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RESEARCH ARTICLE

Optimal parabolic upper bound for the energy-momentum relation of a strongly coupled polaron

David Mitrouskas[1], Krzysztof Myśliwy[2,3] and Robert Seiringer[4]

[1]Institute of Science and Technology Austria, Am Campus 1, Klosterneuburg 3400, Austria; E-mail: david.mitrouskas@ist.ac.at.
[2]Institute of Science and Technology Austria, Am Campus 1, Klosterneuburg 3400, Austria.
[3]Currently University of Warsaw, ul. Pasteura 5, Warsaw 02-093, Poland; E-mail: Krzysztof.Mysliwy@fuw.edu.pl.
[4]Institute of Science and Technology Austria, Am Campus 1, Klosterneuburg 3400, Austria; E-mail: robert.seiringer@ist.ac.at.

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Abstract
We consider the large polaron described by the Fröhlich Hamiltonian and study its energy-momentum relation defined as the lowest possible energy as a function of the total momentum. Using a suitable family of trial states, we derive an optimal parabolic upper bound for the energy-momentum relation in the limit of strong coupling. The upper bound consists of a momentum independent term that agrees with the predicted two-term expansion for the ground state energy of the strongly coupled polaron at rest and a term that is quadratic in the momentum with coefficient given by the inverse of twice the classical effective mass introduced by Landau and Pekar.

Contents

1. Introduction

1.1. The Model

The large polaron provides an idealized description for the motion of a slow band electron through a polarizable crystal. The analysis of the polaron is a classic problem in solid-state physics that first appeared in 1933 when Landau introduced the idea of self-trapping of an electron in a polarizable environment [30]. Since it provides a simple model for a particle interacting with a nonrelativistic quantum field, the polaron has been of interest also in field theory and mathematical physics. In particular, the strong coupling theory of the polaron and Pekar's adiabatic approximation have been the source of interesting and challenging mathematical problems.

Following H. Fröhlich [20], the Hamiltonian of the model acts on the Hilbert space

$$\mathscr{H} = L^2(\mathbb{R}^3, \mathrm{d}x) \otimes \mathcal{F}, \tag{1.1}$$

with $\mathcal{F}$ the bosonic Fock space over $L^2(\mathbb{R}^3)$ and is given by

$$H_\alpha = -\Delta_x + \alpha^{-2}\mathbb{N} + \alpha^{-1}\phi(h_x). \tag{1.2}$$

Here, $x \in \mathbb{R}^3$ is the coordinate of the electron, $\mathbb{N}$ denotes the number operator on Fock space and the field operator $\phi(h_x) = a^\dagger(h_x) + a(h_x)$ with coupling function

$$h_x(y) = -\frac{1}{2\pi^2|x-y|^2} \tag{1.3}$$

accounts for the interaction between the electron and the quantum field. The creation and annihilation operators satisfy the usual canonical commutation relations

$$\big[a(f), a^\dagger(g)\big] = \langle f|g\rangle_{L^2}, \quad \big[a(f), a(g)\big] = 0. \tag{1.4}$$

Since we set $\hbar = 1$ and the mass of the electron equal to $1/2$, the only free parameter is the coupling constant $\alpha > 0$.

By rescaling all lengths by a factor $1/\alpha$, one can show that $\alpha^2 H_\alpha$ is unitarily equivalent to the Hamiltonian

$$H_\alpha^{\mathrm{Polaron}} = -\Delta_x + \mathbb{N} + \sqrt{\alpha}\phi(h_x), \tag{1.5}$$

which is more common in the polaron literature and also explains why $\alpha \to \infty$ is called the strong coupling limit.

The Fröhlich Hamiltonian defines a translation invariant model, that is, it commutes with the total momentum operator,

$$[H_\alpha, -i\nabla_x + P_f] = 0, \tag{1.6}$$

where $P_f = \mathrm{d}\Gamma(-i\nabla)$ denotes the momentum operator of the phonons. This allows the definition of the energy-momentum relation $E_\alpha(P)$ as the lowest possible energy of H_α when restricted to states with total momentum $P \in \mathbb{R}^3$. To this end, it is convenient to switch to the Lee–Low–Pines representation

$$H_\alpha(P) = (P_f - P)^2 + \alpha^{-2}\mathbb{N} + \alpha^{-1}\phi(h_0), \tag{1.7}$$

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where $H_\alpha(P)$ acts on the Fock space only [32]. The Fröhlich Hamiltonian H_α is unitarily equivalent to the fiber decomposition $\int_{\mathbb{R}^3}^{\oplus} H_\alpha(P)\mathrm{d}P$, which follows easily from transforming H_α with $e^{iP_f x}$ and diagonalizing the obtained operator in the electron coordinate. The energy-momentum relation is then defined as the ground state energy of the fiber Hamiltonian,

$$E_\alpha(P) = \inf \sigma(H_\alpha(P)), \tag{1.8}$$

which by construction satisfies $E_\alpha(RP) = E_\alpha(P)$ for all rotations $R \in \mathrm{SO}(3)$. It is known [26] that $E_\alpha(0) \leq E_\alpha(P)$ and hence $E_\alpha(0) = \inf \sigma(H_\alpha)$ (in fact, $E_\alpha(0) < E_\alpha(P)$ for all $P \neq 0$ [29, 52]). Further properties, such as the domain of analyticity, existence of ground states and the value of the bottom of the essential spectrum, were analyzed in [44, 21, 58, 45, 23, 10].

The aim of this work is to analyze the quantitative behavior of the energy-momentum relation for large coupling $\alpha \to \infty$. Our main result provides an upper bound for $E_\alpha(P)$. The upper bound consists of a momentum independent part coinciding with the optimal upper bound for the ground state energy of the strongly coupled polaron at rest and a momentum-dependent part. In more detail, the momentum-independent part is given by the classical Pekar energy and the corresponding quantum fluctuations that are described by the energy of a system of harmonic oscillators with frequencies determined by the Hessian of the corresponding classical field functional. This part agrees with the expected asymptotic form of $E_\alpha(0)$; see equation (1.25). The momentum-dependent part, on the other hand, describes the energy of a free particle with mass $M(\alpha) = \frac{2\alpha^4}{3}\int |\nabla\varphi|^2$, where φ denotes the self-consistent polarization field, which coincides with the classical polaron mass introduced by Landau and Pekar [31]; see equation (1.24). As will be explained in Section 1.3, our result confirms the heuristic picture of the polaron (the electron and the accompanying classical field) as a free quasi-particle with largely enhanced mass. To our best knowledge, the upper bound we present in this work is the first rigorous result about the connection between the energy-momentum relation $E_\alpha(P)$ and the classical polaron mass $M(\alpha)$.

Starting from the works in the 1930s and 1940s [30, 31, 19], there has been a large number of publications in the physics literature that studied the ground state energy $E_\alpha(0)$ and the effective mass, that is, the inverse curvature of $E_\alpha(P)$ at $P = 0$. For a comprehensive summary of the earlier results, we refer to [41]. More recent developments are reviewed in [1].

Mathematically rigorous results for the leading-order asymptotics of $E_\alpha(0)$, for α large, were obtained by Lieb and Yamazaki [40] (with nonmatching upper and lower bounds) and by Donsker and Varadhan [11] as well as Lieb and Thomas [39]. The effective mass has been studied in [57, 12, 14, 38, 37, 4]. Other works have considered confined polarons or polaron models with more regular interaction [18, 15, 48]. For completeness, let us also mention recent progress in the understanding of the polaron path measure [47, 3] as well as the increased interest in the analysis of the Schrödinger time evolution of strongly coupled polarons [25, 34, 35, 42, 13, 16, 17].

1.2. Pekar functionals

The semiclassical theory of the polaron has been introduced by Pekar [51]. It arises naturally in the context of strong coupling, based on the expectation that the electron and the phonons are adiabatically decoupled, similarly as the electrons are adiabatically decoupled from the heavy nuclei in the well-known Born–Oppenheimer theory [6, 5]. With this in mind, one can minimize the Fröhlich Hamiltonian over product states of the form

$$\Psi_{u,v} = u \otimes e^{a^\dagger(\alpha v)}\Omega, \tag{1.9}$$

where $u \in H^1(\mathbb{R}^3)$ is a normalized electron wave function, $\Omega = (1, 0, 0, \ldots)$ the Fock space vacuum and $e^{a^\dagger(\alpha v)}\Omega$ the coherent state, up to normalization, that is associated with a classical field $\alpha v \in L^2(\mathbb{R}^3)$. A simple computation leads to the Pekar energy functional

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$$\mathcal{G}(u,v) = \frac{\langle \Psi_{u,v} | H_\alpha \Psi_{u,v} \rangle_{\mathscr{H}}}{\langle \Psi_{u,v} | \Psi_{u,v} \rangle_{\mathscr{H}}} = \langle u | (-\Delta + V^v) u \rangle_{L^2} + \|v\|_{L^2}^2 \tag{1.10}$$

with polarization potential

$$V^v(x) = 2\,\mathrm{Re}\,\langle v | h_x \rangle_{L^2} = -\mathrm{Re} \int \frac{v(y)}{\pi^2 |x-y|^2} \mathrm{d}y. \tag{1.11}$$

By completing the square, one can further remove the field variable and obtain the energy functional for the electron wave function,

$$\mathcal{E}(u) = \inf_{v \in L^2} \mathcal{G}(u,v) = \int |\nabla u(x)|^2 \mathrm{d}x - \frac{1}{4\pi} \iint \frac{|u(x)|^2 |u(y)|^2}{|x-y|} \mathrm{d}x\mathrm{d}y, \tag{1.12}$$

which is known [36] to admit a unique rotational invariant minimizer $\psi > 0$ (the minimizing property is unique only up to translations and multiplication by a constant phase). Alternatively, one can minimize the Pekar energy functional w.r.t. the electron wave function first. This leads to the classical field functional

$$\mathcal{F}(v) = \inf_{\|u\|_{L^2}=1} \mathcal{G}(u,v) = \inf \mathrm{spec}\,(-\Delta + V^v) + \|v\|_{L^2}^2 \tag{1.13}$$

whose unique rotational invariant minimizer is readily shown to be

$$\varphi(z) = -\langle \psi | h_\cdot(z) \psi \rangle_{L^2} = \int \frac{|\psi(y)|^2}{2\pi^2 |z-y|^2} \mathrm{d}y. \tag{1.14}$$

The corresponding classical ground state energy is called the Pekar energy

$$e^{\mathrm{Pek}} = \mathcal{E}(\psi) = \mathcal{F}(\varphi), \quad e^{\mathrm{Pek}} < 0, \tag{1.15}$$

and by the variational principle it provides an upper bound for $\inf \sigma(H_\alpha)$. The validity of Pekar's ansatz was rigorously verified by Donsker and Varadhan [11] who proved that $\lim_{\alpha\to\infty} \inf \sigma(H_\alpha) = e^{\mathrm{Pek}}$ and subsequently by Lieb and Thomas [39] who added a quantitative bound for the error by showing that

$$\inf \sigma(H_\alpha^{\mathrm{F}}) \geq e^{\mathrm{Pek}} + O(\alpha^{-1/5}). \tag{1.16}$$

Given the potential V^φ for the field φ, one can define the Schrödinger operator

$$h^{\mathrm{Pek}} = -\Delta + V^\varphi(x) - \lambda^{\mathrm{Pek}}, \quad \lambda^{\mathrm{Pek}} = e^{\mathrm{Pek}} - \|\varphi\|_{L^2}^2 \tag{1.17}$$

with $\lambda^{\mathrm{Pek}} = \inf \sigma(-\Delta + V^\varphi(x)) < 0$ and ψ the corresponding unique ground state. It follows from general arguments for Schrödinger operators that h^{Pek} has a finite spectral gap above zero, and thus the reduced resolvent

$$R = Q_\psi (h^{\mathrm{Pek}})^{-1} Q_\psi \quad \text{with} \quad Q_\psi = 1 - P_\psi, \quad P_\psi = |\psi\rangle\langle\psi|, \tag{1.18}$$

defines a bounded operator (P_ψ denotes the orthogonal projection onto the state ψ).

The last object to be introduced in this section is the Hessian H^{Pek} of the energy functional $\mathcal{F}$ at its minimizer φ, defined by

$$\langle v | H^{\mathrm{Pek}} v \rangle_{L^2} = \lim_{\varepsilon\to 0} \frac{1}{\varepsilon^2} \big(\mathcal{F}(\varphi + \varepsilon v) - \mathcal{F}(\varphi) \big) \quad \forall v \in L^2_{\mathbb{R}}(\mathbb{R}^3). \tag{1.19}$$

In the following lemma, we collect some important properties of H^{Pek}.

Lemma 1.1. *The linear operator* $H^{\mathrm{Pek}} : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ *has integral kernel*

$$H^{\mathrm{Pek}}(y,z) = \delta(y-z) - 4\,\mathrm{Re}\,\big\langle \psi \big| h_\cdot(y) R h_\cdot(z) \psi \big\rangle_{L^2} \tag{1.20}$$

and satisfies the following properties.

(i) $0 \le H^{\mathrm{Pek}} \le 1$
(ii) $\mathrm{Ker} H^{\mathrm{Pek}} = \mathrm{Span}\{\partial_i \varphi \,:\, i = 1,2,3\}$
(iii) $H^{\mathrm{Pek}} \ge \tau > 0$ *when restricted to* $(\mathrm{Ker} H^{\mathrm{Pek}})^\perp$
(iv) $\mathrm{Tr}_{L^2}(1 - \sqrt{H^{\mathrm{Pek}}}) < \infty$.

The proof of the lemma, in particular item (ii), is based on the analysis of the Hessian of the energy functional $\mathcal{E}$ [33]. The details are given in Section 4.

1.3. Motivation and goal of this work

In this work, we are interested in the behavior of the energy-momentum relation $E_\alpha(P)$ for large values of the coupling α. In general, $E_\alpha(P)$ is expected to interpolate between two distinct regimes (see, for instance, [24, 22, 60, 58]): The *quasi-particle regime* and the *radiative regime*. The former corresponds to small momenta, and the expectation is that the system behaves effectively like a free particle with energy

$$E_\alpha^{\mathrm{eff}}(P) = E_\alpha(0) + \frac{P^2}{2M^{\mathrm{eff}}(\alpha)}, \tag{1.21}$$

where the effective mass is determined by the inverse curvature of $E_\alpha(P)$ at $P = 0$ (which is known to be well defined),

$$M^{\mathrm{eff}}(\alpha) := \frac{1}{2} \lim_{P\to 0} \left(\frac{E_\alpha(P) - E_\alpha(0)}{P^2} \right)^{-1}. \tag{1.22}$$

It is easy to verify that $M^{\mathrm{eff}}(\alpha) \ge 1/2$ (the mass of the electron in our units), and one can further show that the inequality is strict if $\alpha > 0$ so that the emerging quasi-particle is heavier than the bare electron. The heuristic idea is that the electron drags along a cloud of phonons when it moves through the crystal and thus appears to be heavier than it would be without the interaction. The radiative regime, on the other hand, describes a polaron at rest and an unbound/radiative phonon carrying the total momentum P. It is expected to be valid for large momenta and it is characterized by a flat energy-momentum relation that equals or approaches the bottom of the essential spectrum [45] (see also [29, Lemma 1.1])

$$\sigma_{\mathrm{ess}}(H_\alpha(P)) = [E_\alpha(0) + \alpha^{-2}, \infty). \tag{1.23}$$

The two regimes cross at $|P| = P_{\mathrm{c}}(\alpha) := \sqrt{2M^{\mathrm{eff}}(\alpha)}/\alpha$ which marks a characteristic momentum scale of the polaron. While the quasi-particle picture is expected to be accurate for $|P| \lesssim P_{\mathrm{c}}(\alpha)$, the radiative regime should hold for $|P| \gtrsim P_{\mathrm{c}}(\alpha)$ (see also Remark 1.3 below). Between the two regimes there is no concrete prediction for the behavior of $E_\alpha(P)$. A schematic plot is provided in Figure 1.

One aspect of this work is to show that the quasi-particle picture is mathematically rigorous, insofar as it provides a parabolic upper bound on $E_\alpha(P)$ that coincides with the expected form of the quasi-particle energy in the limit of large coupling. Since the quasi-particle energy (1.21) is determined by the values of $E_\alpha(0)$ and $M^{\mathrm{eff}}(\alpha)$, it is instructive to recall two long-standing open conjectures concerning their behavior for $\alpha \to \infty$. As explained in the previous section, the phonon field behaves classically for large coupling, and thus it is expected that $M^{\mathrm{eff}}(\alpha)$ should asymptotically tend to the expression that follows from the corresponding semiclassical counterpart of the problem. This semiclassical theory of

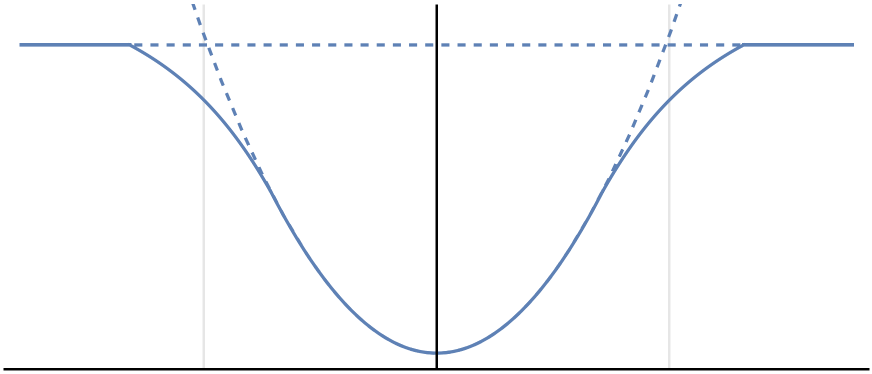

Figure 1. *The energy-momentum relation $E_\alpha(P)$ is expected to have two characteristic regimes: The parabolic quasi-particle regime for $|P| \lesssim P_c(\alpha) = \sqrt{2M^{\mathrm{eff}}(\alpha)}/\alpha$ and the flat radiative regime for larger momenta. For the transition between the two there is no precise prediction. The dashed lines denote the quasi-particle energy (1.21) and the bottom of the essential spectrum (1.23). Their intersection defines the momentum scale $P_c(\alpha)$ that is proportional to α for large coupling. Note that the y-axis is measured in units of order α^{-2}.*

the effective mass was introduced by Landau and Pekar in 1948 [31], and, based on this work (see also [57, 14]), it is conjectured that

$$\lim_{\alpha\to\infty} \frac{M^{\mathrm{eff}}(\alpha)}{\alpha^4} = M^{\mathrm{LP}} \quad \text{with} \quad M^{\mathrm{LP}} = \frac{2}{3}\|\nabla\varphi\|^2_{L^2}. \tag{1.24}$$

Although this problem is many decades old, the best rigorous result available at the time of writing is that $M^{\mathrm{eff}}(\alpha)$ is divergent [38] at least as fast as $\alpha^{2/5}$ [4]. Regarding the ground state energy $E_\alpha(0)$ the prediction from the physics literature (see, e.g., [2, 43, 59, 27]) is that

$$E_\alpha(0) = e^{\mathrm{Pek}} + \frac{1}{2\alpha^2}\mathrm{Tr}_{L^2}\big(\sqrt{H^{\mathrm{Pek}}} - 1\big) + O(\alpha^{-2-\delta}) \quad \text{as} \quad \alpha \to \infty \tag{1.25}$$

for some $\delta > 0$ (in fact it is predicted that $\delta = 2$ [27]). Compared to the semiclassical expansion this includes a subleading correction of order α^{-2}, which we call the *Bogoliubov energy*, and which arises from quantum fluctuations of the field around its classical value. For a nice heuristic derivation of this correction, we recommend the study of [43]. An upper bound of the form (1.25) is an immediate consequence of the results in this paper. We also note that a corresponding lower bound on $E_\alpha(0)$ was recently established in [8].

Now inserting equations (1.24) and (1.25) into equation (1.21), and based on the expectation that the quasi-particle regime is restricted to $|P| \lesssim \sqrt{2M^{\mathrm{eff}}(\alpha)}/\alpha \sim \alpha$, it is clear that the Bogoliubov energy needs to be taken into account in order to see the quasi-particle energy shift given by $P^2/(2\alpha^4 M^{\mathrm{LP}}) \le \alpha^{-2}$.

To put it concisely, we can summarize the heuristics discussed above in the claim that

$$\lim_{\alpha\to\infty} \alpha^2\left(E_\alpha(\alpha P) - e^{\mathrm{Pek}} - \frac{1}{2\alpha^2}\mathrm{Tr}_{L^2}\big(\sqrt{H^{\mathrm{Pek}}} - 1\big)\right) = \min\left\{\frac{P^2}{2M^{\mathrm{LP}}}, 1\right\}. \tag{1.26}$$

Our main result, Theorem 2.1 below, provides an upper bound for $E_\alpha(\alpha P)$ that is compatible with this claim. To be more precise, our result implies that the left side of equation (1.26), with the limit replaced by the lim sup, is bounded from above by the expression on the right side. This shows in particular that the corrections to the quasi-particle energy are always negative, a conclusion that is not entirely obvious a priori.

During the publication process of this work, a corresponding lower bound on $E_\alpha(\alpha P)$ was presented in [9]. When combined with the upper bound presented in this work, the two bounds establish the validity of equation (1.26).

Furthermore, we would like to mention the recent progress made in the analysis of the large coupling limit of the effective mass, as reported in [9, 55]. These advancements represent a significant step forward towards solving the Landau–Pekar conjecture (1.24).

Remark 1.2. An immediate consequence of equation (1.26) is that

$$\frac{1}{2}\lim_{P\to 0}\lim_{\alpha\to\infty}\alpha^2\left(\frac{E_\alpha(\alpha P)-E_\alpha(0)}{P^2}\right)^{-1} = M^{\mathrm{LP}} \tag{1.27}$$

which is to be compared with equation (1.24) where the limits are taken in reversed order. In light of this, we interpret equation (1.26) as an additional confirmation of the polaron's quasi-particle nature, which complements the picture suggested by equation (1.24).

Remark 1.3. An unresolved problem of interest is whether the ground state energy $E_\alpha(P)$ enters the essential spectrum for some finite momentum P, which may depend on the dimension and possibly also on the value of α. It is known that in two dimensions $E_\alpha(P)$ remains an isolated eigenvalue for all P, meaning that the curve approaches $\inf\sigma_{\mathrm{ess}}(H_\alpha(P))$ only in the limit as $|P|$ goes to infinity [58]. However, in three dimensions the question is unsettled. In Corollary 2.2 below, we prove that for large α, $E_\alpha(P)$ remains an isolated eigenvalue for all $|P| \lesssim \sqrt{2M^{\mathrm{LP}}}\alpha$. Nonetheless, there is evidence from results obtained for weak coupling that $E_\alpha(P)$ agrees with the bottom of the essential spectrum when $|P|$ is sufficiently large [10].

2. Main result

We are now ready to state the main result.

Theorem 2.1. *Let $E_\alpha(P) = \inf\sigma(H_\alpha(P))$ and $M^{\mathrm{LP}} = \frac{2}{3}\|\nabla\varphi\|^2_{L^2}$ with φ defined in equation (1.14). For every $\varepsilon > 0$, there exists a constant $C_\varepsilon > 0$ such that*

$$E_\alpha(P) \le e^{\mathrm{Pek}} + \frac{\mathrm{Tr}_{L^2}(\sqrt{H^{\mathrm{Pek}}}-1)}{2\alpha^2} + \min\left\{\frac{P^2}{2\alpha^4 M^{\mathrm{LP}}}, \frac{1}{\alpha^2}\right\} + C_\varepsilon\,\alpha^{-\frac{5}{2}+\varepsilon} \tag{2.1}$$

for all $P \in \mathbb{R}^3$ and all α large enough.

As a consequence of Lemma 1.1, the operator $\sqrt{H^{\mathrm{Pek}}}-1$ is trace-class and nonpositive, implying that the second term on the right-hand side is finite and lowers the energy. This term corresponds to the quantum corrections to the ground state energy of the Fröhlich Hamiltonian, as discussed in Section 1.3. Since $E_\alpha(0) = \inf\sigma(H_\alpha)$, our theorem implies a two-term upper bound for the ground state energy of the Fröhlich Hamiltonian. A complementary lower bound for $E_\alpha(0)$ has been recently proved in [8].

The result for $|P|/\alpha \ge \sqrt{2M^{\mathrm{LP}}}$ can be obtained from equations (1.22) and (2.1) for $P = 0$. The relevant range for the momentum dependent term is $|P|/\alpha \le \sqrt{2M^{\mathrm{LP}}}$. For momenta satisfying $\alpha^{-\frac{1}{4}+\frac{\varepsilon}{2}} \ll |P|/\alpha \le \sqrt{2M^{\mathrm{LP}}}$, the last term in equation (2.1) is subleading for large α when compared to the momentum dependent term. In this region, the upper bound describes a quadratic dispersion relation for a free quasi-particle with mass $\alpha^4 M^{\mathrm{LP}}$. The lower restriction $|P|/\alpha \gg \alpha^{-\frac{1}{4}+\frac{\varepsilon}{2}}$ could in principle be improved by deriving a better error term in equation (2.1).

For a long time, the only rigorous lower bound available for nonzero P was the one derived by Lieb and Yamazaki [40] in 1958, which states that $E_\alpha(P) \ge c_1 e^{\mathrm{Pek}} + c_2 P^2/(2\alpha^4 M^{\mathrm{LP}})$ with $c_1 \approx 3.07$ and $c_2 \approx 0.11$ (where e^{Pek} is negative). After the completion of our paper, a lower bound that matches our

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upper bound was obtained in [9]. It should be noted that the approach in [9] is different from ours, as it does not utilize the fiber decomposition of H_α.

Combining a suitable lower bound on the bottom of the essential spectrum (1.23) with Theorem 2.1 yields an extension of known results regarding the existence of a unique ground state of $H_\alpha(P)$. Fröhlich [21] showed that a unique ground state exists for $|P| < \sqrt{2}$, which was later extended by Spohn [58] to a larger but unspecified domain. More recently, Polzer [52] established the existence of the ground state for all $|P| < \sqrt{2M^{\mathrm{eff}}(\alpha)}/\alpha$ with $M^{\mathrm{eff}}(\alpha)$ defined by equation (1.22). Our new result demonstrates that the ground state exists for $|P| < \sqrt{2M^{\mathrm{LP}}}\alpha$.

Corollary 2.2. *For every $s \in (0, \frac{1}{29})$, there exists a constant $\alpha(s) > 0$ such that $E_\alpha(P)$ is a nondegenerate eigenvalue of $H_\alpha(P)$ for all $|P| < (1 - 2\alpha^{-s})^{1/2}\sqrt{2M^{\mathrm{LP}}}\alpha$ and $\alpha \geq \alpha(s)$.*

To prove this statement, we combine equations (2.1) and (1.21) and [8, Theorem 1.1] to show that $E_\alpha(P) < \inf \sigma_{\mathrm{ess}}(H_\alpha(P))$ for the specified values of $|P|$ and α. This implies that $E_\alpha(P)$ is part of the discrete spectrum, meaning it is an isolated eigenvalue of finite multiplicity. The nondegeneracy of this eigenvalue can then be established using a Perron–Frobenius type argument, as shown in [44, 29].

In the next two sections, we provide the definition of a suitable trial state and formulate our main statement as an energy estimate for this trial state. The remainder of the paper is devoted to the proof of this energy estimate. A sketch of the strategy of the proof is given in Section 3.2.

2.1. Bogoliubov Hamiltonian

In this section, we introduce and discuss a quadratic Hamiltonian defined on the Fock space. For its definition, we set Π_0 and Π_1 to be the orthogonal projectors onto $\mathrm{Ker}H^{\mathrm{Pek}} = \mathrm{Span}\{\partial_i\varphi : i = 1, 2, 3\}$ and $(\mathrm{Ker}H^{\mathrm{Pek}})^\perp$, that is,

$$\mathrm{Ran}(\Pi_0) = \mathrm{Ker}H^{\mathrm{Pek}}, \quad \mathrm{Ran}(\Pi_1) = (\mathrm{Ker}H^{\mathrm{Pek}})^\perp. \tag{2.2}$$

Even though we will not make explicit use of it, it is convenient to keep in mind that the decomposition $L^2(\mathbb{R}^3) = \mathrm{Ran}(\Pi_0) \oplus \mathrm{Ran}(\Pi_1)$ implies the factorization

$$\mathcal{F} = \mathcal{F}_0 \otimes \mathcal{F}_1 \quad \text{with} \quad \mathcal{F}_0 = \mathcal{F}(\mathrm{Ran}(\Pi_0)) \quad \text{and} \quad \mathcal{F}_1 = \mathcal{F}(\mathrm{Ran}(\Pi_1)). \tag{2.3}$$

For technical reasons, which are explained in Section 3.4.3, we introduce the Bogoliubov Hamiltonian $\mathbb{H}_K$ with a momentum cutoff $K \in (0, \infty]$. Setting $\mathbb{N}_1 = \mathrm{d}\Gamma(\Pi_1)$ (the number operator on $\mathcal{F}_1$) and recalling equation (1.18) we define

$$\mathbb{H}_K = \mathbb{N}_1 - \left\langle \psi \middle| \phi(h^1_{K,\cdot}) R \phi(h^1_{K,\cdot}) \psi \right\rangle_{L^2}, \tag{2.4}$$

where the new coupling function

$$h^1_{K,x}(y) = \int \mathrm{d}z\, \Pi_1(y, z) h_{K,x}(z) \quad \text{with} \quad h_{K,x}(y) = -\frac{1}{(2\pi)^3} \int_{|k| \leq K} \frac{e^{ik(x-y)}}{|k|} \mathrm{d}k \tag{2.5}$$

results from the coupling function h_x by removing all momenta larger than K and then projecting to $\mathrm{Ran}(\Pi_1)$. The second term in equation (2.4) defines the quadratic operator given by

$$\left\langle \psi \middle| \phi(h^1_{K,\cdot}) R \phi(h^1_{K,\cdot}) \psi \right\rangle_{L^2} = \iint \mathrm{d}y \mathrm{d}z \left\langle \psi \middle| (h^1_{K,\cdot})(y) R (h^1_{K,\cdot})(z) \psi \right\rangle_{L^2} (a^\dagger_y + a_y)(a^\dagger_z + a_z). \tag{2.6}$$

By definition, $\mathbb{H}_K$ acts nontrivially only on the tensor component $\mathcal{F}_1$. Below we will show that $\mathbb{H}_K$ is bounded from below and diagonalizable by a unitary Bogoliubov transformation. For the precise statement, we need some further preparations.

