^2}\\ &\lesssim \langle \Psi | \mathbb{H}_K | \Psi \rangle - e^{\mathrm{Pek}} + \frac{N_*}{\alpha^2} + D\alpha^{-s}\left(\langle \Psi | \mathbb{H}_K | \Psi\rangle + d + 1\right),\end{aligned}$$

for a suitable $D > 0$. This concludes the proof, since we have $N_* \lesssim \alpha^{\frac{27}{2}s}$. □

The bound in Eq. (7.19) suggests that $\varphi_{y,\xi}$ is close to $\varphi^{\mathrm{Pek}}_{x^{y,\xi}}$ with a high probability, where $x^{y,\xi}$ is the minimizer of $x \mapsto \|\varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_x\|$. Motivated by this observation we expect $\iint F\left(\left|\varphi_{y,\xi}\right|^2\right)\mathrm{d}\mathbb{P}_y\mathrm{d}y \approx \iint F\left(\left|\varphi^{\mathrm{Pek}}_{x^{y,\xi}}\right|^2\right)\mathrm{d}\mathbb{P}_y\mathrm{d}y$ for measures $\mathbb{P}_y$ for low energy states Ψ, and therefore it seems natural to define the measure μ in Theorem 3.2 as $\int f\mathrm{d}\mu := \iint f\left(x^{y,\xi}\right)\mathrm{d}\mathbb{P}_y\mathrm{d}y$, allowing us to identify $\iint F\left(\left|\varphi^{\mathrm{Pek}}_{x^{y,\xi}}\right|^2\right)\mathrm{d}\mathbb{P}_y\mathrm{d}y = \int F\left(\left|\varphi^{\mathrm{Pek}}_x\right|^2\right)\mathrm{d}\mu$. This expression is however ill-defined, since the infimum $\inf_{x\in\mathbb{R}^3}\|\varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_x\|$ is not necessarily attained and it is not necessarily unique. In order to avoid these difficulties, we will slightly modify the definition of the measure μ in the proof of Lemma 7.5.

Lemma 7.5. *Given $m \in \mathbb{N}$, $C > 0$ and $g \in L^2\left(\mathbb{R}^3\right)$ we can find a constant $T > 0$, such that for all states Ψ satisfying $\chi\left(\mathcal{N} \le C\right)\Psi = \Psi$ and $\langle\Psi|\mathbb{H}_K|\Psi\rangle \le e^{\mathrm{Pek}} + \delta e$, with $\delta e \ge 0$ and $K \ge \Lambda_*$, there exists a probability measure μ on $\mathbb{R}^3$ with the property*

$$\frac{1}{T\|f\|_\infty}\left|\iiint F\left(\left|\varphi_{y,\xi}\right|^2\right)\mathrm{d}\mathbb{P}_y(\xi)\,\mathrm{d}y - \int F\left(\left|\varphi^{\mathrm{Pek}}_x\right|^2\right)\mathrm{d}\mu(x)\right| \le \sqrt{\delta e} + \alpha^{-\frac{s}{2}} + \alpha^{\frac{27}{4}s-1}, \tag{7.22}$$

for all F of the form (7.2), and furthermore

$$\frac{1}{T}\left|\iint \|\varphi_{y,\xi} - g\|^2\mathrm{d}\mathbb{P}_y(\xi)\,\mathrm{d}y - \int\|\varphi^{\mathrm{Pek}}_x - g\|^2\mathrm{d}\mu(x)\right| \le \sqrt{\delta e} + \alpha^{-\frac{s}{2}} + \alpha^{\frac{27}{4}s-1}. \tag{7.23}$$

Proof. For $\epsilon > 0$, let $\bigcup_{n=1}^{\infty} A_{\epsilon,n} = \mathbb{C}^{N_*}$ be a partition of $\mathbb{C}^{N_*}$ consisting of non-empty measurable sets $A_{\epsilon,n}$ having a diameter bounded by $d(A_{\epsilon,n}) \le \epsilon$. Furthermore choose $\xi_{\epsilon,n} \in A_{\epsilon,n}$ and $x_{\epsilon,n} \in \mathbb{R}^3$ satisfying $\|\varphi_{0,\xi_{\epsilon,n}} - \varphi^{\mathrm{Pek}}_{x_{\epsilon,n}}\| \le \inf_{x\in\mathbb{R}^3}\|\varphi_{0,\xi_{\epsilon,n}} - \varphi^{\mathrm{Pek}}_x\| + \epsilon$. Then

$$\begin{aligned}\|\varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_{y+x_{\epsilon,n}}\| &= \|\varphi_{0,\xi} - \varphi^{\mathrm{Pek}}_{x_{\epsilon,n}}\| \le \|\varphi_{0,\xi_{\epsilon,n}} - \varphi^{\mathrm{Pek}}_{x_{\epsilon,n}}\| + \|\varphi_{0,\xi} - \varphi_{0,\xi_{\epsilon,n}}\| \\ &\le \|\varphi_{0,\xi_{\epsilon,n}} - \varphi^{\mathrm{Pek}}_{x_{\epsilon,n}}\| + \epsilon \\ &\le \inf_{x\in\mathbb{R}^3}\|\varphi_{0,\xi_{\epsilon,n}} - \varphi^{\mathrm{Pek}}_x\| + 2\epsilon \le \inf_{x\in\mathbb{R}^3}\|\varphi_{0,\xi} - \varphi^{\mathrm{Pek}}_x\| + 3\epsilon = \inf_{x\in\mathbb{R}^3}\|\varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_x\| + 3\epsilon.\end{aligned} \tag{7.24}$$

Let us now define the probability measure μ on $\mathbb{R}^3$ by specifying its action on functions $f \in C\left(\mathbb{R}^3\right)$ as

$$\int f\mathrm{d}\mu := \sum_{n=1}^{\infty}\int f\left(y + x_{\epsilon,n}\right)\mathbb{P}_y\left(A_{\epsilon,n}\right)\mathrm{d}y = \sum_{n=1}^{\infty}\int\int_{A_{\epsilon,n}} f\left(y + x_{\epsilon,n}\right)\mathrm{d}\mathbb{P}_y\mathrm{d}y.$$

Since $\int F\left(\left|\varphi_{y,\xi}\right|^2\right)\mathrm{d}\mathbb{P}_y(\xi) = \sum_{n=1}^{\infty}\int_{A_{\epsilon,n}} F\left(\left|\varphi_{y,\xi}\right|^2\right)\mathrm{d}\mathbb{P}_y(\xi)$, we can estimate the left hand side of Eq. (7.22) with the aid of the triangle inequality by

$$\sum_{n=1}^{\infty}\int\int_{A_{\epsilon,n}}\left|F\left(\left|\varphi_{y,\xi}\right|^2\right) - F\left(\left|\varphi^{\mathrm{Pek}}_{y+x_{\epsilon,n}}\right|^2\right)\right|\mathrm{d}\mathbb{P}_y(\xi)\,\mathrm{d}y. \tag{7.25}$$

