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

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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.

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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 [26]. 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 [18] the Hamiltonian of the model acts on the Hilbert space

\[ \mathcal{H} = L^2(\mathbb{R}^3, dx) \otimes \mathcal{F}, \]

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

\[ H_\alpha = -\Delta_x + \alpha^{-2}N + \alpha^{-1}\phi(h_x). \]

Here \( x \in \mathbb{R}^3 \) is the coordinate of the electron, \( N \) denotes the number operator on Fock space, and the field operator \( \phi(h_x) = a^1(h_x) + a(h_x) \) with coupling function

\[ h_x(y) = -\frac{1}{2\pi^2|x-y|^2} \]

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

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

\[ H_\alpha^{\text{Polaron}} = -\Delta_x + N + \sqrt{\alpha} \phi(h_0), \] (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, i.e., it commutes with the total momentum operator,

\[ [H_\alpha, -i\nabla_x + P_f] = 0 \] (1.6)

where \( P_f = d\Gamma(-i\nabla) \) 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 \( H_\alpha \) 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

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

where \( H_\alpha(P) \) acts on the Fock space only [28]. The Fröhlich Hamiltonian \( H_\alpha \) is unitarily equivalent to the fiber decomposition \( \int_{\mathbb{R}^3} H_\alpha(P) dP \), which follows easily from transforming \( H_\alpha \) 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,

\[ E_\alpha(P) = \inf \sigma(H_\alpha(P)), \] (1.8)

which by construction satisfies \( E_\alpha(RP) = E_\alpha(P) \) for all rotations \( R \in \text{SO}(3) \). It is known that \( E_\alpha(0) \leq E_\alpha(P) \) and hence \( E_\alpha(0) = \inf \sigma(H_\alpha) \) (in fact it is expected that \( E_\alpha(0) < E_\alpha(P) \) for all \( P \neq 0 \) [10]). Further properties, such as the domain of analyticity, existence of ground states and the value of the bottom of the continuous spectrum, were analyzed in [8, 19, 21, 40, 49].

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 (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 $\varphi$ denotes the self-consistent polarization field, which coincides with the classical polaron mass introduced by Landau and Pekar [27], see (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 30’s and 40’s [17, 26, 27] 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 [37]. More recent developments are reviewed in [1]. Mathematically rigorous results for the leading order asymptotics of $E_\alpha(0)$, for $\alpha$ large, were obtained by Lieb and Yamazaki [36] (with non-matching upper and lower bounds) and by Donsker and Varadhan [9] as well as Lieb and Thomas [35]. The effective mass has been studied in [4, 10, 12, 33, 34, 48]. Further improvements have been obtained for confined polarons or polaron models with more regular interaction [13, 16, 43]. For completeness, let us also mention recent progress in the understanding of the polaron path measure [3, 42] as well as the increased interest in the analysis of the Schrödinger time evolution of strongly coupled polarons [11, 14, 15, 23, 30, 31, 38].

1.2 Pekar functionals

The semiclassical theory of the polaron has been introduced by Pekar [46]. 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 famous Born–Oppenheimer theory [5, 6]. With this in mind, one can minimize the Fröhlich Hamiltonian over product states of the form

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

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

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

(1.10)
with polarization potential

\[ V^v(x) = -2 \text{Re} \langle v|h_x \rangle_{L^2} = - \text{Re} \int \frac{v(y)}{\pi^2|x-y|^2} \, dy. \]  

(1.11)

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

\[ E(u) = \inf_{v \in L^2} G(u,v) = \int |u(x)|^2 \, dx - \frac{1}{4\pi} \iint \frac{|u(x)|^2|u(y)|^2}{|x-y|} \, dx \, dy, \]  

(1.12)

which is known [32] to admit a unique rotational invariant minimizer \( \psi > 0 \) (the minimizing property is unique only up to translations and multiplications 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

\[ F(v) = \inf_{||u||_{L^2} = 1} G(u,v) = \inf \text{spec} (-\Delta + V^v) + ||v||_{L^2}^2 \]  

(1.13)

whose unique rotational invariant minimizer is readily shown to be

\[ \varphi(z) = -\langle \psi|h.(z)\psi \rangle_{L^2} = \int \frac{\psi(y)^2}{2\pi^2|z-y|^2} \, dy. \]  

(1.14)

The corresponding classical ground state energy is called the Pekar energy

\[ e_{\text{Pek}} = E(\psi) = F(\varphi), \quad e_{\text{Pek}} < 0, \]  

(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 [9] who proved that \( \lim_{\alpha \to \infty} \inf \sigma(H^\alpha) = e_{\text{Pek}} \) and subsequently by Lieb and Thomas [35] who added a quantitative bound for the error by showing that

\[ \inf \sigma(H^F_\alpha) \geq e_{\text{Pek}} + O(\alpha^{-1/5}). \]  

(1.16)

Given the potential \( V^\varphi \) for the field \( \varphi \), one can define the Schrödinger operator

\[ h_{\text{Pek}} = -\Delta + V^\varphi(x) - \lambda_{\text{Pek}}, \quad \lambda_{\text{Pek}} = e_{\text{Pek}} - ||\varphi||_{L^2}^2 \]  

(1.17)

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

\[ R = Q_\psi(h_{\text{Pek}})^{-1}Q_\psi \quad \text{with} \quad Q_\psi = 1 - P_\psi, \quad P_\psi = \langle \psi \rangle \langle \psi |, \]  

(1.18)
defines a bounded operator \((P_\psi)\) denotes the orthogonal projection onto the state \(\psi\).

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

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

In the following lemma we collect some important properties of \(H^{\text{Pek}}\).

**Lemma 1.1.** The operator \(H^{\text{Pek}}\) has integral kernel

\[
H^{\text{Pek}}(y, z) = \delta(y - z) - 4 \operatorname{Re} \left\langle \psi | h \cdot (y) Rh \cdot (z) \psi \right\rangle_{L^2} \tag{1.20}
\]

and satisfies the following properties.

(i) \(0 \leq H^{\text{Pek}} \leq 1\)

(ii) \(\ker H^{\text{Pek}} = \text{Span}\{\partial_i \varphi : i = 1, 2, 3\}\)

(iii) \(H^{\text{Pek}} \geq \tau > 0\) when restricted to \((\ker H^{\text{Pek}})^{\perp}\)

(iv) \(\operatorname{Tr}_{L^2}(1 - \sqrt{H^{\text{Pek}}}) < \infty\).

The proof of the lemma, in particular Item (ii), is based on the analysis of the Hessian of the energy functional \(E\) [29]. 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 \(\alpha\). In general, \(E_\alpha(P)\) is expected to interpolate between two distinct regimes (see for instance [20, 22, 49, 51]): 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

\[
E^{\text{eff}}_\alpha(P) = E_\alpha(0) + \frac{P^2}{2M^{\text{eff}}(\alpha)} \tag{1.21}
\]

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

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

It is easy to verify that \(M^{\text{eff}}(\alpha) \geq 1/2\) (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
Figure 1.1: The energy-momentum relation $E_\alpha(P)$ is expected to have two characteristic regimes: The parabolic quasi-particle regime for small momenta (dark area) and the radiative regime for large momenta (light area). For the transition between the two there is no concrete prediction. The dashed lines denote the quasi-particle energy (1.21) and the bottom of the continuous spectrum (1.23). Their intersection defines the momentum scale $P_c(\alpha)$ that is proportional to $\alpha$ for large coupling.

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 continuous spectrum [40],

$$\inf \sigma_{\text{cont}}(H_\alpha(P)) = E_\alpha(0) + \alpha^{-2}. \quad (1.23)$$

The two regimes cross at $|P| = P_c(\alpha) := \sqrt{2M_{\text{eff}}(\alpha)/\alpha}$ which marks a characteristic momentum scale of the polaron. While the quasi-particle picture is expected to be accurate for $|P| \ll P_c(\alpha)$, the radiative regime should hold for $|P| \gtrsim P_c(\alpha)$ (see also Remark 1.2 below). Between the two regimes there is no concrete prediction for the behavior of $E_\alpha(P)$. A schematic plot is provided in Figure 1.1.