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For $K \in (0, \infty]$, we introduce H_K^{Pek} as the operator on $L^2(\mathbb{R}^3)$ defined by

$$H_K^{\mathrm{Pek}} \upharpoonright \mathrm{Ran}(\Pi_1) = \Pi_1 - 4T_K \tag{2.7a}$$

$$H_K^{\mathrm{Pek}} \upharpoonright \mathrm{Ran}(\Pi_0) = 0, \tag{2.7b}$$

where T_K is defined by the integral kernel

$$T_K(y, z) = \mathrm{Re} \left\langle \psi \middle| h^1_{K,\cdot}(y) R h^1_{K,\cdot}(z) \psi \right\rangle_{L^2}. \tag{2.8}$$

By definition $H_\infty^{\mathrm{Pek}} = H^{\mathrm{Pek}}$; see equation (1.20). Moreover, we set $\Theta_K = (H_K^{\mathrm{Pek}})^{1/4}$ and

$$A_K \upharpoonright \mathrm{Ran}(\Pi_1) = \frac{\Theta_K^{-1} + \Theta_K}{2} \qquad B_K \upharpoonright \mathrm{Ran}(\Pi_1) = \frac{\Theta_K^{-1} - \Theta_K}{2} \tag{2.9a}$$

$$A_K \upharpoonright \mathrm{Ran}(\Pi_0) = \Pi_0 \qquad B_K \upharpoonright \mathrm{Ran}(\Pi_0) = 0. \tag{2.9b}$$

The next lemma, whose proof can be found in Section 4, implies some useful properties of these operators, among others, that there are constants $C, K_0 > 0$ such that

$$\sup_{K \geq K_0} \left(\|A_K\|_{\mathrm{op}} + \|B_K\|_{\mathrm{HS}} \right) \leq C. \tag{2.10}$$

Lemma 2.3. *For K_0 large enough, there exist constants $\beta \in (0, 1)$ and $C > 0$ such that for all $K \in (K_0, \infty]$*

(i) $0 \leq H_K^{\mathrm{Pek}} \leq 1$ *and* $(H_K^{\mathrm{Pek}} - \beta) \upharpoonright \mathrm{Ran}(\Pi_1) \geq 0$
(ii) $(B_K)^2 \leq C(1 - H_K^{\mathrm{Pek}})$
(iii) $\mathrm{Tr}_{L^2}(1 - H_K^{\mathrm{Pek}}) \leq C$.

Moreover, for all $K \in (K_0, \infty)$

(iv) $\mathrm{Tr}_{L^2}((-i\nabla)(1 - H_K^{\mathrm{Pek}})(-i\nabla)) \leq CK$.

Remark 2.4. Since H_K^{Pek} has a real-valued kernel it satisfies $H_K^{\mathrm{Pek}} f = \mathrm{Re}(H_K^{\mathrm{Pek}} f) + i\,\mathrm{Im}(H_K^{\mathrm{Pek}} f)$ for all $f \in L^2(\mathbb{R}^3)$, and the same holds for Π_0 and Π_1. By the spectral calculus for self-adjoint operators, this property extends to Θ_K and Θ_K^{-1}.

To make the relation between $\mathbb{H}_K$ and H_K^{Pek} precise, we introduce the transformation

$$\mathbb{U}_K a(f) \mathbb{U}_K^\dagger = a(A_K f) + a^\dagger(B_K \overline{f}) \quad \text{for all } f \in L^2(\mathbb{R}^3). \tag{2.11}$$

That this transformation defines a unitary operator $\mathbb{U}_K$ for all $K \in (K_0, \infty]$ is a consequence of equation (2.10) and $A_K^2 = 1 + B_K^2$ by the well-known Shale–Stinespring condition (see [54, 56, 53]). Also, note that $\mathbb{U}_K$ does not mix the two factors in $\mathcal{F} = \mathcal{F}_0 \otimes \mathcal{F}_1$.

Lemma 2.5. *For $K \in (K_0, \infty]$ with K_0 large enough and $\mathbb{U}_K$, the unitary operator defined by equation (2.11), we have*

$$\mathbb{U}_K \mathbb{H}_K \mathbb{U}_K^\dagger = \mathrm{d}\Gamma\left(\sqrt{H_K^{\mathrm{Pek}}}\right) + \frac{1}{2} \mathrm{Tr}_{L^2}\left(\sqrt{H_K^{\mathrm{Pek}}} - \Pi_1\right) \tag{2.12}$$

with H_K^{Pek} defined by equations (2.7a) and (2.7b).

The proof is obtained by an explicit computation and postponed to Section 4. From this lemma, we can infer that the ground state energy of $\mathbb{H}_K$ is given by

$$\inf \sigma(\mathbb{H}_K) = \frac{1}{2} \mathrm{Tr}_{L^2}\left(\sqrt{H_K^{\mathrm{Pek}}} - \Pi_1\right) = \frac{1}{2} \mathrm{Tr}_{L^2}\left(\sqrt{H_K^{\mathrm{Pek}}} - 1\right) + \frac{3}{2}, \tag{2.13}$$

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where we also used $\Pi_1 = 1 - \Pi_0$ and $\mathrm{Tr}_{L^2}(\Pi_0) = 3$. Moreover, since $H_K^{\mathrm{Pek}} \leq \Pi_1$ we have $\inf \sigma(\mathbb{H}_K) < 0$ and from item (iv) of Lemma 2.3 we find that $\inf \sigma(\mathbb{H}_K) > -\infty$ uniformly in $K \to \infty$.

For the ground state of $\mathbb{H}_K$, we shall use the notation

$$\Upsilon_K = \mathbb{U}_K^\dagger \Omega, \tag{2.14}$$

where it is important to keep in mind that the state Υ_K has excitations only in $\mathcal{F}_1$ (i.e., no zero-mode excitations) since $\mathbb{U}_K^\dagger$ acts as the identity on $\mathcal{F}_0$; see equation (2.9b).

From now on, we shall always assume $K \geq K_0$ large enough such that Lemmas 2.3 and 2.5 are applicable.

2.2. *Trial state and energy estimate*

As starting point for the definition of our trial state, consider the Fock space wave function obtained from the fiber decomposition of the classical Pekar product state $\Psi_{\psi,\varphi}$, that is,

$$\Psi_\alpha^{\mathrm{Pek}}(P) = \int \mathrm{d}x\, e^{i(P_f - P)x} \psi(x) e^{a^\dagger(\alpha\varphi)} \Omega. \tag{2.15}$$

Testing the energy of $H_\alpha(P)$ with $\Psi_\alpha^{\mathrm{Pek}}(P)$, one would in fact obtain that $E_\alpha(P)$ is bounded from above by

$$e^{\mathrm{Pek}} - \frac{3}{2\alpha^2} + \frac{P^2}{\alpha^4 M^{\mathrm{LP}}} + o(\alpha^{-2}). \tag{2.16}$$

For $E_\alpha(0)$, this provides already a better bound compared to the semiclassical approximation for $\inf \sigma(H_\alpha)$. The improvement comes from taking into account the translational symmetry and can be interpreted as the missing zero-point energy of three quantum oscillators (that turned into translational degrees of freedom). As a side remark, we find it somewhat surprising that fiber decompositions of this form have been employed very rarely in the polaron literature, exceptions being [28] and [49]. We think they could be of interest also for other translation-invariant polaron type models.

To obtain the desired bound for $E_\alpha(P)$, we need to add several modifications to the integrand in equation (2.15). On the one hand, we have to replace the classical field φ by a suitably shifted φ_P in order to get the correct momentum dependent term (note that equation (2.16) is missing a factor $\frac{1}{2}$ in the quadratic term). The missing part of the rest energy (compare with equation (2.13)), on the other hand, is caused by two types of correlations that need to be added to the Pekar product state. First, we include correlations between the electron and the phonons. This is done in the spirit of first-order adiabatic perturbation theory. Second, we rotate the vacuum by the unitary transformation (2.11) that diagonalizes the Bogoliubov Hamiltonian (2.4). As discussed, the latter describes the quantum fluctuations of the phonons around the classical field. For technical reasons, briefly explained in Section 3.2, we also need to introduce suitable momentum and space cutoffs in the trial state.

Explicitly, we consider the family of Fock space wave functions $\Psi_{K,\alpha}(P) \in \mathcal{F}$, depending on the coupling α, the total momentum $P \in \mathbb{R}^3$ and the cutoff $K \in (K_0, \infty)$, given by

$$\Psi_{K,\alpha}(P) = \int \mathrm{d}x\, e^{i(P_f - P)x}\, e^{a^\dagger(\alpha\varphi_P) - a(\alpha\varphi_P)} \big(G_{K,x}^0 - \alpha^{-1} G_{K,x}^1\big), \tag{2.17}$$

where

$$\varphi_P = \varphi + i\xi_P \quad \text{with} \quad \xi_P = \frac{1}{\alpha^2 M^{\mathrm{LP}}}(P\nabla)\varphi, \quad M^{\mathrm{LP}} = \frac{2}{3}\|\nabla\varphi\|_{L^2}^2, \tag{2.18}$$

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and (recall equations (1.18) and (2.5))

$$G^0_{K,x} = \psi(x)\Upsilon_K, \quad G^1_{K,x} = u_\alpha(x)(R\phi(h^1_{K,\cdot})\psi)(x)\Upsilon_K \quad \text{and} \quad \Upsilon_K = \mathbb{U}^\dagger_K\Omega. \tag{2.19}$$

Here, $u_\alpha : \mathbb{R}^3 \to [0,1]$ is a radial function, satisfying

$$u_\alpha(x) = \begin{cases} 1 & \forall\, |x| \le \alpha \\ 0 & \forall\, |x| \ge 2\alpha \end{cases} \quad \text{and} \quad \|\nabla u_\alpha\|_{L^\infty} + \|\Delta u_\alpha\|_{L^\infty} \le C\alpha^{-1} \tag{2.20}$$

for some $C > 0$. For completeness, we recall that $\psi > 0$ and φ are the unique rotational invariant minimizers of the Pekar functionals (1.12) and (1.13).

Remark 2.6. Writing $G^i_{K,x}$, we think of these states as elements in $L^2(\mathbb{R}^3,\mathcal{F})$ and of

$$(R\phi(h^1_{K,\cdot})\psi)(x) = \iint \mathrm{d}z\mathrm{d}y\, R(x,y)h^1_{K,y}(z)\psi(y)\left(a^\dagger_z + a_z\right) \tag{2.21}$$

as an x-dependent Fock space operator. Via the isomorphism $L^2(\mathbb{R}^3,\mathcal{F}) \simeq \mathscr{H}$, we can view $G^i_{K,x}$ also as a wave function in $\mathscr{H}$. In this case, we shall write

$$G^0_K = \psi \otimes \Upsilon_K, \quad G^1_K = u_\alpha R\phi(h^1_{K,\cdot})\psi \otimes \Upsilon_K. \tag{2.22}$$

Remark 2.7. Let us note that in equation (2.17), we anticipated the fact that the integrand is in $L^1(\mathbb{R}^3,\mathcal{F})$ and thus $\Psi_{K,\alpha}(\cdot) \in C_b(\mathbb{R}^3,\mathcal{F})$. For G^0_K, the integrability follows directly from the exponential decay of ψ (as shown in Lemma 3.7), while for G^1_K it can be seen from

$$\int \mathrm{d}x\, |u_\alpha(x)|\, \|(R\phi(h^1_{K,\cdot})\psi)(x)\Upsilon_K\|_{\mathcal{F}} \le \|u_\alpha\|_{L^2}\|R\phi(h^1_{K,\cdot})\psi \otimes \Upsilon_K\|_{\mathcal{F}} < \infty, \tag{2.23}$$

where we used Cauchy–Schwarz and Lemmas 3.8, 3.9 and 3.13. A more precise estimate for the norm of $\Psi_{K,\alpha}(P)$ for large α will be given in Proposition 3.17.

For the introduced trial states, we prove the following energy estimate, where $\mathbb{H}_\infty$ denotes the Bogoliubov Hamiltonian (2.4) for $K = \infty$.

Proposition 2.8. *Let $\Psi_{K,\alpha}(P) \in \mathcal{F}$ as in equation (2.17), choose $c, \tilde{c} > 0$ and set $r(K,\alpha) = K^{-1/2}\alpha^{-2} + \sqrt{K}\alpha^{-3}$. For every $\varepsilon > 0$, there exists a constant $C_\varepsilon > 0$ (we omit the dependence on c and $\tilde{c}$) such that*

$$\frac{\left\langle \Psi_{K,\alpha}(P) | H_\alpha(P)\Psi_{K,\alpha}(P)\right\rangle_{\mathcal{F}}}{\left\langle \Psi_{K,\alpha}(P)|\Psi_{K,\alpha}(P)\right\rangle_{\mathcal{F}}} \le e^{\mathrm{Pek}} + \frac{\inf\sigma(\mathbb{H}_\infty) - \frac{3}{2}}{\alpha^2} + \frac{P^2}{2\alpha^4 M^{\mathrm{LP}}} + C_\varepsilon\alpha^\varepsilon r(K,\alpha) \tag{2.24}$$

for all $|P|/\alpha \le c$, $K/\alpha \le \tilde{c}$ and α large enough.

The next section, which constitutes the bulk of the paper, is devoted to proving this proposition. Before embarking on the proof, let us now deduce its main consequence and conclude the proof of Theorem 2.1.

Proof of Theorem 2.1. With equation (2.13) and $H^{\mathrm{Pek}}_\infty = H^{\mathrm{Pek}}$ we can rewrite the term of order α^{-2} as

$$\inf\sigma(\mathbb{H}_\infty) - \frac{3}{2} = \frac{1}{2}\mathrm{Tr}_{L^2}\left(\sqrt{H^{\mathrm{Pek}}} - 1\right). \tag{2.25}$$

Choosing K proportional to α optimizes the asymptotics of the error in equation (2.24) and thus proves equation (2.1) for $|P| \le \sqrt{2M^{\mathrm{LP}}}\alpha$ by the variational principle. For larger $|P|$, we use $E_\alpha(P) \le E_\alpha(0) + \alpha^{-2}$ as a consequence of equation (1.24) and apply equation (2.1) for $P = 0$. □

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3. Proof of Proposition 2.8

We recall the definition of the field operators

$$\phi(f) = a^\dagger(f) + a(f), \quad \pi(f) = \phi(if) \tag{3.1}$$

and the Weyl operator

$$W(f) = e^{-i\pi(f)} = e^{a^\dagger(f)-a(f)} = e^{a^\dagger(f)}e^{-a(f)}e^{-\frac{1}{2}\|f\|^2_{L^2}}. \tag{3.2}$$

The Weyl operator is unitary and satisfies

$$W^\dagger(f) = W(-f), \quad W(f)W(g) = W(g)W(f)e^{2i\,\mathrm{Im}\langle g|f\rangle_{L^2}} = W(f+g)e^{i\,\mathrm{Im}\langle g|f\rangle_{L^2}}. \tag{3.3}$$

3.1. The total energy

The proof of Proposition 2.8 starts with a convenient formula for the energy evaluated in the trial state. For the precise statement, we introduce the y-dependent function in $L^2(\mathbb{R}^3)$,

$$w_{P,y} = (1-e^{-y\nabla})\varphi_P, \tag{3.4}$$

and the y-dependent Fock space operator

$$A_{P,y} = iP_f y + ig_P(y), \quad g_P(y) = -\frac{2}{M^{\mathrm{LP}}}\int_0^1 \mathrm{d}s\,\langle\varphi|e^{-sy\nabla}(y\nabla)^3(P\nabla)\varphi\rangle_{L^2}. \tag{3.5}$$

Since $g_P(y)$ is real-valued, we have $(A_{P,y})^\dagger = -A_{P,y}$.

We further consider the shift operator $T_y = e^{y\nabla}$ on $L^2(\mathbb{R}^3)$, that is, $(T_y f)(x) = f(x+y)$ for every $f \in L^2(\mathbb{R}^3)$, and the Hamiltonian acting on $\mathscr{H}$

$$\widetilde{H}_{\alpha,P} = h^{\mathrm{Pek}} + \alpha^{-2}\mathbb{N} + \alpha^{-1}\phi(h_x + \varphi_P), \tag{3.6}$$

where we recall that $h^{\mathrm{Pek}} = -\Delta + V^\varphi - \lambda^{\mathrm{Pek}}$.

Lemma 3.1. *For $\Psi_{K,\alpha}(P)$ defined in equation (2.17), we have*

$$\left\langle\Psi_{K,\alpha}(P)|H_\alpha(P)\Psi_{K,\alpha}(P)\right\rangle_{\mathcal{F}} = \left(e^{\mathrm{Pek}} + \frac{P^2}{2\alpha^4 M^{\mathrm{LP}}}\right)\mathcal{N} + \mathcal{E} + \mathcal{G} + \mathcal{K}, \tag{3.7}$$

where $\mathcal{N} = \|\Psi_{K,\alpha}(P)\|^2_{\mathcal{F}}$ and

$$\mathcal{E} = \int \mathrm{d}y\,\left\langle G_K^0|\widetilde{H}_{\alpha,P}T_y e^{A_{P,y}}W(\alpha w_{P,y})G_K^0\right\rangle_{\mathscr{H}} \tag{3.8a}$$

$$\mathcal{G} = -\frac{2}{\alpha}\int \mathrm{d}y\;\mathrm{Re}\left\langle G_K^0|\widetilde{H}_{\alpha,P}T_y e^{A_{P,y}}W(\alpha w_{P,y})G_K^1\right\rangle_{\mathscr{H}} \tag{3.8b}$$

$$\mathcal{K} = \frac{1}{\alpha^2}\int \mathrm{d}y\,\left\langle G_K^1|\widetilde{H}_{\alpha,P}T_y e^{A_{P,y}}W(\alpha w_{P,y})G_K^1\right\rangle_{\mathscr{H}}. \tag{3.8c}$$

For the proof, we recall that the Weyl operator shifts the creation and annihilation operators by complex numbers,

$$W(g)^\dagger a^\dagger(f)W(g) = a^\dagger(f) + \langle g|f\rangle_{L^2}, \quad W(g)^\dagger a(f)W(g) = a(f) + \overline{\langle g|f\rangle_{L^2}}, \tag{3.9}$$

and, as a simple consequence,

$$W(g)^\dagger \phi(f) W(g) \;=\; \phi(f) + 2\,\mathrm{Re}\,\langle f|g\rangle_{L^2}, \tag{3.10a}$$

$$W(g)^\dagger \mathbb{N} W(g) \;=\; \mathbb{N} + \phi(g) + \|g\|_{L^2}^2, \tag{3.10b}$$

$$W(g)^\dagger P_f W(g) \;=\; P_f - a^\dagger(i\nabla g) - a(i\nabla g) - \langle g|i\nabla g\rangle_{L^2}. \tag{3.10c}$$

Moreover, we need the following identity.

Lemma 3.2. *Let $\varphi_P = \varphi + i\xi_P$ with ξ_P defined by (2.18). Then*

$$W^\dagger(\alpha\varphi_P) e^{i(P_f - P)y} W(\alpha\varphi_P) \;=\; e^{A_{P,y}} W(\alpha w_{P,y}). \tag{3.11}$$

Proof of Lemma 3.2. We first observe that

$$e^{-iP_f y} a^\dagger(f) e^{iP_f y} \;=\; a^\dagger(e^{-y\nabla} f) \tag{3.12}$$

which follows from $\frac{d}{ds} e^{-isP_f y} a^\dagger(e^{(s-1)y\nabla} f) e^{isP_f y} = 0$. In combination with equation (3.3), this leads to

$$W^\dagger(\alpha\varphi_P) e^{iP_f y} W(\alpha\varphi_P) \;=\; e^{iP_f y} W(\alpha(1 - e^{-y\nabla})\varphi_P) \exp\left(i\alpha^2\,\mathrm{Im}\langle\varphi_P|e^{-y\nabla}\varphi_P\rangle_{L^2}\right). \tag{3.13}$$

Recalling $\varphi_P = \varphi + i\frac{1}{\alpha^2 M^{\mathrm{LP}}}(P\nabla)\varphi$, we compute

$$\begin{aligned}
\alpha^2\,\mathrm{Im}\langle\varphi_P|e^{-y\nabla}\varphi_P\rangle_{L^2} &= \frac{2}{M^{\mathrm{LP}}}\langle\varphi|e^{-y\nabla}(P\nabla)\varphi\rangle_{L^2}\\
&= -\frac{2}{M^{\mathrm{LP}}}\langle\varphi|(y\nabla)(P\nabla)\varphi\rangle_{L^2} - \frac{2}{M^{\mathrm{LP}}}\int_0^1 \mathrm{d}s\,\langle\varphi|e^{-sy\nabla}(y\nabla)^3(P\nabla)\varphi\rangle_{L^2},
\end{aligned} \tag{3.14}$$

where we inserted $e^{-y\nabla} = 1 - (y\nabla) + \frac{1}{2}(y\nabla)^2 - \int_0^1 \mathrm{d}s\, e^{-sy\nabla}(y\nabla)^3$ and used that, due to rotational invariance of φ, $\langle\varphi|(P\nabla)\varphi\rangle_{L^2} = 0 = \langle\varphi|(y\nabla)^2(P\nabla)\varphi\rangle_{L^2}$. Also, because of rotational invariance,

$$\langle\varphi|(y\nabla)(P\nabla)\varphi\rangle_{L^2} \;=\; -\frac{(Py)}{3}\|\nabla\varphi\|_{L^2}^2 \;=\; -\frac{(Py)}{2}M^{\mathrm{LP}}, \tag{3.15}$$

and thus, $\alpha^2\,\mathrm{Im}\langle\varphi_P|e^{-y\nabla}\varphi_P\rangle_{L^2} = Py + g_P(y)$. □

Proof of Lemma 3.1. Throughout this proof, let $\Xi_i = W(\alpha\varphi_P)G_K^i \in L^2(\mathbb{R}^3) \otimes \mathcal{F}$, $i = 0, 1$, with G_K^i defined in equation (2.19) and set $\Psi_i = \int \mathrm{d}x\, e^{i(P_f - P)x}\Xi_i(x)$. First, note that $\Psi_i \in D(H_\alpha(P)^{1/2})$ for $i, j \in \{0, 1\}$ which follows from $D(H_\alpha(P)^{1/2}) = D(|P_f| + \mathbb{N}^{1/2})$ [40] together with $|P_f|\Xi_i \in L^1(\mathbb{R}^3, \mathcal{F})$ and $\mathbb{N}^{1/2}\Xi_i \in L^1(\mathbb{R}^3, \mathcal{F})$. The integrability of these states is verified using Lemmas 3.16 and 3.14.

Below, we shall employ the identities[1]

$$\langle\Psi_i|\Psi_j\rangle_{\mathcal{F}} = \int \mathrm{d}y\,\langle\Xi_i|e^{i(P_f - P)y}T_y\Xi_j\rangle_{\mathscr{H}} \tag{3.16a}$$

$$\langle\Psi_i|H_\alpha(P)\Psi_j\rangle_{\mathcal{F}} = \int \mathrm{d}y\,\langle\Xi_i|H_\alpha e^{i(P_f - P)y}T_y\Xi_j\rangle_{\mathscr{H}}, \tag{3.16b}$$

[1]Strictly speaking, Ψ_i does not belong to the operator domain of $H_\alpha(P)$ (and similarly for Ξ_i and H_α). Nonetheless, the following steps are justified by the well-known fact that the quadratic form with momentum cutoff (that is, with h_x replaced by $h_{\Lambda,x}$ given in equation (2.5)) converges to the quadratic form associated with $H_\alpha(P)$ [40, 25].

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where H_α is the Fröhlich Hamiltonian given by equation (1.2). To obtain the first identity, write

$$\left\langle \Psi_i | \Psi_j \right\rangle_{\mathcal{F}} = \int \mathrm{d}x \left\langle \Xi_i(x) \right| \int \mathrm{d}y \, e^{i(P_f - P)(y-x)} \Xi_j(y) \Big\rangle_{\mathcal{F}} = \Big\langle \Xi_i \Big| \int \mathrm{d}y \, e^{i(P_f - P)y} T_y \Xi_j \Big\rangle_{\mathcal{H}}$$

and for the second one, use $e^{-i(P_f - P)x} \phi(v_0) = \phi(v_x) e^{-i(P_f - P)x}$ so that

$$\left\langle \Psi_i | \phi(v_0) \Psi_j \right\rangle_{\mathcal{F}} = \int \mathrm{d}x \left\langle \Xi_i(x) | \phi(v_x) \int \mathrm{d}y \, e^{i(P_f - P)(y-x)} \Xi_j(y) \right\rangle_{\mathcal{F}} \tag{3.17a}$$

$$\left\langle \Psi_i | \mathbb{N} \Psi_j \right\rangle_{\mathcal{F}} = \int \mathrm{d}x \left\langle \Xi_i(x) | \mathbb{N} \int \mathrm{d}y \, e^{i(P_f - P)(y-x)} \Xi_j(y) \right\rangle_{\mathcal{F}} \tag{3.17b}$$

$$\begin{aligned} \left\langle \Psi_i | (P_f - P)^2 \Psi_j \right\rangle_{\mathcal{F}} &= \int \mathrm{d}x \left\langle \Xi_i(x) | (P_f - P)^2 \int \mathrm{d}y \, e^{i(P_f - P)(y-x)} \Xi_j(y) \right\rangle_{\mathcal{F}} \\ &= \int \mathrm{d}x \left\langle \Xi_i(x) | (-\Delta_x) \int \mathrm{d}y \, e^{i(P_f - P)(y-x)} \Xi_j(y) \right\rangle_{\mathcal{F}}. \end{aligned} \tag{3.17c}$$

With equations (3.16a) and (3.16b), the norm and the energy of the trial state are given by

$$\begin{aligned} \|\Psi_{K,\alpha}(P)\|_{\mathcal{F}}^2 = &\sum_{i \in \{0,1\}} \alpha^{-2i} \int \mathrm{d}y \left\langle \Xi_i | e^{i(P_f - P)y} T_y \Xi_i \right\rangle_{\mathcal{H}} \\ &- 2\alpha^{-1} \operatorname{Re} \int \mathrm{d}y \left\langle \Xi_0 | e^{i(P_f - P)y} T_y \Xi_1 \right\rangle_{\mathcal{H}} \end{aligned} \tag{3.18a}$$

$$\begin{aligned} \left\langle \Psi_{K,\alpha}(P) | H_\alpha(P) \Psi_{K,\alpha}(P) \right\rangle_{\mathcal{F}} = &\sum_{i \in \{0,1\}} \alpha^{-2i} \int \mathrm{d}y \left\langle \Xi_i | H_\alpha e^{i(P_f - P)y} T_y \Xi_i \right\rangle_{\mathcal{H}} \\ &- 2\alpha^{-1} \operatorname{Re} \int \mathrm{d}y \left\langle \Xi_0 | H_\alpha e^{i(P_f - P)y} T_y \Xi_1 \right\rangle_{\mathcal{H}}. \end{aligned} \tag{3.18b}$$

Inserting $\Xi_i = W(\alpha \varphi_P) G_K^i$ and applying Lemma 3.2, we find for $i, j \in \{0, 1\}$

$$\left\langle \Xi_i | e^{i(P_f - P)y} T_y \Xi_j \right\rangle_{\mathcal{H}} = \left\langle G_K^i | e^{A_{P,y}} W(\alpha w_{P,y}) T_y G_K^j \right\rangle_{\mathcal{H}} \tag{3.19a}$$

$$\left\langle \Xi_i | H_\alpha e^{i(P_f - P)y} T_y \Xi_j \right\rangle_{\mathcal{H}} = \left\langle G_K^i | W(\alpha \varphi_P)^\dagger H_\alpha W(\alpha \varphi_P) e^{A_{P,y}} W(\alpha w_{P,y}) T_y G_K^j \right\rangle_{\mathcal{H}}. \tag{3.19b}$$

Using equations (3.10a) and (3.10b) and $2 \operatorname{Re}\langle \varphi_P | h_x \rangle_{L^2} = 2 \operatorname{Re}\langle \varphi | h_x \rangle_{L^2} = V^\varphi(x)$ (see equation (1.11)) the Weyl-transformed Hamiltonian becomes

$$\begin{aligned} W(\alpha \varphi_P)^\dagger H_\alpha W(\alpha \varphi_P) &= -\Delta_x + V^\varphi(x) + \alpha^{-2} \mathbb{N} + \alpha^{-1} \phi(h_x + \varphi_P) + \|\varphi_P\|_{L^2}^2 \\ &= \widetilde{H}_{\alpha,P} + e^{\mathrm{Pek}} + \|\varphi_P\|_{L^2}^2 - \|\varphi\|_{L^2}^2 \end{aligned} \tag{3.20}$$

with $\widetilde{H}_{\alpha,P}$ defined by equation (3.6). Note that we added and subtracted $e^{\mathrm{Pek}} = \lambda^{\mathrm{Pek}} + \|\varphi\|_{L^2}^2$ and used equation (3.6). Altogether, this implies

$$\left\langle \Psi_{K,\alpha}(P) | H_\alpha(P) \Psi_{K,\alpha}(P) \right\rangle_{\mathcal{F}} = \left(e^{\mathrm{Pek}} + \|\varphi_P\|_{L^2}^2 - \|\varphi\|_{L^2}^2 \right) \mathcal{N} + \mathcal{E} + \mathcal{G} + \mathcal{K}. \tag{3.21}$$

The claimed result now follows from

$$\|\varphi_P\|_{L^2}^2 - \|\varphi\|_{L^2}^2 = \frac{1}{\alpha^4 (M^{\mathrm{LP}})^2} \|(P\nabla)\varphi\|_{L^2}^2 = \frac{P^2}{2\alpha^4 M^{\mathrm{LP}}}, \tag{3.22}$$

where we used $\|(P\nabla)\varphi\|_{L^2}^2 = \frac{P^2}{3} \|\nabla\varphi\|_{L^2}^2 = \frac{P^2}{2} M^{\mathrm{LP}}$ because of rotational invariance of φ. □

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3.2. A short guide to the proof