From the concrete form of the function F given in Eq. (7.2), as well as the facts that $\|\varphi^{\mathrm{Pek}}_{y+x_{\epsilon,n}}\| = \|\varphi^{\mathrm{Pek}}_0\|$ is finite and $\|\varphi_{y,\xi}\| = |\xi|$, one readily concludes that

$$\left|F\left(|\varphi_{y,\xi}|^2\right) - F\left(\left|\varphi^{\mathrm{Pek}}_{y+x_{\epsilon,n}}\right|^2\right)\right| \lesssim \|f\|_\infty \left\|\varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_{y+x_{\epsilon,n}}\right\| (1+|\xi|)^{2m-1}.$$

Using Eq. (7.24) we further obtain for any $\kappa > 0$ and $\xi \in A_{\epsilon,n}$

$$\begin{aligned}\left\|\varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_{y+x_{\epsilon,n}}\right\| (1+|\xi|)^{2m-1} &\le \left(\inf_{x\in\mathbb{R}^3} \|\varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_x\| + 3\epsilon\right)(1+|\xi|)^{2m-1} \\ &\le \kappa^{-1} \inf_{x\in\mathbb{R}^3} \|\varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_x\|^2 + \frac{\kappa}{4}(1+|\xi|)^{4m-2} + 3\epsilon\,(1+|\xi|)^{2m-1},\end{aligned}$$

and therefore the expression in Eq. (7.25) can be bounded from above by

$$\begin{aligned}\|f\|_\infty \Bigg(&\kappa^{-1}\iint \inf_{x\in\mathbb{R}^3}\|\varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_x\|^2 \mathrm{d}\mathbb{P}_y(\xi)\,\mathrm{d}y + \frac{\kappa}{4}\iint (1+|\xi|)^{4m-2}\,\mathrm{d}\mathbb{P}_y(\xi)\,\mathrm{d}y \\ &+ 3\epsilon \iint (1+|\xi|)^{2m-1}\,\mathrm{d}\mathbb{P}_y(\xi)\,\mathrm{d}y\Bigg).\end{aligned}$$

By Lemma 7.4 this concludes the proof of (7.22) with $\epsilon := \kappa := \sqrt{\delta e + \alpha^{-s} + \alpha^{\frac{27}{2}s-2}}$. Equation (7.23) can be proven analogously, using the estimate

$$\left|\|\varphi_{y,\xi} - g\|^2 - \|\varphi^{\mathrm{Pek}}_{y+x_{\epsilon,n}} - g\|^2\right| \lesssim \left\|\varphi_{y,\xi} - \varphi^{\mathrm{Pek}}_{y+x_{\epsilon,n}}\right\| (1+|\xi|)$$

for $\xi \in A_{\epsilon,n}$. □

Combining Eq. (7.13), respectively Eq. (7.14), with Eq. (7.22), respectively Eq. (7.23), immediately yields that the left hand side of Eq. (3.2), respectively Eq. (3.3), is of the order $\sqrt{\delta e} + \alpha^{-\frac{s}{2}} + \alpha^{\frac{27}{4}s-1}$. Optimizing in the parameter $0 < s \le \frac{4}{27}$ concludes the proof of Theorem 3.2 with the concrete choice $s := \frac{4}{29}$.

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A. Properties of the Pekar Minimizer

In the following section we derive certain useful properties concerning the minimizer φ^{Pek} of the Pekar functional $\mathcal{F}^{\text{Pek}}$ in (5.4). We start with Lemma A.1, where we quantify the error of applying the cut-off Π to a minimizer, where Π is the projection defined in Eq. (4.1) for a given parameter $0 < \sigma < \frac{1}{4}$. The subsequent Lemmas A.2 and A.3 then concern the concentration of the density $\left|\varphi^{\text{Pek}}\right|^2$ around the origin.

Lemma A.1. *For all $r > 0$ we have the estimates* $\sup_{|x|\leq r} \left\|(1-\Pi)\,\varphi_x^{\text{Pek}}\right\| \lesssim \alpha^{-\frac{6}{5}(1+\sigma)}$. *Moreover,* $\left\|(1-\Pi)\,\partial_{x_n}\varphi^{\text{Pek}}\right\| \lesssim \alpha^{-\frac{2}{5}(1+\sigma)}$ *for* $n \in \{1,2,3\}$.

Proof. We can write $\varphi^{\text{Pek}} = 4\sqrt{\pi}\,(-\Delta)^{-\frac{1}{2}}\left|\psi^{\text{Pek}}\right|^2$ where ψ^{Pek} is the ground state of the operator $H_{V^{\text{Pek}}}$. Consequently $\varphi_x^{\text{Pek}} = 4\sqrt{\pi}\,(f_x + g_x)$ with the definitions $\widehat{f_x}(k) = \mathbb{1}_{B_\Lambda}(k)\frac{\widehat{|\psi^{\text{Pek}}|^2}(k)}{|k|}e^{ik\cdot x}$ and $\widehat{g_x}(k) = \mathbb{1}_{\mathbb{R}^3\setminus B_\Lambda}(k)\frac{\widehat{|\psi^{\text{Pek}}|^2}(k)}{|k|}e^{ik\cdot x}$, where $\widehat{\cdot}$ denotes the Fourier transform. In the first step we are going to estimate $\|\,(1-\Pi)\,g_x\| = \|g_x\|$ by

$$\|g_x\|^2 = \int_{|k|\geq\Lambda}\frac{\left|\widehat{\left|\psi^{\text{Pek}}\right|^2}(k)\right|^2}{|k|^2}\mathrm{d}k \leq \left\||k|^2\widehat{\left|\psi^{\text{Pek}}\right|^2}(k)\right\|_\infty^2 \int_{|k|\geq\Lambda}\frac{1}{|k|^6}\mathrm{d}k \lesssim \frac{1}{\Lambda^3} = \alpha^{-\frac{12}{5}(1+\sigma)}, \tag{A.1}$$

where we have used that $\psi^{\text{Pek}} \in H^2(\mathbb{R}^3)$, [17,24] and therefore $\left\||k|^2\widehat{\left|\psi^{\text{Pek}}\right|^2}(k)\right\|_\infty < \infty$. In order to estimate the remaining part $\|\,(1-\Pi)\,f_x\|$, let us first compute

$$\begin{aligned} f_x(y) &= \frac{1}{\sqrt{(2\pi)^3}}\int_{|k|\leq\Lambda}\frac{\widehat{\left|\psi^{\text{Pek}}\right|^2}(k)}{|k|}e^{ik\cdot(x-y)}\mathrm{d}k \\ &= \frac{1}{(2\pi)^3}\int_{|k|\leq\Lambda}\frac{e^{ik\cdot(x-y)}}{|k|}\int_{\mathbb{R}^3}\left|\psi^{\text{Pek}}(z)\right|^2 e^{ik\cdot z}\mathrm{d}z\mathrm{d}k \\ &= \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\left|\psi^{\text{Pek}}(z)\right|^2\int_{|k|\leq\Lambda}\frac{e^{ik\cdot(x+z-y)}}{|k|}\mathrm{d}k\,\mathrm{d}z \\ &= \frac{1}{\sqrt{4\pi}}\int_{\mathbb{R}^3}\left|\psi^{\text{Pek}}(z)\right|^2\,\Pi_\Lambda w_{x+z}(y)\,\mathrm{d}z \end{aligned}$$