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 $M_{\text{eff}}(\alpha)$, it is instructive to recall two longstanding 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 $M_{\text{eff}}(\alpha)$ should asymptotically tend to the expression that follows from the corresponding semiclassical counterpart of the problem. This semiclassical theory of the effective mass was introduced by Landau and Pekar in 1948 [27], and, based on this work (see also [12, 48]), it is conjectured that

$$\lim_{\alpha \to \infty} \frac{M_{\text{eff}}(\alpha)}{\alpha^4} = M^{\text{LP}} \quad \text{with} \quad M^{\text{LP}} = \frac{2}{3} \|\nabla \varphi\|_{L^2}^2. \quad (1.24)$$
Although this problem is many decades old, the best available rigorous result is that $M^{\text{eff}}(\alpha)$ is divergent \cite{34}, with a recent proof that it diverges at least as fast as $\alpha^{2/5}$ \cite{4}. Regarding the ground state energy $E_\alpha(0)$ the prediction from the physics literature (see e.g. \cite{2, 24, 39, 50}) is that

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

for some $\delta > 0$ (in fact it is predicted that $\delta = 2$ \cite{24}). Compared to the semiclassical expansion this includes a subleading correction of order $\alpha^{-2}$, 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 \cite{39}. Now inserting (1.24) and (1.25) into (1.21), and based on the expectation that the quasi-particle regime is restricted to $|P| \ll \sqrt{2M^{\text{eff}}(\alpha)/\alpha} \sim \alpha$, it is clear that the Bogoliubov energy needs to be taken into account in order to see the quasi-particle energy shift given by $P^2/(2\alpha^4M^{\text{LP}}) \ll \alpha^{-2}$.

Mathematically, the validity of (1.25) has been established only for confined polaron models \cite{13, 16}. The corresponding upper bound for the unconfined model is a corollary of our main result.

As a summary of the above we arrive at the following claim.

**Conjecture.** Let $M^{\text{LP}}$ be the Landau–Pekar mass defined in (1.24). There exists a continuous function $f : [0, \infty) \to [0, \infty)$, satisfying $f(s) \to 1$ as $s \to \infty$ and

$$f(s) = \frac{s}{2M^{\text{LP}}} + O(s^2) \quad \text{as} \quad s \to 0, \quad (1.26)$$

such that for all $P \in \mathbb{R}^3$

$$\lim_{\alpha \to \infty} \alpha^2 \left( E_\alpha(\alpha P) - e^{\text{Pek}} - \frac{1}{2\alpha^2} \text{Tr}_{L^2}(\sqrt{H^{\text{Pek}}} - 1) \right) = f(P^2). \quad (1.27)$$

Our main result, Theorem 2.1 below, provides an upper bound for $E_\alpha(\alpha P)$ that is compatible with the conjecture in the quasi-particle regime. To be more precise, our result implies that the left side of (1.27), with the limit replaced by the lim sup, is bounded from above by $P^2/(2M^{\text{LP}})$ for all $P \in \mathbb{R}^3$. This shows that the corrections to the quasi-particle energy are always negative, a conclusion that is not entirely obvious a priori.

**Remark 1.1.** An immediate consequence of the conjecture would be that

$$\frac{1}{2} \lim_{P \to 0} \lim_{\alpha \to \infty} \alpha^2 \left( \frac{E_\alpha(\alpha P) - E_\alpha(0)}{P^2} \right)^{-1} = M^{\text{LP}} \quad (1.28)$$

which is to be compared with (1.24) where the limits are taken in reversed order.

**Remark 1.2.** Even though our analysis is focused on the quasi-particle regime, let us mention an interesting problem concerning the radiative regime. The question is whether $E_\alpha(P)$ enters the continuous part of the spectrum, i.e. whether the spectral gap closes at some finite
momentum, or not. The answer may in fact depend on the dimension and possibly also on the value of $\alpha$. It is known that in two dimensions $E_\alpha(P)$ remains an isolated eigenvalue for all $P$, meaning that the curve approaches $\inf \sigma_{\text{cont}}(H_\alpha(P))$ only in the limit $|P| \to \infty$ [49]. To our knowledge in three dimensions the question is not completely settled. While for small momenta it is known that $E_\alpha(P)$ corresponds to a simple eigenvalue [49], there is indication from results obtained for weak coupling that $E_\alpha(P)$ agrees with the bottom of the continuous spectrum when $|P|$ is sufficiently large [8].

2 Main Result

We are now ready to state the main result.

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

$$E_\alpha(P) \leq e^{\text{pek}} + \frac{\text{Tr}_{L^2}(\sqrt{H^\text{pek}} - 1)}{2\alpha^2} + \frac{P^2}{2\alpha^4 M_{LP}} + C_{c, \varepsilon} \alpha^{-\frac{3}{2} + \varepsilon}$$

(2.1)

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

Since the operator $\sqrt{H^\text{pek}} - 1$ is trace class, non-zero and non-positive (see Lemma 1.1), the second term on the right side is finite and lowers the energy. It corresponds to the predicted quantum corrections of the ground state energy of the Fröhlich Hamiltonian [2, 24, 39, 50]. 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 that agrees with this prediction. For momenta in the range $\alpha^{-\frac{1}{4} + \frac{\varepsilon}{2}} \ll |P|/\alpha \leq c$, the last term in (2.1) is subleading for large $\alpha$ 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 $\alpha^4 M_{LP}$. The upper restriction on the range of $|P|$ is natural, since for $|P|/\alpha \geq \sqrt{2M_{LP}}$ the right side of (2.1) would be larger than the value of the bottom of the continuous spectrum (1.23). The lower restriction $|P|/\alpha \gg \alpha^{-\frac{1}{4} + \frac{\varepsilon}{2}}$, on the other hand, could in principle be improved by deriving a better error term in (2.1).

The derivation of a matching lower bound is, of course, more involved. To our knowledge the best known parabolic lower bound is still the one obtained by Lieb and Yamazaki [36] in 1958 stating that $E_\alpha(P) \geq c_1 e^{\text{pek}} + c_2 P^2/(2\alpha^4 M_{LP})$ with $c_1 \approx 3.07$ and $c_2 \approx 0.11$. Even for $P = 0$ it remains a challenging problem to improve the Lieb–Thomas bound (1.15) such that it includes the quantum corrections of order $\alpha^{-2}$. Progress in this direction has been achieved in [13, 16] for simplified polaron models in which the electron and the quantum field are confined to suitable finite size regions.

In the next two sections we provide the definition of our trial state and formulate our main statement as a variational estimate. The remainder of the paper is devoted to the proof of the variational 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 $\Pi_0$ and $\Pi_1$ to be the orthogonal projectors onto $\text{Ker}H_{\text{Pek}} = \text{Span}\{\partial_i \varphi : i = 1, 2, 3\}$ and $(\text{Ker}H_{\text{Pek}})^\perp$, that is

$$\text{Ran}(\Pi_0) = \text{Ker}H_{\text{Pek}}, \quad \text{Ran}(\Pi_1) = (\text{Ker}H_{\text{Pek}})^\perp.$$  \hspace{1cm} (2.2)

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

$$\mathcal{F} = \mathcal{F}_0 \otimes \mathcal{F}_1 \quad \text{with} \quad \mathcal{F}_0 = \mathcal{F}(\text{Ran}(\Pi_0)) \quad \text{and} \quad \mathcal{F}_1 = \mathcal{F}(\text{Ran}(\Pi_1)).$$  \hspace{1cm} (2.3)

For technical reasons, which are explained in Section 3.4.3, we introduce the Bogoliubov Hamiltonian $H_K$ with a momentum cutoff $K \in (0, \infty]$. Setting $N_1 = d\Gamma(\Pi_1)$ (the number operator on $\mathcal{F}_1$) we define

$$H_K = N_1 - \langle \psi | \phi(h_{K,x}^1)R\phi(h_{K,x}^1)\psi \rangle_{L^2},$$  \hspace{1cm} (2.4)

where the new coupling function

$$h_{K,x}^1(y) = \int dz \Pi_1(y, z)h_{K,x}(z) \quad \text{with} \quad h_{K,x}(y) = \frac{1}{(2\pi)^3} \int_{|k| \leq K} \frac{e^{ik(x-y)}}{|k|} dk$$  \hspace{1cm} (2.5)