3.2.1. Heuristic picture

Given Lemma 3.1, the remaining task is to show that $(\mathcal{E}+\mathcal{G}+\mathcal{K})/\mathcal{N}$ coincides, up to small errors, with the energy contribution of order α^{-2} in equation (2.24). Although our proof is somewhat technical, the main idea is a simple one, and we explain the corresponding heuristics here in order to facilitate the reading. The main point is that the integrals appearing in the terms given in Lemma 3.1 turn out to be, as $\alpha \to \infty$ and $|P|/\alpha \le c$, sharply localized around zero at the length scale of order α^{-1}. In this regime, as formally $w_{P,y}(z) \approx y\nabla\varphi(z)$ for y small, the Weyl operator $W(\alpha w_{P,y})$ effectively acts nontrivially only on the $\mathcal{F}_0$ part of the Fock space (at this point, it is convenient to recall the factorization (2.3)). Moreover, we shall show that $e^{A_{P,y}}$ can be effectively replaced by the identity operator and it suffices to consider $T_y \approx 1 + y\nabla$. Since our trial state coincides with the vacuum on $\mathcal{F}_0$, we thus expect for $|y|$ small that

$$T_y e^{A_{P,y}} W(\alpha w_{P,y}) G_K^i \approx e^{-\lambda\alpha^2 y^2}(1+y\nabla)e^{a^\dagger(\alpha y\nabla\varphi)} G_K^i, \quad i = 0, 1 \tag{3.23}$$

with $\lambda = \frac{1}{6}\|\nabla\varphi\|_{L^2}^2$. (Since T_y acts on the electron coordinate, it commutes with $e^{A_{P,y}}$ and $W(\alpha w_{P,y})$). Taking this approximation for granted, and considering only the term with $i = j = 0$ in equations (3.18a) and (3.19a), would lead to

$$\mathcal{N} \approx \int \mathrm{d}y \, \langle G_K^0 | T_y e^{A_{P,y}} W(\alpha w_{P,y}) G_K^0 \rangle_{\mathscr{H}} = \int \mathrm{d}y \, e^{-\lambda\alpha^2 y^2} + \text{Errors}. \tag{3.24}$$

With the above replacement and keeping only the terms of order α^{-2} (relative to the factor from the norm), the energy terms are found to be given by

$$\mathcal{E} = \frac{1}{\alpha^2}\langle \psi\otimes\Upsilon_K | \mathbb{N}_1 \psi\otimes\Upsilon_K\rangle_{\mathscr{H}} \int \mathrm{d}y \, e^{-\lambda\alpha^2 y^2} + \text{Errors} \tag{3.25a}$$

$$+\frac{1}{\alpha}\int \mathrm{d}y\, e^{-\lambda\alpha^2y^2}\langle \psi\otimes\Upsilon_K | \big(\phi(h_\cdot + \varphi)(1+(y\nabla)a^\dagger(\alpha y\nabla\varphi))\big)\psi\otimes\Upsilon_K\rangle_{\mathscr{H}} \tag{3.25b}$$

$$\mathcal{G} = -\frac{2}{\alpha^2}\operatorname{Re}\langle \psi\otimes\Upsilon_K | \phi(h_\cdot^1)u_\alpha R\phi(h_{K,\cdot}^1)\psi\otimes\Upsilon_K\rangle_{\mathscr{H}} \int \mathrm{d}y\, e^{-\lambda\alpha^2y^2} + \text{Errors} \tag{3.25c}$$

$$\mathcal{K} = \frac{1}{\alpha^2}\langle \psi\otimes\Upsilon_K | \phi(h_\cdot^1)Ru_\alpha h^{\text{Pek}}u_\alpha R\phi(h_{K,\cdot}^1)\psi\otimes\Upsilon_K\rangle_{\mathscr{H}} \int \mathrm{d}y\, e^{-\lambda\alpha^2y^2} + \text{Errors}. \tag{3.25d}$$

From here, the Bogoliubov energy is obtained by setting $u_\alpha = 1$ and $K = \infty$ in the leading-order terms and using $Rh^{\text{Pek}}R = R$, since this would imply (omitting the errors)

$$\begin{aligned}(3.25\text{a}) + (3.25\text{c}) + (3.25\text{d}) &= \langle \psi\otimes\Upsilon_\infty | (\mathbb{N}_1 - \phi(h_\cdot^1)R\phi(h_{\infty,\cdot}^1))\psi\otimes\Upsilon_\infty\rangle_{\mathscr{H}} \frac{1}{\alpha^2}\int \mathrm{d}y\, e^{-\lambda\alpha^2y^2} \\ &= \frac{\inf\sigma(\mathbb{H}_\infty)}{\alpha^2}\int \mathrm{d}y\, e^{-\lambda\alpha^2y^2}.\end{aligned} \tag{3.26}$$

The remaining $-\frac{3}{2\alpha^2}$ term stems from the part of the interaction involving the zero modes. In equation (3.25b), the term not involving $y\nabla$ vanishes due to $\langle\psi|h_\cdot\psi\rangle_{L^2} = -\varphi$. Moreover, $\langle\psi|h_\cdot\nabla\psi\rangle_{L^2} = -\frac{1}{2}\nabla\varphi$ using $\nabla h_\cdot = -(\nabla h)_\cdot$ via integration by parts (in the sense of distributions). Thus, since $[a^\dagger(y\nabla\varphi), \mathbb{U}_\infty^\dagger] = 0$,

$$\begin{aligned}(3.25\text{b}) &= \int \mathrm{d}y\, e^{-\lambda\alpha^2y^2}\langle\Omega|\phi(\langle\psi|h_\cdot y\nabla\psi\rangle)a^\dagger(y\nabla\varphi)\Omega\rangle_{\mathcal{F}} \\ &= -\frac{1}{2}\int \mathrm{d}y\, e^{-\lambda\alpha^2y^2}\|y\nabla\varphi\|_{L^2}^2 = -\frac{3}{2\alpha^2}\int \mathrm{d}y\, e^{-\lambda\alpha^2y^2}.\end{aligned} \tag{3.27}$$

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Equations (3.26) and (3.27) now add up to the desired energy of order α^{-2}; see equation (2.25). Note that for estimating the error induced by replacing $e^{A_{P,y}}$ by unity we require the momentum cutoff K in the definition of the trial state; see Lemma 3.16.

The main issue in equation (3.23) is that, while for small enough y one can use the first-order approximation $W(\alpha w_{P,y}) \approx W(\alpha y \nabla\varphi)$, for y large, on the other hand, the higher-order terms in $w_{P,y}$ begin to play an important part, ultimately killing the Gaussian factor. Writing

$$\begin{aligned}&\big\langle G_K^i|\widetilde{H}_\alpha(P)e^{A_{P,y}}W(\alpha w_{P,y})T_yG_K^j\big\rangle_{\mathscr{H}} \\ &\quad= e^{-\frac{\alpha^2}{2}\|w_{P,y}\|_{L^2}^2}\big\langle G_K^i|\widetilde{H}_\alpha(P)e^{A_{P,y}}e^{a^\dagger(\alpha w_{P,y})}e^{-a(\alpha w_{P,y})}T_yG_K^j\big\rangle_{\mathscr{H}}, \quad i,j=0,1,\end{aligned} \tag{3.28}$$

we notice that, since

$$\|w_{P,y}\|_{L^2}^2 = 2\int \mathrm{d}k\,|\hat{\varphi}_P(k)|^2(1-\cos(ky)) \to 2\|\varphi_P\|_{L^2}^2 \quad \text{for} \quad |y|\to\infty, \tag{3.29}$$

the prefactor should lead to a y-independent, exponentially small constant. In order to make use of this exponential decay in α, however, we need to ensure that

$$\Big|\big\langle G_K^i|\widetilde{H}_\alpha(P)e^{A_{P,y}}e^{a^\dagger(\alpha w_{P,y})}e^{-a(\alpha w_{P,y})}T_yG_K^j\big\rangle_{\mathscr{H}}\Big| \le C\alpha^n g(y) \tag{3.30}$$

is polynomially bounded in α with some integrable function $g(y)$, which heuristically can be expected to be true since the average number of particles in the state $\widetilde{H}_\alpha(P)G_K^i$ is of order one w.r.t. α. To obtain the required integrability in y is also the reason for introducing the cutoff function u_α in the definition of G_K^1.

3.2.2. Outline of the proof

Although the replacement (3.23) illustrates the main idea behind extracting the leading order terms, in our proof we do not directly perform this replacement and estimate the resulting error. Instead, when taking inner products, we commute the exponential operators $e^{a^\dagger(\alpha w_P)}$ and $e^{-a(\alpha w_P)}$ in $W(\alpha w_{P,y})$ to the left resp. to the right until they hit the vacuum state in G_K^i. This involves the Bogoliubov transformation, cf. Lemma 3.12 and gives rise to a slight modification of $w_{P,y}$, which we denote by $\widetilde{w}_{P,y}$. These manipulations naturally lead to a multiplicative factor $\exp(-\frac{\alpha^2}{2}\|\widetilde{w}_{P,y}\|_{L^2}^2)$ which, as we shall see, indeed behaves like the Gaussian function in equation (3.23) for $|y|$ small and tends to a constant exponentially small in α as $|y|\to\infty$. In Lemma 3.5, we prove the large α asymptotics of integrals of the type $\int g(y)\exp(-\frac{\alpha^2}{2}\|\widetilde{w}_{P,y}\|_{L^2}^2)\mathrm{d}y$ for a suitable class of functions g. The major part of the proof, apart from extracting the leading order terms, is to establish that the resulting error terms in the integrands are, in fact, functions in this class. This is, for the most part, achieved by use of elementary estimates combined with the commutator method by Lieb and Yamazaki [40] in the form stated in Lemma 3.9. As already mentioned, for certain terms this makes the introduction of the space cutoff u_α and the momentum cutoff K necessary, while for others, it is enough to use the well-known regularity properties of ψ, the relevant consequences of which are summarized in Lemma 3.7.

In the next two sections, we state the remaining necessary lemmas. The main proof is then carried out in Sections 3.5–3.9.

Throughout the remainder of the proof, we will abbreviate constants by the letter C and write C_τ whenever we want to specify that it depends on a parameter τ. As usual, the value of a constant may change from one line to the next.

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3.3. The Gaussian lemma

We recall that $w_{P,y} = (1 - e^{-y\nabla})\varphi_P$ and $\Theta_K = (H_K^{\mathrm{Pek}})^{1/4}$ and set

$$w^0_{P,y} = \Pi_0 w_{P,y} \in \mathrm{Ker} H^{\mathrm{Pek}} \tag{3.31a}$$

$$w^1_{P,y} = \Pi_1 w_{P,y} \in (\mathrm{Ker} H^{\mathrm{Pek}})^{\perp} \tag{3.31b}$$

$$\widetilde{w}^1_{P,y} = \Theta_K \,\mathrm{Re}(w^1_{P,y}) + i\Theta_K^{-1}\,\mathrm{Im}(w^1_{P,y}) \tag{3.31c}$$

$$\widetilde{w}_{P,y} = w^0_{P,y} + \widetilde{w}^1_{P,y}. \tag{3.31d}$$

Remark 3.3. Note that $(y,z) \mapsto \mathrm{Re}(w_{P,y})(z)$ is even as a function on $\mathbb{R}^6$, while $\mathrm{Im}(w_{P,y})(z)$ is odd on the same space. Since Π_0 and Θ_K both commute with the reflection operator $(\pi f)(x) = f(-x)$, they preserve the parity properties just mentioned. That Π_0 has the desired properties follows directly from its explicit form. To see this for Θ_K, it is enough to check this for H_K^{Pek}, which can be easily done using the fact that the resolvent R commutes with the reflection operator, which, on the other hand, follows from the invariance of h^{Pek} and P_ψ under parity, cf. the definition of R (1.18). Thus, $(y,z) \mapsto \mathrm{Re}(w^i_{P,y})(z)$ is even as a function on $\mathbb{R}^6$ for $i = 0, 1$ while the corresponding imaginary parts are odd on the same space. These facts will be of relevance below where they lead to the vanishing of several integrals.

The following lemma is proven in Section 4.

Lemma 3.4. *Let $\lambda = \frac{1}{6}\|\nabla\varphi\|^2_{L^2}$. For every $c > 0$, there exists a constant $C > 0$ such that*

$$\|w^1_{P,y}\|^2_{L^2} + \|\widetilde{w}^1_{P,y}\|^2_{L^2} \le C\big(\alpha^{-2}y^2 + y^4\big) \tag{3.32a}$$

$$\Big|\|w^0_{P,y}\|^2_{L^2} - 2\lambda y^2\Big| \le C\big(\alpha^{-2}y^2 + y^4 + y^6\big) \tag{3.32b}$$

$$\Big|\|\widetilde{w}_{P,y}\|^2_{L^2} - 2\lambda y^2\Big| \le C\big(\alpha^{-2}y^2 + y^4 + y^6\big) \tag{3.32c}$$

for all $y \in \mathbb{R}^3$, $|P|/\alpha \le c$ and $\alpha > 0$.

For $0 \le \delta < 1$ and $\eta > 0$, we introduce the weight function

$$n_{\delta,\eta}(y) = \exp\left(-\frac{\eta\alpha^{2(1-\delta)}\|\widetilde{w}_{P,y}\|^2_{L^2}}{2}\right), \tag{3.33}$$

where, for ease of notation, the dependence on α, P and K is omitted. Using the arguments laid down in Remark 3.3, it is easy to see that $n_{\delta,\eta}(y)$ is even as a function of y. Moreover, in the limit of large α the dominant part of the weight function when integrated against suitably decaying functions comes from the term in the exponent that is quadratic in y, cf. equation (3.32c). This is a crucial ingredient in our proofs and the content of the next lemma.

Lemma 3.5. *Let $\eta_0 > 0$, $c > 0$, $\lambda = \frac{1}{6}\|\nabla\varphi\|^2_{L^2}$ and $n_{\delta,\eta}$ defined in equation (3.33). For every $n \in \mathbb{N}_0$, there exist constants $d, C_n > 0$ such that*

$$\int |y|^n g(y)\left|n_{\delta,\eta}(y) - e^{-\eta\lambda\alpha^{2(1-\delta)}y^2}\right|\mathrm{d}y \le C_n\frac{\|g\|_{L^\infty}}{\alpha^{(4+n)(1-\delta)+\delta}} + e^{-d\alpha^{-2\delta+1}}\||\cdot|^n g\|_{L^1} \tag{3.34}$$

for all nonnegative functions $g \in L^\infty(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$, $\eta \ge \eta_0$, $\delta \in [0,1)$, $|P|/\alpha \le c$ and all α large enough.

At first reading, one should think of $n = 0$, $\delta = 0$, $\eta = 1$ and g a suitable α-independent nonnegative function. In this case, the integral involving the Gaussian is of order α^{-3} whereas the term on the right-hand side is of order α^{-4} and thus contributing a subleading error. The proof of the lemma is given in Section 4. As a direct consequence that will be useful to estimate error terms, we find

Corollary 3.6. *Given the same assumptions as in Lemma 3.5, for every $n \in \mathbb{N}_0$ there exist constants $d, C_n > 0$ such that*

$$\int |y|^n g(y) n_{\delta,\eta}(y)\mathrm{d}y \le C_n \frac{\|g\|_{L^\infty}}{\alpha^{(3+n)(1-\delta)}} + e^{-d\alpha^{-2\delta+1}} \| |\cdot|^n g\|_{L^1} \tag{3.35}$$

for all nonnegative functions $g \in L^\infty(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$, $\eta \ge \eta_0$, $\delta \in [0, 1)$, $|P|/\alpha \le c$ and all K, α large enough.

Proof of Corollary 3.6. Since

$$\int \mathrm{d}y\, |y|^n e^{-\eta\lambda\alpha^{2(1-\delta)} y^2} = (\eta\lambda\alpha^{2(1-\delta)})^{-\frac{3+n}{2}} \int \mathrm{d}y\, |y|^n e^{-y^2} = C_n \alpha^{-(3+n)(1-\delta)}, \tag{3.36}$$

the statement follows immediately from Lemma 3.5. □

3.4. Further preliminaries

3.4.1. Estimates involving the Pekar minimizers

Lemma 3.7. *Let $\psi > 0$ be the (normalized) rotational invariant unique minimizer of the Pekar functional (1.12), and let*

$$H(x) := \langle \psi | T_x \psi \rangle_{L^2} = (\psi * \psi)(x). \tag{3.37}$$

We have that ψ, $|\nabla\psi|$ and H are $L^p(\mathbb{R}^3, (1 + |x|^n)\mathrm{d}x)$ functions for all $1 \le p \le \infty$ and all $n \ge 0$. Moreover, there exists a constant $C > 0$ such that for all x we have

$$|H(x) - 1| \le Cx^2. \tag{3.38}$$

Proof. As follows from [36], $\psi(x)$ is monotone decreasing in $|x|$; moreover, it is smooth and bounded and vanishes exponentially at infinity, that is, there exists a constant $C > 0$ such that $\psi(x) \le Ce^{-|x|/C}$ for all $|x|$ large enough (for the precise asymptotics see [46]). This clearly implies the statement for ψ. It further implies that all the derivatives of ψ are bounded. Hence, in order to show the desired result for $|\nabla\psi|$, it suffices to show that $\int \mathrm{d}x |x|^n |\nabla\psi(x)|$ is finite for all $n \ge 0$. Since ψ is radial, that is, there is a function $\psi^{\mathrm{rad}} : [0, \infty) \to (0, \infty)$ such that $\psi(x) = \psi^{\mathrm{rad}}(|x|)$, and monotone decreasing, we have

$$\begin{aligned}\int \mathrm{d}x\, |x|^n |\nabla\psi(x)| &= -4\pi \int_0^\infty \frac{\mathrm{d}\psi^{\mathrm{rad}}(r)}{\mathrm{d}r} r^{n+2}\mathrm{d}r = (n+2)\int \frac{|\psi(x)|}{|x|}|x|^n \mathrm{d}x \\ &\le 4\pi\left(R_0^{n+2}\|\psi\|_{L^\infty} + \frac{n+2}{R_0}\| |\cdot|^n \psi\|_{L^1}\right)\end{aligned} \tag{3.39}$$

for all $R_0 > 0$. Clearly, H is bounded, and hence, by $|x + y|^n \le 2^{n-1}(|x|^n + |y|^n)$, we can easily bound

$$\int |x|^n H(x)\mathrm{d}x \le 2^{n-2}\|\psi\|_{L^1} \| |\cdot|^n \psi\|_{L^1} \tag{3.40}$$

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from which the statement follows also for H. To show (3.38), use the Fourier representation

$$H(x) = \int |\widehat{\psi}(k)|^2 \cos(kx)\mathrm{d}k, \tag{3.41}$$

together with $H(x) \le 1$, $\cos(2\pi kx) \ge 1 - \frac{(kx)^2}{2}$, $\|\psi\|_{L^2} = 1$ and $\nabla\psi \in L^2$. □

The next lemma contains suitable bounds for the potential V^φ and the resolvent R introduced in equations (1.11), (1.14) and (1.18).

Lemma 3.8. *There is a constant $C > 0$ such that*

$$(V^\varphi)^2 \le C(1-\Delta), \quad \pm V^\varphi \le \frac{1}{2}(-\Delta) + C \quad \textit{and} \quad \|\nabla R^{1/2}\|_{\mathrm{op}} \le C. \tag{3.42}$$

Proof. For the proof of the first two inequalities, we refer to [35, Lemma III.2]. The bound for the resolvent is obtained through

$$0 \le R^{\frac{1}{2}}(-\Delta)R^{\frac{1}{2}} \le R^{\frac{1}{2}}h^{\mathrm{Pek}}R^{\frac{1}{2}} - R^{\frac{1}{2}}(V^\varphi - \lambda^{\mathrm{Pek}})R^{\frac{1}{2}} \le CR + \frac{1}{2}R^{\frac{1}{2}}(-\Delta)R^{\frac{1}{2}}, \tag{3.43}$$

where we made use of the second inequality in equation (3.42). □

3.4.2. The commutator method

In the course of the proof, we are frequently faced with bounding field operators like $\phi(h_x)$. From the standard estimates for creation and annihilation operators, we would obtain

$$\|a(f)\Psi\|_{\mathscr{H}} \le \|f\|_{L^2}\|\mathbb{N}^{1/2}\Psi\|_{\mathscr{H}}, \ \|a^\dagger(f)\Psi\|_{\mathscr{H}} \le \|f\|_{L^2}\|(\mathbb{N}+1)^{1/2}\Psi\|_{\mathscr{H}}, \ \Psi \in \mathscr{H}, \tag{3.44}$$

which is not sufficient since $h_0(y)$ is not square-integrable. With the aid of the commutator method introduced by Lieb and Yamazaki [40] one obtains suitable upper bounds by using in addition some regularity in the electron variable of the wave function Ψ. For our purpose, the version summarized in the following lemma will be sufficient.

Lemma 3.9. *Let $h_{K,\cdot}$ for $K \in (1,\infty]$ as defined in equation (2.5), let A denote a bounded operator in $L^2(\mathbb{R}^3)$ (acting on the field variable) and $a^\bullet \in \{a, a^\dagger\}$. Further, let X, Y be bounded symmetric operators in $L^2(\mathbb{R}^3)$ (acting on the electron variable) that satisfy $D_0 := \|X\|_{\mathrm{op}}\|Y\|_{\mathrm{op}} + \|\nabla X\|_{\mathrm{op}}\|Y\|_{\mathrm{op}} + \|X\|_{\mathrm{op}}\|\nabla Y\|_{\mathrm{op}} < \infty$. There exists a constant $C > 0$ such that*

$$\|Xa^\bullet(Ah_{K,\cdot+y})Y\Psi\|_{\mathscr{H}} \le CD_0\|(\mathbb{N}+1)^{1/2}\Psi\|_{\mathscr{H}} \tag{3.45a}$$

$$\|Xa^\bullet(Ah_{\Lambda,\cdot+y} - Ah_{K,\cdot+y})Y\Psi\|_{\mathscr{H}} \le \frac{CD_0}{\sqrt{K}}\|(\mathbb{N}+1)^{1/2}\Psi\|_{\mathscr{H}} \tag{3.45b}$$

for all $y \in \mathbb{R}^3$, $\Psi \in \mathscr{H}$ and $1 \le K \le \Lambda \le \infty$.

Remark 3.10. Note that $Ah_{K,\cdot+y} = T_y(Ah_{K,\cdot})$ and in case that A has an integral kernel,

$$(Ah_{K,x})(z) = \int \mathrm{d}u\, A(z,u)h_{K,x}(u). \tag{3.46}$$

Proof of Lemma 3.9. To obtain the first inequality, write $h_{K,\cdot} = (h_{K,\cdot} - h_{1,\cdot}) + h_{1,\cdot}$ and apply the second inequality (with Λ and K interchanged) to the term in parenthesis. The bound for the term involving $h_{1,\cdot}$

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follows from equation (3.44), as

$$\|a^\bullet(Ah_{1,\cdot+y})Y\Psi\|_{\mathscr{H}}^2 = \int \mathrm{d}x\, \|a^\bullet(Ah_{1,x+y})(Y\Psi)(x)\|_{\mathcal{F}}^2 \le \int \mathrm{d}x \|Ah_{1,x+y}\|_{L^2}^2 \, \|(\mathbb{N}+1)^{1/2}(Y\Psi)(x)\|_{\mathcal{F}}^2 \le \|A\|_{\mathrm{op}}^2 \|h_{1,0}\|_{L^2}^2 \|Y\|_{\mathrm{op}}^2 \|(\mathbb{N}+1)^{1/2}\Psi\|_{\mathscr{H}}^2. \tag{3.47}$$

To verify the second inequality, write the difference as a commutator

$$h_{\Lambda,x}(z) - h_{K,x}(z) = [-i\nabla_x, j_{K,\Lambda,x}(z)], \quad j_{K,\Lambda,x}(z) = \frac{1}{(2\pi)^3} \int_{K\le|k|\le\Lambda} \mathrm{d}k \frac{k e^{ik(x-z)}}{|k|^3} \tag{3.48}$$

and use that ∇ and A commute (they act on different variables). Then similarly as in equation (3.47) we obtain

$$\begin{aligned}\|Xa^\bullet([\nabla, Aj_{K,\Lambda,\cdot+y}])Y\Psi\|_{\mathscr{H}} &\le \|X\nabla a^\bullet(Aj_{K,\Lambda,\cdot+y})Y\Psi\|_{\mathscr{H}} + \|Xa^\bullet(Aj_{K,\Lambda,\cdot+y})\nabla Y\Psi\|_{\mathscr{H}} \\ &\le \|X\nabla\|_{\mathrm{op}} \|a^\bullet(Aj_{K,\Lambda,\cdot+y})Y\Psi\|_{\mathscr{H}} + \|X\|_{\mathrm{op}} \|a^\bullet(Aj_{K,\Lambda,\cdot+y})\nabla Y\Psi\|_{\mathscr{H}} \\ &\le \|A\|_{\mathrm{op}} \big(\|X\nabla\|_{\mathrm{op}}\|Y\|_{\mathrm{op}} + \|X\|_{\mathrm{op}}\|\nabla Y\|_{\mathrm{op}}\big) \, \|j_{K,\Lambda,0}\|_{L^2} \, \|(\mathbb{N}+1)^{1/2}\Psi\|_{\mathscr{H}}.\end{aligned} \tag{3.49}$$

The desired bound now follows from $\sup_{\Lambda>K} \|j_{K,\Lambda,0}\|_{L^2}^2 \le C/K$. □

A simple but useful corollary is given by

Corollary 3.11. *Under the same conditions as in Lemma 3.9, with the additional assumption that Y is a rank-one operator, there exists a constant $C > 0$ such that*

$$\int \mathrm{d}z\, \|X(Ah_{K,\cdot+y})(z)Y\|_{\mathrm{op}}^2 \ \le\ CD_0^2 \tag{3.50a}$$

$$\int \mathrm{d}z\, \|X\big((Ah_{K,\cdot+y})(z) - (Ah_{\Lambda,\cdot+y})(z)\big)Y\|_{\mathrm{op}}^2 \ \le\ \frac{CD_0^2}{K} \tag{3.50b}$$

for all $y \in \mathbb{R}^3$ and $1 \le K \le \Lambda \le \infty$.

Proof. Since Y has rank one, we can use

$$\int \mathrm{d}z\, \|X(Ah_{K,\cdot+y})(z)w\|_{L^2}^2 \ =\ \|Xa^\dagger(Ah_{K,\cdot+y})w \otimes \Omega\|_{\mathscr{H}}^2, \tag{3.51}$$

for any $w \in L^2(\mathbb{R}^3)$, and similarly for equation (3.50b), and apply Lemma 3.9. □

3.4.3. Transformation properties of $\mathbb{U}_K$

The next lemma collects some useful relations for the Bogoliubov transformation $\mathbb{U}_K$. The proof follows directly from the definition (2.11) and the properties explained in Remark 2.4. We omit the details.

Lemma 3.12. *Let $f \in L^2(\mathbb{R}^3)$, $f^0 = \Pi_0 f$, $f^1 = \Pi_1 f$ with Π_i defined in equation (2.2), and set*

$$\underline{f} \ =\ f^0 + \Theta_K^{-1}\,\mathrm{Re}(f^1) + i\Theta_K\,\mathrm{Im}(f^1) \tag{3.52a}$$

$$\widetilde{f} \ =\ f^0 + \Theta_K\,\mathrm{Re}(f^1) + i\Theta_K^{-1}\,\mathrm{Im}(f^1). \tag{3.52b}$$

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The unitary operator $\mathbb{U}_K$ *defined in equation (2.11) satisfies the relations*

$$\mathbb{U}_K a(f)\mathbb{U}_K^\dagger = a(f^0) + a(A_K f^1) + a^\dagger(B_K \overline{f^1}) \tag{3.53a}$$

$$\mathbb{U}_K^\dagger a(f)\mathbb{U}_K = a(f^0) + a(A_K f^1) - a^\dagger(B_K \overline{f^1}) \tag{3.53b}$$

$$\mathbb{U}_K \phi(f)\mathbb{U}_K^\dagger = \phi(\underline{f}), \quad \mathbb{U}_K \pi(f)\mathbb{U}_K^\dagger = \pi(\widetilde{f}) \tag{3.53c}$$

$$\mathbb{U}_K W(f)\mathbb{U}_K^\dagger = W(\widetilde{f}). \tag{3.53d}$$

Note that equation (3.31d) is consistent with the general notation introduced in equation (3.52b). The following statements provide helpful bounds involving the number operator when transformed with the Bogoliubov transformation.

Lemma 3.13. *There exists a constant* $b > 0$ *such that*

$$\mathbb{U}_K(\mathbb{N}+1)^n\mathbb{U}_K^\dagger \le b^n n^n (\mathbb{N}+1)^n, \quad \mathbb{U}_K^\dagger(\mathbb{N}+1)^n\mathbb{U}_K \le b^n n^n (\mathbb{N}+1)^n \tag{3.54}$$

for all $n \in \mathbb{N}$.

Proof. With b replaced by $b_K = 2\|B_K\|_{\mathrm{HS}}^2 + \|A_K\|_{\mathrm{op}}^2 + 1$, both estimates follow from [7, Lemma 4.4] together with equations (3.53a) and (3.53b). That $b_K \le b$ for some K-independent $b > 0$ is inferred from Lemma 2.3. □

In the next two statements, we denote by $\mathbb{1}(\mathbb{N} > c)$ (resp. $\mathbb{1}(\mathbb{N} \le c)$) the orthogonal projector in $\mathcal{F}$ to all states with phonon number larger than (resp. less or equal to) c.

Corollary 3.14. *Let* $\Upsilon_K = \mathbb{U}_K^\dagger\Omega$ *and* $\Upsilon_K^{>} := \mathbb{1}(\mathbb{N} > \alpha^\delta)\Upsilon_K$ *for* $\delta > 0$. *There exist constants* $b, C_{\delta,n} > 0$ *such that*

$$\left\langle \Upsilon_K | (\mathbb{N}+1)^n \Upsilon_K \right\rangle_{\mathcal{F}} \le b^n n^n \tag{3.55a}$$

$$\left\langle \Upsilon_K^{>} | (\mathbb{N}+1)^n \Upsilon_K^{>} \right\rangle_{\mathcal{F}} \le C_{\delta,n}\, \alpha^{-20} \tag{3.55b}$$

for all $n \in \mathbb{N}_0$.