using the projection Π_Λ from Definition 2.1 and the function w_x from Lemma 2.2. Consequently we obtain by Lemma 2.2

$$\begin{aligned} \|\,(1-\Pi)\,f_x\| &\leq \frac{1}{\sqrt{4\pi}}\int_{\mathbb{R}^3}\left|\psi^{\text{Pek}}(z)\right|^2\|\Pi_\Lambda w_{x+z} - \Pi w_{x+z}\|\,\mathrm{d}z \\ &\lesssim \ell\sqrt{\Lambda}\int_{\mathbb{R}^3}|z|\left|\psi^{\text{Pek}}(z)\right|^2\mathrm{d}z + \ell\sqrt{\Lambda}|x| + \sqrt{\ell}, \end{aligned}$$

where we have used $(1-\Pi)\,\Pi_\Lambda = \Pi_\Lambda - \Pi$ and $\int_{\mathbb{R}^3}\left|\psi^{\text{Pek}}(z)\right|^2\mathrm{d}z = 1$. This concludes the proof of the first part, since the terms $\ell\sqrt{\Lambda}$ and $\sqrt{\ell}$ are all bounded by $\alpha^{-\frac{6}{5}(1+\sigma)}$, and the state ψ^{Pek} satisfies $\int_{\mathbb{R}^3}|z|^p\left|\psi^{\text{Pek}}(z)\right|^2\mathrm{d}z < \infty$ for any $p \geq 0$, see [24].

In order to verify the second part, we write again $\partial_{x_n}\varphi^{\mathrm{Pek}} = 4\sqrt{\pi}\left(\partial_{x_n} f_0 + \partial_{x_n} g_0\right)$. In analogy to Eq. (A.1) we have $\|\partial_{x_n} g_0\|^2 \lesssim \frac{1}{\Lambda} = \alpha^{-\frac{4}{5}(1+\sigma)}$. Furthermore $\partial_{x_n} f_0(x) = -\frac{1}{\sqrt{4\pi}}\int_{\mathbb{R}^3}\partial_{z_n}\left(\left|\psi^{\mathrm{Pek}}(z)\right|^2\right)\Pi_\Lambda w_z(x)\,\mathrm{d}z$, hence proceeding as above yields

$$\|(1-\Pi)\,\partial_{x_n} f_0\| \lesssim \ell\sqrt{\Lambda}\int_{\mathbb{R}^3}|z|\left|\partial_{z_n}\left(\left|\psi^{\mathrm{Pek}}(z)\right|^2\right)\right|\mathrm{d}z + \left(\ell\sqrt{\Lambda}|x| + \sqrt{\ell}\right)\int_{\mathbb{R}^3}\left|\partial_{z_n}\left(\left|\psi^{\mathrm{Pek}}(z)\right|^2\right)\right|\mathrm{d}z.$$

This concludes the proof, since

$$\int_{\mathbb{R}^3}|z|\left|\partial_{x_n}\left(\left|\psi^{\mathrm{Pek}}(z)\right|^2\right)\right|\mathrm{d}z = 2\int_{\mathbb{R}^3}|z||\psi^{\mathrm{Pek}}(z)||\partial_{z_n}\psi^{\mathrm{Pek}}(z)|\,\mathrm{d}z \leq \int_{\mathbb{R}^3}|z|^2|\psi^{\mathrm{Pek}}(z)|^2\,\mathrm{d}z + \int_{\mathbb{R}^3}|\nabla\psi^{\mathrm{Pek}}(z)|^2\,\mathrm{d}z < \infty$$

and similarly with $|z|$ replaced by 1. □

Lemma A.2. *There exists a constant C such that $\int_{t\leq x_i\leq t+\epsilon}\left|\varphi^{\mathrm{Pek}}(x)\right|^2\mathrm{d}x \leq C\epsilon$ for all $t\in\mathbb{R}$, $\epsilon>0$ and $i\in\{1,2,3\}$.*

Proof. By the reflection symmetry of the Pekar minimizer, it is enough to prove the statement for $i=1$. For this purpose, let us define the function $D:\mathbb{R}\to\mathbb{R}$ as

$$D(t) := \int_{\mathbb{R}^2}\left|\varphi^{\mathrm{Pek}}(t,x_2,x_3)\right|^2\mathrm{d}x_2\mathrm{d}x_3$$

In order to prove the Lemma, we are going to show that D is a bounded function. Since $D(t)\underset{t\to\pm\infty}{\longrightarrow}0$, we have $\|D\|_\infty \leq \int|D'(t)|\mathrm{d}t$ and furthermore

$$\int|D'(t)|\mathrm{d}t \leq \int\int_{\mathbb{R}^2}\left|\partial_t\left|\varphi^{\mathrm{Pek}}(t,x_2,x_3)\right|^2\right|\mathrm{d}x_2\mathrm{d}x_3\mathrm{d}t \leq \int_{\mathbb{R}^3}\left|\nabla_x\left|\varphi^{\mathrm{Pek}}\right|^2\right|\mathrm{d}x = 2\int_{\mathbb{R}^3}\varphi^{\mathrm{Pek}}(x)\left|\nabla_x\varphi^{\mathrm{Pek}}\right|\mathrm{d}x \leq \|\varphi^{\mathrm{Pek}}\|^2 + \|\nabla\varphi^{\mathrm{Pek}}\|^2 < \infty,$$

where we have used that $\varphi^{\mathrm{Pek}}\in H^1\left(\mathbb{R}^3\right)$. □

Lemma A.3. *The Pekar minimizers φ_x^{Pek} satisfy $\left\|\varphi_x^{\mathrm{Pek}} - \varphi^{\mathrm{Pek}}\right\|^2 \lesssim \sum_{i=1}^3 P_i^\epsilon\left(\left|\varphi_x^{\mathrm{Pek}}\right|^2\right) + \alpha^{-u}$, where P_i^ϵ is defined in Eq. (3.17).*