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

$$\langle \psi | \phi(h_{K,x}^1)R\phi(h_{K,x}^1)\psi \rangle_{L^2} = \int dym dyd\psi \langle (h_{K,x}^1)(y)R(h_{K,x}^1)(z)\psi \rangle_{L^2}(a_y^\dagger a_y + a_z^\dagger a_z).$$  \hspace{1cm} (2.6)

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

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

$$H_{\text{Pek}}^K \mid \text{Ran}(\Pi_1) = \Pi_1 - 4T_K$$  \hspace{1cm} (2.7a)

$$H_{\text{Pek}}^K \mid \text{Ran}(\Pi_0) = 0$$  \hspace{1cm} (2.7b)

where $T_K$ is defined by the integral kernel

$$T_K(y, z) = \text{Re} \langle \psi | h_{K,x}^1(y)Rh_{K,x}^1(z)\psi \rangle_{L^2}.$$  \hspace{1cm} (2.8)
By definition $H_K^\text{Pek} = H^\text{Pek}$, see (1.20). Moreover we set $\Theta_K = (H_K^\text{Pek})^{1/4}$ and

$$
A_K \upharpoonright \text{Ran}(\Pi_1) = \frac{\Theta_K^{-1} + \Theta_K}{2} \quad B_K \upharpoonright \text{Ran}(\Pi_1) = \frac{\Theta_K^{-1} - \Theta_K}{2}
$$

$$
A_K \upharpoonright \text{Ran}(\Pi_0) = \Pi_0 \quad B_K \upharpoonright \text{Ran}(\Pi_0) = 0.
$$

(2.9a) (2.9b)

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

$$
\sup_{K \geq K_0} (\|A_K\|_{\text{op}} + \|B_K\|_{\text{HS}}) \leq C
$$

(2.10)

for some $K_0$ large enough.

**Lemma 2.2.** For $K_0$ large enough there exist constants $\beta \in (0, 1)$ and $C > 0$ such that

(i) $0 \leq H_K^\text{Pek} \leq 1$ and $(H_K^\text{Pek} - \beta) \upharpoonright \text{Ran}(\Pi_1) \geq 0$

(ii) $(B_K)^2 \leq C(1 - H_K^\text{Pek})$

(iii) $\text{Tr}_{L^2}(1 - H_K^\text{Pek}) \leq C$

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

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

Up to normal ordering the Hamiltonian $H_K$ corresponds to the second quantization of $H_K^\text{Pek}$. From the properties of the latter we can deduce that $H_K$ is diagonizable by a unitary Bogoliubov transformation. To this end we introduce the transformation

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

(2.11)

That this transformation defines a unitary operator $\mathbb{U}_K$ for all $K \in (K_0, \infty]$ is a consequence of (2.10). This is known as the Shale-Stinespring condition and we refer to [47] for more details. Also note that $\mathbb{U}_K$ does not mix the two components in $\mathcal{F} = \mathcal{F}_0 \otimes \mathcal{F}_1$.

**Lemma 2.3.** For $K \in (K_0, \infty]$ with $K_0$ large enough and $\mathbb{U}_K$ the unitary operator defined by (2.11), we have

$$
\mathbb{U}_K H_K \mathbb{U}_K^\dagger = \text{d}\Gamma(\sqrt{H_K^\text{Pek}}) + \frac{1}{2} \text{Tr}_{L^2}(\sqrt{H_K^\text{Pek}} - \Pi_1)
$$

(2.12)

with $H_K^\text{Pek}$ defined by (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 $H_K$ is given by

$$
\inf \sigma(H_K) = \frac{1}{2} \text{Tr}_{L^2}(\sqrt{H_K^\text{Pek}} - \Pi_1) = \frac{1}{2} \text{Tr}_{L^2}(\sqrt{H_K^\text{Pek}} - 1) + \frac{3}{2}.
$$

(2.13)
where we also used $\Pi_1 = 1 - \Pi_0$ and $\text{Tr}_{L^2}(\Pi_0) = 3$. Moreover, since $H^{\text{Pek}}_K \leq \Pi_1$ we have $\inf \sigma(\mathbb{H}_K) < 0$ and from Item (iv) of Lemma 2.2 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

$$\Upsilon_K = \mathbb{U}^\dagger_K \Omega,$$  \hfill (2.14)

where it is important to keep in mind that the state $\Upsilon_K$ has excitations only in $F_1$ (i.e., no zero-mode excitations) since $\mathbb{U}^\dagger_K$ acts as the identity on $F_0$, see (2.9b).

### 2.2 Trial state and variational 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 $\Psi_{\psi,\phi}$, that is

$$\Psi_{\alpha}^{\text{Pek}}(P) = \int dx e^{i(P_f - P)x} \psi(x) e^{a^\dagger(\alpha \phi)} \Omega.$$  \hfill (2.15)

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

$$e^{\text{Pek}} - \frac{3}{2\alpha^2} + \frac{P^2}{\alpha^4 M_{\text{LP}}} + o(\alpha^{-2}).$$  \hfill (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 [25] and [44]. 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 (2.15). On the one hand, we have to replace the classical field $\phi$ by a suitably shifted $\varphi_F$ in order to get the correct momentum dependent term (note that (2.16) is missing a factor $\frac{1}{2}$ in the quadratic term). The missing part of the rest energy (compare with (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 \( \alpha \), the total momentum \( P \in \mathbb{R}^3 \) and the cutoff \( K \in (K_0, \infty) \), given by

\[
\Psi_{K,\alpha}(P) = \int dx e^{i(P_f^\dagger - P_s^\dagger) \alpha} e^{a(\alpha \varphi_P)} \left( G^0_{K,x} - \alpha^{-1} G^1_{K,x} \right)
\]  

(2.17)

where

\[
\varphi_P = \varphi + i\xi_P \quad \text{with} \quad \xi_P = \frac{1}{\alpha^2 M_{LP}} \nabla \varphi, \quad M_{LP} = \frac{2}{3} \| \nabla \varphi \|_{L^2}^2,
\]  

(2.18)

and

\[
G^0_{K,x} = \psi(x) \Upsilon_K, \quad G^1_{K,x} = u_\alpha(x) (R\phi(h^K_{K,x}) \psi)(x) \Upsilon_K \quad \text{and} \quad \Upsilon_K = \Upsilon_K^\dagger \Omega.
\]  

(2.19)

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

\[
u = \begin{cases}
1 & \forall |x| \leq \alpha \\
0 & \forall |x| \geq 2\alpha
\end{cases}
\]

and

\[
\| \nabla u_\alpha \|_{L^\infty} + \| \Delta u_\alpha \|_{L^\infty} \leq C\alpha^{-1}
\]  

(2.20)

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

Remark 2.1. Writing \( G^i_{K,x} \) we think of these states as elements in \( L^2(\mathbb{R}^3, \mathcal{F}) \) and of

\[
\langle R\phi(h^K_{K,x}) \psi(x) = \int \int dz dy R(x,y) h^K_{K,y}(z) \psi(y) (a^\dagger_z + a_z)
\]  

(2.21)

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

\[
G^0_K = \psi \otimes \Upsilon_K, \quad G^1_K = u_\alpha R\phi(h^K_{K,x}) \psi \otimes \Upsilon_K.
\]  

(2.22)

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

Proposition 2.4. Let \( \Psi_{K,\alpha}(P) \in \mathcal{F} \) as in (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

\[
\frac{\langle \Psi_{K,\alpha}(P) | H_\alpha(P) \Psi_{K,\alpha}(P) \rangle_{\mathcal{F}}}{\langle \Psi_{K,\alpha}(P) | \Psi_{K,\alpha}(P) \rangle_{\mathcal{F}}} \leq e^{P_{\text{pek}}} + \frac{\inf \sigma(\mathbb{H}_\infty) - \frac{\varepsilon}{2}}{\alpha^2} + \frac{P^2}{2\alpha^4 M_{LP}} + C_\varepsilon \alpha \varepsilon r(K, \alpha)
\]  

(2.23)

for all \( |P|/\alpha \leq c \) and all \( K, \alpha \) large enough with \( K/\alpha \leq \tilde{c} \).
With (2.13) and $H_{\infty}^{\text{Pek}} = H^{\text{Pek}}$ we can rewrite the term of order $\alpha^{-2}$ as
\[
\inf \sigma(H_{\infty}) - \frac{3}{2} = \frac{1}{2} \text{Tr}_{L^2}(\sqrt{H^{\text{Pek}}} - 1).
\] (2.24)
Choosing $K$ now proportional to $\alpha$ optimizes the asymptotics of the error in (2.23) and proves Theorem 2.1.