Proof. The first bound follows directly from Lemma 3.13. The second one is obtained from

$$\begin{aligned}\left\langle \Upsilon_K^{>} | (\mathbb{N}+1)^n \Upsilon_K^{>} \right\rangle_{\mathcal{F}} &\le \|\mathbb{N}^m(\mathbb{N}+1)^n\Upsilon_K^{>}\|_{\mathcal{F}}\, \|\mathbb{N}^{-m}\Upsilon_K^{>}\|_{\mathcal{F}} \\ &\le \|(\mathbb{N}+1)^{n+m}\Upsilon_K\|_{\mathcal{F}}\, \alpha^{-m\delta} \le (2(n+m)b)^{n+m}\alpha^{-m\delta}\end{aligned} \tag{3.56}$$

with $m \ge 20/\delta$. □

Lemma 3.15. *For* $\delta > 0$ *and* $\kappa = 1/(16eb\alpha^\delta)$ *with* $b > 0$ *the constant from Lemma 3.13, the operator inequality*

$$\mathbb{1}(\mathbb{N} \le 2\alpha^\delta)\mathbb{U}_K^\dagger \exp(2\kappa\mathbb{N})\mathbb{U}_K \mathbb{1}(\mathbb{N} \le 2\alpha^\delta) \le 2 \tag{3.57}$$

holds for all α *large enough.*

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Proof. We write out the Taylor series for the exponential and invoke Lemma 3.13,

$$\begin{aligned}\mathbb{1}(\mathbb{N} \le 2\alpha^\delta)\mathbb{U}_K^\dagger e^{2\kappa\mathbb{N}}\mathbb{U}_K \mathbb{1}(\mathbb{N} \le 2\alpha^\delta) &= \sum_{n=0}^{\infty} \frac{(2\kappa)^n}{n!} \mathbb{1}(\mathbb{N} \le 2\alpha^\delta)\mathbb{U}_K^\dagger (\mathbb{N}+1)^n \mathbb{U}_K \mathbb{1}(\mathbb{N} \le 2\alpha^\delta)\\ &\le \sum_{n=0}^{\infty} \frac{(2\kappa b n)^n}{n!} \mathbb{1}(\mathbb{N} \le 2\alpha^\delta)(\mathbb{N}+1)^n \mathbb{1}(\mathbb{N} \le 2\alpha^\delta)\\ &\le \sum_{n=0}^{\infty} \frac{(8\alpha^\delta \kappa b n)^n}{n!}, \end{aligned} \tag{3.58}$$

where we used $1 \le 2\alpha^\delta$ in the last step. The stated bound now follows from the elementary inequality $n! \ge (\frac{n}{e})^n$. □

The reason for introducing the momentum cutoff in $\mathbb{H}_K$ is to obtain a finite upper bound for the norm of the state $P_f \Upsilon_K$. This is the content of the next lemma, whose proof is given in Section 4.

Lemma 3.16. *Let $P_f = \int \mathrm{d}k\, k\, a_k^\dagger a_k$ and K_0 large enough. There is a $C > 0$ such that*

$$\left\langle \Omega \middle| \mathbb{U}_K (P_f)^2 \mathbb{U}_K^\dagger \Omega \right\rangle_{\mathcal{F}} \le CK \tag{3.59}$$

for all $K \in (K_0, \infty)$.

3.5. Norm of the trial state

In this section, we provide the computation of the norm $\mathcal{N} = \|\Psi_{K,\alpha}(P)\|_{\mathcal{F}}^2$.

Proposition 3.17. *Let $\lambda = \frac{1}{6}\|\nabla\varphi\|_{L^2}^2$ and $c > 0$. For every $\varepsilon > 0$, there exist a constant $C_\varepsilon > 0$ (we omit the dependence on c) such that*

$$\left| \mathcal{N} - \left(\frac{\pi}{\lambda\alpha^2}\right)^{3/2} \right| \le C_\varepsilon \sqrt{K} \alpha^{-4+\varepsilon} \tag{3.60}$$

for all $|P|/\alpha \le c$ and all α large enough.

Proof. It follows from equations (3.18a) and (3.19a) that $\mathcal{N} = \mathcal{N}_0 + \mathcal{N}_1 + \mathcal{N}_2$ with

$$\mathcal{N}_0 = \int \mathrm{d}y\, \left\langle G_K^0 \middle| T_y e^{A_{P,y}} W(\alpha w_{P,y}) G_K^0 \right\rangle_{\mathscr{H}} \tag{3.61a}$$

$$\mathcal{N}_1 = -\frac{2}{\alpha} \int \mathrm{d}y\, \operatorname{Re} \left\langle G_K^0 \middle| T_y e^{A_{P,y}} W(\alpha w_{P,y}) G_K^1 \right\rangle_{\mathscr{H}} \tag{3.61b}$$

$$\mathcal{N}_2 = \frac{1}{\alpha^2} \int \mathrm{d}y\, \left\langle G_K^1 \middle| T_y e^{A_{P,y}} W(\alpha w_{P,y}) G_K^1 \right\rangle_{\mathscr{H}}. \tag{3.61c}$$

Term $\mathcal{N}_0$. This part contains the leading order contribution $(\frac{\pi}{\lambda\alpha^2})^{3/2}$. With H defined in equation (3.37), let us write

$$\begin{aligned}\mathcal{N}_0 = &\int \mathrm{d}y\, H(y) \left\langle \Upsilon_K \middle| W(\alpha w_{P,y}) \Upsilon_K \right\rangle_{\mathcal{F}}\\ &+ \int \mathrm{d}y\, H(y) \left\langle \Upsilon_K \middle| (e^{A_{P,y}} - 1) W(\alpha w_{P,y}) \Upsilon_K \right\rangle_{\mathcal{F}} = \mathcal{N}_{01} + \mathcal{N}_{02}. \end{aligned} \tag{3.62}$$

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In the first term, we use $\Upsilon_K = \mathbb{U}_K^\dagger \Omega$ and apply equation (3.53d) to transform the Weyl operator with the Bogoliubov transformation. This gives

$$\mathbb{U}_K W(\alpha w_{P,y}) \mathbb{U}_K^\dagger = W(\alpha \widetilde{w}_{P,y}) \tag{3.63}$$

with $\widetilde{w}_{P,y}$ defined in equation (3.31d). From equations (3.2) and (3.33), we thus obtain

$$\mathcal{N}_{01} = \int \mathrm{d}y\, H(y) \big\langle \Omega \big| W(\alpha \widetilde{w}_{P,y}) \Omega \big\rangle_{\mathcal{F}} = \int \mathrm{d}y\, H(y) n_{0,1}(y). \tag{3.64}$$

Since $\|H\|_{L^1} + \|H\|_{L^\infty} \leq C$, cf. Lemma 3.7, we can apply Lemma 3.5 in order to replace the weight function $n_{0,1}(y)$ by the Gaussian $e^{-\lambda\alpha^2 y^2}$. More precisely,

$$\left| \int \mathrm{d}y\, H(y) n_{0,1}(y) - \int \mathrm{d}y\, H(y) e^{-\lambda\alpha^2 y^2} \right| \leq C\alpha^{-4} \tag{3.65}$$

for all $|P|/\alpha \leq c$ and all K, α large enough. Then we use $|H(y) - 1| \leq Cy^2$ in order to obtain

$$\left| \mathcal{N}_{01} - \left(\frac{\pi}{\lambda\alpha^2} \right)^{3/2} \right| \leq C\alpha^{-4}. \tag{3.66}$$

To treat $\mathcal{N}_{02}$, it is convenient to decompose the state Υ_K into a part with bounded particle number and a remainder. To this end, we choose a small $\delta > 0$ and write

$$\Upsilon_K = \Upsilon_K^{<} + \Upsilon_K^{>} = \mathbb{1}(\mathbb{N} \leq \alpha^\delta)\Upsilon_K + \mathbb{1}(\mathbb{N} > \alpha^\delta)\Upsilon_K. \tag{3.67}$$

Inserting this into $\mathcal{N}_{02}$ and using unitarity of $e^{A_{P,y}}$ and $\|H\|_{L^1} \leq C$, we can estimate

$$|\mathcal{N}_{02}| \leq \int \mathrm{d}y\, H(y) \left| \big\langle \Upsilon_K^{<} \big| (e^{A_{P,y}} - 1) W(\alpha w_{P,y}) \Upsilon_K \big\rangle_{\mathcal{F}} \right| + C\|\Upsilon_K^{>}\|_{\mathcal{F}}. \tag{3.68}$$

By Corollary 3.14 for $n = 0$, $\|\Upsilon_K^{>}\| \leq C_\delta\, \alpha^{-10}$. In the remaining expression, we use equation (3.63),

$$\big\langle \Upsilon_K^{<} \big| (e^{A_{P,y}} - 1) W(\alpha w_{P,y}) \Upsilon_K \big\rangle_{\mathcal{F}} = \big\langle \Upsilon_K^{<} \big| (e^{A_{P,y}} - 1) \mathbb{U}_K^\dagger W(\alpha \widetilde{w}_{P,y}) \Omega \big\rangle_{\mathcal{F}}, \tag{3.69}$$

and insert the identity

$$\mathbb{1} = e^{\kappa\mathbb{N}} e^{-\kappa\mathbb{N}} \quad \text{with} \quad \kappa = \frac{1}{16eb\alpha^\delta} \tag{3.70}$$

on the left of the Weyl operator (where $b > 0$ is the constant from Lemma 3.13). After applying the Cauchy–Schwarz inequality, this leads to

$$\left| \big\langle \Upsilon_K^{<} \big| (e^{A_{P,y}} - 1) W(\alpha w_{P,y}) \Upsilon_K \big\rangle_{\mathcal{F}} \right| \leq \|e^{\kappa\mathbb{N}} \mathbb{U}_K (e^{-A_{P,y}} - 1) \Upsilon_K^{<}\|_{\mathcal{F}} \|e^{-\kappa\mathbb{N}} W(\alpha \widetilde{w}_{P,y}) \Omega\|_{\mathcal{F}}. \tag{3.71}$$

In the second factor, we then employ

$$\|e^{-\kappa\mathbb{N}} W(\alpha \widetilde{w}_{P,y}) \Omega\|_{\mathcal{F}} = e^{-\frac{\alpha^2}{2}\|\widetilde{w}_{P,y}\|_{L^2}^2} \|e^{-\kappa\mathbb{N}} e^{a^\dagger(\alpha \widetilde{w}_{P,y})} e^{\kappa\mathbb{N}} \Omega\|_{\mathcal{F}} \tag{3.72}$$

and use $e^{-\kappa\mathbb{N}} a^\dagger(f) e^{\kappa\mathbb{N}} = a^\dagger(e^{-\kappa} f)$ to write

$$e^{-\kappa\mathbb{N}} e^{a^\dagger(\alpha \widetilde{w}_{P,y})} e^{\kappa\mathbb{N}} \Omega = e^{a^\dagger(e^{-\kappa}\alpha \widetilde{w}_{P,y})} \Omega = e^{\frac{\alpha^2 e^{-2\kappa}}{2}\|\widetilde{w}_{P,y}\|_{L^2}^2} W(e^{-\kappa}\alpha \widetilde{w}_{P,y}) \Omega. \tag{3.73}$$

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Combining the previous two lines, we obtain

$$\|e^{-\kappa\mathbb{N}}W(\alpha\widetilde{w}_{P,y})\Omega\|_{\mathcal{F}} \;=\; \exp\Big(-\frac{\alpha^2}{2}(1-e^{-2\kappa})\|\widetilde{w}_{P,y}\|_{L^2}^2\Big) \le n_{\delta,\eta}(y) \tag{3.74}$$

for some α-independent $\eta > 0$ and α large enough. To estimate the first factor in equation (3.71), we apply Lemma 3.15 (note that $(e^{A_{P,y}}-1)\Upsilon_K^< \in \mathrm{Ran}(\mathbb{1}(\mathbb{N}\le 2\alpha^\delta))$)

$$\|e^{\kappa\mathbb{N}}\mathbb{U}_K(e^{-A_{P,y}}-1)\Upsilon_K^<\|_{\mathcal{F}} \le \sqrt{2}\|(e^{-A_{P,y}}-1)\Upsilon_K\|_{\mathcal{F}}. \tag{3.75}$$

On the right side, we use the functional calculus for self-adjoint operators

$$\|(e^{-A_{P,y}}-1)\Upsilon_K\|_{\mathcal{F}} \le \|A_{P,y}\Upsilon_K\|_{\mathcal{F}} \le \|(yP_f)\Upsilon_K\|_{\mathcal{F}} + |g_P(y)| \le C\big(\sqrt{K}|y| + \alpha|y|^3\big), \tag{3.76}$$

where in the last step we applied Lemma 3.16 and used

$$|g_P(y)| \;\le\; C\alpha|y|^3, \tag{3.77}$$

which is inferred from equation (3.5) using $\|\Delta\varphi\|_{L^2} < \infty$. Returning to equation (3.71), we have shown that

$$|\mathcal{N}_{02}| \;\le\; C\int \mathrm{d}y\, H(y)\big(\sqrt{K}|y| + \alpha|y|^3\big)n_{\delta,\eta}(y) + C_\delta\,\alpha^{-10}, \tag{3.78}$$

and hence we are in a position to apply Corollary 3.6. This implies for all α large

$$|\mathcal{N}_{02}| \;\le\; C\big(\sqrt{K}\alpha^{-4(1-\delta)} + \alpha^{-6(1-\delta)+1}\big) + C_\delta\,\alpha^{-10} \le C_\delta\,\sqrt{K}\alpha^{-4(1-\delta)}. \tag{3.79}$$

<u>Term $\mathcal{N}_1$</u>. We start by inserting equation (2.22) for G_K^1 in expression (3.61b). Since the Weyl operator commutes with u_α, R and $P_\psi = |\psi\rangle\langle\psi|$, we can apply equation (3.10a) to obtain

$$W(\alpha w_{P,y})G_K^1 \;=\; u_\alpha R\big(\phi(h_{K,\cdot}^1) + 2\alpha\langle h_{K,\cdot}|\,\mathrm{Re}(w_{P,y}^1)\rangle_{L^2}\big)P_\psi W(\alpha w_{P,y})G_K^0, \tag{3.80}$$

where we used that $h_{K,x}$ is real-valued. Note that $\langle h_{K,\cdot}|\,\mathrm{Re}(w_{P,y}^1)\rangle_{L^2}$ is a y-dependent multiplication operator in the electron variable. With $(T_y e^{A_{P,y}})^\dagger = T_{-y}e^{-A_{P,y}}$ and equation (3.67), we can thus write

$$\mathcal{N}_1 \;=\; -\frac{2}{\alpha}\int \mathrm{d}y\;\mathrm{Re}\,\big\langle R_{1,y}\psi\otimes\big(\Upsilon_K^< + \Upsilon_K^>\big)\big|W(\alpha w_{P,y})G_K^0\big\rangle_{\mathscr{H}} = \mathcal{N}_1^< + \mathcal{N}_1^>, \tag{3.81}$$

where we introduced the operator $R_{1,y} = R_{1,y}^1 + R_{1,y}^2$ with

$$R_{1,y}^1 \;=\; P_\psi\phi(h_{K,\cdot}^1)Ru_\alpha T_{-y}P_\psi e^{-A_{P,y}}, \tag{3.82a}$$

$$R_{1,y}^2 \;=\; 2\alpha P_\psi\big\langle h_{K,\cdot}|\,\mathrm{Re}(w_{P,y}^1)\big\rangle_{L^2}Ru_\alpha T_{-y}P_\psi e^{-A_{P,y}}. \tag{3.82b}$$

Using Lemma 3.9 in combination with $\|\nabla P_\psi\|_{\mathrm{op}} + \|\nabla R^{1/2}\|_{\mathrm{op}} < \infty$ (see Lemmas 3.7 and 3.8), we can bound the first operator, for any $\Psi\in\mathscr{H}$, by

$$\|R_{1,y}^1\Psi\|_{\mathscr{H}} \le C\|(\mathbb{N}+1)^{1/2}u_\alpha T_{-y}P_\psi e^{-A_{P,y}}\Psi\|_{\mathscr{H}} \le C\|u_\alpha T_{-y}P_\psi\|_{\mathrm{op}}\|(\mathbb{N}+1)^{1/2}\Psi\|_{\mathscr{H}}. \tag{3.83}$$

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To estimate the second operator, we write out the inner product, use Cauchy–Schwarz twice, apply Corollary 3.11 (with $A = 1$, $X = R$ and $Y = P_\psi$) and use equation (3.32a),

$$\begin{aligned}
\|R^2_{1,y}\Psi\|^2_{\mathscr{H}} &= 4\alpha^2 \Big\| \int \mathrm{d}z \, \mathrm{Re}(w^1_{P,y}(z)) P_\psi h_{K,\cdot}(z) R u_\alpha T_{-y} P_\psi e^{-A_{P,y}} \Psi \Big\|^2_{\mathscr{H}} \\
&\le 4\alpha^2 \int \mathrm{d}u \, |w^1_{P,y}(u)|^2 \int \mathrm{d}z \, \|P_\psi h_{K,\cdot}(z) R\|^2_{\mathrm{op}} \, \|u_\alpha T_{-y} P_\psi e^{-A_{P,y}} \Psi\|^2_{\mathscr{H}} \\
&\le C\alpha^2 \|w^1_{P,y}\|^2_{L^2} \|u_\alpha T_{-y} P_\psi e^{-A_{P,y}} \Psi\|^2_{\mathscr{H}} \\
&\le C\alpha^2 (y^4 + \alpha^{-4}) \|u_\alpha T_{-y} P_\psi\|^2_{\mathrm{op}} \|\Psi\|^2_{\mathscr{H}}.
\end{aligned} \tag{3.84}$$

Combining the above estimates we arrive at

$$\|R_{1,y}\Psi\|_{\mathscr{H}} \le C \|u_\alpha T_{-y} P_\psi\|_{\mathrm{op}} (1 + \alpha y^2) \|(\mathbb{N}+1)^{1/2}\Psi\|_{\mathscr{H}}. \tag{3.85}$$

Since $\psi(x)$ decays exponentially for large $|x|$, the function $f_\alpha(y) := \|u_\alpha T_{-y} P_\psi\|_{\mathrm{op}}$ satisfies

$$\| |\cdot|^n f_\alpha \|_{L^1} \le \int \mathrm{d}y \, |y|^n \Big(\int \mathrm{d}x \, \psi(x+y)^2 u_\alpha(x)^2 \Big)^{1/2} \le C_n \alpha^{3+n} \quad \text{for all } n \in \mathbb{N}_0. \tag{3.86}$$

With this at hand, we can estimate the part containing the tail. Invoking Corollary 3.14

$$|\mathcal{N}_1^>| \le \frac{C}{\alpha} \|(\mathbb{N}+1)^{1/2} \Upsilon_K^>\|_{\mathcal{F}} \int \mathrm{d}y \, f_\alpha(y)(1+\alpha y^2) \le C_\delta \, \alpha^{-5}. \tag{3.87}$$

To estimate the first term in equation (3.81), we proceed similarly as in the bound for $\mathcal{N}_{02}$. We insert the identity (3.70), apply Cauchy–Schwarz and employ equation (3.74). This leads to

$$\begin{aligned}
|\mathcal{N}_1^<| &\le \frac{2}{\alpha} \int \mathrm{d}y \, \|e^{\kappa\mathbb{N}} \mathbb{U}_K (e^{-A_{P,y}} R_{1,y}\psi \otimes \Upsilon_K^<)\|_{\mathcal{F}} \, \|e^{-\kappa\mathbb{N}} W(\alpha \widetilde{w}_{P,y})\Omega\|_{\mathcal{F}} \\
&\le \frac{2}{\alpha} \int \mathrm{d}y \, \|e^{\kappa\mathbb{N}} \mathbb{U}_K (e^{-A_{P,y}} R_{1,y}\psi \otimes \Upsilon_K^<)\|_{\mathcal{F}} \, n_{\delta,\eta}(y).
\end{aligned} \tag{3.88}$$

In the remaining norm, we use the fact that $R_{1,y}$ changes the number of phonons at most by one, and thus we can apply Lemma 3.15 and equation (3.85), together with equation (3.55a), to get

$$\|e^{\kappa\mathbb{N}} \mathbb{U}_K (e^{-A_{P,y}} R_{1,y}\psi \otimes \Upsilon_K^<)\|_{\mathcal{F}} \le \sqrt{2} \|R_{1,y}\psi \otimes \Upsilon_K^<\|_{\mathcal{F}} \le C f_\alpha(y) \big(1 + \alpha y^2\big). \tag{3.89}$$

With Corollary 3.6, equation (3.86) and $\|f_\alpha\|_{L^\infty} \le 1$, this leads to

$$|\mathcal{N}_1^<| \le \frac{C}{\alpha} \int \mathrm{d}y \, f_\alpha(y) \big(1 + \alpha y^2\big) \, n_{\delta,\eta}(y) \le C\alpha^{-1-3(1-\delta)}. \tag{3.90}$$

Term $\mathcal{N}_2$. The strategy for estimating this term is similar to the one for $\mathcal{N}_1$. Proceeding as described before equation (3.81), one obtains

$$\mathcal{N}_2 = \frac{1}{\alpha^2} \int \mathrm{d}y \, \big\langle R_{2,y}\psi \otimes \big(\Upsilon_K^< + \Upsilon_K^>\big) \big| W(\alpha w_{P,y}) G_K^0 \big\rangle_{\mathscr{H}} = \mathcal{N}_2^< + \mathcal{N}_2^> \tag{3.91}$$

with $R_{2,y} = R^1_{2,y} + R^2_{2,y}$ and

$$R^1_{2,y} = P_\psi \phi(h^1_{K,\cdot}) R e^{-A_{P,y}} u_\alpha T_{-y} u_\alpha R \phi(h^1_{K,\cdot}) P_\psi, \tag{3.92a}$$

$$R^2_{2,y} = 2\alpha P_\psi \langle h_{K,\cdot} | \operatorname{Re}(w^1_{P,y}) \rangle_{L^2} R e^{-A_{P,y}} u_\alpha T_{-y} u_\alpha R \phi(h^1_{K,\cdot}) P_\psi. \tag{3.92b}$$

It follows in close analogy as for $R_{1,y}$ in equations (3.82a) and (3.82b) that given any $\Psi \in \mathscr{H}$,

$$\|R_{2,y}\Psi\|_{\mathscr{H}} \le C \|u_\alpha T_{-y} u_\alpha\|_{\mathrm{op}} (1 + \alpha y^2) \|(\mathbb{N}+1)\Psi\|_{\mathscr{H}}, \tag{3.93}$$

and since $\|u_\alpha T_{-y} u_\alpha\|_{\mathrm{op}} \le \mathbb{1}(|y| \le 4\alpha)$, we can use Corollary 3.14 to estimate

$$|\mathcal{N}_2^>| \le \frac{C}{\alpha^2} \|(\mathbb{N}+1)\Upsilon_K^>\|_{\mathcal{F}} \int \mathrm{d}y\, \mathbb{1}(|y| \le 4\alpha)(1+\alpha y^2) \le C_\delta\, \alpha^{-6}. \tag{3.94}$$

To bound the first term in equation (3.91), we proceed similarly as for $\mathcal{N}_{01}$,

$$\begin{aligned} |\mathcal{N}_2^<| &\le \alpha^{-2} \int \mathrm{d}y\, \|e^{\kappa\mathbb{N}} \mathbb{U}_K (R_{2,y}\psi \otimes \Upsilon_K^<)\|_{\mathcal{F}}\, \|e^{-\kappa\mathbb{N}} W(\alpha \widetilde{w}_{P,y})\Omega\|_{\mathcal{F}} \\ &\le \frac{\sqrt{2}}{\alpha^2} \int \mathrm{d}y\, \|R_{2,y}\psi \otimes \Upsilon_K^<\|_{\mathscr{H}}\, n_{\delta,\eta}(y) \le \frac{C}{\alpha^2} \int \mathrm{d}y\, \mathbb{1}(|y| \le 4\alpha)(1+\alpha y^2)\, n_{\delta,\eta}(y). \end{aligned} \tag{3.95}$$

The last integral is estimated again via Corollary 3.6, and thus $|\mathcal{N}_2^<| \le C\alpha^{-5+3\delta}$.

Collecting all relevant estimates and choosing $\delta > 0$ small enough completes the proof of the proposition. □

3.6. Energy contribution $\mathcal{E}$

In this section, we prove the following estimate for the energy contribution $\mathcal{E}$ defined in equation (3.8a).

Proposition 3.18. *Let* $\mathbb{N}_1 = \mathrm{d}\Gamma(\Pi_1)$ *and choose* $c > 0$. *For every* $\varepsilon > 0$, *there is a constant* $C_\varepsilon > 0$ *(we omit the dependence on c) such that*

$$\left| \mathcal{E} - \frac{1}{\alpha^2}\left(\left\langle \Upsilon_K | \mathbb{N}_1 \Upsilon_K \right\rangle_{\mathcal{F}} - \frac{3}{2} \right) \mathcal{N} \right| \le C_\varepsilon \sqrt{K} \alpha^{-6+\varepsilon} \tag{3.96}$$

for all $|P|/\alpha \le c$ *and* α *large enough.*

Proof. Since $G_K^0 = \psi \otimes \Upsilon_K$, $h^{\mathrm{Pek}}\psi = 0$ and $\mathbb{N}\Upsilon_K = \mathbb{N}_1\Upsilon_K$, one has

$$\mathcal{E} = \int \mathrm{d}y\, \left\langle G_K^0 \middle| \left(\alpha^{-2}\mathbb{N}_1 + \alpha^{-1}\phi(h_\cdot + \varphi_P)\right) T_y e^{A_{P,y}} W(\alpha w_{P,y}) \middle| G_K^0 \right\rangle_{\mathscr{H}} = \mathcal{E}_1 + \mathcal{E}_2, \tag{3.97}$$

where both terms provide contributions to the energy of order α^{-2}.

Term $\mathcal{E}_1$. Recall that $H(y) = \langle \psi | T_y \psi \rangle_{L^2}$, and use this to write

$$\begin{aligned} \mathcal{E}_1 &= \frac{1}{\alpha^2} \int \mathrm{d}y\, H(y) \left\langle \Upsilon_K | \mathbb{N}_1 W(\alpha w_{P,y}) \Upsilon_K \right\rangle_{\mathcal{F}} \\ &\quad + \frac{1}{\alpha^2} \int \mathrm{d}y\, H(y) \left\langle \Upsilon_K | \mathbb{N}_1 (e^{A_{P,y}} - 1) W(\alpha w_{P,y}) \Upsilon_K \right\rangle_{\mathcal{F}} = \mathcal{E}_{11} + \mathcal{E}_{12}. \end{aligned} \tag{3.98}$$

With equations (3.63), (3.3) and (3.33), it follows that

$$W(\alpha w_{P,y})\Upsilon_K = \mathbb{U}_K^\dagger W(\alpha \widetilde{w}_{P,y})\Omega = n_{0,1}(y) \mathbb{U}_K^\dagger\, e^{a^\dagger(\alpha w^0_{P,y})} e^{a^\dagger(\alpha \widetilde{w}^1_{P,y})} \Omega, \tag{3.99}$$

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and since $e^{a^\dagger(\alpha w^0_{P,y})}$ commutes with $\mathbb{U}_K\mathbb{N}_1\mathbb{U}_K^\dagger$ and $e^{a(\alpha w^0_{P,y})}\Upsilon_K = \Upsilon_K$ (we use $\mathbb{U}_K a^\dagger(f^0)\mathbb{U}_K^\dagger = a^\dagger(f^0)$ for $f^0 \in \mathrm{Ran}(\Pi_0)$), this leads to

$$\mathcal{E}_{11} = \frac{1}{\alpha^2}\int \mathrm{d}y\, H(y) n_{0,1}(y) \big\langle \Omega | \mathbb{U}_K \mathbb{N}_1 \mathbb{U}_K^\dagger e^{a^\dagger(\alpha \widetilde{w}^1_{P,y})}\Omega\big\rangle_{\mathcal{F}}. \tag{3.100}$$

Because $\mathbb{U}_K\mathbb{N}_1\mathbb{U}_K^\dagger$ is quadratic in creation and annihilation operators, we can expand the exponential in the inner product and use that only the zeroth- and second-order terms give a nonvanishing contribution,

$$\begin{aligned}\mathcal{E}_{11} &= \frac{1}{\alpha^2}\int \mathrm{d}y\, H(y) n_{0,1}(y)\big\langle \Upsilon_K | \mathbb{N}_1 \Upsilon_K\big\rangle_{\mathcal{F}}\\ &\quad + \frac{1}{2\alpha^2}\int \mathrm{d}y\, H(y) n_{0,1}(y)\big\langle \Upsilon_K | \mathbb{N}_1 \mathbb{U}_K^\dagger a^\dagger(\alpha\widetilde{w}^1_{P,y}) a^\dagger(\alpha\widetilde{w}^1_{P,y})\Omega\big\rangle_{\mathcal{F}} = \mathcal{E}_{111} + \mathcal{E}_{112}.\end{aligned} \tag{3.101}$$

Next, we add and subtract the Gaussian to separate the leading-order term,

$$\begin{aligned}\mathcal{E}_{111} &= \frac{1}{\alpha^2}\int \mathrm{d}y\, H(y)\, e^{-\lambda\alpha^2 y^2}\big\langle \Upsilon_K | \mathbb{N}_1 \Upsilon_K\big\rangle_{\mathcal{F}}\\ &\quad + \frac{1}{\alpha^2}\int \mathrm{d}y\, H(y)\big(n_{0,1}(y) - e^{-\lambda\alpha^2y^2}\big)\big\langle \Upsilon_K | \mathbb{N}_1 \Upsilon_K\big\rangle_{\mathcal{F}} = \mathcal{E}^{\mathrm{lo}}_{111} + \mathcal{E}^{\mathrm{err}}_{111}.\end{aligned} \tag{3.102}$$

In $\mathcal{E}^{\mathrm{lo}}_{111}$, we use $|H(y)-1| \le Cy^2$ and Corollary 3.14 to replace $H(y)$ by unity at the cost of an error of order α^{-7}. In the term where $H(y)$ is replaced by unity, we perform the Gaussian integral and use Proposition 3.17 and again Corollary 3.14. This leads to

$$\left|\mathcal{E}^{\mathrm{lo}}_{111} - \mathcal{N}\frac{1}{\alpha^2}\big\langle \Upsilon_K | \mathbb{N}_1 \Upsilon_K\big\rangle_{\mathcal{F}}\right| \le C_\varepsilon \sqrt{K}\alpha^{-6+\varepsilon}. \tag{3.103}$$

The error in equation (3.102) is bounded with the help of Lemma 3.5,

$$|\mathcal{E}^{\mathrm{err}}_{111}| \le \frac{C}{\alpha^2}\int \mathrm{d}y\, H(y)|n_{0,1}(y) - e^{-\lambda\alpha^2y^2}| \le C\alpha^{-6}. \tag{3.104}$$