Proof. Since $\left\|\varphi_x^{\mathrm{Pek}} - \varphi^{\mathrm{Pek}}\right\| \leq \left\|\varphi_x^{\mathrm{Pek}}\right\| + \left\|\varphi^{\mathrm{Pek}}\right\| = 2\left\|\varphi^{\mathrm{Pek}}\right\|$ and $\left\|\varphi_x^{\mathrm{Pek}} - \varphi^{\mathrm{Pek}}\right\|^2 \leq |x|^2\left\|\nabla\varphi^{\mathrm{Pek}}\right\|^2$, we have $\left\|\varphi_x^{\mathrm{Pek}} - \varphi^{\mathrm{Pek}}\right\|^2 \lesssim \min\{|x|^2, 1\}$. Therefore it is enough to show that we have $\min\{x_i^2, 1\} \lesssim P_i^\epsilon\left(\left|\varphi_x^{\mathrm{Pek}}\right|^2\right) + \epsilon$. By the reflection symmetry of φ^{Pek}, we can assume w.l.o.g. that $i = 1$. We identify $\frac{1}{\|\varphi^{\mathrm{Pek}}\|^4} P_1^{\epsilon}\left(\left|\varphi_x^{\mathrm{Pek}}\right|^2\right)$ as

$$\begin{aligned}
&\frac{1}{4} - \frac{1}{\|\varphi^{\mathrm{Pek}}\|^2} \int\limits_{y_1 \leq x_1+\epsilon} \left|\varphi^{\mathrm{Pek}}(y)\right|^2 \mathrm{d}y \left(1 - \frac{1}{\|\varphi^{\mathrm{Pek}}\|^2} \int\limits_{y_1 \leq x_1-\epsilon} \left|\varphi^{\mathrm{Pek}}(y)\right|^2 \mathrm{d}y\right) \\
&= \left(\frac{1}{2} - F(x_1)\right)^2 + F(x_1)\big(F(x_1-\epsilon) - F(x_1)\big) + \big(F(x_1) - F(x_1+\epsilon)\big)\big(1 - F(x_1-\epsilon)\big) \\
&\geq \left(\frac{1}{2} - F(x_1)\right)^2 + \big(F(x_1-\epsilon) - F(x_1)\big) + \big(F(x_1) - F(x_1+\epsilon)\big) \\
&\geq \left(\frac{1}{2} - F(x_1)\right)^2 - 2C\epsilon
\end{aligned}$$

with $F(t) := \frac{1}{\|\varphi^{\mathrm{Pek}}\|^2} \int_{y_1 \leq t} \left|\varphi^{\mathrm{Pek}}(y)\right|^2 \mathrm{d}y$, where C is the constant from Lemma A.2. Since φ^{Pek} is radially decreasing, see [17], it is clear that $|\varphi^{\mathrm{Pek}}(x)|^2 \geq c > 0$ for all $x \in [-\delta, \delta]^3$ where $\delta, c > 0$ are suitable constants. Assuming $x_1 > 0$ w.l.o.g. we conclude that $\left\|\varphi^{\mathrm{Pek}}\right\|^2 \left(F(x_1) - \frac{1}{2}\right) \geq c \int_{0 \leq y_1 \leq x_1} \mathbb{1}_{[-\delta,\delta]^3}(y)\, \mathrm{d}y = 4c\delta^2 \min\{x_1, \delta\} \gtrsim \min\{x_1, 1\}$. □

B. Properties of the Projection Π

In the following section we discuss properties of the Projections Π defined in Eq. (4.1) and Π_K defined in Definition 2.1. The first two results in Lemma B.1 and Corollary B.2 concern the space confinement of elements in the range of Π, to be precise we show that the associated potentials V_φ defined in Eq. (5.1) are concentrated in a ball of radius α^q for a suitable $q > 0$. While Lemma B.3 is an auxiliary result, we will show in the subsequent Lemmas B.4 and B.5 that the operator $J_{t,\epsilon}$ is an approximation of the Hessian $\mathrm{Hess}|_{\varphi^{\mathrm{Pek}}} \mathcal{F}^{\mathrm{Pek}}$, where $J_{t,\epsilon}$ is the operator defined in Eq. (5.14). Finally, we will show in Lemma B.6 that the functions $\Pi_K w_x$, which appear in the definition of $\mathbb{H}_K$ in Eq. (2.2), are confined in space around the origin. We will then use this result in order to quantify the energy cost of having the electron and the phonon field localized in different regions of space, see Corollary B.7.

The proof of the following auxiliary Lemma B.1 is an easy analysis exercise and is left to the reader.

Lemma B.1. *There exists a constant $C > 0$ such that for $f \in C^3\left(\mathbb{R}^3\right)$ and $K := (k_1, k_1') \times (k_2, k_2') \times (k_3, k_3') \subset \mathbb{R}^3$ with $k_i < k_i' < k_i + 2$*

$$\left|\widehat{(\mathbb{1}_K f)}(x)\right| \leq C \frac{\|f\|_{C^3(K)}}{(1+|x_1|)(1+|x_2|)(1+|x_3|)}$$

for all $x = (x_1, x_2, x_3) \in \mathbb{R}^3$, where $\|f\|_{C^3(K)} := \max_{|\alpha| \leq 3} \sup_{x \in K} |\partial^\alpha f(x)|$ and $\widehat{\cdot}$ denotes the Fourier transform.

Corollary B.2. *There exists a constant $v > 0$, such that for all $r > 0$ and $\varphi \in \Pi L^2\left(\mathbb{R}^3\right)$*

$$\left\|\mathbb{1}_{\mathbb{R}^3 \setminus B_r(0)} V_\varphi\right\| \lesssim \frac{\alpha^v \|\varphi\|}{\sqrt{r}}, \tag{B.1}$$

where Π is defined in Eq. (4.1) and V_φ is defined in Eq. (5.1).

Proof. Let e_n be the basis from Definition 2.1 corresponding to concrete choices of Λ and ℓ defined above Eq. (4.1). Given $\varphi = \sum_{n=1}^{N} \lambda_n e_n \in \Pi L^2(\mathbb{R}^3)$, $\lambda_n \in \mathbb{C}$, we have the rough estimate

$$\left\| \mathbb{1}_{\mathbb{R}^3 \setminus B_r(0)} V_\varphi \right\| \leq \sum_{n=1}^{N} |\lambda_n| \left\| \mathbb{1}_{\mathbb{R}^3 \setminus B_r(0)} V_{e_n} \right\| \leq \sqrt{N} \|\varphi\| \sup_{n \in \{1,\ldots,N\}} \left\| \mathbb{1}_{\mathbb{R}^3 \setminus B_r(0)} V_{e_n} \right\| .$$

Since $N \leq \alpha^p$ for a suitable constant p, it is enough to verify Eq. (B.1) for $\varphi = e_n$. Making use of $V_{e_n} = \widehat{\mathbb{1}_{K_n} f}$ with $K_n := \left(z_1^n - \ell, z_1^n + \ell\right) \times \left(z_2^n - \ell, z_2^n + \ell\right) \times \left(z_3^n - \ell, z_3^n + \ell\right)$ and $f(k) = \frac{-2}{\sqrt{(2\pi)^3 \int_{K_n} \frac{1}{|k|^2} \mathrm{d}k}} \frac{1}{|k|^2}$, and the fact that $(z_k^n + \ell) - (z_k^n - \ell) = 2\ell \leq 2$, we obtain by Lemma B.1

$$\left\| \mathbb{1}_{\mathbb{R}^3 \setminus B_r(0)} V_{e_n} \right\|^2 \lesssim \alpha^{2p'} \int_{|x|>r} \frac{1}{(1+|x_1|)^2 (1+|x_3|)^2 (1+|x_3|)^2} \mathrm{d}x \lesssim \alpha^{2p'} \frac{1}{r},$$

where we have used $K_n \subset \mathbb{R}^3 \setminus B_{2\ell}(0)$ and therefore $\|f\|_{C^3(K)} \lesssim \ell^{-\frac{3}{2}} \Lambda(\ell)^{-5} = \alpha^{p'}$ for a suitable $p' > 0$. $\square$