3 Proof of Proposition 2.4

We recall the definition of the field operators
\[
\phi(f) = a^\dagger(f) + a(f), \quad \pi(f) = \phi(if)
\] (3.1)
and the Weyl operator
\[
W(f) = e^{-i\pi(f)} = e^{a^\dagger(f) - a(f)} = e^{a^\dagger(f)}e^{-a(f)}e^{-\frac{1}{2}||f||^2_{L^2}}.
\] (3.2)
The Weyl operator is unitary and satisfies
\[
W^\dagger(f) = W(-f), \quad W(f)W(g) = W(g)W(f)e^{2i\text{Im}(gf)_{L^2}} = W(f + g)e^{i\text{Im}(gf)_{L^2}}.
\] (3.3)

3.1 The total energy

The proof of Proposition 2.4 starts with a convenient formula for the energy evaluated in the trial state. For the precise statement, we introduce the $y$-dependent function in $L^2(\mathbb{R}^3)$,
\[
w_{P,y} = (1 - e^{-y\nabla})\varphi_P,
\] (3.4)
and the $y$-dependent Fock space operator
\[
A_{P,y} = iP_fy + ig_P(y), \quad g_P(y) = -\frac{2}{M_{\text{LP}}} \int_0^1 ds \langle \varphi | e^{-sy\nabla} (y\nabla)^3 (P\nabla) \varphi \rangle_{L^2}.
\] (3.5)
Since $g_P(y)$ is real-valued we have $(A_{P,y})^\dagger = -A_{P,y}$. We further consider the Weyl-transformed Fröhlich Hamiltonian,
\[
\tilde{H}_{\alpha,P} = W(\alpha \varphi_P)^\dagger(H_\alpha - e^{\text{Pek}})W(\alpha \varphi_P) = h^{\text{Pek}} + \alpha^{-2}N + \alpha^{-1}\varphi(h_x + \varphi_P),
\] (3.6)
where we recall $h^{\text{Pek}} = -\Delta + V^\varphi - \lambda^{\text{Pek}}$, and denote the shift operator acting on $L^2(\mathbb{R}^3)$ by $T_y = e^{y\nabla}$ with $y \in \mathbb{R}^3$. 
Lemma 3.1. For $\Psi_{K,\alpha}(P)$ defined in (2.17) we have

$$\langle \Psi_{K,\alpha}(P) | H_\alpha(P) | \Psi_{K,\alpha}(P) \rangle_x = \left( e^{Pek} + \frac{P^2}{2\alpha^4MLP} \right) N + \mathcal{E} + \mathcal{G} + \mathcal{K}$$

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

$$\mathcal{E} = \int dy \langle G_K^0 | \tilde{H}_{\alpha,P} T_y e^{A_{P,y}} W(\alpha w_{P,y}) G_K^0 \rangle_x$$

$$\mathcal{G} = -\frac{2}{\alpha} \int dy \text{ Re} \langle G_K^0 | \tilde{H}_{\alpha,P} T_y e^{A_{P,y}} W(\alpha w_{P,y}) G_K^1 \rangle_x$$

$$\mathcal{K} = \frac{1}{\alpha^2} \int dy \langle G_K^1 | \tilde{H}_{\alpha,P} T_y e^{A_{P,y}} W(\alpha w_{P,y}) G_K^1 \rangle_x.$$

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

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

and, as a simple consequence,

$$W(g)^\dagger \phi(f) W(g) = \phi(f) + 2 \text{ Re} \langle f|g\rangle_{L^2},$$

$$W(g)^\dagger N W(g) = N + \phi(g) + \|g\|_{L^2}^2,$$

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

Moreover we need the following identity.

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

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

Proof of Lemma 3.2. We first observe that

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

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 (3.3) this leads to

$$W^\dagger(\alpha \varphi_P) e^{iP_f y} W(\alpha \varphi_P) = e^{iP_f y} W(\alpha(1 - e^{-y\nabla})\varphi_P) \exp\{i\alpha^2 \text{ Im} \langle \varphi_P | e^{-y\nabla} \varphi_P \rangle_{L^2}\}.$$

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

$$\alpha^2 \text{ Im} \langle \varphi_P | e^{-y\nabla} \varphi_P \rangle_{L^2} = \frac{2}{MLP} \langle \varphi | e^{-y\nabla} (P\nabla) \varphi \rangle_{L^2}$$

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

\[
\langle \varphi | (y\nabla)(P\nabla)\varphi \rangle_{L^2} = -\frac{(Py)}{3} \|
\nabla \varphi \|^2_{L^2} = -\frac{(Py)}{2} M_{LP}, \tag{3.15}
\]

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

**Proof of Lemma 3.1.** The norm squared is given by

\[
\mathcal{N} = \left\| \int dx e^{i(P_j - P)x} W(\alpha \varphi_P)(G_{K,x}^0 - \alpha^{-1}G_{K,x}^1) \right\|^2_x
= \sum_{i \in \{0,1\}} \alpha^{-2i} \int dy dx \langle G_{K,x}^i | W(\alpha \varphi_P)^\dagger e^{i(P_j - P)(y - x)} W(\alpha \varphi_P) G_{K,y}^j \rangle_x
- 2\alpha^{-1} \text{Re} \int dy dx \langle G_{K,x}^0 | e^{i(P_j - P)(y - x)} W(\alpha \varphi_P) G_{K,y}^1 \rangle_x, \tag{3.16}
\]

Shifting \( y \to y + x \) and writing the \( x \)-integration as an inner product in the electron coordinate, cf. Remark 2.1, we can proceed for \( i, j \in \{0,1\} \) with

\[
\int dy dx \langle G_{K,x}^i | W(\alpha \varphi_P)^\dagger e^{i(P_j - P)(y - x)} W(\alpha \varphi_P) G_{K,y}^j \rangle_x
= \int dy dx \langle G_{K,x}^i | W(\alpha \varphi_P)^\dagger e^{i(P_j - P)y} W(\alpha \varphi_P) G_{K,y}^j \rangle_x
= \int dy \langle G_{K}^i | e^{A_{P,y}^\dagger} W(\alpha \varphi_P) T_y G_{K}^j \rangle_x,
\]

where we applied Lemma 3.2 in the last step. Similarly for the energy

\[
\langle \Psi_{K,\alpha}(P) | H_{\alpha}(P) \Psi_{K,\alpha}(P) \rangle_x
= \sum_{i \in \{0,1\}} \alpha^{-2i} \int dy dx \langle G_{K,x}^i | W(\alpha \varphi_P)^\dagger e^{-i(P_j - P)x} H_{\alpha}(P) e^{i(P_j - P)y} W(\alpha \varphi_P) G_{K,y}^j \rangle_x
- 2\alpha^{-1} \text{Re} \int dy dx \langle G_{K,x}^0 | e^{-i(P_j - P)x} H_{\alpha}(P) e^{i(P_j - P)y} W(\alpha \varphi_P) G_{K,y}^1 \rangle_x \tag{3.18}
\]

where we also used self-adjointness of \( H_{\alpha}(P) \). Next we invoke

\[
e^{-i(P_j - P)x} H_{\alpha}(P) = \left( -\Delta_x + \alpha^{-2}N + \alpha^{-1}\phi(h_x) \right) e^{-i(P_j - P)x} \tag{3.19}
\]
to proceed for $i,j \in \{0,1\}$ with

$$
\int\int dydx \left\langle G^i_{K,x} | W(\alpha \varphi_P)^\dagger \left( - \Delta_x + \alpha^{-2}N + \alpha^{-1}\phi(h_x) \right)e^{i(P_P - P)(y-x)}W(\alpha \varphi_P)G^j_{K,y} \right\rangle_x
= \int dy \left\langle G^i_K | W(\alpha \varphi_P)^\dagger H_\alpha W(\alpha \varphi_P)T_y G^j_K \right\rangle_x
= \int dy \left\langle G^i_K | W(\alpha \varphi_P)^\dagger H_\alpha W(\alpha \varphi_P)e^{A_{P,y}}W(\alpha w_{P,y})T_y G^j_K \right\rangle_x.
$$