In $\mathcal{E}_{112}$, we use the Cauchy–Schwarz inequality, Corollary 3.14 and Lemma 3.4, to obtain

$$\begin{aligned}&\big|\big\langle \Upsilon_K | \mathbb{N}_1 \mathbb{U}_K^\dagger a^\dagger(\alpha\widetilde{w}^1_{P,y}) a^\dagger(\alpha\widetilde{w}^1_{P,y})\Omega\big\rangle_{\mathcal{F}}\big|\\ &\quad\le \|\mathbb{N}_1\Upsilon_K\|_{\mathcal{F}}\, \|a^\dagger(\alpha\widetilde{w}^1_{P,y}) a^\dagger(\alpha\widetilde{w}^1_{P,y})\Omega\|_{\mathcal{F}} \le 2\alpha^2\|\widetilde{w}^1_{P,y}\|^2_{L^2} \le C\alpha^2(y^4+\alpha^{-4}).\end{aligned} \tag{3.105}$$

With $\||\cdot|^n H\|_{L^1} \le C_n$, we can now apply Corollary 3.6 to obtain

$$|\mathcal{E}_{112}| \le C\int \mathrm{d}y\, H(y)(y^4+\alpha^{-4}) n_{0,1}(y) \le C\alpha^{-7}. \tag{3.106}$$

In order to bound $\mathcal{E}_{12}$ in equation (3.98), we decompose $\Upsilon_K = \Upsilon_K^< + \Upsilon_K^>$ for some $\delta > 0$ (see equation (3.67)) and then follow similar steps as described below equation (3.69). This way we can estimate

$$|\mathcal{E}_{12}| \le \frac{1}{\alpha^2}\int \mathrm{d}y\, H(y)\|e^{\kappa\mathbb{N}}\mathbb{U}_K(e^{-A_{P,y}}-1)\mathbb{N}_1\Upsilon_K^<\|_{\mathcal{F}}\, n_{\delta,\eta}(y) + \frac{2}{\alpha^2}\|\mathbb{N}_1\Upsilon_K^>\|_{\mathcal{F}}\int \mathrm{d}y\, H(y). \tag{3.107}$$

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While the second term is bounded via equation (3.55b) by $C_\delta\,\alpha^{-12}$, in the first term we apply Lemma 3.15 and use the functional calculus for self-adjoint operators,

$$\begin{aligned}\|e^{\kappa\mathbb{N}}\mathbb{U}_K(e^{-A_{P,y}}-1)\mathbb{N}_1\Upsilon_K^{<}\|_{\mathcal{F}} &\le \sqrt{2}\|(e^{-A_{P,y}}-1)\mathbb{N}_1\Upsilon_K^{<}\|_{\mathcal{F}}\\ &\le \sqrt{2}\|(P_f\,y+g_P(y))\mathbb{N}_1\Upsilon_K^{<}\|_{\mathcal{F}}.\end{aligned}\tag{3.108}$$

Since P_f changes the number of phonons in $\mathcal{F}_1$ at most by one, we can proceed by

$$\|(P_f\,y+g_P(y))\mathbb{N}_1\Upsilon_K^{<}\|_{\mathcal{F}} \le (\alpha^\delta+1)\|(P_f\,y+g_P(y))\Upsilon_K\|_{\mathcal{F}} \le C\alpha^\delta(\sqrt{K}|y|+\alpha|y|^3),\tag{3.109}$$

where we used $1\le\alpha^\delta$, Lemma 3.16 and equation (3.77) in the second step. We conclude via Corollary 3.6 that

$$|\mathcal{E}_{12}| \le \frac{C}{\alpha^2}\int \mathrm{d}y\,H(y)(\sqrt{K}|y|+\alpha|y|^3)n_{\delta,\eta}(y)+C_\delta\,\alpha^{-12} \le C_\delta\sqrt{K}\alpha^{-6+4\delta}.\tag{3.110}$$

Term $\mathcal{E}_2$. Here, we start with

$$\begin{aligned}\mathcal{E}_2 &= \alpha^{-1}\int \mathrm{d}y\,\big\langle\Upsilon_K|L_{1,y}W(\alpha w_{P,y})\Upsilon_K\big\rangle_{\mathcal{F}}\\ &\quad+\alpha^{-1}\int \mathrm{d}y\,\big\langle\Upsilon_K|L_{1,y}(e^{A_{P,y}}-1)W(\alpha w_{P,y})\Upsilon_K\big\rangle_{\mathcal{F}} = \mathcal{E}_{21}+\mathcal{E}_{22},\end{aligned}\tag{3.111}$$

where

$$L_{1,y} = \big\langle\psi|\phi(h_\cdot+\varphi_P)T_y\psi\big\rangle_{L^2}=\phi(l_y)+\pi(j_y)\tag{3.112}$$

with

$$l_y = H(y)\varphi+\big\langle\psi|h_\cdot T_y\psi\big\rangle_{L^2},\quad j_y = H(y)\xi_P,\tag{3.113}$$

and ξ_P defined in equation (2.18). We record the following properties of l_y and its derivative. The proof of the lemma is postponed until the end of the present section.

Lemma 3.19. *For $k=0,1$ and for all $n\in\mathbb{N}_0$,*

$$\sup_y\|\nabla^k l_y\|_{L^2} < \infty,\qquad \int |y|^n\|\nabla^k l_y\|_{L^2}\,\mathrm{d}y < \infty.\tag{3.114}$$

Note that, by Lemma 3.7, j_y clearly has these properties as well. We proceed by writing $\mathcal{E}_{21}=\mathcal{E}_{21}^0+\mathcal{E}_{21}^P$ with

$$\mathcal{E}_{21}^0 = \alpha^{-1}\int \mathrm{d}y\,\big\langle\Upsilon_K|\phi(l_y)W(\alpha w_{P,y})\Upsilon_K\big\rangle_{\mathcal{F}}\tag{3.115a}$$

$$\mathcal{E}_{21}^P = \alpha^{-1}\int \mathrm{d}y\,\big\langle\Upsilon_K|\pi(j_y)W(\alpha w_{P,y})\Upsilon_K\big\rangle_{\mathcal{F}},\tag{3.115b}$$

and estimate the two parts separately. Using the canonical commutation relations and (3.53c), we evaluate

$$\begin{aligned}\mathcal{E}_{21}^0 &= \int \big\langle\underline{l_y}|\widetilde{w}_{P,y}\big\rangle_{L^2}n_{0,1}(y)\mathrm{d}y\\ &= \int\Big(\big\langle l_y^0|w_{P,y}^0\big\rangle_{L^2}+\big\langle l_y^1|\mathrm{Re}(w_{P,y}^1)\big\rangle_{L^2}+i\big\langle l_y^1|\Theta_K^{-2}\mathrm{Im}(w_{P,y}^1)\big\rangle_{L^2}\Big)n_{0,1}(y)\mathrm{d}y,\end{aligned}\tag{3.116}$$

where we used that l_y is real-valued. Note that $l_{-y}(-z) = l_y(z)$. As discussed in Remark 3.3, $n_{0,1}(y)$ is even, and using the arguments therein one can conclude that $\Theta_K^{-2}\mathrm{Im}(w^1_{P,y})$ and $\mathrm{Im}(w^0_{P,y})$ are odd functions on $\mathbb{R}^6$ since $(y,z) \mapsto \mathrm{Im}(w_{P,y})(z)$ is odd on this space, and hence

$$\int \left\langle l^0_y | \mathrm{Im}(w^0_{P,y}) \right\rangle_{L^2} n_{0,1}(y)\mathrm{d}y \;=\; \int \left\langle l^1_y | \Theta_K^{-2}\mathrm{Im}(w^1_{P,y}) \right\rangle_{L^2} n_{0,1}(y)\mathrm{d}y \;=\; 0. \tag{3.117}$$

Thus, with $\mathrm{Re}(w_{P,y}) = w_{0,y}$, and with

$$v(y) \;:=\; \left\langle l_y | w_{0,y} \right\rangle_{L^2} \tag{3.118}$$

we finally have

$$\mathcal{E}^0_{21} \;=\; \int \left\langle l^0_y + l^1_y \,|\, \mathrm{Re}(w^0_{P,y}) + \mathrm{Re}(w^1_{P,y}) \right\rangle_{L^2} n_{0,1}(y)\mathrm{d}y \;=\; \int v(y) n_{0,1}(y)\mathrm{d}y. \tag{3.119}$$

Note that $v \in L^1 \cap L^\infty$ since $y \mapsto \|l_y\|_{L^2}$ is, while $\|w_{0,y}\|_{L^2}$ is uniformly bounded in y. Because of $\varphi(z) = -\langle \psi | h_\cdot(z)\psi \rangle_{L^2}$ and $\nabla_z h(x-z) \;=\; -\nabla_x h(x-z)$, we have by integration by parts

$$\nabla\varphi \;=\; -2\left\langle \nabla\psi | h_\cdot \psi \right\rangle_{L^2}. \tag{3.120}$$

Thus,

$$l_y \;=\; -\frac{1}{2} y\nabla\varphi + \varphi(H(y)-1) + \left\langle \psi | h_\cdot (T_y\psi - \psi - y\nabla\psi) \right\rangle_{L^2}. \tag{3.121}$$

Since ψ is a smooth function with uniformly bounded derivatives, there exists a $C > 0$ such that for all y

$$\|T_y\psi - \psi - y\nabla\psi\|_{L^\infty} \;\le\; C y^2. \tag{3.122}$$

Moreover, for $k = 0, 1$ and every $z \in \mathbb{R}^3$,

$$x \mapsto (h_\cdot(z)\nabla^k\psi)(x) \in L^1(\mathbb{R}^3, \mathrm{d}x) \quad \text{and} \quad z \mapsto \|h_\cdot(z)\nabla^k\psi\|_{L^1} \in L^2(\mathbb{R}^3, \mathrm{d}z). \tag{3.123}$$

The first statement follows easily from Lemma 3.7; to show the second one, use

$$\int \mathrm{d}z \, \frac{1}{|u-z|^2|v-z|^2} \;=\; \frac{1}{\pi^3|u-v|} \tag{3.124}$$

and apply the Hardy–Littlewood–Sobolev inequality. This, together with equation (3.38), shows that there exists a function f in $L^2(\mathbb{R}^3, \mathrm{d}z)$ such that

$$|l_y(z) + \frac{1}{2} y\nabla\varphi(z)| \;\le\; f(z)y^2. \tag{3.125}$$

Now, let

$$b_y(z) \;:=\; w_{0,y}(z) - y\nabla\varphi(z) \;=\; \int_0^1 \mathrm{d}s \int_0^s \mathrm{d}t \, (y\nabla)^2\varphi(z - ty) \tag{3.126}$$

and note that $\|b_y\|^2_{L^2} \le \frac{1}{4} y^4 \|\Delta\varphi\|^2_{L^2}$ which is finite since $\Delta\varphi \in L^2$. This equation, together with equation (3.125), implies

$$\left| v(y) + \frac{1}{2}\|y\nabla\varphi\|^2_{L^2} \right| \;\le\; C(|y|^3 + |y|^4). \tag{3.127}$$

From this and from $v \in L^1 \cap L^\infty$, it is also easy to deduce that $|\cdot|^{-2} v \in L^1 \cap L^\infty$. We can thus write

$$\int \mathrm{d}y\, v(y) n_{0,1}(y) = \int \mathrm{d}y\, v(y) e^{-\alpha^2 \lambda y^2} + \int \mathrm{d}y\, |y|^{-2} v(y) y^2 \left(n_{0,1}(y) - e^{-\alpha^2 \lambda y^2}\right) \tag{3.128}$$

and use Lemma 3.5 for $g = |\cdot|^{-2}|v|$ to bound

$$\left| \int \mathrm{d}y\, |y|^{-2} v(y) y^2 (n_{0,1}(y) - e^{-\alpha^2 \lambda y^2}) \right| \leq C\alpha^{-6}. \tag{3.129}$$

Using equation (3.127), the definition of $\lambda = \frac{1}{6}\|\nabla\varphi\|_{L^2}^2$ as well as $\int y^2 e^{-y^2} \mathrm{d}y = \frac{3}{2}\pi^{3/2}$, we further have that

$$\left| \int \mathrm{d}y\, v(y) e^{-\alpha^2 \lambda y^2} + \frac{3}{2\alpha^2} \left(\frac{\pi}{\lambda \alpha^2}\right)^{3/2} \right| \leq C\alpha^{-6} \tag{3.130}$$

which finally gives the estimate

$$\left| \mathcal{E}_{21}^0 + \left(\frac{3}{2\alpha^2}\right) \mathcal{N} \right| \leq C_\varepsilon \sqrt{K} \alpha^{-6+\varepsilon} \tag{3.131}$$

using Proposition 3.17.

In a similar fashion as for $\mathcal{E}_{21}^0$, we obtain

$$\mathcal{E}_{21}^P = \frac{1}{\alpha^2 M^{\mathrm{LP}}} \int \left\langle iP\nabla\varphi | w_{P,y}^0 \right\rangle_{L^2} H(y) n_{0,1}(y) \mathrm{d}y. \tag{3.132}$$

Explicit computation, using $\Pi_0 = \frac{3}{\|\nabla\varphi\|_{L^2}^2} \sum_{i=1}^3 |\partial_i \varphi\rangle\langle\partial_i\varphi|$ and $\langle\varphi|\nabla\varphi\rangle_{L^2} = 0$, gives

$$\frac{1}{3} w_{P,y}^0(z) = -\frac{(\varphi * \nabla\varphi)(y)}{\|\nabla\varphi\|_{L^2}^2} \nabla\varphi(z) + \frac{iP}{\alpha^2 M^{\mathrm{LP}}} \left(\|\nabla\varphi\|_{L^2}^2 - (\nabla\varphi * \nabla\varphi)(y) \right) \frac{\nabla\varphi(z)}{\|\nabla\varphi\|_{L^2}^2}. \tag{3.133}$$

Note that the real part of the above is odd as a function of y and hence

$$\int \left\langle \nabla\varphi | \mathrm{Re}(w_{P,y}^0) \right\rangle_{L^2} n_{0,1}(y) H(y) \mathrm{d}y = 0, \tag{3.134}$$

and, taking rotational invariance of φ into account, we arrive at

$$\mathcal{E}_{21}^P = \frac{P^2}{\alpha^4 (M^{\mathrm{LP}})^2} \int \left(\|\nabla\varphi\|_2^2 - (\nabla\varphi * \nabla\varphi)(y) \right) n_{0,1}(y) H(y) \mathrm{d}y. \tag{3.135}$$

Further, note that $|\|\nabla\varphi\|_{L^2}^2 - (\nabla\varphi * \nabla\varphi)(y)| \leq Cy^2$ and thus, by Lemma 3.7 and Corollary 3.6, one obtains

$$|\mathcal{E}_{21}^P| \leq C\frac{P^2}{\alpha^9} \leq \frac{C}{\alpha^7}. \tag{3.136}$$

This completes the analysis of $\mathcal{E}_{21}$.

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In order to estimate the term $\mathcal{E}_{22}$, we proceed as before by splitting $\Upsilon_K = \Upsilon_K^< + \Upsilon_K^>$. Using equation (3.44), we can estimate

$$\left|\alpha^{-1}\int \mathrm{d}y \left\langle \Upsilon_K^> | (\phi(l_y) + \pi(j_y))(e^{A_{P,y}} - 1)W(\alpha w_{P,y})\Upsilon_K \right\rangle_{\mathcal{F}}\right| \leq C\alpha^{-1}\int \mathrm{d}y\, (\|l_y\|_{L^2} + \|j_y\|_{L^2})\|(\mathbb{N}+1)^{1/2}\Upsilon_K^>\|_{\mathcal{F}} \leq C_\delta\, \alpha^{-11} \tag{3.137}$$

where we used Corollary 3.14 and Lemmas 3.7 and 3.19. The term involving $\Upsilon_K^<$ is split again into two contributions,

$$\mathcal{E}_{22}^0 = \alpha^{-1}\int \mathrm{d}y \left\langle \Upsilon_K^< | \phi(l_y)(e^{A_{P,y}} - 1)W(\alpha w_{P,y})\Upsilon_K \right\rangle_{\mathcal{F}} \tag{3.138a}$$

$$\mathcal{E}_{22}^P = \alpha^{-1}\int \mathrm{d}y \left\langle \Upsilon_K^< | \pi(j_y)(e^{A_{P,y}} - 1)W(\alpha w_{P,y})\Upsilon_K \right\rangle_{\mathcal{F}}. \tag{3.138b}$$

To bound the first one, we proceed as in equation (3.107), that is, use Lemma 3.15 and the fact that $\phi(l_y)$ changes the number of phonons at most by one. This leads to

$$|\mathcal{E}_{22}^0| \leq \alpha^{-1}\int \mathrm{d}y\, \|e^{\kappa\mathbb{N}}\mathbb{U}_K(e^{-A_{P,y}} - 1)\phi(l_y)\Upsilon_K^<\|_{\mathcal{F}}\, n_{\delta,\eta}(y) \leq \sqrt{2}\alpha^{-1}\int \mathrm{d}y\, \|(e^{-A_{P,y}} - 1)\phi(l_y)\Upsilon_K^<\|_{\mathcal{F}}\, n_{\delta,\eta}(y). \tag{3.139}$$

Furthermore, we have

$$\|(e^{-A_{P,y}} - 1)\phi(l_y)\Upsilon_K^<\|_{\mathcal{F}} \leq \|A_{P,y}\phi(l_y)\Upsilon_K^<\|_{\mathcal{F}} \leq \|\phi(l_y)A_{P,y}\Upsilon_K^<\|_{\mathcal{F}} + \|[A_{P,y}, \phi(l_y)]\Upsilon_K^<\|_{\mathcal{F}} \leq C\alpha^{\delta/2}\big(\|l_y\|_{L^2}\|A_{P,y}\Upsilon_K\|_{\mathcal{F}} + \|y\nabla l_y\|_{L^2}\big), \tag{3.140}$$

where we used $[iP_f\, y, \phi(f)] = \pi(y\nabla f)$ and $\Upsilon_K^< = \mathbb{1}(\mathbb{N} \leq \alpha^\delta)\Upsilon_K$. Note that in order to estimate the remaining expression, it is not sufficient to directly apply Corollary 3.6. To obtain a better bound, we first replace $n_{\delta,\eta}(y)$ by $e^{-\eta\lambda\alpha^{2(1-\delta)}y^2}$ and then, for the part containing the Gaussian, we use that $\|l_y\|_{L^2}$ and $\|\nabla l_y\|_{L^2}$ provide additional factors of $|y|$, as is shown below. More precisely, with Lemma 3.19 and the aid of Lemmas 3.5 and 3.16, we bound

$$\alpha^{\frac{\delta}{2}-1}\int \mathrm{d}y\, \|l_y\|_{L^2}\|A_{P,y}\Upsilon_K\|_{\mathcal{F}}\, n_{\delta,\eta}(y) \tag{3.141}$$

$$\leq C\alpha^{\frac{\delta}{2}-1}\int \mathrm{d}y\, \|l_y\|_{L^2}(\sqrt{K}|y| + \alpha|y|^3)n_{\delta,\eta}(y) \leq C\alpha^{\frac{\delta}{2}-1}\int \mathrm{d}y\, \|l_y\|_{L^2}(\sqrt{K}|y| + \alpha|y|^3)e^{-\eta\lambda\alpha^{2(1-\delta)}y^2} + C\sqrt{K}\alpha^{-6+\frac{9\delta}{2}}. \tag{3.142}$$

Next, we use that by equation (3.125) there exists an L^2 function f such that

$$|l_y(z)| \leq \frac{1}{2}|y\nabla\varphi(z)| + f(z)y^2. \tag{3.143}$$

Hence, by integration

$$\alpha^{\delta/2-1}\int \mathrm{d}y\, \|l_y\|_{L^2}\Big(\sqrt{K}|y| + \alpha|y|^3\Big)e^{-\lambda\eta\alpha^{2(1-\delta)}y^2} \leq C\sqrt{K}\alpha^{-6+11/2\delta}. \tag{3.144}$$

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Regarding the second term in equation (3.140), we need to bound

$$\alpha^{\delta/2-1}\int \mathrm{d}y\,|y|\|\nabla l_y\|_{L^2} n_{\delta,\eta}(y), \tag{3.145}$$

where we proceed in a similar way as above, using that

$$\|\nabla l_y\|_{L^2}\ \le\ C(|y|+y^2). \tag{3.146}$$

In fact, since $\nabla\varphi(z)=-\langle\psi|h_{\cdot}(z)\nabla\psi\rangle_{L^2}-\langle\nabla\psi|h_{\cdot}(z)\psi\rangle_{L^2}$, we have the identity

$$\begin{aligned}\nabla l_y(z)\ &=\ H(y)\nabla\varphi(z)+\left\langle\nabla\psi|h_{\cdot}(z)T_y\psi\right\rangle_{L^2}+\left\langle\psi|h_{\cdot}(z)\nabla T_y\psi\right\rangle_{L^2}\\ &=\ (H(y)-1)\nabla\varphi(z)+\left\langle\nabla\psi|h_{\cdot}(z)(T_y-1)\psi\right\rangle_{L^2}+\left\langle\psi|h_{\cdot}(z)(T_y-1)\nabla\psi\right\rangle_{L^2}.\end{aligned} \tag{3.147}$$

Again, using that ψ has bounded derivatives, we have

$$\|(T_y-1)\psi\|_{L^\infty}+\|(T_y-1)\nabla\psi\|_{L^\infty}\le C|y|, \tag{3.148}$$

and the desired inequality now follows from $|H(y)-1|\le Cy^2$ and equation (3.123). Given equation (3.114), we can use Lemma 3.5 to replace $n_{\delta,\eta}(y)$ in equation (3.145) with $e^{-\lambda\eta\alpha^{2(1-\delta)}y^2}$ at the energy penalty $C\alpha^{-6+9\delta/2}$, and then use equation (3.146) to bound the remaining integral involving the Gaussian factor, which yields an error of the same order. Altogether, this gives the estimate

$$|\mathcal{E}_{22}^0|\ \le\ C\sqrt{K}\alpha^{-6+\frac{11}{2}\delta}. \tag{3.149}$$

For the term $\mathcal{E}_{22}^P$, we proceed in exactly the same way as in equation (3.139):

$$\begin{aligned}|\mathcal{E}_{22}^P|\ &\le\ \sqrt{2}\alpha^{-1}\int \mathrm{d}y\,\left\|\left(e^{-A_{P,y}}-1\right)\pi(j_y)\Upsilon_K^{<}\right\|_{\mathcal{F}}\,n_{\delta,\eta}(y)\\ &\le\ C\alpha^{\delta/2-1}\int \mathrm{d}y\,\|j_y\|_{L^2}\|A_{P,y}\Upsilon_K\|_{\mathcal{F}}\,n_{\delta,\eta}(y)+C\alpha^{\delta/2-1}\int \mathrm{d}y\,\|y\nabla j_y\|_{L^2}n_{\delta,\eta}(y)\\ &\le\ C\alpha^{\delta/2-1}\frac{|P|}{\alpha^2}\int \mathrm{d}y\,H(y)\,(\sqrt{K}|y|+\alpha|y|^3)n_{\delta,\eta}(y)\\ &\quad +C\alpha^{\delta/2-1}\frac{|P|}{\alpha^2}\int \mathrm{d}y\,|y|H(y)\,n_{\delta,\eta}(y)\\ &\le\ C\alpha^{-6+\frac{9}{2}\delta}\sqrt{K},\end{aligned} \tag{3.150}$$

where the last estimate follows from Corollary 3.6 and the assumption $|P|\le c\alpha$.

Combining the relevant estimates, that is, equations (3.103), (3.104), (3.106) and (3.110) for $\mathcal{E}_1$ as well as equations (3.131), (3.136), (3.137), (3.149) and (3.150) for $\mathcal{E}_2$, we arrive at the statement of Proposition 3.18, thus providing an appropriate bound for $\mathcal{E}$. □

Proof of Lemma 3.19. Since H has the desired properties, we need to show them for

$$l_y^{(1)}\ =\ \left\langle\psi|h_{\cdot}T_y\psi\right\rangle_{L^2}. \tag{3.151}$$

To this end, we introduce

$$\mathcal{S}\ =\ \{f\in L^p(\mathbb{R}^3,(1+|y|^n)\mathrm{d}y)\quad\forall 1\le p\le\infty,\quad\forall n\ge 0\} \tag{3.152}$$

and start with the following observation: Suppose f_1, f_2, f_3 and f_4 are functions in $\mathcal{S}$. Then

$$S(y) := \iint \mathrm{d}u\mathrm{d}v \frac{f_1(u)f_2(v)f_3(u+y)f_4(v+y)}{|u-v|} \in \mathcal{S}. \tag{3.153}$$

In fact, $|S(y)| \le C\|f_4\|_{L^\infty}\|f_3\|_{L^\infty}\|f_1\|_{L^p}\|f_2\|_{L^q}$ for all $1 < p < 3/2, q = 3p/(5p-3)$ by the Hardy–Littlewood–Sobolev inequality. Since $\int \mathrm{d}y|y|^n f_3(u+y) \le 2^{n-1}(|u|^n\|f_3\|_{L^1} + \||\cdot|^n f_3\|_{L^1})$, we have also

$$\int \mathrm{d}y|y|^n S(y) \le C\|f_4\|_{L^\infty}(\||\cdot|^n f_1\|_{L^p}\|f_2\|_{L^q}\|f_3\|_{L^1} + \|f_1\|_{L^p}\|f_2\|_{L^q}\||\cdot|^n f_3\|_{L^1}) \tag{3.154}$$

from which (3.153) follows. Moreover,

$$f \in \mathcal{S} \implies \sqrt{|f|} \in \mathcal{S}. \tag{3.155}$$

Indeed, we have for all $n \ge 0$,

$$\int |y|^n\sqrt{|f|}\mathrm{d}y \le \sqrt{\|f\|_{L^\infty}}\int_{|y|\le 1}|y|^n\mathrm{d}y + \frac{1}{2}\int |y|^{n+m}|f|\mathrm{d}y + \frac{1}{2}\int_{|y|>1}|y|^{n-m}\mathrm{d}y < \infty \tag{3.156}$$

since m can be chosen arbitrarily large by assumption. Thus, it suffices to prove the desired statement for the functions $\|\nabla^k l_y^{(1)}\|_{L^2}^2$. For $k = 0$, we use equation (3.124) to compute

$$\|l_y^{(1)}\|_{L^2}^2 = \frac{1}{4\pi}\iint \mathrm{d}u\mathrm{d}v \frac{\psi(u)\psi(v)\psi(y+u)\psi(v+y)}{|u-v|}. \tag{3.157}$$

The statement now follows easily from equation (3.153) and Lemma 3.7. Arguing again via equation (3.155), for $k = 1$ it suffices to show the statement for

$$\begin{aligned}\|\nabla l_y^{(1)}\|_{L^2}^2 &= \|\langle\nabla\psi|h.T_y\psi\rangle_{L^2} + \langle\psi|h.\nabla T_y\psi\rangle_{L^2}\|_{L^2}^2 \\ &\le 2\|\langle\nabla\psi|h.T_y\psi\rangle_{L^2}\|_{L^2}^2 + 2\|\langle\psi|h.\nabla T_y\psi\rangle_{L^2}\|_{L^2}^2\end{aligned} \tag{3.158}$$

(the first equality follows from $\nabla_z h_x(z) = -\nabla_x h_x(z)$ and integration by parts). Using (3.124), we find

$$\|\langle\nabla\psi|h.T_y\psi\rangle_{L^2}\|_{L^2}^2 \le C\iint \mathrm{d}u\mathrm{d}v \frac{|\nabla\psi(u)||\nabla\psi(v)|\psi(v+y)\psi(u+y)}{|u-v|}, \tag{3.159a}$$

$$\|\langle\psi|h.\nabla T_y\psi\rangle_{L^2}\|_{L^2}^2 \le C\iint \mathrm{d}u\mathrm{d}v \frac{|\nabla\psi(u+y)||\nabla\psi(v+y)|\psi(v)\psi(u)}{|u-v|}. \tag{3.159b}$$

We arrive at the desired conclusion by Lemma 3.7 and equation (3.153). □

3.7. *Energy contribution $\mathcal{G}$*

The energy contribution $\mathcal{G}$, defined in equation (3.8b), is evaluated by the following proposition.

Proposition 3.20. *Let $\mathbb{H}_K$ as in equation (2.4), $\mathbb{N}_1 = \mathrm{d}\Gamma(\Pi_1)$ and choose $c > 0$. For every $\varepsilon > 0$, there exists a constant $C_\varepsilon > 0$ (we omit the dependence on c) such that*

$$\left|\mathcal{G} - \mathcal{N}\frac{2}{\alpha^2}\langle\Upsilon_K|(\mathbb{H}_K - \mathbb{N}_1)\Upsilon_K\rangle_{\mathcal{F}}\right| \le C_\varepsilon\,\alpha^\varepsilon\left(\sqrt{K}\alpha^{-6} + K^{-1/2}\alpha^{-5}\right) \tag{3.160}$$

for all $|P|/\alpha \le c$ and all α large enough.