Lemma B.3. *For $\psi \in L^2(\mathbb{R}^3)$ and $T > 0$,*

$$\int \int_{|k'| \leq T} \frac{|\widehat{\psi}(k-k')|^2}{(1+|k|^2)\,|k'|^2} \mathrm{d}k' \mathrm{d}k \lesssim \|\psi\|^2 T, \tag{B.2}$$

$$\int \int_{|k'| > T} \frac{|\widehat{\psi}(k-k')|^2}{(1+|k|^2)\,|k'|^2} \mathrm{d}k' \mathrm{d}k \lesssim \frac{\|\psi\|^2}{\sqrt{T}}. \tag{B.3}$$

Furthermore, interpreting ψ as a multiplication operator we have

$$\left\| (1-\Delta)^{-\frac{1}{2}} \, \psi \, (-\Delta)^{-\frac{1}{2}} \right\|_{\mathrm{HS}} \lesssim \|\psi\|, \tag{B.4}$$

$$\left\| (1-\Delta)^{-\frac{1}{2}} \, (-\Delta)^{-\frac{1}{2}} \, \psi \right\|_{\mathrm{HS}} = \sqrt{2}\pi \|\psi\|. \tag{B.5}$$

Proof. Equations (B.2) and (B.3) immediately follow from the estimates

$$\int \int_{|k'| \leq T} \frac{|\widehat{\psi}(k-k')|^2}{(1+|k|^2)\,|k'|^2} \mathrm{d}k' \mathrm{d}k \leq \int \int_{|k'| \leq T} \frac{|\widehat{\psi}(k-k')|^2}{|k'|^2} \mathrm{d}k' \mathrm{d}k = \|\psi\|^2 4\pi T,$$

$$\int \int_{|k'| > T} \frac{|\widehat{\psi}(k-k')|^2}{(1+|k|^2)\,|k'|^2} \mathrm{d}k' \mathrm{d}k \leq \frac{1}{2} \int \int_{|k'| > T} \left(\frac{1}{\sqrt{T}(1+|k|^2)^2} + \frac{\sqrt{T}}{|k'|^4} \right) |\widehat{\psi}(k-k')|^2 \mathrm{d}k' \mathrm{d}k$$
$$\leq \frac{1}{2} \left(\int \frac{1}{(1+|k|^2)^2} \mathrm{d}k + 4\pi \right) \frac{\|\psi\|^2}{\sqrt{T}}.$$

By making use of the fact that the integral kernel of $(1-\Delta)^{-\frac{1}{2}} \, \psi \, (-\Delta)^{-\frac{1}{2}}$ in Fourier space is given as $\frac{\widehat{\psi}(k-k')}{\sqrt{1+|k|^2}|k'|}$, Eq. (B.4) immediately follows from Eqs. (B.3) and (B.2) with the concrete choice $T = 1$. Finally Eq. (B.5) follows from the fact that the corresponding integral kernel is given by $\frac{\widehat{\psi}(k-k')}{\sqrt{1+|k|^2}|k|}$ and the identity $\int \int \frac{|\widehat{\psi}(k-k')|^2}{|k|^2(1+|k|^2)} \mathrm{d}k' \mathrm{d}k = \int \frac{1}{|k|^2(1+|k|^2)} \mathrm{d}k \, \|\psi\|^2 = 2\pi^2 \|\psi\|^2$. $\square$

Lemma B.4. *We have* $\mathrm{Tr}\left[(1-\Pi)\, L_x^{\mathrm{Pek}}\,(1-\Pi)\right] \lesssim \alpha^{-\frac{2}{5}}$ *for* $|x| \lesssim 1$, *where* L_x^{Pek} *is the operator defined above Eq.* (5.13).

Proof. With the definition $\psi_x^{\mathrm{Pek}}(y) := \psi^{\mathrm{Pek}}(y-x)$, we can express the operator L_x^{Pek} as $L_x^{\mathrm{Pek}} = 2\left|(1-\Delta)^{-\frac{1}{2}}\,\psi_x^{\mathrm{Pek}}\,(-\Delta)^{-\frac{1}{2}}\right|^2$. Since the integral kernel of $(1-\Delta)^{-\frac{1}{2}}\,\psi_x^{\mathrm{Pek}}\,(-\Delta)^{-\frac{1}{2}}$ is given by $\frac{\widehat{\psi}_x^{\mathrm{Pek}}(k-k')}{\sqrt{1+|k|^2}|k'|}$ in Fourier space and since the one of Π reads $\sum_{n=1}^N \frac{\mathbb{1}_{C_{z^n}}(k)\mathbb{1}_{C_{z^n}}(k')}{\int_{C_{z^n}}\frac{1}{|q|^2}\mathrm{d}q\,|k|\,|k'|}$, where C_{z^n} is as in Definition 2.1, we can further express the integral kernel of the operator $(1-\Delta)^{-\frac{1}{2}}\,\psi_x^{\mathrm{Pek}}\,(-\Delta)^{-\frac{1}{2}}\,(1-\Pi)$ as

$$\sum_{n=1}^N \frac{\int_{C_{z^n}} \frac{\widehat{\psi}_x^{\mathrm{Pek}}(k-k')-\widehat{\psi}_x^{\mathrm{Pek}}(k-q)}{\sqrt{1+|k|^2}|k'|}\frac{1}{|q|^2}\mathrm{d}q}{\int_{C_{z^n}}\frac{1}{|q'|^2}\mathrm{d}q}\mathbb{1}_{C_{z^n}}(k') + \frac{\widehat{\psi}_x^{\mathrm{Pek}}(k-k')}{\sqrt{1+|k|^2}|k'|}\mathbb{1}_{\mathbb{R}^3\setminus(\bigcup_n C_{z^n})}(k'). \quad (\mathrm{B.6})$$

In the following we need to show that the $L^2(\mathbb{R}^3\times\mathbb{R}^3)$ norm of the expression in Eq. (B.6) is of order $\alpha^{-\frac{1}{5}}$. As in the proof of Lemma 2.2, we will use $\mathbb{R}^3\setminus\left(\bigcup_n C_{z^n}\right) \subset B_{2\ell}\cup\left(\mathbb{R}^3\setminus B_{\Lambda-4\ell}\right)$, where Λ and ℓ are defined above Eq. (4.1). Applying Eq. (B.2) with $T=2\ell$ and Eq. (B.3) with $T=\Lambda-4\ell$ yields

$$\int\int_{\mathbb{R}^3\setminus(\bigcup_n C_{z^n})} \frac{|\widehat{\psi}_x^{\mathrm{Pek}}(k-k')|^2}{(1+|k|^2)|k'|^2}\mathrm{d}k'\mathrm{d}k \lesssim 2\ell + \frac{1}{\sqrt{\Lambda-4\ell}} \lesssim \alpha^{-\frac{2}{5}}.$$