(3.20)

Using (3.10a), (3.10b) and $-2 \text{Re}\langle \varphi_P | h_x | L^2 = -2 \text{Re}\langle \varphi | h_x | L^2 = V\varphi(x)$ we have

$$
W(\alpha \varphi_P)^\dagger H_\alpha W(\alpha \varphi_P) = -\Delta_x + V\varphi(x) + \alpha^{-2}N + \alpha^{-1}\phi(h_x + \varphi_P) + \|\varphi_P\|_L^2
= \tilde{H}_\alpha + e_{\text{Pek}} + \|\varphi_P\|_L^2 - \|\varphi\|_L^2,
$$

(3.21)

where we added and subtracted $e_{\text{Pek}} = \lambda_{\text{Pek}} + \|\varphi\|_L^2$. It remains to compute

$$
\|\varphi_P\|_L^2 - \|\varphi\|_L^2 = \frac{1}{\alpha^4(M_{\text{LP}})^2} \|P\nabla\|_L^2 = \frac{P^2}{2\alpha^4M_{\text{LP}}}
$$

(3.22)

since $\|P\nabla\|_L^2 = \frac{P^2}{2} \|\nabla\|_L^2 = \frac{P^2}{2}M_{\text{LP}}$ because of rotational invariance of $\varphi$. With (3.21) inserted into (3.20), the stated formula for the energy follows from (3.16) and (3.18).

\[\square\]

3.2 A short guide to the proof

3.2.1 Heuristic picture

Given Lemma 3.1, the remaining task is to show that $(\mathcal{E} + \mathcal{G} + \mathcal{K})/N$ coincides, up to small errors, with the energy contribution of order $\alpha^{-2}$ in (2.23). 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 $|P|/\alpha \leq c$, sharply localized around zero at the length scale of order $\alpha^{-1}$. 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 non-trivially 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

$$
T_y e^{A_{P,y}} W(\alpha w_{P,y}) G^i_K \approx e^{-\lambda/2} (1 + y \nabla) e^{a_1(y \nabla \varphi)} G^i_K,
$$

(3.23)

with $\lambda = \frac{1}{6} \|\nabla\varphi\|_L^2$. (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 $i = 0$.
\[ j = 0 \text{ in (3.17), would lead to} \]
\[
N \approx \int dy \langle G^0_K | T_y e^{A_{P,y}} W(\alpha w_{P,y}) G^0_K \rangle_{\mathcal{H}} = \int dy e^{-\lambda_\alpha^2 y^2} + \text{Errors.} \tag{3.24}
\]

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

\[
\mathcal{E} = \frac{1}{\alpha^2} \langle \psi \otimes \Upsilon_K | N_1 \psi \otimes \Upsilon_K \rangle_{\mathcal{H}} \int dy e^{-\lambda_\alpha^2 y^2} + \text{Errors} \tag{3.25a}
\]
\[
+ \frac{1}{\alpha} \int dy e^{-\lambda_\alpha^2 y^2} \langle \psi \otimes \Upsilon_K | (\phi(h. + \varphi)(1 + (y \nabla)a^\dagger(\alpha y \nabla \varphi))) \psi \otimes \Upsilon_K \rangle_{\mathcal{H}} \tag{3.25b}
\]
\[
\mathcal{G} = -\frac{2}{\alpha^2} \text{Re} \langle \psi \otimes \Upsilon_K | \phi(h^i) u_\alpha R \phi(h^i_{K,\alpha}) \psi \otimes \Upsilon_K \rangle_{\mathcal{H}} \int dy e^{-\lambda_\alpha^2 y^2} + \text{Errors} \tag{3.25c}
\]
\[
\mathcal{K} = \frac{1}{\alpha^2} \langle \psi \otimes \Upsilon_K | \phi(h^i) R u_\alpha \psi \otimes \Upsilon_K \rangle_{\mathcal{H}} \int dy e^{-\lambda_\alpha^2 y^2} + \text{Errors.} \tag{3.25d}
\]

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)

\[
(3.25a) + (3.25c) + (3.25d) = \langle \psi \otimes \Upsilon_\infty | (N_1 - \phi(h^i_{K,\alpha})) \psi \otimes \Upsilon_\infty \rangle_{\mathcal{H}} \frac{1}{\alpha^2} \int dy e^{-\lambda_\alpha^2 y^2} = \frac{\text{inf}_{\Upsilon} \sigma(\mathbb{H}_\infty)}{\alpha^2} \int dy e^{-\lambda_\alpha^2 y^2}. \tag{3.26}
\]

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

\[
(3.25b) = \int dy e^{-\lambda_\alpha^2 y^2} \langle \Omega | \phi(\langle \psi | h_\alpha y \nabla \psi \rangle a^\dagger(y \nabla \varphi) \Omega \rangle_{\mathcal{H}} \]
\[
= -\frac{1}{2} \int dy e^{-\lambda_\alpha^2 y^2} \| y \nabla \varphi \|^2_{L^2} = -\frac{3}{2\alpha^2} \int dy e^{-\lambda_\alpha^2 y^2}. \tag{3.27}
\]

Equations (3.26) and (3.27) now add up to the desired energy of order \(\alpha^{-2}\), see (2.24). 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 3.14.

The main issue in (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

\[
\langle G^0_K | \tilde{H}_\alpha(P) e^{A_{P,y}} W(\alpha w_{P,y}) T_y G^0_K \rangle_{\mathcal{H}} \tag{3.28}
\]
\[
e^{-\frac{\alpha^2}{2}\|w_P,y\|^2_{L^2}} \langle G_K | \tilde{H}_\alpha(P)e^{A_{P,y}}e^{a^\dagger(\alpha w_P,y)} e^{-a(\alpha w_P,y)} T_y G^i_K \rangle_{\mathcal{F}}, \quad i,j = 0,1,
\]
we notice that, since
\[
\|w_P,y\|^2_{L^2} = 2 \int dk |\tilde{\varphi}_P(k)|^2 (1 - \cos(ky)) \to 2\|\varphi_P\|^2_{L^2} \quad \text{for} \quad |y| \to \infty,
\]
the prefactor should lead to a \(y\)-independent, exponentially small constant. In order to make use of this exponential decay in \(\alpha\), however, we need to ensure that
\[
|\langle G^i_K | \tilde{H}_\alpha(P)e^{A_{P,y}}e^{a^\dagger(\alpha w_P,y)} e^{-a(\alpha w_P,y)} T_y G^j_K \rangle_{\mathcal{F}}| \leq C\alpha^n g(y) \tag{3.30}
\]
is polynomially bounded in \(\alpha\) with some integrable function \(g(y)\), which heuristically can be expected to be true since the average number of particles in the state \(\tilde{H}_\alpha(P)G^i_K\) is of order one w.r.t. \(\alpha\). To obtain the required integrability in \(y\) is also the reason for introducing the cutoff function \(u_\alpha\) in the definition of \(G^i_K\).

### 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 \(G^i_K\). This involves the Bogoliubov transformation, cf. Lemma 3.10, and gives rise to a slight modification of \(w_{P,y}\), which we denote by \(\tilde{w}_{P,y}\). These manipulations naturally lead to a multiplicative factor \(\exp(-\frac{\alpha^2}{2}\|\tilde{w}_{P,y}\|^2_{L^2})\) which, as we shall see, indeed behaves like the Gaussian function in (3.23) for \(|y|\) small and tends to a constant exponentially small in \(\alpha\) as \(|y| \to \infty\). In Lemma 3.4 we prove the large \(\alpha\) asymptotics of integrals of the type \(\int g(y) \exp(-\frac{\alpha^2}{2}\|\tilde{w}_{P,y}\|^2_{L^2}) dy\) 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 [36] in the form stated in Lemma 3.8. As already mentioned, for certain terms this makes the introduction of the space cutoff \(u_\alpha\) and the momentum cutoff \(K\) necessary, while for others, it is enough to use the well-known regularity properties of \(\psi\), the relevant consequences of which are summarized in Lemma 3.6.