Proof. Using $h^{\mathrm{Pek}}G^0_K = 0$ and $\mathbb{N}G^0_K = \mathbb{N}_1 G^0_K$, we can decompose $\mathcal{G}$ into two terms

$$\begin{aligned}\mathcal{G} &= -\frac{2}{\alpha}\int \mathrm{d}y\ \mathrm{Re}\left\langle G^0_K|(\alpha^{-2}\mathbb{N}_1 + \alpha^{-1}\phi(h_{\cdot} + \varphi_P))T_y e^{A_{P,y}} W(\alpha w_{P,y})G^1_K\right\rangle_{\mathscr{H}} \\ &= \mathcal{G}_1 + \mathcal{G}_2,\end{aligned} \tag{3.161}$$

where the first term will contribute to the error while the second one provides an energy contribution of order α^{-2}. We proceed for each one separately.
Term $\mathcal{G}_1$. With the aid of equations (3.67) and (3.80) and $(T_y e^{A_{P,y}})^\dagger = T_{-y}e^{-A_{P,y}}$, one finds

$$\mathcal{G}_1 = -\frac{2}{\alpha^3}\int \mathrm{d}y\ \mathrm{Re}\left\langle R_{3,y}\psi\otimes\left(\Upsilon^<_K + \Upsilon^>_K\right)|W(\alpha w_{P,y})G^0_K\right\rangle_{\mathscr{H}} = \mathcal{G}^<_1 + \mathcal{G}^>_1, \tag{3.162}$$

where we introduced the operator $R_{3,y} = R^1_{3,y} + R^2_{3,y}$ with

$$R^1_{3,y} = P_\psi \phi(h^1_{K,\cdot})Ru_\alpha T_{-y}P_\psi e^{-A_{P,y}}\mathbb{N}_1 \tag{3.163a}$$

$$R^2_{3,y} = 2\alpha P_\psi \left\langle h_{K,\cdot}|\,\mathrm{Re}(w^1_{P,y})\right\rangle_{L^2} Ru_\alpha T_{-y}P_\psi e^{-A_{P,y}}\mathbb{N}_1. \tag{3.163b}$$

Proceeding similarly as for $R^1_{1,y}$ and $R^2_{2,y}$ in equations (3.82a) and (3.82b), one further verifies

$$\|R_{3,y}\Psi\|_{\mathscr{H}} \le C\|u_\alpha T_{-y}P_\psi\|_{\mathrm{op}}\left(1+\alpha y^2\right)\|(\mathbb{N}+1)^{3/2}\Psi\|_{\mathscr{H}}. \tag{3.164}$$

Recalling the definition $f_\alpha(y) = \|u_\alpha T_{-y}P_\psi\|_{\mathrm{op}}$ and equation (3.86), we can use Corollary 3.14 to find

$$|\mathcal{G}^>_1| \le \frac{C}{\alpha^3}\|(\mathbb{N}+1)^{3/2}\Upsilon^>_K\|_{\mathcal{F}}\int \mathrm{d}y\ f_\alpha(y)(1+\alpha y^2) \le C_\delta\,\alpha^{-7}. \tag{3.165}$$

In the first term, we proceed with equation (3.74) and Lemma 3.15 to obtain

$$\begin{aligned}|\mathcal{G}^<_1| &\le \frac{2}{\alpha^3}\int \mathrm{d}y\ \|e^{\kappa\mathbb{N}}\mathbb{U}_K(R_{3,y}\psi\otimes\Upsilon^<_K)\|_{\mathscr{H}}\,\|e^{-\kappa\mathbb{N}}W(\alpha\widetilde{w}_{P,y})\Omega\|_{\mathcal{F}} \\ &\le \frac{2\sqrt{2}}{\alpha^3}\int \mathrm{d}y\ \|R_{3,y}\psi\otimes\Upsilon_K\|_{\mathscr{H}}\,n_{\delta,\eta}(y) \le \frac{C}{\alpha^3}\int \mathrm{d}y\ f_\alpha(y)(1+\alpha y^2)\,n_{\delta,\eta}(y),\end{aligned} \tag{3.166}$$

which brings us again into a position to apply Corollary 3.6. Hence,

$$|\mathcal{G}^<_1| \le C\alpha^{-6+3\delta}. \tag{3.167}$$

Term $\mathcal{G}_2$. Here, we have

$$\begin{aligned}\mathcal{G}_2 = &-\frac{2}{\alpha^2}\int \mathrm{d}y\ \mathrm{Re}\left\langle G^0_K|\phi(h_{\cdot}+\varphi_P)T_y W(\alpha w_{P,y})G^1_K\right\rangle_{\mathscr{H}} \\ &-\frac{2}{\alpha^2}\int \mathrm{d}y\ \mathrm{Re}\left\langle G^0_K|\phi(h_{\cdot}+\varphi_P)T_y(e^{A_{P,y}}-1)W(\alpha w_{P,y})G^1_K\right\rangle_{\mathscr{H}} = \mathcal{G}_{21}+\mathcal{G}_{22}.\end{aligned} \tag{3.168}$$

To separate the leading order contribution in $\mathcal{G}_{21}$, we insert $1 = \mathbb{U}^\dagger_K\mathbb{U}_K$ next to G^0_K and bring $\mathbb{U}^\dagger_K$ to the right side of the inner product. With $\mathbb{U}_K\Upsilon_K = \Omega$, equation (3.53c) and equation (3.63) this gives

$$\mathcal{G}_{21} = -\frac{2}{\alpha^2}\int \mathrm{d}y\ \mathrm{Re}\left\langle \psi\otimes\Omega|a(\underline{h_{\cdot}+\varphi_P})T_y W(\alpha\widetilde{w}_{P,y})u_\alpha Ra^\dagger(\underline{h^1_{K,\cdot}})\psi\otimes\Omega\right\rangle_{\mathscr{H}}, \tag{3.169}$$

where $\underline{\cdot}$ is defined in equation (3.52a). Next, we write $W(\alpha\widetilde{w}_{P,y}) = n_{0,1}(y)e^{a^\dagger(\alpha\widetilde{w}_{P,y})}e^{-a(\alpha\widetilde{w}_{P,y})}$ and move the first exponential to the left side and the second exponential to the right side until they act both on the Fock space vacuum. Using $e^{-a(f)}a^\dagger(g)e^{a(f)} = a^\dagger(g) - \langle f|g\rangle$, we find this way

$$\mathcal{G}_{21} = -\frac{2}{\alpha^2}\int \mathrm{d}y\, n_{0,1}(y)\ \mathrm{Re}\left\langle \psi\otimes\Omega|a(\underline{h_\cdot + \varphi_P})T_y u_\alpha R a^\dagger(\underline{h^1_{K,\cdot}})\psi\otimes\Omega\right\rangle_{\mathscr{H}} \tag{3.170a}$$

$$+2\int \mathrm{d}y\, n_{0,1}(y)\ \mathrm{Re}\left\langle \psi\otimes\Omega|\langle\underline{h_\cdot + \varphi_P}|\widetilde{w}_{P,y}\rangle_{L^2} T_y u_\alpha R\langle\widetilde{w}_{P,y}|\underline{h^1_{K,\cdot}}\rangle_{L^2}\psi\otimes\Omega\right\rangle_{\mathscr{H}}. \tag{3.170b}$$

In the first line, we write $h_\cdot + \varphi_P = h^0_\cdot + h^1_\cdot + \varphi + i\xi_P$, with $h^i_\cdot = (\Pi_i h)_\cdot$, and use that

$$\left\langle \psi\otimes\Omega|a(\underline{h^0_\cdot + i\xi_P})T_y u_\alpha R a^\dagger(\underline{h^1_{K,\cdot}})\psi\otimes\Omega\right\rangle_{\mathscr{H}} = 0 \tag{3.171}$$

since $h^0_x + i\xi_P \in \mathrm{Ran}(\Pi_0)$ whereas $h^1_{K,x} \in \mathrm{Ran}(\Pi_1)$. Finally, we can replace a and $a^\dagger$ by ϕ, and then transform back with $\mathbb{U}_K$, using equation (3.53c), in order to obtain

$$(3.170\mathrm{a}) \ = \ -\frac{2}{\alpha^2}\int \mathrm{d}y\, n_{0,1}(y)\ \mathrm{Re}\left\langle \psi\otimes\Upsilon_K|\phi(h^1_\cdot + \varphi)T_y u_\alpha R\phi(h^1_{K,\cdot})\psi\otimes\Upsilon_K\right\rangle_{\mathscr{H}}. \tag{3.172}$$

To summarize, we have shown that

$$\mathcal{G}_{21} = -\frac{2}{\alpha^2}\int \mathrm{d}y\ \mathrm{Re}\left\langle G^0_K|L_{2,y}G^0_K\right\rangle_{\mathscr{H}} n_{0,1}(y) + \int \mathrm{d}y\,\ell_2(y)n_{0,1}(y) = \mathcal{G}_{211} + \mathcal{G}_{212} \tag{3.173}$$

with

$$L_{2,y} \ = \ P_\psi\phi(h^1_\cdot + \varphi)T_y u_\alpha R\phi(h^1_{K,\cdot})P_\psi \tag{3.174a}$$

$$\ell_2(y) \ = \ 2\,\mathrm{Re}\left\langle\psi|\langle\underline{h_\cdot + \varphi_P}|\widetilde{w}_{P,y}\rangle_{L^2} T_y u_\alpha R\langle\widetilde{w}^1_{P,y}|\underline{h^1_{K,\cdot}}\rangle_{L^2}\psi\right\rangle_{L^2}. \tag{3.174b}$$

In the first term, we add and subtract the Gaussian,

$$\begin{aligned}\mathcal{G}_{211} =& -\frac{2}{\alpha^2}\int \mathrm{d}y\ \mathrm{Re}\left\langle G^0_K|L_{2,y}G^0_K\right\rangle_{\mathscr{H}} e^{-\lambda\alpha^2 y^2}\\ &-\frac{2}{\alpha^2}\int \mathrm{d}y\ \mathrm{Re}\left\langle G^0_K|L_{2,y}G^0_K\right\rangle_{\mathscr{H}}\left(n_{0,1}(y) - e^{-\lambda\alpha^2y^2}\right) \ = \ \mathcal{G}^{\mathrm{lo}}_{211} + \mathcal{G}^{\mathrm{err}}_{211},\end{aligned} \tag{3.175}$$

and proceed with $\mathcal{G}^{\mathrm{lo}}_{211}$ by inserting $h^1_\cdot = h^1_{K,\cdot} + (h^1_\cdot - h^1_{K,\cdot})$, $T_y = 1 + (T_y - 1)$ and $u_\alpha = 1 + (u_\alpha - 1)$,

$$\begin{aligned}\mathcal{G}^{\mathrm{lo}}_{211} =& -\frac{2}{\alpha^2}\mathrm{Re}\left\langle G^0_K|\phi(h^1_{K,\cdot} + \varphi)R\phi(h^1_{K,\cdot})G^0_K\right\rangle_{\mathscr{H}}\int \mathrm{d}y\, e^{-\lambda\alpha^2y^2}\\ &-\frac{2}{\alpha^2}\mathrm{Re}\left\langle G^0_K|\phi(h^1_{K,\cdot} + \varphi)(u_\alpha - 1)R\phi(h^1_{K,\cdot})G^0_K\right\rangle_{\mathscr{H}}\int \mathrm{d}y\, e^{-\lambda\alpha^2y^2}\\ &-\frac{2}{\alpha^2}\int \mathrm{d}y\ \mathrm{Re}\left\langle G^0_K|\phi(h^1_{K,\cdot} + \varphi)(T_y - 1)u_\alpha R\phi(h^1_{K,\cdot})G^0_K\right\rangle_{\mathscr{H}} e^{-\lambda\alpha^2y^2}\\ &-\frac{2}{\alpha^2}\int \mathrm{d}y\ \mathrm{Re}\left\langle G^0_K|\phi(h^1_\cdot - h^1_{K,\cdot})T_y u_\alpha R\phi(h^1_{K,\cdot})G^0_K\right\rangle_{\mathscr{H}} e^{-\lambda\alpha^2y^2}\\ =& \sum_{n=1}^{4}\mathcal{G}^{\mathrm{lo},n}_{211}.\end{aligned} \tag{3.176}$$

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Since $P_\psi \phi(\varphi) R = 0$, we have $\mathcal{G}^{\mathrm{lo},1}_{211} = \frac{2}{\alpha^2}\big\langle \Upsilon_K | (\mathbb{H}_K - \mathbb{N}_1)\Upsilon_K \big\rangle_{\mathcal{F}} (\frac{\pi}{\lambda\alpha^2})^{3/2}$, cf. (2.4), and hence we can use Proposition 3.17 to conclude that

$$\left| \mathcal{G}^{\mathrm{lo},1}_{211} - \mathcal{N}\frac{2}{\alpha^2}\big\langle \Upsilon_K | (\mathbb{H}_K - \mathbb{N}_1)\Upsilon_K \big\rangle_{\mathcal{F}} \right| \le C_\varepsilon \sqrt{K}\alpha^{-6+\varepsilon}. \tag{3.177}$$

For the other terms, we shall show the combined error estimate

$$|\mathcal{G}^{\mathrm{lo},2}_{211}| + |\mathcal{G}^{\mathrm{lo},3}_{211}| + |\mathcal{G}^{\mathrm{lo},4}_{211}| \le C\big(\sqrt{K}\alpha^{-6} + K^{-1/2}\alpha^{-5}\big). \tag{3.178}$$

In the last term, we recall $h_\cdot(y) = h_{K=\infty,\cdot}(y)$, and apply Lemma 3.9 in combination with $\|R^{1/2} u_\alpha T_{-y}\nabla\|_{\mathrm{op}} \le C$. This gives

$$\begin{aligned} |\mathcal{G}^{\mathrm{lo},4}_{211}| &\le \frac{2}{\alpha^2}\int \mathrm{d}y\, e^{-\lambda\alpha^2 y^2}\, \|R^{1/2}u_\alpha T_{-y}\phi(h^1_\cdot - h^1_{K,\cdot})P_\psi G^0_K\|_{\mathscr{H}}\, \|R^{1/2}\phi(h^1_{K,\cdot})P_\psi G^0_K\|_{\mathscr{H}} \\ &\le C\alpha^{-5}K^{-1/2}. \end{aligned} \tag{3.179}$$

Next, we write $T_y - 1 = \int_0^1 \mathrm{d}s T_{sy}(y\nabla)$ in the third term to obtain an additional $|y|$,

$$\begin{aligned} |\mathcal{G}^{\mathrm{lo},3}_{211}| &\le \frac{2}{\alpha^2}\left(\int \mathrm{d}y\, |y| e^{-\lambda\alpha^2 y^2}\right)\|\nabla u_\alpha R^{1/2}\|_{\mathrm{op}}\, \|\phi(h^1_{K,\cdot} + \varphi)G^0_K\|_{\mathscr{H}} \|R^{1/2}\phi(h^1_{K,\cdot})G^0_K\|_{\mathscr{H}} \\ &\le C\alpha^{-6}\sqrt{K}, \end{aligned} \tag{3.180}$$

where the factor $\sqrt{K}$ comes from the L^2 norm of $h^1_{K,0}$ in the bound on the first field operator (since $\Delta R^{1/2}$ is unbounded, we cannot apply the commutator method to this part). In the second term, we use $\psi(x) \le Ce^{-|x|/C}$ for some $C > 0$, and thus $\|(u_\alpha - 1)\psi\|_{L^2} \le Ce^{-\alpha/C}$, to estimate

$$|\mathcal{G}^{\mathrm{lo},2}_{211}| \le \frac{C}{\alpha^5}\|(u_\alpha - 1)\psi\|_{L^2}\, \|\phi(h^1_{K,\cdot} + \varphi)R\phi(h^1_{K,\cdot})G^0_K\|_{\mathscr{H}} \le C\sqrt{K}e^{-\alpha/C}. \tag{3.181}$$

This proves equation (3.178).

To bound the remaining contributions in $\mathcal{G}^{\mathrm{err}}_{211}$ and $\mathcal{G}_{212}$, we shall use

$$\big|\big\langle G^0_K | L_{2,y} G^0_K \big\rangle\big| \le C f_{2,\alpha}(y) \tag{3.182a}$$

$$|\ell_2(y)| \le C f_{2,\alpha}(y)(y^2 + \alpha^{-2})(|y| + |y|^3 + \alpha^{-2}), \tag{3.182b}$$

where

$$f_{2,\alpha}(y) = \|u_\alpha T_{-y}P_\psi\|_{\mathrm{op}} + \|\nabla u_\alpha T_{-y}P_\psi\|_{\mathrm{op}}. \tag{3.183}$$

Using the exponential decay of ψ and $|\nabla^k u_\alpha|(y) \le \mathbb{1}(|y| \le 2\alpha)$, for $k = 0, 1$, it is easy to show that

$$\|f_{2,\alpha}\|_{L^\infty} \le C \quad \text{and} \quad \||\cdot|^n f_{2,\alpha}\|_{L^1} \le C_n \alpha^{3+n} \quad \text{for all } n \in \mathbb{N}_0. \tag{3.184}$$

To verify equations (3.182a) and (3.182b), use $u_\alpha T_{-y}\phi(h_\cdot) = \phi(h_{\cdot - y})u_\alpha T_{-y}$ and Cauchy–Schwarz to bound

$$\big|\big\langle G^0_K | L_{2,y} G^0_K \big\rangle_{\mathscr{H}}\big| \le \|R^{1/2}\phi(h^1_{\cdot - y} + \varphi)u_\alpha T_{-y}P_\psi G^0_K\|_{\mathscr{H}}\, \|R^{1/2}\phi(h^1_{K,\cdot})P_\psi G^0_K\|_{\mathscr{H}}. \tag{3.185}$$

Now, we can use equation (3.44) and Lemma 3.9 to obtain equation (3.182a). To estimate $\ell_2(y)$, defined in equation (3.174b), we proceed with

$$|\ell_2(y)| \le 2\Big|\big\langle \psi|T_y u_\alpha \langle \underline{h_{\cdot-y}}|\widetilde{w}_{P,y}\rangle_{L^2} R\langle \widetilde{w}^1_{P,y}|\underline{h^1_{K,\cdot}}\rangle_{L^2}\psi\big\rangle_{L^2}\Big| \tag{3.186a}$$

$$+\ 2\Big|\big\langle \psi|T_y u_\alpha \langle \underline{\varphi_P}|\widetilde{w}_{P,y}\rangle_{L^2} R\langle \widetilde{w}^1_{P,y}|\underline{h^1_{K,\cdot}}\rangle_{L^2}\psi\big\rangle_{L^2}\Big|, \tag{3.186b}$$

and considering the first line, we use Cauchy–Schwarz, write out the two inner products (in the phonon variable) and then use Cauchy–Schwarz again,

$$\begin{aligned} |((3.186a)| &\le 2\int \mathrm{d}u\, |\widetilde{w}_{P,y}(u)|\, \|P_\psi T_y u_\alpha \underline{h_{\cdot-y}}(u) R^{1/2}\|_{\mathrm{op}} \int \mathrm{d}z\, |\widetilde{w}^1_{P,y}(z)|\, \|R^{1/2}\underline{h^1_{K,\cdot}}(z)\psi\| \\ &\le 2\|\widetilde{w}_{P,y}\|_{L^2}\|\widetilde{w}^1_{P,y}\|_{L^2}\left(\int \mathrm{d}u \|P_\psi T_y u_\alpha \underline{h_{\cdot-y}}(u)R^{1/2}\|^2_{\mathrm{op}} \int \mathrm{d}z \|R^{1/2}\underline{h^1_{K,\cdot}}(z)\psi\|^2_{L^2}\right)^{1/2} \\ &\le C f_{2,\alpha}(y)(|y| + y^3 + \alpha^{-2})(y^2 + \alpha^{-2}), \end{aligned} \tag{3.187}$$

where the last step follows from Lemma 3.4 and Corollary 3.11 together with $\underline{h_{K,\cdot}} = h^0_{K,\cdot} + \Theta_K^{-1} h^1_{K,\cdot}$. Since the second line is estimated similarly, we arrive at equation (3.182b). With equation (3.182a) at hand, we can apply Lemma 3.5 and equation (3.184) to get

$$|\mathcal{G}^{\mathrm{err}}_{211}| \le \frac{2}{\alpha^2}\int \mathrm{d}y\, \big|\big\langle G^0_K|L_{2,y}G^0_K\big\rangle_{\mathscr{H}}\big|\, \big|n_{0,1}(y) - e^{-\lambda\alpha^2 y^2}\big| \le C\alpha^{-6}, \tag{3.188}$$

and further, using equation (3.182b) and Corollary 3.6, we obtain

$$|\mathcal{G}_{212}| \le C\int \mathrm{d}y\, |\ell_2(y)|\, n_{0,1}(y) \le C\alpha^{-6}. \tag{3.189}$$

This completes the analysis of $\mathcal{G}_{21}$.

Next, we introduce $R_{4,y} = R^1_{4,y} + R^2_{4,y}$ with

$$R^1_{4,y} = P_\psi \phi(h^1_{K,\cdot}) R^{\frac12}(e^{-A_{P,y}} - 1) R^{\frac12}\phi(h_{\cdot-y} + \varphi_P) u_\alpha T_{-y} P_\psi \tag{3.190a}$$

$$R^2_{4,y} = 2\alpha P_\psi \big\langle h_{K,\cdot}|\operatorname{Re}(w^1_{P,y})\big\rangle_{L^2} R^{\frac12}(e^{-A_{P,y}} - 1) R^{\frac12}\phi(h_{\cdot-y} + \varphi_P) u_\alpha T_{-y} P_\psi. \tag{3.190b}$$

Inserting equations (3.67) and (3.80) into equation (3.168) it follows that

$$\mathcal{G}_{22} = -\frac{2}{\alpha^2}\int \mathrm{d}y\, \operatorname{Re}\big\langle R_{4,y}\psi \otimes (\Upsilon^<_K + \Upsilon^>_K)|W(\alpha w_{P,y})G^0_K\big\rangle_{\mathscr{H}} = \mathcal{G}^<_{22} + \mathcal{G}^>_{22}. \tag{3.191}$$

With the aid of Lemma 3.9, we obtain

$$\|R^1_{4,y}\Psi\|_{\mathscr{H}} \le C\|(e^{-A_{P,y}} - 1)(\mathbb{N}+1)^{1/2} R^{1/2}\phi(h_{\cdot-y} + \varphi_P) u_\alpha T_{-y} P_\psi \Psi\|_{\mathscr{H}}, \tag{3.192}$$

and proceeding similarly as in equation (3.84), we find

$$\|R^2_{4,y}\Psi\|_{\mathscr{H}} \le C\alpha(y^2 + \alpha^{-2})\|(e^{-A_{P,y}} - 1) R^{1/2}\phi(h_{\cdot-y} + \varphi_P) u_\alpha T_{-y} P_\psi \Psi\|_{\mathscr{H}}. \tag{3.193}$$

For $\Psi = \psi \otimes \Upsilon_K^{>}$, a second application of Lemma 3.9 (after using unitarity of $e^{-A_{P,y}}$) together with $\|\varphi_P\|_{L^2}^2 \le C$ for $|P|/\alpha \le c$ and Corollary 3.14 is sufficient to find

$$\begin{aligned}\|R_{4,y}\psi \otimes \Upsilon_K^{>}\|_{\mathscr{H}} &\le C\big(\|u_\alpha T_{-y} P_\psi\|_{\mathrm{op}} + \|\nabla u_\alpha T_{-y} P_\psi\|_{\mathrm{op}}\big)(1+\alpha y^2)\|(\mathbb{N}+1)\Upsilon_K^{>}\|_{\mathcal{F}}\\ &\le C_\delta\, \alpha^{-10} f_{2,\alpha}(y)(1+\alpha y^2)\end{aligned} \tag{3.194}$$

with $f_{2,\alpha}$ defined in equation (3.183). Using this bound in $G_{22}^{>}$ and recalling Corollary 3.14 and equation (3.184) we thus obtain

$$|\mathcal{G}_{22}^{>}| \le C_\delta\, \alpha^{-6}. \tag{3.195}$$

In $\mathcal{G}_{22}^{<}$, we proceed by inserting equation (3.70) and use equation (3.74) and Lemma 3.15. This gives

$$|\mathcal{G}_{22}^{<}| \le \frac{2\sqrt{2}}{\alpha^2}\int \mathrm{d}y\, \|R_{4,y}\psi \otimes \Upsilon_K^{<}\|_{\mathscr{H}}\, n_{\delta,\eta}(y). \tag{3.196}$$

The derivation of a suitable bound for the norm in the integrand is more cumbersome, so we go through it step by step. To shorten the notation let $G_K^{0<} = \psi \otimes \Upsilon_K^{<}$. We start from equations (3.192) and (3.193) where we insert $h_\cdot = h_{K,\cdot} + (h_\cdot - h_{K,\cdot})$ and use the triangle inequality,

$$\|R_{4,y}^1 G_K^{0<}\|_{\mathscr{H}} \le C\|(e^{-A_{P,y}}-1)(\mathbb{N}+1)^{1/2}R^{\frac12}\phi(h_{K,\cdot-y}+\varphi_P)u_\alpha T_{-y}G_K^{0<}\|_{\mathscr{H}} \tag{3.197a}$$

$$+\, C\|(e^{-A_{P,y}}-1)(\mathbb{N}+1)^{1/2}R^{\frac12}\phi(h_{\cdot-y}-h_{K,\cdot-y})u_\alpha T_{-y}G_K^{0<}\|_{\mathscr{H}}, \tag{3.197b}$$

$$\|R_{4,y}^2 G_K^{0<}\|_{\mathscr{H}} \le C\alpha(y^2+\alpha^{-2})\|(e^{-A_{P,y}}-1)R^{\frac12}\phi(h_{K,\cdot-y}+\varphi_P)u_\alpha T_{-y}G_K^{0<}\|_{\mathscr{H}} \tag{3.197c}$$

$$+\, C\alpha(y^2+\alpha^{-2})\|(e^{-A_{P,y}}-1)R^{\frac12}u_\alpha\phi(h_{\cdot-y}-h_{K,\cdot-y})u_\alpha T_{-y}G_K^{0<}\|_{\mathscr{H}}. \tag{3.197d}$$

For the second and fourth line, we apply Lemma 3.9 a second time (after bringing $(\mathbb{N}+1)^{1/2}$ to the right of a and $a^\dagger$) to find

$$\begin{aligned}(3.197\mathrm{b}) + (3.197\mathrm{d}) &\le CK^{-1/2}(1+\alpha y^2)(\|u_\alpha T_{-y}P_\psi\|_{\mathrm{op}} + \|\nabla u_\alpha T_{-y}P_\psi\|_{\mathrm{op}})\|(\mathbb{N}+1)\Upsilon_K^{<}\|_{\mathcal{F}}\\ &\le CK^{-1/2}(1+\alpha y^2)f_{2,\alpha}(y).\end{aligned} \tag{3.198}$$

In the first and third line, we use the functional calculus and write out $A_{P,y} = iP_f y + i g_P(y)$,

$$(3.197\mathrm{a}) + (3.197\mathrm{c}) \le C\|(P_f y)(\mathbb{N}+1)^{1/2}R^{\frac12}\phi(h_{K,\cdot-y}+\varphi_P)u_\alpha T_{-y}G_K^{0<}\|_{\mathscr{H}} \tag{3.199a}$$

$$+\, C\alpha(y^2+\alpha^{-2})\|(P_f y)R^{\frac12}\phi(h_{K,\cdot-y}+\varphi_P)u_\alpha T_{-y}G_K^{0<}\|_{\mathscr{H}} \tag{3.199b}$$

$$+\, C|g_P(y)|\|(\mathbb{N}+1)^{1/2}R^{1/2}\phi(h_{K,\cdot-y}+\varphi_P)u_\alpha T_{-y}G_K^{0<}\|_{\mathscr{H}} \tag{3.199c}$$

$$+\, C\alpha(y^2+\alpha^{-2})|g_P(y)|\|R^{\frac12}\phi(h_{K,\cdot-y}+\varphi_P)u_\alpha T_{-y}G_K^{0<}\|_{\mathscr{H}}. \tag{3.199d}$$

Now, we use $[iP_f y, \phi(f)] = \pi(y\nabla f)$ such that we can estimate the first line by

$$\begin{aligned}(3.199\mathrm{a}) \le C\big(&\|(\mathbb{N}+1)^{1/2}R^{1/2}\phi(h_{K,\cdot-y}+\varphi_P)(P_f y)u_\alpha T_{-y}G_K^{0<}\|_{\mathscr{H}}\\ &+\|(\mathbb{N}+1)^{1/2}R^{1/2}\pi(y\nabla h_{K,\cdot-y}+y\nabla\varphi_P)u_\alpha T_{-y}G_K^{0<}\|_{\mathscr{H}}\big).\end{aligned} \tag{3.200}$$

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To bound the first line, we use again Lemma 3.9, while in the second line we use $(\nabla h_K)_\cdot = -\nabla(h_{K,\cdot}) = -[\nabla, h_{K,\cdot}]$ and (3.44) together with $\|\nabla\varphi_P\|_{L^2} \le C$ for $|P|/\alpha \le c$. Together, we obtain

$$
\begin{aligned}
(3.199a) &\le C|y|\big(\|u_\alpha T_{-y}P_\psi\|_{\mathrm{op}} + \|\nabla u_\alpha T_{-y}P_\psi\|_{\mathrm{op}}\big)\big(\|(\mathbb{N}+1)P_f\Upsilon_K^<\|_{\mathcal{F}} + \sqrt{K}\|(\mathbb{N}+1)\Upsilon_K^<\|_{\mathcal{F}}\big)\\
&\le C\alpha^\delta|y|f_{2,\alpha}(y)\big(\|P_f\Upsilon_K^<\|_{\mathcal{F}} + \sqrt{K}\big)\\
&\le C\alpha^\delta\sqrt{K}|y|f_{2,\alpha}(y), \qquad (3.201)
\end{aligned}
$$

where the factor $\sqrt{K}$ in the first step comes from the L^2-norm of $h_{K,0}$, and the last step follows from Lemma 3.16. In a similar fashion, one shows

$$(3.199b) \le C\alpha^\delta\sqrt{K}|y|(1+\alpha y^2)f_{2,\alpha}(y), \qquad (3.202)$$

and, with equation (3.77), one also verifies

$$(3.199c) + (3.199d) \le C\alpha^\delta(\alpha^2|y|^5 + \alpha|y|^3)f_{2,\alpha}(y). \qquad (3.203)$$

Collecting the estimates (3.198), (3.201), (3.202) and (3.203), we arrive at

$$\|R_{4,y}\psi\otimes\Upsilon_K^<\|_{\mathscr{H}} \le Cf_{2,\alpha}(y)\alpha^\delta\Big(K^{-\frac{1}{2}}(1+\alpha y^2) + \alpha^2|y|^5 + \sqrt{K}(|y| + \alpha|y|^3)\Big). \qquad (3.204)$$

Now, we can apply Corollary 3.6 together with equation (3.184) to bound the right side of equation (3.196). The result is

$$|\mathcal{G}_{22}^<| \le C\alpha^{-2+\delta}\big(K^{-1/2}\alpha^{-3} + \sqrt{K}\alpha^{-4+4\delta}\big). \qquad (3.205)$$

In view of the estimates (3.165), (3.167), (3.177), (3.178), (3.188), (3.189), (3.195) and (3.205), the proof of Proposition 3.20 is now complete. □

3.8. *Energy contribution* $\mathcal{K}$

Recall that $\mathcal{K}$ was defined in (3.8c).

Proposition 3.21. *Let $\mathbb{H}_K$ as in equation (2.4), $\mathbb{N}_1 = \mathrm{d}\Gamma(\Pi_1)$ and choose $c > 0$. For every $\varepsilon > 0$, there exists a constant $C_\varepsilon > 0$ (we omit the dependence on c) such that*

$$\left|\mathcal{K} + \mathcal{N}\frac{1}{\alpha^2}\big\langle\Upsilon_K|(\mathbb{H}_K - \mathbb{N}_1)\Upsilon_K\big\rangle_{\mathcal{F}}\right| \le C_\varepsilon\alpha^\varepsilon\big(\sqrt{K}\alpha^{-6} + K^{-1/2}\alpha^{-5}\big) \qquad (3.206)$$

for all $|P|/\alpha \le c$ and all α large enough.