In order to estimate the L^2 norm of $f(k,k') := \sum_{n=1}^N \frac{\int_{C_{z^n}} \frac{\widehat{\psi}_x^{\mathrm{Pek}}(k-k')-\widehat{\psi}_x^{\mathrm{Pek}}(k-q)}{\sqrt{1+|k|^2}|k'|}\frac{1}{|q|^2}\mathrm{d}q}{\int_{C_{z^n}}\frac{1}{|q|^2}\mathrm{d}q}\mathbb{1}_{C_{z^n}}(k')$, let us define $\psi_{x,s,\eta}(y) := \frac{\eta}{|\eta|}\cdot y e^{is\eta\cdot y}\psi_x^{\mathrm{Pek}}(y)$ for $s\in\mathbb{R}$, $\eta\in\mathbb{R}^3$ and $\xi := q-k'$, and compute

$$\widehat{\psi}_x^{\mathrm{Pek}}(k-k')-\widehat{\psi}_x^{\mathrm{Pek}}(k-q) = \int_0^1 \xi\cdot\nabla\widehat{\psi}_x^{\mathrm{Pek}}(k-k'+s\xi)\mathrm{d}s = |\xi|\int_0^1 \widehat{\psi}_{x,s,\xi}(k-k')\mathrm{d}s.$$

Making use of the inequality $\frac{\frac{1}{|q|^2}}{\int_{C_{z^n}}\frac{1}{|q'|^2}\mathrm{d}q'} \lesssim \ell^{-3}$ for $q\in C_{z^n}$ and the fact that $\xi = q-k' \in K := (-2\ell,2\ell)^3$ for all $k',q\in C_{z^n}$, yields

$$\begin{aligned}
\left|f(k,k')\right|^2 &\lesssim \sum_{n=1}^N \mathbb{1}_{C_{z^n}}(k')\ell^{-4}\left|\int_K\int_0^1 \frac{\left|\widehat{\psi}_{x,s,\xi}(k-k')\right|}{\sqrt{1+|k|^2}|k'|}\mathrm{d}s\mathrm{d}\xi\right|^2 \\
&\le \sum_{n=1}^N \mathbb{1}_{C_{z^n}}(k')8\ell^{-1}\int_K\int_0^1 \frac{\left|\widehat{\psi}_{x,s,\xi}(k-k')\right|^2}{(1+|k|^2)|k'|^2}\mathrm{d}s\mathrm{d}\xi \\
&\le 8\ell^{-1}\int_K\int_0^1 \frac{\left|\widehat{\psi}_{x,s,\xi}(k-k')\right|^2}{(1+|k|^2)|k'|^2}\mathrm{d}s\mathrm{d}\xi,
\end{aligned}$$

where we have applied the Cauchy–Schwarz inequality. An application of Lemma B.3 with $T=1$ then yields

$$\iint \left|f(k,k')\right|^2\mathrm{d}k'\mathrm{d}k \lesssim \ell^{-1}\int_K\int_0^1 \|\psi_{x,s,\xi}\|^2\mathrm{d}s\mathrm{d}\xi \le C\ell^2 \lesssim \alpha^{-8},$$

where we used that $\|\psi_{x,s,\eta}\| \leq C$ for all $|x| \lesssim 1$ and a suitable constant $C < \infty$. □

Lemma B.5. *Recall the operator H^{Pek} from Eq. (1.4). Then there exists a constant $c > 0$ such that $J_{t,\epsilon} \geq c\,\pi$ for ϵ small enough and α large enough. Furthermore*

$$\left|\text{Tr}_{\Pi L^2(\mathbb{R}^3)}\left[1 - \sqrt{J_{t,\epsilon}}\right] - \text{Tr}\left[1 - \sqrt{H^{\text{Pek}}}\right]\right| \lesssim \epsilon + \alpha^{-\frac{1}{5}} \tag{B.7}$$

for $|t| < \epsilon$, ϵ small enough and α large enough.

Proof. Recall the definition of π and $J_{t,\epsilon}$ in, respectively below, Eq. (5.13) for $|t| < \epsilon < \delta_*$, where δ_* is defined before Definition 5.3. In the following we are going to verify that $\|(1+\epsilon)\pi\left(K^{\text{Pek}}_{x_t} + \epsilon L^{\text{Pek}}_{x_t}\right)\pi\|_{\text{op}} \leq 1 - c$ for a suitable constant $c > 0$, small ϵ and $|t| < \epsilon$, which immediately implies $J_{t,\epsilon} \geq c\,\pi$. Let π_x be the orthogonal projection onto $\{\partial_{x_1}\varphi^{\text{Pek}}_x, \partial_{x_2}\varphi^{\text{Pek}}_x, \partial_{x_3}\varphi^{\text{Pek}}_x\}^\perp$ and let φ_n be defined in Eq. (5.11). Then we estimate

$$\begin{aligned}
\text{Tr}\left[|\pi_0 - \pi_x|\right] &\leq 2\sum_{n=1}^{3}\left\|\varphi_n - \frac{\partial_{x_n}\varphi^{\text{Pek}}_x}{\|\partial_{x_n}\varphi^{\text{Pek}}_x\|}\right\| \\
&\leq 2\sum_{n=1}^{3}\left\|\frac{\partial_{x_n}\varphi^{\text{Pek}}}{\|\partial_{x_n}\varphi^{\text{Pek}}\|} - \frac{\partial_{x_n}\varphi^{\text{Pek}}_x}{\|\partial_{x_n}\varphi^{\text{Pek}}_x\|}\right\| + 2\sum_{n=1}^{3}\left\|\varphi_n - \frac{\partial_{x_n}\varphi^{\text{Pek}}}{\|\partial_{x_n}\varphi^{\text{Pek}}\|}\right\| \\
&\lesssim |x| + \alpha^{-\frac{2}{5}},
\end{aligned} \tag{B.8}$$