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 \(C_\tau\) whenever we want to specify that it depends on a parameter \(\tau\). As usual, the value of a constant may change from one line to the next.
3.3 The Gaussian lemma

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

$$w^0_{P,y} = \Pi_0 w_{P,y} \in \text{Ker} H^\text{Pek}_K$$

$$w^1_{P,y} = \Pi_1 w_{P,y} \in (\text{Ker} H^\text{Pek}_K)^\perp$$

$$\tilde{w}_{P,y} = w^0_{P,y} + \Theta_K \text{Re}(w^1_{P,y}) + i\Theta_K^{-1} \text{Im}(w^1_{P,y}).$$

Remark 3.1. Note that $(y,z) \mapsto \text{Re}(w_{P,y})(z)$ is even as a function on $\mathbb{R}^6$, while $\text{Im}(w_{P,y})(z)$ is odd on the same space. Since $\Pi_0$ and $\Theta_K$ have real-valued kernels that are even as functions on $\mathbb{R}^6$, they preserve the parity properties just mentioned. That $\Pi_0$ has the desired properties follows directly from its explicit form. To see this for $\Theta_K$, it is enough to check this for $H^{\text{Pek}}_K$, 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 $h^{\text{Pek}}_K$ and $\Pi_i$ under parity.

Thus $(y,z) \mapsto \text{Re}(w^i_{P,y})(z)$ 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 3.3.** Let $\lambda = \frac{1}{6\|\nabla \varphi\|_2^2}$ and $K_0 > 0$ large enough. For every $c > 0$ there exists a constant $C > 0$ such that

$$\|w^1_{P,y}\|_{L^2}^2 + \|	ilde{w}_{P,y}\|_{L^2}^2 \leq C(\alpha^{-2}y^2 + y^4)$$

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

$$\|	ilde{w}_{P,y}\|_{L^2}^2 - 2\lambda y^2 \leq C(\alpha^{-2}y^2 + y^4 + y^6)$$

for all $y \in \mathbb{R}^3$, $|P|/\alpha \leq c$, $K \in (K_0, \infty]$ and $\alpha > 0$.

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

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

where, for ease of notation, the dependence on $\alpha$, $P$ and $K$ is omitted. Using the arguments laid down in Remark 3.1, it is easy to see that $n_{\delta,\eta}(y)$ is even as a function of $y$. Moreover in the limit of large $\alpha$ 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. (3.32c).

This is a crucial ingredient in our proofs and the content of the next lemma.

**Lemma 3.4.** Let $\eta_0 > 0$, $c > 0$, $\lambda = \frac{1}{6\|\nabla \varphi\|_2^2}$ and $n_{\delta,\eta}(y)$ defined in (3.33). For every $n \in \mathbb{N}_0$
there exist constants \( d, C_n > 0 \) such that

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

for all non-negative functions \( g \in L^\infty(\mathbb{R}^3) \cap L^1(\mathbb{R}^3) \), \( \eta \geq \eta_0, \delta \in [0, 1) \), \( |P|/\alpha \leq c \) and all \( K, \alpha \) large enough.

At first reading, one should think of \( n = 0, \delta = 0, \eta = 1 \) and \( g \) a suitable \( \alpha \)-independent non-negative function. In this case the integral involving the Gaussian is of order \( \alpha^{-3} \) whereas the term on the right hand side is of order \( \alpha^{-4} \) 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 3.5.** Given the same assumptions as in Lemma 3.4, for every \( n \in \mathbb{N}_0 \) there exist constants \( d, C_n > 0 \) such that

\[
\int |y|^n g(y) n_{\delta, \eta}(y) dy \leq C_n \frac{\|g\|_{L^\infty}}{\alpha^{(3+n)(1-\delta)}} + e^{-d\alpha^{-2\delta+1}} \|n\|_{L^1} \tag{3.35}
\]

for all non-negative functions \( g \in L^\infty(\mathbb{R}^3) \cap L^1(\mathbb{R}^3) \), \( \eta \geq \eta_0, \delta \in [0, 1) \), \( |P|/\alpha \leq c \) and all \( K, \alpha \) large enough.

**Proof of Corollary 3.5.** Since

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

the statement follows immediately from Lemma 3.4.

\[\tag*{3.38}\]

\[\tag*{3.38}\]

### 3.4 Further preliminaries

#### 3.4.1 Estimates involving the Pekar minimizers

**Lemma 3.6.** Let \( \psi > 0 \) be the 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 \( \psi, |\nabla \psi| \) and \( H \) are \( L^p(\mathbb{R}^3, (1 + |x|^n)dx) \) functions for all \( 1 \leq p \leq \infty \) and all \( n \geq 0 \). Moreover, there exists a constant \( C > 0 \) such that for all \( x \) we have

\[
|H(x) - 1| \leq Cx^2. \tag{3.38}
\]

**Proof.** As follows from \([32]\), \( \psi(x) \) is monotone decreasing in \( |x| \); moreover, it is smooth and bounded and vanishes exponentially at infinity, i.e. there exists a constant \( C0 \) such that \( \psi(x) \leq
\( C e^{-|x|/C} \) for all \(|x|\) large enough (for the precise asymptotics see [41]). This clearly implies the statement for \( \psi \). It further implies that all the derivatives of \( \psi \) are bounded. Hence, in order to show the desired result for \(|\nabla \psi|\), it suffices to show that \( \int dx |x|^n |\nabla \psi(x)| \) is finite for all \( n \geq 0 \). Since \( \psi \) is radial, i.e. there is a function \( \psi^{rad} : [0, \infty) \to (0, \infty) \) such that \( \psi(x) = \psi^{rad}(|x|) \), and monotone decreasing, we have

\[
\int dx |x|^n |\nabla \psi(x)| = -4\pi \int_0^\infty \frac{d\psi^{rad}(r)}{dr} r^{n+2} dr = (n+2) \int \frac{|\psi(x)|}{|x|} |x|^n dx \\
\leq 4\pi \left( R_0^{n+2} \|\psi\|_{L^\infty} + \frac{n+2}{R_0} \| |n\psi|\|_{L^1} \right)
\]  

(3.39)

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

\[
\int |x|^n H(x) dx \leq 2^{2-n} \|\psi\|_{L^1} \| |n\psi|\|_{L^1}.
\]  

(3.40)

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

\[
H(x) = \int \hat{\psi}(k)^2 \cos(kx) dk,
\]  

(3.41)

together with \( H(x) \leq 1, \cos(kx) \geq 1 - \frac{(kx)^2}{2} \) and \( \nabla \psi \in L^2 \).

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

**Lemma 3.7.** There is a constant \( C > 0 \) such that

\[
(V^\varphi)^2 \leq C(1 - \Delta), \quad \pm V^\varphi \leq \frac{1}{2} (-\Delta) + C \quad \text{and} \quad \| \nabla R^{1/2} \|_{op} \leq C.
\]  

(3.42)

**Proof.** For the proof of the first two inequalities, we refer to [31, Lemma III.2]. The bound for the resolvent is obtained through

\[
0 \leq R^{\frac{1}{2}} (-\Delta) R^{\frac{1}{2}} \leq R^{\frac{1}{2}} h^{Pek} R^{\frac{1}{2}} - R^{\frac{1}{2}} (V^\varphi - \lambda^{Pek}) R^{\frac{1}{2}} \leq CR + \frac{1}{2} R^{\frac{1}{2}} (-\Delta) R^{\frac{1}{2}},
\]  

(3.43)

where we made use of the second inequality in (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

\[
\|a(f)\psi\|_{\mathcal{H}} \leq \|f\|_{L^2} \| N^{1/2} \psi \|_{\mathcal{H}}, \quad \|a^\dagger(f)\psi\|_{\mathcal{H}} \leq \|f\|_{L^2} \| (N + 1)^{1/2} \psi \|_{\mathcal{H}}, \quad \psi \in \mathcal{H},
\]  

(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 [36] one obtains suitable upper bounds by using in addition some regularity in the electron variable of the wave function \( \Psi \). For our purpose, the version summarized in the following lemma will be sufficient.