Proof. We split this contribution into three terms

$$
\begin{aligned}
\mathcal{K} &= \frac{1}{\alpha^2}\int \mathrm{d}y\,\big\langle G_K^1|\big(h^{\mathrm{Pek}} + \alpha^{-2}\mathbb{N} + \alpha^{-1}\phi(h_\cdot + \varphi_P)\big)T_y e^{A_{P,y}}W(\alpha w_{P,y})G_K^1\big\rangle_{\mathscr{H}}\\
&= \mathcal{K}_1 + \mathcal{K}_2 + \mathcal{K}_3, \qquad (3.207)
\end{aligned}
$$

and note that $\mathcal{K}_1$ provides the energy contribution of order α^{-2}.

Term $\mathcal{K}_1$. We start again by writing

$$
\begin{aligned}
\mathcal{K}_1 &= \frac{1}{\alpha^2}\int \mathrm{d}y\,\big\langle G_K^1|h^{\mathrm{Pek}}T_yW(\alpha w_{P,y})G_K^1\big\rangle_{\mathscr{H}}\\
&\quad + \frac{1}{\alpha^2}\int \mathrm{d}y\,\big\langle G_K^1|h^{\mathrm{Pek}}T_y(e^{A_{P,y}} - 1)W(\alpha w_{P,y})G_K^1\big\rangle_{\mathscr{H}} = \mathcal{K}_{11} + \mathcal{K}_{12}, \qquad (3.208)
\end{aligned}
$$

and proceed for the first term similarly as in the computation of $\mathcal{G}_2$; see equation (3.168). This leads to

$$\begin{aligned}\mathcal{K}_{11} &= \frac{1}{\alpha^2}\int \mathrm{d}y\,\langle G_K^0|\phi(h^1_{K,\cdot})Ru_\alpha h^{\mathrm{Pek}}T_yW(\alpha w_{P,y})u_\alpha R\phi(h^1_{K,\cdot})G_K^0\rangle_{\mathscr{H}}\\ &= \frac{1}{\alpha^2}\int \mathrm{d}y\,\langle \psi\otimes\Omega|a(\underline{h^1_{K,\cdot}})Ru_\alpha h^{\mathrm{Pek}}T_yW(\alpha\widetilde{w}_{P,y})u_\alpha Ra^\dagger(\underline{h^1_{K,\cdot}})\psi\otimes\Omega\rangle_{\mathscr{H}}\\ &= \frac{1}{\alpha^2}\int \mathrm{d}y\,\langle G_K^0|L_{3,y}G_K^0\rangle_{\mathscr{H}}n_{0,1}(y) - \int \mathrm{d}y\,\ell_3(y)n_{0,1}(y) \;=\; \mathcal{K}_{111}+\mathcal{K}_{112},\end{aligned} \tag{3.209}$$

where

$$L_{3,y} \;=\; P_\psi\phi(h^1_{K,\cdot})Ru_\alpha h^{\mathrm{Pek}}T_yu_\alpha R\phi(h^1_{K,\cdot})P_\psi \tag{3.210a}$$

$$\ell_3(y) \;=\; \langle\psi|\langle \underline{h^1_{K,\cdot}}|\widetilde{w}^1_{P,y}\rangle_{L^2}Ru_\alpha h^{\mathrm{Pek}}T_yu_\alpha R\langle\widetilde{w}^1_{P,y}|\underline{h^1_{K,\cdot}}\rangle_{L^2}\psi\rangle_{L^2}. \tag{3.210b}$$

We go on with

$$\begin{aligned}\mathcal{K}_{111} &= \frac{1}{\alpha^2}\int \mathrm{d}y\,\langle G_K^0|L_{3,y}G_K^0\rangle_{\mathscr{H}}\,e^{-\lambda\alpha^2y^2}\\ &\quad+\frac{1}{\alpha^2}\int \mathrm{d}y\,\langle G_K^0|L_{3,y}G_K^0\rangle_{\mathscr{H}}\big(n_{0,1}(y)-e^{-\lambda\alpha^2y^2}\big) = \mathcal{K}^{\mathrm{lo}}_{111}+\mathcal{K}^{\mathrm{err}}_{111},\end{aligned} \tag{3.211}$$

and in the leading-order term, we insert $T_y = 1+(T_y-1)$ and $u_\alpha = 1+(u_\alpha-1)$,

$$\begin{aligned}\mathcal{K}^{\mathrm{lo}}_{111} &= \frac{1}{\alpha^2}\langle G_K^0|\phi(h^1_{K,\cdot})Rh^{\mathrm{Pek}}R\phi(h^1_{K,\cdot})G_K^0\rangle_{\mathscr{H}}\int \mathrm{d}y\,e^{-\lambda\alpha^2y^2}\\ &\quad+\frac{1}{\alpha^2}\langle G_K^0|\phi(h^1_{K,\cdot})R(u_\alpha-1)h^{\mathrm{Pek}}R\phi(h^1_{K,\cdot})G_K^0\rangle_{\mathscr{H}}\int \mathrm{d}y\,e^{-\lambda\alpha^2y^2}\\ &\quad+\frac{1}{\alpha^2}\langle G_K^0|\phi(h^1_{K,\cdot})Ru_\alpha h^{\mathrm{Pek}}(u_\alpha-1)R\phi(h^1_{K,\cdot})G_K^0\rangle_{\mathscr{H}}\int \mathrm{d}y\,e^{-\lambda\alpha^2y^2}\\ &\quad+\frac{1}{\alpha^2}\int \mathrm{d}y\,\langle G_K^0|\phi(h^1_{K,\cdot})Ru_\alpha h^{\mathrm{Pek}}(T_y-1)u_\alpha R\phi(h^1_{K,\cdot})G_K^0\rangle_{\mathscr{H}}e^{-\lambda\alpha^2y^2}\\ &= \sum_{n=1}^4\mathcal{K}^{\mathrm{lo,n}}_{111}.\end{aligned} \tag{3.212}$$

Since $Rh^{\mathrm{Pek}}R = R$, one finds $\mathcal{K}^{\mathrm{lo},1}_{111} = -\frac{1}{\alpha^2}\langle\Upsilon_K|(\mathbb{H}_K-\mathbb{N}_1)\Upsilon_K\rangle_{\mathcal{F}}(\frac{\pi}{\lambda\alpha^2})^3$, cf. equation (2.4), and with the aid of Proposition 3.17, this gives the leading-order contribution

$$\Big|\mathcal{K}^{\mathrm{lo},1}_{111}+\mathcal{N}\frac{1}{\alpha^2}\langle\Upsilon_K|(\mathbb{H}_K-\mathbb{N}_1)\Upsilon_K\rangle_{\mathcal{F}}\Big| \;\le\; C_\varepsilon\sqrt{K}\alpha^{-6+\varepsilon}. \tag{3.213}$$

For the other terms, we shall show that

$$|\mathcal{K}^{\mathrm{lo},2}_{111}|+|\mathcal{K}^{\mathrm{lo},3}_{111}|+|\mathcal{K}^{\mathrm{lo},4}_{111}| \le C\sqrt{K}\alpha^{-6}. \tag{3.214}$$

In the second term, we use $h^{\mathrm{Pek}}R = Q_\psi = 1-P_\psi$ to write

$$K^{\mathrm{lo},2}_{111} \;=\; \alpha^{-2}\langle G_K^0|\phi(h^1_{K,\cdot})R(u_\alpha-1)(1-P_\psi)\phi(h^1_{K,\cdot})G_K^0\rangle_{\mathscr{H}}\Big(\frac{\pi}{\lambda\alpha^2}\Big)^{3/2} \tag{3.215}$$

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which is exponentially small in α, since $\|(u_\alpha - 1)\psi\|_{L^2} \leq Ce^{-\alpha/C}$, and thus with Lemma 3.9 one obtains $|\mathcal{K}^{\mathrm{lo},2}_{111}| \leq C\sqrt{K}e^{-\alpha/C}$. In the next term, we use $[h^{\mathrm{Pek}}, u_\alpha - 1] = -[\Delta, u_\alpha]$ and again $h^{\mathrm{Pek}}R = 1 - P_\psi$ to get

$$\begin{aligned}\mathcal{K}^{\mathrm{lo},3}_{111} &= \alpha^{-2}\big\langle G^0_K|\phi(h^1_{K,\cdot})Ru_\alpha(u_\alpha - 1)(1 - P_\psi)\phi(h^1_{K,\cdot})G^0_K\big\rangle_{\mathscr{H}}\left(\frac{\pi}{\lambda\alpha^2}\right)^{3/2}\\ &\quad - \alpha^{-2}\big\langle G^0_K|\phi(h^1_{K,\cdot})R[\Delta, u_\alpha]R\phi(h^1_{K,\cdot})G^0_K\big\rangle_{\mathscr{H}}\left(\frac{\pi}{\lambda\alpha^2}\right)^{3/2}. \end{aligned}\tag{3.216}$$

Here, the first line is bounded again exponentially in α, whereas in the second line we use $[\Delta, u_\alpha] = 2(\nabla u_\alpha)\nabla + (\Delta u_\alpha)$ and $\|\nabla u_\alpha\|_{L^\infty} + \|\Delta u_\alpha\|_{L^\infty} \leq C\alpha^{-1}$, see (2.20). Together with Lemmas 3.8 and 3.9, this implies $|\mathcal{K}^{\mathrm{lo},3}_{111}| \leq C\alpha^{-6}$. In the last term, we employ $T_y - 1 = \int_0^1 \mathrm{d}s T_{sy}(y\nabla)$, $[h^{\mathrm{Pek}}, u_\alpha] = -[\Delta, u_\alpha]$ and $h^{\mathrm{Pek}}R = Q_\psi$ to find

$$\begin{aligned}\mathcal{K}^{\mathrm{lo},4}_{111} &= \alpha^{-2}\int \mathrm{d}y \int_0^1 \mathrm{d}s\,\big\langle G^0_K|\phi(h^1_{K,\cdot})Q_\psi u_\alpha T_{sy}(y\nabla)u_\alpha R\phi(h^1_{K,\cdot})G^0_K\big\rangle_{\mathscr{H}} e^{-\lambda\alpha^2 y^2}\\ &\quad + \alpha^{-2}\int \mathrm{d}y \int_0^1 \mathrm{d}s\,\big\langle G^0_K|\phi(h^1_{K,\cdot})R[\Delta, u_\alpha]T_{sy}(y\nabla)u_\alpha R\phi(h^1_{K,\cdot})G^0_K\big\rangle_{\mathscr{H}} e^{-\lambda\alpha^2 y^2}.\end{aligned}\tag{3.217}$$

In both lines, there is an additional factor y, and together with equation (2.20), we thus obtain

$$\begin{aligned}|\mathcal{K}^{\mathrm{lo},4}_{111}| &\leq C\alpha^{-6}\|\phi(h^1_{K,\cdot})G^0_K\|_{\mathscr{H}}\,\|\nabla u_\alpha R^{1/2}\|_{\mathrm{op}}\|R^{1/2}\phi(h^1_{K,\cdot})G^0_K\|_{\mathscr{H}}\\ &\quad + C\alpha^{-6}\|R^{1/2}\phi(h^1_{K,\cdot})G^0_K\|_{\mathscr{H}}\|R^{1/2}[\Delta, u_\alpha]\|_{\mathrm{op}}\|\nabla u_\alpha R^{1/2}\|_{\mathrm{op}}\|R\phi(h^1_{K,\cdot})G^0_K\|_{\mathscr{H}}\\ &\leq C(\alpha^{-6}\sqrt{K} + \alpha^{-7}).\end{aligned}\tag{3.218}$$

This proves (3.214).

To estimate $\mathcal{K}_{112}$ and $\mathcal{K}^{\mathrm{err}}_{111}$, we make use of

$$\left|\big\langle G^0_K|L_{3,y}G^0_K\big\rangle_{\mathscr{H}}\right| \leq Cf_{3,\alpha}(y) \tag{3.219a}$$

$$|\ell_3(y)| \leq Cf_{3,\alpha}(y)(y^4 + \alpha^{-4}), \tag{3.219b}$$

where

$$f_{3,\alpha}(y) = \|u_\alpha T_y u_\alpha\|_{\mathrm{op}} + \|(\nabla u_\alpha)T_y u_\alpha\|_{\mathrm{op}} + \|u_\alpha T_y(\nabla u_\alpha)\|_{\mathrm{op}} + \|(\nabla u_\alpha)T_y(\nabla u_\alpha)\|_{\mathrm{op}}. \tag{3.220}$$

Recalling that by definition $|\nabla^k u_\alpha(y)| \leq \mathbb{1}(|y| \leq 2\alpha)$ for $k = 0, 1$, it follows that $f_{3,\alpha}(y) \leq 4\mathbb{1}(|y| \leq 4\alpha)$ and thus

$$\|f_{3,\alpha}\|_{L^\infty} \leq 4 \quad \text{and} \quad \||\cdot|^n f_{3,\alpha}\|_{L^1} \leq C_n\alpha^{3+n} \quad \text{for all } n \in \mathbb{N}_0. \tag{3.221}$$

In order to verify equation (3.219a), use $h^{\mathrm{Pek}} = -\Delta + V^\varphi - \lambda^{\mathrm{Pek}}$ to write

$$\begin{aligned}R^{\frac12}u_\alpha T_y h^{\mathrm{Pek}}u_\alpha R^{\frac12} &= R^{\frac12}u_\alpha\big((-i\nabla)T_y(-i\nabla) + T_y(V^\varphi - \lambda^{\mathrm{Pek}})\big)u_\alpha R^{\frac12}\\ &= -R^{\frac12}(-i\nabla u_\alpha)T_y(-i\nabla u_\alpha)R^{\frac12} + R^{\frac12}(-i\nabla)u_\alpha T_y u_\alpha(-i\nabla)R^{\frac12}\\ &\quad + R^{\frac12}(-i\nabla)u_\alpha T_y(-i\nabla u_\alpha)R^{\frac12} - R^{\frac12}(-i\nabla u_\alpha)T_y u_\alpha(-i\nabla)R^{\frac12}\\ &\quad + R^{\frac12}u_\alpha T_y u_\alpha(V^\varphi - \lambda^{\mathrm{Pek}})R^{\frac12}.\end{aligned}\tag{3.222}$$

Since $\|V^{\varphi} R^{1/2}\|_{\mathrm{op}} \leq C(\|R\|_{\mathrm{op}} + \|\nabla R^{1/2}\|_{\mathrm{op}}) \leq C$ (see Lemma 3.8), it thus follows that

$$\|R^{\frac{1}{2}} u_\alpha T_y h^{\mathrm{Pek}} u_\alpha R^{\frac{1}{2}}\|_{\mathrm{op}} \leq C f_{3,\alpha}(y), \tag{3.223}$$

With this at hand, one applies Lemma 3.9 to conclude the bound stated in equation (3.219a). For $\ell_3(y)$, we proceed similarly as in equation (3.187), that is,

$$\begin{aligned} |\ell_3(y)| &\leq \|R^{1/2} u_\alpha h^{\mathrm{Pek}} T_y u_\alpha R^{1/2}\|_{\mathrm{op}} \|R^{1/2} \langle \widetilde{w}^1_{P,y} | \underline{h^1_{K,\cdot}} \rangle_{L^2} \psi\|^2_{L^2} \\ &\leq f_{3,\alpha}(y)\, \|\widetilde{w}^1_{P,y}\|^2_{L^2} \int \mathrm{d}z \|P_\psi \underline{h^1_{K,\cdot}}(z) R^{1/2}\|^2_{\mathrm{op}} \leq C f_{3,\alpha}(y)(y^4 + \alpha^{-4}). \end{aligned} \tag{3.224}$$

Now, we can apply Lemma 3.5 and (3.221) to estimate

$$|\mathcal{K}^{\mathrm{err}}_{111}| \leq \frac{C}{\alpha^2} \int \mathrm{d}y\, f_{3,\alpha}(y)\, |n_{0,1}(y) - e^{-\lambda \alpha^2 y^2}| \leq C\alpha^{-6}, \tag{3.225}$$

and further invoke Corollary 3.6 to obtain

$$|\mathcal{K}_{112}| \leq \int \mathrm{d}y\, f_{3,\alpha}(y)(|y|^4 + \alpha^{-4}) n_{0,1}(y) \leq C\alpha^{-7}. \tag{3.226}$$

Next, we come to $\mathcal{K}_{12}$ which we rewrite with the aid of equations (3.67) and (3.80) as

$$\mathcal{K}_{12} = \frac{1}{\alpha^2} \int \mathrm{d}y \left\langle R_{5,y} \psi \otimes \left(\Upsilon^<_K + \Upsilon^>_K\right) \middle| W(\alpha w_{P,y}) G^0_K \right\rangle_{\mathscr{H}} = \mathcal{K}^<_{12} + \mathcal{K}^>_{12} \tag{3.227}$$

with the operator $R_{5,y} = R^1_{5,y} + R^2_{5,y}$ and

$$R^1_{5,y} = P_\psi \phi(h^1_{K,\cdot}) R u_\alpha (e^{-A_{P,y}} - 1) T_{-y} h^{\mathrm{Pek}} u_\alpha R \phi(h^1_{K,\cdot}) P_\psi \tag{3.228a}$$

$$R^2_{5,y} = 2\alpha P_\psi \left\langle h_{K,\cdot} \middle| \mathrm{Re}(w^1_{P,y}) \right\rangle_{L^2} R u_\alpha (e^{-A_{P,y}} - 1) T_{-y} h^{\mathrm{Pek}} u_\alpha R \phi(h^1_{K,\cdot}) P_\psi. \tag{3.228b}$$

Utilizing Lemma 3.9 and (3.32a), we have

$$\|R^1_{5,y} \Psi\|_{\mathscr{H}} \leq C\|(e^{-A_{P,y}} - 1)(\mathbb{N}+1)^{1/2} R^{\frac{1}{2}} u_\alpha T_{-y} h^{\mathrm{Pek}} u_\alpha R \phi(h^1_{K,\cdot}) P_\psi \Psi\|_{\mathscr{H}}, \tag{3.229}$$

and following the same steps as in equation (3.84),

$$\|R^2_{5,y} \Psi\| \leq C\alpha(y^2 + \alpha^{-2}) \|(e^{-A_{P,y}} - 1) R^{\frac{1}{2}} u_\alpha T_{-y} h^{\mathrm{Pek}} u_\alpha R \phi(h^1_{K,\cdot}) P_\psi \Psi\|_{\mathscr{H}}. \tag{3.230}$$

After using unitarity of $e^{-A_{P,y}}$ and equation (3.221), we can apply Lemma 3.9 another time to obtain

$$\|R_{5,y} \psi \otimes \Upsilon^>_K\|_{\mathscr{H}} \leq C f_{3,\alpha}(-y)(1 + \alpha y^2) \|(\mathbb{N}+1)\Upsilon^>_K\|_{\mathcal{F}}. \tag{3.231}$$

Thus, we can estimate the tail with the aid of Corollary 3.14 and equation (3.221),

$$|\mathcal{K}^>_{12}| \leq \frac{C}{\alpha^2} \|(\mathbb{N}+1)\Upsilon^>_K\|_{\mathcal{F}} \int \mathrm{d}y\, f_{3,\alpha}(-y)(1 + \alpha y^2) \leq C_\delta\, \alpha^{-6}. \tag{3.232}$$

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Then we use equation (3.63), equaiton (3.74) and apply Lemma 3.15 to get

$$\begin{aligned} |\mathcal{K}_{12}^{<}| &\leq \frac{1}{\alpha^2} \int \mathrm{d}y\, \|\mathbb{U}_K e^{\kappa \mathbb{N}} R_{5,y} \psi \otimes \Upsilon_K^{<}\|_{\mathscr{H}} \|e^{-\kappa \mathbb{N}} W(\alpha \widetilde{w}_{P,y}) \Omega\|_{\mathcal{F}} \\ &\leq \frac{\sqrt{2}}{\alpha^2} \int \mathrm{d}y\, \|R_{5,y} \psi \otimes \Upsilon_K^{<}\|_{\mathscr{H}}\, n_{\delta,\eta}(y). \end{aligned} \tag{3.233}$$

To bound the norm in the integral, we proceed in close analogy to the steps following equation (3.196). We abbreviate again $G_K^{0<} = \psi \otimes \Upsilon_K^{<}$ and start from equations (3.229) and (3.230). With equation (3.221), the functional calculus and $A_{P,y} = iP_f y + i g_P(y)$, one finds

$$\begin{aligned} \|R_{5,y} G_K^{0<}\|_{\mathscr{H}} &\leq C\big(f_{3,\alpha}(-y) \|(e^{-A_{P,y}} - 1)(\mathbb{N}+1)^{1/2} R^{\frac{1}{2}} \phi(h^1_{K,\cdot}) G_K^{0<}\|_{\mathscr{H}} \\ &\quad + \alpha(y^2 + \alpha^{-2}) f_{3,\alpha}(-y) \|(e^{-A_{P,y}} - 1) R^{\frac{1}{2}} \phi(h^1_{K,\cdot}) G_K^{0<}\|_{\mathscr{H}}\big) \\ &\leq C\big(f_{3,\alpha}(-y)\big(\|(yP_f)(\mathbb{N}+1)^{1/2} R^{\frac{1}{2}} \phi(h^1_{K,\cdot}) G_K^{0<}\|_{\mathscr{H}} && (3.234a) \\ &\quad + f_{3,\alpha}(-y) |g_P(y)| (\mathbb{N}+1)^{1/2} R^{\frac{1}{2}} \phi(h^1_{K,\cdot}) G_K^{0<}\|_{\mathscr{H}} && (3.234b) \\ &\quad + f_{3,\alpha}(-y)(\alpha y^2 + \alpha^{-1}) \|(P_f y) R^{\frac{1}{2}} \phi(h^1_{K,\cdot}) G_K^{0<}\|_{\mathscr{H}} && (3.234c) \\ &\quad + f_{3,\alpha}(-y)(\alpha y^2 + \alpha^{-1}) |g_P(y)| \|R^{\frac{1}{2}} \phi(h^1_{K,\cdot}) G_K^{0<}\|_{\mathscr{H}}\big). && (3.234d) \end{aligned}$$

In the second and fourth line, we use $|g_P(y)| \leq C\alpha |y|^3$ and Lemma 3.9,

$$\begin{aligned} (3.234b) + (3.234d) &\leq C(\alpha^2 |y|^5 + \alpha |y|^3) f_{3,\alpha}(-y) \|(\mathbb{N}+1) \Upsilon_K^{<}\|_{\mathcal{F}} \\ &\leq C(\alpha^2 |y|^5 + \alpha |y|^3) f_{3,\alpha}(-y). \end{aligned} \tag{3.235}$$

In the first and third line, we employ the commutator $[iP_f y, \phi(f)] = \pi(y \nabla f)$ to get

$$\begin{aligned} (3.234a) + (3.234c) &\leq C\big(f_{3,\alpha}(-y) \|(\mathbb{N}+1)^{1/2} R^{\frac{1}{2}} \phi(h^1_{K,\cdot})(yP_f) G_K^{0<}\|_{\mathscr{H}} && (3.236a) \\ &\quad + f_{3,\alpha}(-y) \|(\mathbb{N}+1)^{1/2} R^{\frac{1}{2}} \pi(y \nabla h^1_{K,\cdot}) G_K^{0<}\|_{\mathscr{H}} && (3.236b) \\ &\quad + f_{3,\alpha}(-y)(\alpha y^2 + \alpha^{-1}) \|R^{\frac{1}{2}} \phi(h^1_{K,\cdot})(yP_f) G_K^{0<}\|_{\mathscr{H}} && (3.236c) \\ &\quad + f_{3,\alpha}(-y)(\alpha y^2 + \alpha^{-1}) \|R^{\frac{1}{2}} \pi(y \nabla h^1_{K,\cdot}) G_K^{0<}\|_{\mathscr{H}}\big). && (3.236d) \end{aligned}$$

After another application of Lemma 3.9, we can use equation (3.67) and then Lemma 3.16 for the terms involving P_f,

$$\begin{aligned} (3.236a) + (3.236c) &\leq C f_{3,\alpha}(-y)(\alpha y^2 + 1)\, |y|\, \|(\mathbb{N}+1) P_f \Upsilon_K^{<}\|_{\mathcal{F}} \\ &\leq C f_{3,\alpha}(-y)(\alpha |y|^3 + |y|) \alpha^{\delta} \sqrt{K},, \end{aligned} \tag{3.237}$$

while in the other two lines, we use $(\nabla h_K)_{\cdot} = -[\nabla, h_{K,\cdot}]$, to obtain

$$\begin{aligned} (3.236b) + (3.236d) &\leq C f_{3,\alpha}(-y)\, |y|\, (\alpha y^2 + 1) \|h_{K,0}\|_{L^2} \|(\mathbb{N}+1) \Upsilon_K^{<}\|_{\mathcal{F}} \\ &\leq C f_{3,\alpha}(-y)(\alpha |y|^3 + |y|) \sqrt{K}. \end{aligned} \tag{3.238}$$

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Collecting all estimates we have thus shown that

$$\|R_{5,y}\psi \otimes \Upsilon_K^{<}\|_{\mathscr{H}} \;\le\; C f_{3,\alpha}(-y)\alpha^{\delta}\Big(\alpha^2|y|^5 + \sqrt{K}(\alpha|y|^3 + |y|)\Big). \tag{3.239}$$

Using this bound in equation (3.233), we can invoke Corollary 3.6 together with equation (3.221) in order to obtain

$$|\mathcal{K}_{12}^{<}| \le C\sqrt{K}\alpha^{-6+5\delta}. \tag{3.240}$$

Term $\mathcal{K}_2$. Using equations (3.67) and (3.80), one finds

$$\mathcal{K}_2 \;=\; \frac{1}{\alpha^4}\int \mathrm{d}y \left\langle R_{6,y}\psi \otimes \left(\Upsilon_K^{<} + \Upsilon_K^{>}\right) | W(\alpha w_{P,y}) G_K^0 \right\rangle_{\mathscr{H}} \;=\; \mathcal{K}_2^{<} + \mathcal{K}_2^{>} \tag{3.241}$$

with the operator $R_{6,y} = R_{6,y}^1 + R_{6,y}^2$ and

$$R_{6,y}^1 \;=\; P_\psi \phi(h_{K,\cdot}^1) R u_\alpha \mathbb{N} T_{-y} e^{-A_{P,y}} u_\alpha R \phi(h_{K,\cdot}^1) P_\psi \tag{3.242a}$$

$$R_{6,y}^2 \;=\; 2\alpha P_\psi \phi(h_{K,\cdot}^1) R u_\alpha \mathbb{N} T_{-y} e^{-A_{P,y}} u_\alpha R \langle \mathrm{Re}(w_{P,y}^1) | h_{K,\cdot}\rangle_{L^2} P_\psi. \tag{3.242b}$$

With Lemma 3.9 and equation (3.32a) it is not difficult to verify

$$\|R_{6,y}\Psi\|_{\mathscr{H}} \;\le\; C\|u_\alpha T_{-y} u_\alpha\|_{\mathrm{op}}(1+\alpha y^2)\|(\mathbb{N}+1)^2\Psi\|_{\mathscr{H}}, \tag{3.243}$$

and since $\|u_\alpha T_{-y} u_\alpha\|_{\mathrm{op}} \le \mathbb{1}(|y| \le 4\alpha)$, we can use Corollary 3.14 to estimate the part with the tail by

$$|\mathcal{K}_2^{>}| \;\le\; \frac{C}{\alpha^4}\|(\mathbb{N}+1)^2\Upsilon_K^{>}\|_{\mathcal{F}} \int \mathrm{d}y\, \mathbb{1}(|y| \le 4\alpha)(1+\alpha y^2) \;\le\; C_\delta\, \alpha^{-8}. \tag{3.244}$$

To treat $\mathcal{K}_2^{<}$ we proceed as in (3.233), that is

$$|\mathcal{K}_2^{<}| \le \frac{\sqrt{2}}{\alpha^4}\int \mathrm{d}y\, \|R_{6,y}\psi \otimes \Upsilon_K^{<}\|_{\mathscr{H}}\, n_{\delta,\eta}(y) \le \frac{C}{\alpha^4}\int \mathrm{d}y\, \mathbb{1}(|y| \le \alpha)(1+\alpha y^2)\, n_{\delta,\eta}(y). \tag{3.245}$$

It now follows from Corollary 3.6 that

$$|\mathcal{K}_2^{<}| \le C\alpha^{-7}. \tag{3.246}$$

Term $\mathcal{K}_3$. This term is similarly estimated as the previous one. With the aid of equations (3.67) and (3.80), we have

$$\mathcal{K}_3 \;=\; \frac{1}{\alpha^3}\int \mathrm{d}y \left\langle R_{7,y}\psi \otimes \left(\Upsilon_K^{<} + \Upsilon_K^{>}\right) | W(\alpha w_{P,y}) G_K^0 \right\rangle_{\mathscr{H}} \;=\; \mathcal{K}_3^{<} + \mathcal{K}_3^{>} \tag{3.247}$$

with the operator $R_{7,y} = R_{7,y}^1 + R_{7,y}^2$ and

$$R_{7,y}^1 \;=\; P_\psi \phi(h_{K,\cdot}^1) R u_\alpha e^{-A_{P,y}} T_{-y} \phi(h_\cdot + \varphi_P) u_\alpha R \phi(h_{K,\cdot}^1) P_\psi \tag{3.248a}$$

$$R_{7,y}^2 \;=\; 2\alpha P_\psi \langle \mathrm{Re}(w_{P,y}^1) | h_{K,\cdot}\rangle_{L^2} R u_\alpha e^{-A_{P,y}} T_{-y} \phi(h_\cdot + \varphi_P) u_\alpha R \phi(h_{K,\cdot}^1) P_\psi. \tag{3.248b}$$

Utilizing again Lemma 3.9 and equation (3.32a), one shows that

$$\|R_{7,y}\Psi\|_{\mathscr{H}} \;\le\; C f_{3,\alpha}(-y)(1+\alpha y^2)\|(\mathbb{N}+1)^{3/2}\Psi\|_{\mathscr{H}} \tag{3.249}$$

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with $f_{3,\alpha}$ defined in (3.220). Invoking Corollary 3.14 and equation (3.221), we thus find

$$|\mathcal{K}_3^{>}| \le \frac{C}{\alpha^3}\|(\mathbb{N}+1)^{3/2}\Upsilon_K^{>}\|_{\mathcal{F}} \int \mathrm{d}y\, f_{3,\alpha}(-y)(1+\alpha y^2) \le C_\delta\, \alpha^{-7}. \tag{3.250}$$

Similarly, as in equation (3.233), we also obtain

$$|\mathcal{K}_3^{<}| \le \frac{\sqrt{2}}{\alpha^3}\int \mathrm{d}y\, \|R_{7,y}\psi\otimes\Upsilon_K^{<}\|_{\mathscr{H}}\, n_{\delta,\eta}(y) \le \frac{C}{\alpha^3}\int \mathrm{d}y\, f_{3,\alpha}(-y)(1+\alpha y^2)n_{\delta,\eta}(y). \tag{3.251}$$

By Corollary 3.6 and equation (3.220) it follows that

$$|\mathcal{K}_3^{<}| \le C\alpha^{-6+3\delta}. \tag{3.252}$$

This completes the analysis of $\mathcal{K}$. The proof of Proposition 3.21 follows from combining equations (3.213), (3.214), (3.225), (3.226), (3.232), (3.240), (3.244), (3.246), (3.250) and (3.252). □

3.9. *Concluding the proof of Proposition 2.8*

Combining Propositions 3.18, 3.20 and 3.21, we arrive at

$$\left|\frac{\mathcal{E}+\mathcal{G}+\mathcal{K}}{\mathcal{N}} - \frac{\inf\sigma(\mathbb{H}_K)}{\alpha^2} + \frac{3}{2\alpha^2}\right| \le C_\varepsilon\,\alpha^\varepsilon\left(\frac{K^{-1/2}\alpha^{-5}+\sqrt{K}\alpha^{-6}}{\mathcal{N}}\right). \tag{3.253}$$

Now, for $K \le \widetilde{c}\alpha$ we know from Proposition 3.17 that $\mathcal{N} \ge C\alpha^3$ for some $C > 0$, such that the right side is bounded by $C_\varepsilon\,\alpha^\varepsilon r(K,\alpha)$. It remains to show that one can replace $\alpha^{-2}\inf\sigma(\mathbb{H}_K)$ by $\alpha^{-2}\inf\sigma(\mathbb{H}_\infty)$ at the cost of an additional error. To this end, recall that $\inf\sigma(\mathbb{H}_K) = \langle\Upsilon_K|\mathbb{H}_K\Upsilon_K\rangle_{\mathcal{F}}$ and use the variational principle to find

$$\left\langle\Upsilon_K|(\mathbb{H}_K-\mathbb{H}_\infty)\Upsilon_K\right\rangle_{\mathcal{F}} \le \inf\sigma(\mathbb{H}_K) - \inf\sigma(\mathbb{H}_\infty) \le \left\langle\Upsilon_\infty|(\mathbb{H}_K-\mathbb{H}_\infty)\Upsilon_\infty\right\rangle_{\mathcal{F}}. \tag{3.254}$$

Writing

$$\mathbb{H}_K - \mathbb{H}_\infty = \left\langle\psi|\phi(h^1_{K,\cdot}-h^1_\cdot)R\phi(h^1_{K,\cdot})\psi\right\rangle_{L^2} - \left\langle\psi|\phi(h^1_\cdot)R\phi(h^1_\cdot-h^1_{K,\cdot})\psi\right\rangle_{L^2}, \tag{3.255}$$

and using Lemma 3.9, we can infer that for any $\Psi\in\mathcal{F}$

$$\left|\left\langle\Psi|(\mathbb{H}_K-\mathbb{H}_\infty)\Psi\right\rangle_{\mathcal{F}}\right| \le CK^{-1/2}\left\langle\Psi|(\mathbb{N}_1+1)\Psi\right\rangle_{\mathcal{F}}. \tag{3.256}$$

By Corollary 3.14, we know that $\left\langle\Upsilon_K|(\mathbb{N}_1+1)\Upsilon_K\right\rangle_{\mathcal{F}} \le C$, and thus $|\inf\sigma(\mathbb{H}_K)-\inf\sigma(\mathbb{H}_\infty)| \le CK^{-1/2}$. In view of equation (3.253) and Lemma 3.1 this completes the proof of Proposition 2.8.