where we have used Lemma A.1 in order to obtain $\|\partial_{x_n}\varphi^{\text{Pek}} - \Pi\partial_{x_n}\varphi^{\text{Pek}}\| \lesssim \alpha^{-\frac{2}{5}}$ and the fact that $\varphi^{\text{Pek}} \in H^2(\mathbb{R}^3)$, which yields $\|\partial_{x_n}\varphi^{\text{Pek}}_x - \partial_{x_n}\varphi^{\text{Pek}}\| \leq |x|\,\left\|\nabla\partial_{x_n}\varphi^{\text{Pek}}\right\| \lesssim |x|$. Hence $\text{Tr}\left[\left|\pi_0 - \pi_{\pm x_t}\right|\right] \lesssim |t| + \alpha^{-\frac{2}{5}}$ for t small enough. It is a straightforward consequence of (7.1) that the operator norm of $\pi_0 K^{\text{Pek}}\pi_0$ is bounded by $\|\pi_0 K^{\text{Pek}}\pi_0\|_{\text{op}} < 1$ (see also [22, Lemma 1.1]). Therefore we obtain, using $\pi = \Pi\pi_0 = \pi_0\Pi$,

$$\begin{aligned}
&\left\|(1+\epsilon)\pi\left(K^{\text{Pek}}_{x_t} + \epsilon L^{\text{Pek}}_{x_t}\right)\pi\right\|_{\text{op}} \leq \left\|(1+\epsilon)\pi_0\left(K^{\text{Pek}}_{x_t} + \epsilon L^{\text{Pek}}_{x_t}\right)\pi_0\right\|_{\text{op}} \\
&= \left\|\pi_0 K^{\text{Pek}}_{x_t}\pi_0\right\|_{\text{op}} + O(\epsilon) \\
&= \left\|\pi_{-x_t}K^{\text{Pek}}\pi_{-x_t}\right\|_{\text{op}} + O(\epsilon) = \left\|\pi_0 K^{\text{Pek}}\pi_0\right\|_{\text{op}} + O(\epsilon) + O\left(\alpha^{-2/5}\right) \leq 1 - c
\end{aligned} \tag{B.9}$$

for a suitable constant $c > 0$, ϵ small enough, $|t| < \epsilon$ and α large enough.

In order to verify Eq. (B.7), let $|t| < \epsilon$ and ϵ be small enough such that $J_{t,\epsilon} \geq 0$, and let us compute

$$\text{Tr}_{\Pi L^2(\mathbb{R}^3)}\left[1 - \sqrt{J_{t,\epsilon}}\right] = \text{Tr}\left[1 + \pi_0^\perp - \sqrt{1 - (1+\epsilon)\pi\left(K^{\text{Pek}}_{x_t} + \epsilon L^{\text{Pek}}_{x_t}\right)\pi}\right],$$

Furthermore we have the identity $\text{Tr}\left[1 - \sqrt{1 - K^{\text{Pek}}}\right] = \text{Tr}\left[1 + \pi_0^\perp - \sqrt{1 - \pi_0 K^{\text{Pek}}\pi_0}\right]$ $= \text{Tr}\left[1 - \sqrt{1 - \pi_{x_t}K^{\text{Pek}}_{x_t}\pi_{x_t}}\right] + \text{Tr}\left[\pi_0^\perp\right]$. Using the definition of K^{Pek} in Eq. (5.6), we can express $\text{Tr}_{\Pi L^2(\mathbb{R}^3)}\left[1 - \sqrt{J_{t,\epsilon}}\right] - \text{Tr}\left[1 - \sqrt{H^{\text{Pek}}}\right]$ as

$$\text{Tr}\left[1 - \sqrt{1 - (1+\epsilon)\pi\left(K^{\text{Pek}}_{x_t} + \epsilon L^{\text{Pek}}_{x_t}\right)\pi}\right] - \text{Tr}\left[1 - \sqrt{1 - \pi_{x_t}K^{\text{Pek}}_{x_t}\pi_{x_t}}\right]. \tag{B.10}$$

In the following let f be a smooth function with compact support satisfying $f(x) = 1 - \sqrt{1-x}$ for $0 \leq x \leq 1-c$, where c is as in Eq. (B.9), and let us define the operators $A := (1+\epsilon)\pi\left(K^{\text{Pek}}_{x_t} + \epsilon L^{\text{Pek}}_{x_t}\right)\pi$ and $B := \pi_{x_t} K^{\text{Pek}}_{x_t} \pi_{x_t}$. Using Eq. (B.10) and $\left\|(1+\epsilon)\pi\left(K^{\text{Pek}}_{x_t} + \epsilon L^{\text{Pek}}_{x_t}\right)\pi\right\|_{\text{op}} \leq 1-c$ for t and ϵ small enough, we obtain

$$\left|\operatorname{Tr}_{\Pi L^2(\mathbb{R}^3)}\left[1 - \sqrt{J_{t,\epsilon}}\right] - \operatorname{Tr}\left[1 - \sqrt{H^{\text{Pek}}}\right]\right| = \left|\operatorname{Tr}\left[f(A) - f(B)\right]\right|$$
$$\leq \|f(A) - f(B)\|_1 \leq \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} |t\widehat{f}(t)|\,\mathrm{d}t\, \|A - B\|_1\,, \tag{B.11}$$

where $\|\cdot\|_1$ is the trace norm and $\widehat{f}$ is the Fourier transformation of f. In order to estimate the right hand side of Eq. (B.11), we write $A - B = T_1 + \pi_0 T_2 \pi_0 + \pi T_3 \pi$ with $T_1 := (\pi_0 - \pi_{x_t})K^{\text{Pek}}_{x_t}\pi_0 + \pi_{x_t}K^{\text{Pek}}_{x_t}(\pi_0 - \pi_{x_t})$, $T_2 := (\Pi - 1)K^{\text{Pek}}_{x_t}\Pi + K^{\text{Pek}}_{x_t}(\Pi - 1)$ and $T_3 := \epsilon\left(K^{\text{Pek}}_{x_t} + (1+\epsilon)L^{\text{Pek}}_{x_t}\right)$. Clearly we have the estimates $\|\pi T_3 \pi\|_1 \leq \|T_3\|_1 \lesssim \epsilon$ and $\|T_1\|_1 \lesssim \|\pi_0 - \pi_{x_t}\|_1 \lesssim t + \alpha^{-\frac{2}{5}}$ by Eq. (B.8), using the fact that $K^{\text{Pek}}_{x_t}$ is trace-class, which follows from $K^{\text{Pek}}_{x_t} \lesssim L^{\text{Pek}}_{x_t}$ and the fact that $L^{\text{Pek}}_{x_t}$ is trace-class, see Eq. (B.4) with $\psi := \psi^{\text{Pek}}$. Using Lemma B.4 together with a Cauchy–Schwarz estimate for the trace norm, we can bound the final contribution $\pi_0 T_2 \pi_0$ by

$$\|\pi_0 T_2 \pi_0\|_1 \leq \|T_2\|_1 \leq 2\operatorname{Tr}\left[\Pi K^{\text{Pek}}_{x_t}\Pi\right]^{\frac{1}{2}} \operatorname{Tr}\left[(1-\Pi)\,K^{\text{Pek}}_{x_t}\,(1-\Pi)\right]^{\frac{1}{2}} \lesssim \alpha^{-\frac{1}{5}}.$$

□

The following Lemma B.6 is an auxiliary result, which we will use to quantify the energy cost of having the electron and the phonon field localized in different regions of space, see Corollary B.7.