**Lemma 3.8.** Let \( h_{K,} \) for \( K \in (1, \infty] \) as defined in (2.5), let \( A \) denote a bounded operator in \( L^2(\mathbb{R}^3) \) (acting on the field variable) and \( a^* \in \{a, a^\dagger\} \). Further let \( X, Y \) be bounded symmetric operators in \( L^2(\mathbb{R}^3) \) (acting on the electron variable) that satisfy \( D_0 := \|X\|_{op}Y\|_{op} + \|\nabla X\|_{op}Y\|_{op} + \|X\|_{op}\|\nabla Y\|_{op} < \infty \). There exists a constant \( C > 0 \) such that

\[
\|X a^*(A_{h_{K,}+y})Y\Psi\|_{\mathcal{H}} \leq CD_0\|N + 1\|^{1/2}\Psi\|_{\mathcal{H}} \tag{3.45a}
\]

\[
\|X a^*(A_{\Lambda,}-y - A_{h_{K,}+y})Y\Psi\|_{\mathcal{H}} \leq \frac{CD_0\|N + 1\|^{1/2}\Psi\|_{\mathcal{H}}}{\sqrt{K}} \tag{3.45b}
\]

for all \( y \in \mathbb{R}^3, \Psi \in \mathcal{H} \) and \( \Lambda > K > 1 \).

**Remark 3.2.** Note that \( A_{h_{K,}+y} = T_y(A_{h_{K,}}) \) and in case that \( A \) has an integral kernel,

\[
(A_{h_{K,x}})(z) = \int du A(z, u)h_{K,x}(u). \tag{3.46}
\]

**Proof of Lemma 3.8.** To obtain the first inequality, write \( h_{K,} = (h_{K,} - h_{1,}) + h_{1,} \) and apply the second inequality (with \( \Lambda \) and \( K \) interchanged) to the term in parenthesis. The bound for the term involving \( h_{1,} \) follows from (3.44), as

\[
\|a^*(A_{1,y})Y\Psi\|_{\mathcal{H}}^2 = \int dx \|a^*(A_{1,x+y})Y\Psi(x)\|^2_{\mathcal{H}} \leq \int dx \|A_{1,x+y}\|^2_{L^2} (N + 1)^{1/2}(Y\Psi)(x)\|^2_{\mathcal{H}} \leq \|A\|_{op}^2 h_{1,0}^2 \|Y\|_{op}^2 \|(N + 1)^{1/2}\Psi\|_{\mathcal{H}}^2. \tag{3.47}
\]

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

\[
h_{\Lambda,x}(z) - h_{K,x}(z) = [-i\nabla, j_{K,\Lambda,x}(z)], \quad j_{K,\Lambda,x}(z) = \frac{1}{(2\pi)^3} \int_{k \leq |k| \leq \Lambda} dk \frac{k e^{ik(x-z)}}{|k|^3} \tag{3.48}
\]

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

\[
\|X a^*([\nabla, A_{j_{K,\Lambda,y}}])Y\Psi\|_{\mathcal{H}} \leq \|X \nabla a^*(A_{j_{K,\Lambda,y}})Y\Psi\|_{\mathcal{H}} + \|X a^*(A_{j_{K,\Lambda,y}})\nabla Y\Psi\|_{\mathcal{H}} \leq \|X\|_{op}\|a^*(A_{j_{K,\Lambda,y}})Y\Psi\|_{\mathcal{H}} + \|X\|_{op}\|a^*(A_{j_{K,\Lambda,y}})\nabla Y\Psi\|_{\mathcal{H}} \leq \|A\|_{op}(\|X\|_{op}\|Y\|_{op} + \|X\|_{op}\|\nabla Y\|_{op}) \|j_{K,\Lambda,0}\|_{L^2}^2 (N + 1)^{1/2}\Psi\|_{\mathcal{H}}. \tag{3.49}
\]

The desired bound now follows from \( \sup_{\Lambda > K} \|j_{K,\Lambda,0}\|_{L^2} \leq C/K \).
A simple but useful corollary is given by

**Corollary 3.9.** Under the same conditions as in Lemma 3.8, with the additional assumption that $Y$ is a rank-one operator, there exists a constant $C > 0$ such that

\[
\int \, dz \, \| X((Ah_{K, y})(z) - (Ah_{\Lambda, y})(z)) Y \|_{op}^2 \leq \frac{CD_0^2}{\Lambda}
\]

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

**Proof.** Since $Y$ has rank one, we can use

\[
\int \, dz \, \| X(\overline{Ah_{K, y}}(z) w) \|_{L^2}^2 = \| Xa_\dagger(\overline{Ah_{K, y}}) w \otimes \Omega \|_{H}^2,
\]

for any $w \in L^2(\mathbb{R}^3)$, and similarly for (3.50b), and apply Lemma 3.8. \qed

### 3.4.3 Transformation properties of $U_K$

The next lemma collects relations for the Bogoliubov transformation $U_K$ defined in (2.11). Its proof follows directly from this definition and the fact that $\Theta_K = (H_{K_{\text{Pek}}})^{1/4}$ is real-valued. We omit the details.

**Lemma 3.10.** Let $f \in L^2(\mathbb{R}^3)$, $f^0 = \Pi_0 f$, $f^1 = \Pi_1 f$ defined in (2.2) and set

\[
f = f^0 + \Theta_K^{-1} \text{Re}(f^1) + i\Theta_K \text{Im}(f^1) \quad (3.52a)
\]

\[
\tilde{f} = f^0 + \Theta_K \text{Re}(f^1) + i\Theta_K^{-1} \text{Im}(f^1). \quad (3.52b)
\]

The unitary operator $U_K$ defined in (2.11) satisfies the relations

\[
U_K a(f) U_K^\dagger = a(f^0) + a(A_K f^1) + a^\dagger(B_K \overline{f^1}) \quad (3.53a)
\]

\[
U_K^\dagger a(f) U_K = a(f^0) + a(A_K f^1) - a^\dagger(B_K \overline{f^1}) \quad (3.53b)
\]

\[
U_K \phi(f) U_K^\dagger = \phi(f), \quad U_K \pi(f) U_K^\dagger = \pi(\tilde{f}) \quad (3.53c)
\]

\[
U_K W(f) U_K^\dagger = W(\tilde{f}). \quad (3.53d)
\]

The following statements provide helpful bounds involving the number operator when transformed with the Bogoliubov transformation.

**Lemma 3.11.** There exists a constant $b > 0$ such that

\[
U_K(N + 1)^n U_K^\dagger \leq b^n n^n (N + 1)^n, \quad U_K^\dagger (N + 1)^n U_K \leq b^n n^n (N + 1)^n
\]

for all $n \in \mathbb{N}$ and $K \in (K_0, \infty]$ with $K_0$ large enough.
Proof. With $b$ replaced by $b_K = 2\|B_K\|_{\text{HS}}^2 + \|A_K\|_{\text{op}}^2 + 1$, both estimates follow from [7, Lemma 4.4] together with (3.53a) and (3.53b). That $b_K \leq b$ for some $K$-independent $b > 0$ is inferred from Lemma 2.2.

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

**Corollary 3.12.** Let $\Upsilon_K = U_K^\dagger \Omega$ and $\Upsilon_K^\geq := 1(N > \alpha \delta)\Upsilon_K$ for $\delta > 0$. There exist constants $b, C_{\delta,n} > 0$ such that

$$\langle \Upsilon_K | (N+1)^n \Upsilon_K \rangle_{\mathcal{F}} \leq b^n n^n$$

(3.55a)

$$\langle \Upsilon_K^\geq | (N+1)^n \Upsilon_K^\geq \rangle_{\mathcal{F}} \leq C_{\delta,n} \alpha^{-20}.$$  

(3.55b)

for all $n \in \mathbb{N}_0$ and all $K \in (K_0, \infty]$ with $K_0$ large enough.

**Proof.** The first bound follows directly from Lemma 3.11. The second one is obtained from

$$\langle \Upsilon_K^\geq | (N+1)^n \Upsilon_K^\geq \rangle_{\mathcal{F}} \leq \|N^m(N+1)^n \Upsilon_K^\geq \|_{\mathcal{F}} \|N^{-m} \Upsilon_K^\geq \|_{\mathcal{F}}$$

$$\leq \|(N+1)^n \Upsilon_K \|_{\mathcal{F}} \alpha^{-m\delta} \leq (2(n+m)b)^{n+m} \alpha^{-m\delta}$$

(3.56)

with $m \geq 20/\delta$.