4. Remaining Proofs

Proof of Lemma 1.1. The form of the kernel is readily found using second order perturbation theory (we omit the details). (i) The lower bound $H^{\mathrm{Pek}} \ge 0$ follows from (1.19) whereas $H^{\mathrm{Pek}} \le 1$ is a consequence of

$$\left\langle v|(1-H^{\mathrm{Pek}})v\right\rangle_{L^2} = 4\left\|\int \mathrm{d}y\, v(y)R^{1/2}h_\cdot(y)\psi\right\|^2_{L^2}. \tag{4.1}$$

(ii) That $\mathrm{Span}\{\partial_i\varphi : i=1,2,3\} \subseteq \mathrm{Ker}H^{\mathrm{Pek}}$ follows from translation invariance of the energy functional $\mathcal{F}$ (1.15). To show equality, we argue that there is a $\tau > 0$ such that $\langle v|H^{\mathrm{Pek}}v\rangle_{L^2} \ge \tau\|v\|^2_{L^2}$ for all $v\in L^2(\mathbb{R}^3)$ with $\langle v|\nabla\varphi\rangle_{L^2} = 0$ (note that this also implies (iii)). Since H^{Pek} has real-valued kernel, it

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is sufficient to consider $v \in L^2_{\mathbb{R}}(\mathbb{R}^3)$. We start by quoting [13, Lemma 2.7] stating that there exists a constant $\tau > 0$ such that

$$\mathcal{F}(v) - \mathcal{F}(\varphi) \geq \tau \inf_{y \in \mathbb{R}^3} \|v - \varphi(\cdot - y)\|^2_{L^2} \tag{4.2}$$

for all $v \in L^2(\mathbb{R}^3)$. (A key ingredient in the proof of this quadratic lower bound are the results about the Hessian of the Pekar energy functional (1.12) that were obtained in [33]; see [13] for a detailed derivation). Combined with equation (1.19), and using that for small ε the infimum over $y \in \mathbb{R}^3$ exists, this implies

$$\langle v | H^{\mathrm{Pek}} v \rangle_{L^2} \geq \tau \liminf_{\varepsilon \to 0} \min_{y \in \mathbb{R}^3} f_v(y, \varepsilon), \tag{4.3a}$$

$$f_v(y, \varepsilon) = \|v\|^2_{L^2} + \varepsilon^{-2} \|\varphi - \varphi(\cdot - y)\|^2_{L^2} + 2\varepsilon^{-1} \operatorname{Re}\langle v | \varphi - \varphi(\cdot - y)\rangle_{L^2}. \tag{4.3b}$$

Given any v satisfying $\langle v | \nabla \varphi \rangle_{L^2} = 0$, we choose $y^*(\varepsilon)$ such that $f_v(y^*(\varepsilon), \varepsilon)$ is minimal. Furthermore, note that for every zero sequence $(\varepsilon_n)_{n \in \mathbb{N}}$ such that

$$\liminf_{n \to \infty} \|\varphi - \varphi(\cdot - y^*(\varepsilon_n))\|_{L^2} > 0, \tag{4.4}$$

it follows that $\liminf_{n \to \infty} f_v(y^*(\varepsilon_n), \varepsilon_n) = \infty$, and hence, we can conclude that $|y^*(\varepsilon)| \to 0$ as $\varepsilon \to 0$. To proceed, let $\eta(\varepsilon) := \varphi - \varphi(\cdot - y^*(\varepsilon))$ and assume $|y^*(\varepsilon)| > 0$ (for if $y^*(\varepsilon) = 0$ it follows directly that $f_v(y^*(\varepsilon), \varepsilon) = \|v\|^2_{L^2}$). With this, we can estimate

$$f_v(y^*(\varepsilon), \varepsilon) \geq \|v\|^2_{L^2} + \varepsilon^{-2} \|\eta(\varepsilon)\|^2_{L^2} - 2\varepsilon^{-1} |\langle v | \eta(\varepsilon)\rangle_{L^2}| \geq \|v\|^2_{L^2} - \left| \langle v | \frac{\eta(\varepsilon)}{\|\eta(\varepsilon)\|_{L^2}} \rangle_{L^2} \right|^2. \tag{4.5}$$

To bound the right side, write

$$\eta(\varepsilon)(z) = \int_0^1 \mathrm{d}s \, (y^*(\varepsilon)\nabla)\varphi(z - s y^*(\varepsilon)) \tag{4.6}$$

and use, by dominated convergence, that

$$\frac{\| \int_0^1 \mathrm{d}s \, (y\nabla)\varphi(\cdot - sy) - (y\nabla)\varphi \|_{L^2}}{\| \int_0^1 \mathrm{d}s \, (y\nabla)\varphi(\cdot - sy) \|_{L^2}} \to 0 \quad \text{as} \quad |y| \to 0. \tag{4.7}$$

Combining the last statement with $|y^*(\varepsilon)| \to 0$ as $\varepsilon \to 0$ and $\langle v | \nabla \varphi \rangle_{L^2} = 0$, we conclude that

$$\liminf_{\varepsilon \to 0} f_v(y^*(\varepsilon), \varepsilon) \geq \|v\|^2_{L^2}. \tag{4.8}$$

This completes the proof of items (ii) and (iii). Property (iv) follows from $H^{\mathrm{Pek}} \leq (H^{\mathrm{Pek}})^{1/2}$ and $\operatorname{Tr}_{L^2}(1 - H^{\mathrm{Pek}}) < \infty$; see Lemma 2.3 for $K = \infty$. □

Proof of Lemma 2.3. (i) The bound $H^{\mathrm{Pek}}_K \restriction \operatorname{Ran}(\Pi_1) \leq 1$ follows analogously to equation (4.1) and $H^{\mathrm{Pek}}_K \restriction \operatorname{Ran}(\Pi_0) = 0$ holds by definition. The lower bound on $\operatorname{Ran}(\Pi_1)$ is a consequence of $(H^{\mathrm{Pek}} - \tau) \restriction \operatorname{Ran}(\Pi_1) \geq 0$ for some $\tau > 0$; see Lemma 1.1, in combination with

$$\pm (H^{\mathrm{Pek}} - H^{\mathrm{Pek}}_K) \leq C K^{-1/2}. \tag{4.9}$$

To verify the latter, let $v \in \mathrm{Ran}(\Pi_1)$, $\Pi_v = |v\rangle\langle v|$ and write

$$\begin{aligned}\left\langle v|(H_K^{\mathrm{Pek}} - H^{\mathrm{Pek}})v\right\rangle_{L^2} &= 4\int \mathrm{d}y \ \mathrm{Re}\left\langle \psi|\big(h_{K,\cdot}(y) - h_\cdot)(y)\big)R(\Pi_v h_{K,\cdot})(y)\psi\right\rangle_{L^2} \\ &\quad + 4\int \mathrm{d}y \ \mathrm{Re}\left\langle \psi|(\Pi_v h_\cdot)(y)R\big(h_{K,\cdot}(y) - h_\cdot(y)\big)\psi\right\rangle_{L^2}. \end{aligned} \tag{4.10}$$

With Cauchy–Schwarz, it follows that

$$\begin{aligned}\left|\left\langle v|(H_K^{\mathrm{Pek}} - H^{\mathrm{Pek}})v\right\rangle_{L^2}\right| &\le 4K^{1/2}\int \mathrm{d}y \,\|R^{1/2}(h_{K,\cdot}(y) - h_\cdot(y))P_\psi\|_{\mathrm{op}}^2 \\ &\quad + 4K^{-1/2}\int \mathrm{d}y \left(\|R^{1/2}(\Pi_v h_{K,\cdot})(y)P_\psi\|_{\mathrm{op}}^2 + \|R^{1/2}(\Pi_v h_\cdot)(y)P_\psi\|_{\mathrm{op}}^2\right), \end{aligned} \tag{4.11}$$

and from Corollary 3.11, we obtain

$$\left|\left\langle v|(H_K^{\mathrm{Pek}} - H^{\mathrm{Pek}})v\right\rangle_{L^2}\right| \le CK^{-1/2}. \tag{4.12}$$

(ii) On $\mathrm{Ran}(\Pi_0)$ the inequality holds trivially, whereas on $\mathrm{Ran}(\Pi_1)$, it follows from $\Theta_K \le 1$, $B_K^2 \le \frac{1}{4}(\Theta_K^{-2} - 1)$, $\Theta_K^{-2} = (1 - (1 - H_K^{\mathrm{Pek}}))^{-1/2}$ and the elementary inequality $(1-x)^{-1/2} \le 1 + \beta^{-3/2}x$ for all $x \in (0, 1-\beta)$.

(iii) Here, we use $\mathrm{Tr}_{\mathrm{Ran}(\Pi_0)}(1 - H_K^{\mathrm{Pek}}) = 3$, write

$$\mathrm{Tr}_{\mathrm{Ran}(\Pi_1)}(1 - H_K^{\mathrm{Pek}}) = \int \mathrm{d}y \left\langle \psi|h^1_{K,\cdot}(y)Rh^1_{K,\cdot}(y)\psi\right\rangle_{L^2} = \int \mathrm{d}y \,\|R^{1/2}h^1_{K,\cdot}(y)P_\psi\|_{\mathrm{op}}^2 \tag{4.13}$$

and apply Corollary 3.11.

(iv) Since $1 - H_K^{\mathrm{Pek}} = \Pi_0 + \Pi_1(1 - H_K^{\mathrm{Pek}})\Pi_1 = \Pi_0 + 4T_K$, cf. equations (2.7a) and (2.7b), we can write

$$\mathrm{Tr}_{L^2}((-i\nabla)(1 - H_K^{\mathrm{Pek}})(-i\nabla)) = \mathrm{Tr}_{L^2}\left(\nabla\Pi_0\nabla\right) + 4\mathrm{Tr}_{L^2}\left(\nabla T_K\nabla\right). \tag{4.14}$$

Using the explicit form of Π_0, one shows that the first term is given by

$$\mathrm{Tr}_{L^2}\left(\nabla\Pi_0\nabla\right) = \frac{3}{\|\nabla\varphi\|_{L^2}^2}\sum_{j=1}^{3}\mathrm{Tr}_{L^2}\left(\nabla|\nabla_j\varphi\rangle\langle\nabla_j\varphi|\nabla\right) \le 3\frac{\|\Delta\varphi\|_{L^2}^2}{\|\nabla\varphi\|_{L^2}^2}, \tag{4.15}$$

which is finite since $\Delta\varphi \in L^2$. For the second term, it follows from a short computation that

$$\mathrm{Tr}_{L^2}\left(\nabla T_K\nabla\right) = \int \mathrm{d}y \left\langle \psi|[\nabla, h^1_{K,\cdot}(y)]R[\nabla, h^1_{K,\cdot}(y)]|\psi\right\rangle_{L^2}. \tag{4.16}$$

Using the Cauchy–Schwarz inequality and $\|\nabla\psi\|_{L^2} + \|R^{1/2}\|_{\mathrm{op}} + \|R^{1/2}\nabla\|_{\mathrm{op}} < \infty$, see Lemmas 3.7 and 3.8, we can estimate the last expression by

$$\begin{aligned}\int \mathrm{d}y \,\|R^{1/2}[\nabla, h^1_{K,\cdot}(y)]\psi\|_{L^2}^2 &\le C\int \mathrm{d}y \left(\|h^1_{K,\cdot}(y)\psi\|_{L^2}^2 + \|h^1_{K,\cdot}(y)\nabla\psi\|_{L^2}^2\right) \\ &\le C\int \mathrm{d}y \,|h^1_{K,0}(y)|^2 \le C\|h_{K,0}\|_{L^2}^2 = CK. \end{aligned} \tag{4.17}$$

This completes the proof of the lemma. □

Proof of Lemma 2.5. We recall that $H_K^{\mathrm{Pek}} \restriction \mathrm{Ran}(\Pi_0) = 0$ and $T_K = \frac{1}{4}(H_K^{\mathrm{Pek}} - \Pi_1)$, and set $S_K = \frac{1}{2}(\Pi_1 + H_K^{\mathrm{Pek}})$. For $(u_n)_{n\in\mathbb{N}}$ an orthonormal basis of $\mathrm{Ran}(\Pi_1)$, we further set $a_n = a(u_n)$ and use this to write the Bogoliubov Hamiltonian as

$$\mathbb{H}_K = \sum_{n,m=1}^{\infty} \Big(\big\langle u_n | S_K u_m \big\rangle_{L^2} a_n^\dagger a_m + \big(\big\langle u_n | T_K \overline{u_m} \big\rangle_{L^2} a_n^\dagger a_m^\dagger + \text{h.c.} \big) \Big) + \mathrm{Tr}_{L^2}(T_K). \tag{4.18}$$

Applying the transformation (2.11), a straightforward computation leads to

$$\begin{aligned} \mathbb{U}_K \mathbb{H}_K \mathbb{U}_K^\dagger = \sum_{n,m=1}^{\infty} \Big(& \big\langle u_n | (A_K S_K A_K + B_K S_K B_K + 4 A_K T_K B_K) u_m \big\rangle_{L^2} a_n^\dagger a_m \\ & + \big(\big\langle u_n | (A_K S_K B_K + A_K T_K A_K + B_K T_K B_K) \overline{u_m} \big\rangle_{L^2} a_n^\dagger a_m^\dagger + \text{h.c.} \big) \Big) \\ & + \mathrm{Tr}_{\mathrm{Ran}(\Pi_1)} \big(T_K + B_K S_K B_K + 2 A_K T_K B_K \big). \end{aligned} \tag{4.19}$$

The statement of the lemma now follows from

$$\Pi_1 (A_K S_K A_K + B_K S_K B_K + 4 A_K T_K B_K) \Pi_1 = \sqrt{H_K^{\mathrm{Pek}}} \tag{4.20a}$$

$$\Pi_1 (A_K S_K B_K + A_K T_K A_K + B_K T_K B_K) \Pi_1 = 0 \tag{4.20b}$$

$$\Pi_1 (T_K + B_K S_K B_K + 2 A_K T_K B_K) \Pi_1 = \frac{1}{2} \Big(\sqrt{H_K^{\mathrm{Pek}}} - \Pi_1 \Big). \tag{4.20c}$$

□

Proof of Lemma 3.4. To bound $\| w_{P,y}^1 \|_{L^2}^2$, we expand

$$\begin{aligned} w_{P,y}^1 = \Pi_1 (1 - e^{-y\nabla})(\varphi + i \xi_P) = & \int_0^1 \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2 \, \Pi_1 e^{-s_2 y \nabla} (y \nabla)^2 \varphi \\ & + \frac{i}{\alpha^2 M^{\mathrm{LP}}} \int_0^1 \mathrm{d}s \, \Pi_1 e^{-s y \nabla} (y \nabla)(P \nabla) \varphi, \end{aligned} \tag{4.21}$$

where we used $\Pi_1 (y\nabla)\varphi = 0$. Thus, since $\Delta \varphi \in L^2$, we easily arrive at

$$\| w_{P,y}^1 \|_{L^2}^2 \le C \big(y^4 + \alpha^{-4} y^2 P^2 \big) \tag{4.22}$$

for some constant $C > 0$, and with $|P| \le \alpha c$ we obtain the stated estimated. The bound for $\| \widetilde{w}_{P,y}^1 \|_{L^2}^2$ follows from

$$\| \widetilde{w}_{P,y}^1 \|_{L^2}^2 = \| \Theta_K \, \mathrm{Re}(w_{P,y}^1) \|_{L^2}^2 + \| \Theta_K^{-1} \, \mathrm{Im}(w_{P,y}^1) \|_{L^2}^2 \le C \| w_{P,y}^1 \|_{L^2}^2, \tag{4.23}$$

where we used that Θ_K is real-valued and satisfies

$$0 < \beta \le \Theta_K^2 \le 1 \tag{4.24}$$

when restricted to $\mathrm{Ran}(\Pi_1)$; see Lemma 2.3. To bound $\| w_{P,y}^0 \|_{L^2}^2$ we use

$$\| w_{P,y}^0 \|_{L^2}^2 = \| w_{0,y}^0 \|_{L^2}^2 + \| \Pi_0 (1 - e^{-y\nabla}) \xi_P \|_{L^2}^2, \tag{4.25}$$

since φ, ξ_P and Π_0 are all real-valued. Expanding $1 - e^{-y\nabla}$ as in equation (4.21), it is easy to conclude that $\|\Pi_0(1 - e^{-y\nabla})\xi_P\|^2_{L^2} \leq CP^2y^2\alpha^{-4}$. Using the explicit form of Π_0 and $\langle\nabla\varphi|\varphi\rangle_{L^2} = 0$, we can write

$$\|w^0_{0,y}\|^2_{L^2} = \frac{3}{\|\nabla\varphi\|^2_{L^2}} \sum_{i=1}^{3} \left|\left\langle\nabla_i\varphi|e^{-y\nabla}\varphi\right\rangle_{L^2}\right|^2. \tag{4.26}$$

Using the Fourier representation and rotation invariance, we have

$$\left|\left\langle\nabla_i\varphi|e^{-y\nabla}\varphi\right\rangle_{L^2}\right| = \left|\int p_i|\hat{\varphi}(p)|^2 \sin(py)\, \mathrm{d}y\right|. \tag{4.27}$$

By the elementary inequality $|\sin z - z| \leq Cz^3$, the formula $\|(y\nabla)\varphi\|^2_{L^2} = 2\lambda y^2$ and the finiteness of $\|\Delta\varphi\|_{L^2}$, we conclude that

$$\left|\|w^0_{P,y}\|^2_{L^2} - 2\lambda y^2\right| \leq C\left(y^4 + y^6 + \alpha^{-4}y^2P^2\right). \tag{4.28}$$

To prove the last bound, we use

$$\|\widetilde{w}_{P,y}\|^2_{L^2} = \|w^0_{P,y}\|^2_{L^2} + \|\Theta_K \operatorname{Re}(w^1_{P,y})\|^2_{L^2} + \|\Theta_K^{-1} \operatorname{Im}(w^1_{P,y})\|^2_{L^2}, \tag{4.29}$$

and hence with equation (4.24),

$$\beta\|w^1_{P,y}\|^2_{L^2} \leq \|\widetilde{w}_{P,y}\|^2_{L^2} - \|w^0_{P,y}\|^2_{L^2} \leq \beta^{-1}\|w^1_{P,y}\|^2_{L^2}. \tag{4.30}$$

The desired bound now follows from equations (4.22) and (4.28). □

Proof of Lemma 3.5. From Lemma 3.4, we have

$$\left|\|\widetilde{w}_{P,y}\|^2_{L^2} - 2\lambda y^2\right| \leq C(\alpha^{-2}y^2 + y^4 + y^6) \leq C\frac{y^2}{\alpha} \quad \text{for all} \quad \frac{|P|}{\alpha} \leq c,\ y^2 \leq \alpha^{-1}. \tag{4.31}$$

Hence, there is a constant $\mu > 0$ such that for all $y^2 \leq \alpha^{-1}$ the weight function (3.33) satisfies

$$n_{\delta,\eta}(y) \leq \exp(-(\lambda\eta\alpha^{2(1-\delta)} - \mu\alpha^{-2\delta+1})y^2) \tag{4.32a}$$

$$n_{\delta,\eta}(y) \geq \exp(-(\lambda\eta\alpha^{2(1-\delta)} + \mu\alpha^{-2\delta+1})y^2). \tag{4.32b}$$

In the remainder, let us abbreviate $f_n(y) = |y|^n g(y)$ and $Z(y) = |n_{\delta,\eta}(y) - e^{-\lambda\eta\alpha^{2(1-\delta)}y^2}|$. We then decompose the integral into

$$\int \mathrm{d}y\, f_n(y)Z(y) = \int_{B_\alpha} \mathrm{d}y\, f_n(y)Z(y) + \int_{B^c_\alpha} \mathrm{d}y\, f_n(y)Z(y) \tag{4.33}$$

with $B_\alpha = \{y \in \mathbb{R}^3 : y^2 \leq \alpha^{-1}\}$. The bounds (4.32a) and (4.32b) imply that

$$|Z(y)| \leq e^{-\lambda\eta\alpha^{2(1-\delta)}}\left(e^{\mu\alpha^{-2\delta+1}y^2} - 1\right) \quad \forall y \in B_\alpha \tag{4.34}$$

and thus by $|e^z - 1| \leq ze^z$ for $z > 0$, we obtain

$$\int_{B_\alpha} \mathrm{d}y\, f_n(y)Z(y) \leq \mu\alpha^{-2\delta+1} \int \mathrm{d}y\, f_n(y)y^2 e^{-(\eta\lambda-\mu\alpha^{-1})\alpha^{2(1-\delta)}y^2}. \tag{4.35}$$

The last expression is further bounded by

$$\int \mathrm{d}y\, f_n(y) y^2 e^{-(\eta\lambda-\mu\alpha^{-1})\alpha^{2(1-\delta)}y^2} \le \|g\|_{L^\infty} \int \mathrm{d}y\, |y|^{n+2} e^{-(\eta\lambda-\mu\alpha^{-1})\alpha^{2(1-\delta)}y^2} = \frac{C_n \|g\|_{L^\infty}}{\alpha^{(5+n)(1-\delta)}} \left(\eta\lambda - \mu\alpha^{-1}\right)^{-(n+5)/2} \tag{4.36}$$

and since the resulting expression is uniformly bounded in $\eta \ge \eta_0$ and α large, we get

$$\int_{B_\alpha} \mathrm{d}y\, f_n(y) Z(y) \le C_n \frac{\|g\|_{L^\infty}}{\alpha^{(4+n)(1-\delta)+\delta}}. \tag{4.37}$$

To bound the second term in equation (4.33), we estimate

$$\int_{B_\alpha^c} \mathrm{d}y\, f_n(y) Z(y) \le \int_{B_\alpha^c} \mathrm{d}y\, f_n(y) n_{\delta,\eta}(y) + e^{-\lambda\eta\alpha^{-2\delta+1}} \int \mathrm{d}y\, f_n(y). \tag{4.38}$$

To see that the first summand is exponentially small as well, we use equation (4.29), equation (4.24) and $\mathrm{Re}(w^i_{P,y}) = \Pi_i \,\mathrm{Re}(w_{P,y}) = \Pi_i \,\mathrm{Re}(w_{0,y})$ for $i = 0, 1$,

$$\|\widetilde{w}_{P,y}\|^2_{L^2} \ge \|\,\mathrm{Re}(w^0_{P,y})\|^2_{L^2} + \beta \|\,\mathrm{Re}(w^1_{P,y})\|^2_{L^2} \ge \beta \|\mathrm{Re}(w_{0,y})\|^2_{L^2} = \beta \|(1 - e^{-y\nabla})\varphi\|^2_{L^2}, \tag{4.39}$$

and hence

$$n_{\delta,\eta}(y) \le \exp\Big(-\eta\beta\alpha^{2(1-\delta)} q(y)\Big) \quad \text{with} \quad q(y) = \frac{1}{2}\|(1 - e^{-y\nabla})\varphi\|^2_{L^2}. \tag{4.40}$$

Since φ is real-valued, we have $\langle \varphi | e^{-y\nabla} | \varphi \rangle_{L^2} = \langle \varphi | e^{y\nabla} | \varphi \rangle_{L^2} = (\varphi * \varphi)(y)$ and thus

$$q(y) = \|\varphi\|^2_{L^2} - (\varphi * \varphi)(y). \tag{4.41}$$

Recall that, as shown in [36], the electronic Pekar minimizer ψ is radial and nonincreasing and hence φ, cf. equation (1.14), is radial and nonincreasing as well, as convolutions of radial nonincreasing functions are themselves radial nonincreasing functions. Consequently, $q(y)$ is radial and monotone nondecreasing, and thus $q(y) \ge q(y')$ for all $y \in B^c_\alpha$, $y' \in B_\alpha$. On the other hand, by a simple computation, using the regularity of φ, one finds that $q(y) \ge C_0 y^2$ for some $C_0 > 0$ and all $|y|$ small enough, and thus $q(y) \ge C_0 \alpha^{-1}$ for all $y \in B^c_\alpha$ and α large. Therefore,

$$\begin{aligned}\int_{B_\alpha^c} \mathrm{d}y\, f_n(y) n_{\delta,\eta}(y) &\le \int_{B_\alpha^c} \mathrm{d}y\, f_n(y) e^{-\eta\beta\alpha^{2(1-\delta)} q(y)} \\ &\le e^{-C_0\eta\beta\alpha^{2(1-\delta)-1}} \int \mathrm{d}y\, f_n(y) \le e^{-d\alpha^{-2\delta+1}} \int \mathrm{d}y\, f_n(y)\end{aligned} \tag{4.42}$$

for some $d > 0$, which completes the proof of the lemma. □

Proof of Lemma 3.16. Let $p = -i\nabla$. By a straightforward computation using equation (2.11), we arrive at

$$\mathbb{U}_K P_f \mathbb{U}_K^\dagger \Omega = \sum_n a^\dagger(A_K u_n) a^\dagger(B_K p \overline{u_n})\Omega + \mathrm{Tr}_{L^2}(B_K p B_K)\Omega \tag{4.43}$$

for some orthonormal basis $(u_n)_{n\in\mathbb{N}}$ of $L^2(\mathbb{R}^3)$. That $B_K p B_K$ is trace-class can be seen via

$$\mathrm{Tr}_{L^2} |B_K p B_K| \le \|B_K\|_{\mathrm{HS}} \|p B_K\|_{\mathrm{HS}} \le CK, \tag{4.44}$$

where the second step follows from Lemma 2.3, implying $\|B_K\|_{\mathrm{HS}} \leq C$, and

$$\|pB_K\|_{\mathrm{HS}}^2 = \mathrm{Tr}_{L^2}(pB_KB_Kp) \leq \mathrm{Tr}_{L^2}(p(1 - H_K^{\mathrm{Pek}})p) \leq CK. \tag{4.45}$$

By rotation invariance $\mathrm{Tr}_{L^2}(B_KpB_K) = 0$. The first term in equation (4.43), on the other hand, is seen to be a two-particle wave function Φ_K given by

$$\Phi_K(x, y) = \frac{1}{\sqrt{2}}(A_KpB_K + B_KpA_K)(x, y). \tag{4.46}$$

Thus,

$$\left\langle \Upsilon_K \middle| (P_f)^2 \Upsilon_K \right\rangle_{\mathcal{F}} = \frac{1}{2}\|A_KpB_K + B_KpA_K\|_{\mathrm{HS}}^2 \leq 2\|A_K\|_{\mathrm{op}}^2 \|pB_K\|_{\mathrm{HS}}^2 \leq CK, \tag{4.47}$$

where we invoked again equation (4.45). □

Competing Interest. The authors have no competing interest to declare.

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