Lemma B.6. *Let $w_0(y) = \pi^{-\frac{3}{2}}\frac{1}{|y|^2}$ and let Π_K be the projection defined in Definition 2.1. Then there exist a constant D such that*

$$\|\mathbb{1}_{\mathbb{R}^3\setminus B_r(0)}\Pi_K w_0\| \leq \frac{D}{\sqrt{r}}$$

for all $K, r > 0$.

Proof. The Fourier transform of $\Pi_K w_0$ is given by $\frac{\chi(|k|\leq K)}{\sqrt{2\pi^2}|k|}$. Defining the function u via its Fourier transform as $\widehat{u}(k) := \frac{\chi^\epsilon(2\epsilon\leq|k|\leq K)}{\sqrt{2\pi^2}|k|}$, where $\epsilon > 0$ and χ^ϵ is defined in Eq. (3.1), we have

$$\|\Pi_K w_0 - u\|^2 \leq \frac{1}{2\pi^2}\int_{|k|\leq 3\epsilon}\frac{1}{|k|^2}\mathrm{d}k + \frac{1}{2\pi^2}\int_{K-\epsilon\leq|k|\leq K+\epsilon}\frac{1}{|k|^2}\mathrm{d}k = \frac{6\epsilon}{\pi},$$

and consequently $\|\mathbb{1}_{\mathbb{R}^3\setminus B_r(0)}\Pi_K w_0\| \leq \sqrt{\frac{6\epsilon}{\pi}} + \|\mathbb{1}_{\mathbb{R}^3\setminus B_r(0)}u\|$. Making use of the observation that $\frac{1}{|y|}\mathbb{1}_{\mathbb{R}^3\setminus B_r(0)}(y) \leq \frac{1}{r}$ yields

$$\|\mathbb{1}_{\mathbb{R}^3\setminus B_r(0)}u\|^2 \leq \frac{1}{r^2}\int_{\mathbb{R}^3}|y|^2|u(y)|^2\mathrm{d}y = \frac{1}{r^2}\left\|\nabla_k\hat{u}\right\|^2 = \frac{1}{2\pi^2 r^2}\|f_1 - f_2\|^2$$

with $f_1(k) := \frac{\chi^\epsilon(2\epsilon\leq|k|\leq K)}{|k|^2}$ and $f_2(k) := \frac{\nabla_k\chi^\epsilon(2\epsilon\leq|k|\leq K)}{|k|}$. Clearly we can bound $\|f_1\|^2 \leq \int_{|k|\geq\epsilon}\frac{1}{|k|^4}\mathrm{d}k = \frac{4\pi}{\epsilon}$. Furthermore we obtain, using $\|\nabla_k\chi^\epsilon(2\epsilon\leq|k|\leq K)\|_\infty \lesssim \frac{1}{\epsilon}$,

$$\|f_2\|^2 \lesssim \frac{1}{\epsilon^2}\left(\int_{\epsilon\leq|k|\leq 3\epsilon}\frac{1}{|k|^2}\mathrm{d}k + \int_{K-\epsilon\leq|k|\leq K+\epsilon}\frac{1}{|k|^2}\mathrm{d}k\right) = \frac{4}{\epsilon}.$$

In combination this yields $\|\mathbb{1}_{\mathbb{R}^3\setminus B_r(0)}\Pi_K w_0\|^2 \lesssim \epsilon + \frac{1}{r^2\epsilon}$, which concludes the proof with the concrete choice $\epsilon := \frac{1}{r}$. □

Corollary B.7. *Given $A\subset\mathbb{R}^3$, let us define the operator $\mathcal{N}_A := \widehat{D_A}$ with $D_A(\rho) := \int_A \mathrm{d}\rho(y)$, using the notation of Definition 3.1, i.e. $\alpha^2\mathcal{N}_A$ counts the number of particles in the region A. Furthermore let $A'\subset\mathbb{R}^3$. Then given a constant $C>0$, there exists a constant $D>0$ such that for all states Ψ with* $\mathrm{supp}(\Psi)\subset A'$ *and* $\chi(\mathcal{N}\leq C)\Psi=\Psi$

$$\langle\Psi|\mathbb{H}_K|\Psi\rangle \geq E_\alpha + \langle\Psi|\mathcal{N}_A|\Psi\rangle - \sqrt{\frac{D}{\mathrm{dist}(A,A')}},$$

where $K>0$.

Proof. Let us define the function $v_x := \mathbb{1}_A\Pi_K w_x$ and rewrite $\mathbb{H}_K - \mathcal{N}_A$ as

$$\mathbb{H}_K - \mathcal{N}_A = -\Delta_x - a(\Pi_K w_x - v_x) - a^\dagger(\Pi_K w_x - v_x) + \mathcal{N} - \mathcal{N}_A - a(v_x) - a^\dagger(v_x).$$

Identifying $L^2\Big(\mathbb{R}^3,\mathcal{F}\big(L^2(\mathbb{R}^3)\big)\Big) \cong L^2\Big(\mathbb{R}^3,\mathcal{F}\Big(L^2\big(\mathbb{R}^3\setminus A\big)\Big)\Big)\otimes\mathcal{F}\Big(L^2(A)\Big)$, we observe that $-\Delta_x - a(\Pi_K w_x - v_x) - a^\dagger(\Pi_K w_x - v_x) + \mathcal{N} - \mathcal{N}_A$ is the restriction (in the sense of quadratic forms) of $\mathbb{H}_K$ to states of the form $\Psi'\otimes\Omega$, where Ω is the vacuum in $\mathcal{F}\Big(L^2(A)\Big)$, and therefore we have the operator inequality $-\Delta_x - a(\Pi_K w_x - v_x) - a^\dagger(\Pi_K w_x - v_x) + \mathcal{N} - \mathcal{N}_A \geq E_\alpha$. Consequently

$$\langle\Psi|\mathbb{H}_K - \mathcal{N}_A|\Psi\rangle \geq E_\alpha - \langle\Psi|a(v_x) + a^\dagger(v_x)|\Psi\rangle \geq E_\alpha - \sup_{x\in A'}\|v_x\|(1+C),$$

where we have used the operator inequality $a(v_x) + a^\dagger(v_x) \geq -\|v_x\|(1+\mathcal{N})$, as well as the assumptions $\mathrm{supp}(\Psi)\subset A'$ and $\chi(\mathcal{N}\leq C)\Psi=\Psi$, in the second inequality. This concludes the proof, since $\|v_x\|^2 = \int_A|\Pi_K w_0(y-x)|^2\mathrm{d}y \leq \int_{|y|\geq\mathrm{dist}(A,A')}|\Pi_K w_0(y)|^2\mathrm{d}y$ for all $x\in A'$ and $\int_{|y|\geq\mathrm{dist}(A,A')}|\Pi_K w_0(y)|^2\mathrm{d}y \lesssim \frac{1}{\mathrm{dist}(A,A')}$, see Lemma B.6. □

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