**Lemma 3.13.** For $\delta > 0$ and $\kappa = 1/(16eb \alpha \delta)$ with $b > 0$ the constant from Lemma 3.11, the operator inequality

$$1(N \leq 2\alpha \delta) U_K^\dagger \exp(2\kappa N) U_K 1(N \leq 2\alpha \delta) \leq 2$$

(3.57)

holds for all $K, \alpha$ large enough.

**Proof.** We write out the Taylor series for the exponential and invoke Lemma 3.11,

$$1(N \leq 2\alpha \delta) U_K^\dagger e^{2\kappa N} U_K 1(N \leq 2\alpha \delta) = \sum_{n=0}^{\infty} \frac{(2\kappa)^n}{n!} 1(N \leq 2\alpha \delta) U_K^\dagger (N+1)^n U_K 1(N \leq 2\alpha \delta)$$

$$\leq \sum_{n=0}^{\infty} \frac{(2\kappa b)^n}{n!} 1(N \leq 2\alpha \delta) (N+1)^n 1(N \leq 2\alpha \delta)$$

$$\leq \sum_{n=0}^{\infty} \frac{(8\alpha \delta kb)^n}{n!}$$

(3.58)

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

The reason for introducing the momentum cutoff in $\mathcal{H}_K$ 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 3.14. Let $P_f = \int dk k a_k^\dagger a_k$ and $K_0$ large enough. There is a $C > 0$ such that

$$\langle \Omega | U_K(P_f)^2 U_K^\dagger \Omega \rangle_x \leq CK \quad (3.59)$$

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

3.5 The norm

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

Proposition 3.15. 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

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

for all $|P|/\alpha \leq c$ and all $K, \alpha$ large enough.

Proof. It follows from (3.16) and (3.17) that $N = N_0 + N_1 + N_2$ with

$$N_0 = \int dy \langle G^0_K | T_y e^{A_{P,y}} W(\alpha w_{P,y}) G^0_K \rangle_x$$

$$N_1 = -\frac{2}{\alpha} \int dy \, \text{Re} \langle G^0_K | T_y e^{A_{P,y}} W(\alpha w_{P,y}) G^1_K \rangle_x$$

$$N_2 = \frac{1}{\alpha^2} \int dy \langle G^1_K | T_y e^{A_{P,y}} W(\alpha w_{P,y}) G^1_K \rangle_x \quad (3.61)$$

Term $N_0$. This part contains the leading order contribution $\left( \frac{\pi}{\lambda \alpha^2} \right)^{3/2}$. With $H$ defined in (3.37), let us write

$$N_0 = \int dy \, H(y) \langle \Upsilon_K | W(\alpha w_{P,y}) \Upsilon_K \rangle_x$$

$$+ \int dy \, H(y) \langle \Upsilon_K | (e^{A_{P,y}} - 1) W(\alpha w_{P,y}) \Upsilon_K \rangle_x = N_{01} + N_{02}. \quad (3.62)$$

In the first term we use $\Upsilon_K = U_K^\dagger \Omega$ and apply (3.53d) to transform the Weyl operator with the Bogoliubov transformation. This gives

$$U_K W(\alpha w_{P,y}) U_K^\dagger = W(\alpha \tilde{w}_{P,y}) \quad (3.63)$$

with $\tilde{w}_{P,y}$ defined in (3.31c). From (3.2) and (3.33), we thus obtain

$$N_{01} = \int dy \, H(y) \langle \Omega | W(\alpha \tilde{w}_{P,y}) \Omega \rangle_x = \int dy \, H(y) n_{0,1}(y). \quad (3.64)$$

Since $\|H\|_{L^1} + \|H\|_{L^\infty} \leq C$, cf. Lemma 3.6, we can apply Lemma 3.4 in order to replace the
weight function $n_{0,1}(y)$ by the Gaussian $e^{-\lambda y^2}$. More precisely,

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

for all $|P|/\alpha \leq c$ and all $K, \alpha$ 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 $\Upsilon_K$ into a part with bounded particle number and a remainder. To this end, we choose a small $\delta > 0$ and write

$$\Upsilon_K = \Upsilon^K_\prec + \Upsilon^K_\succ = \{ N \leq \alpha \delta \} \Upsilon_K + \{ N > \alpha \delta \} \Upsilon_K. \tag{3.67}$$

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

$$|\mathcal{N}_{02}| \leq \int dy \, H(y) \left| \langle \Upsilon^K_\prec | (e^{AP,y} - 1)W(\alpha w_{P,y}) \Upsilon_K \rangle_F \right| + C \| \Upsilon^K_\succ \|_F. \tag{3.68}$$

By Corollary 3.12 for $n = 0$, $\| \Upsilon^K_\succ \| \leq C_\delta \alpha^{-10}$. In the remaining expression we use (3.63),

$$\langle \Upsilon^K_\prec | (e^{AP,y} - 1)W(\alpha w_{P,y}) \Upsilon_K \rangle_F = \langle \Upsilon^K_\prec | (e^{AP,y} - 1)U^\dagger_K W(\alpha \tilde{w}_{P,y}) \Omega \rangle_F, \tag{3.69}$$

and insert the identity

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

on the left of the Weyl operator (where $b > 0$ is the constant from Lemma 3.11). After applying the Cauchy–Schwarz inequality, this leads to

$$\left| \langle \Upsilon^K_\prec | (e^{AP,y} - 1)W(\alpha w_{P,y}) \Upsilon_K \rangle_F \right| \leq \| e^{zn}U_K (e^{-AP,y} - 1) \Upsilon^K_\prec \|_F \| e^{-zn}W(\alpha \tilde{w}_{P,y}) \Omega \|_F. \tag{3.71}$$

In the second factor we then employ

$$\| e^{-zn}W(\alpha \tilde{w}_{P,y}) \Omega \|_F = e^{-\frac{\alpha^2}{2} \| \tilde{w}_{P,y} \|_2^2} \| e^{-zn}e^{a^\dagger(\alpha \tilde{w}_{P,y})}e^{zn} \Omega \|_F \tag{3.72}$$

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

$$e^{-zn}e^{a^\dagger(\alpha \tilde{w}_{P,y})}e^{zn} \Omega = e^{a^\dagger(\kappa^{-1} \alpha \tilde{w}_{P,y})} \Omega = e^{\frac{\alpha^2}{2} \| \tilde{w}_{P,y} \|_2^2} W(e^{-\kappa \alpha \tilde{w}_{P,y}}) \Omega. \tag{3.73}$$
Combining the previous two lines we obtain

\[ \|e^{-\kappa N}W(\alpha \bar{w}_{P,y})\Omega_x\|_x = \exp \left( -\frac{\alpha^2}{2}(1 - e^{-2\kappa})\|\bar{w}_{P,y}\|_L^2 \right) \leq n_{\delta,\eta}(y) \]  

(3.74)

for some \(\alpha\)-independent \(\eta > 0\) and \(\alpha\) large enough. To estimate the first factor in (3.71), we apply Lemma 3.13 (note that \((e^{A_{P,y}} - 1)Y_K^{\leq} \in \text{Ran}(1(\mathbb{N} \leq 2\alpha^\delta)))\)

\[ \|e^{\kappa N}U_K(e^{-A_{P,y}} - 1)Y_K^{\leq}\|_x \leq \sqrt{2}\|(e^{-A_{P,y}} - 1)Y_K\|_x. \]  

(3.75)

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

\[ \|(e^{-A_{P,y}} - 1)Y_K\|_x \leq \|A_{P,y}Y_K\|_x \leq \|(yP_f)Y_K\|_x + |g_P(y)| \leq C(\sqrt{K}|y| + \alpha|y|^3), \]  

(3.76)

where in the last step we applied Lemma 3.14 and used

\[ |g_P(y)| \leq C\alpha|y|^3, \]  

(3.77)

which is inferred from (3.5) using \(\|\Delta\phi\|_L^2 < \infty\). Returning to (3.71) we have shown that

\[ |N_{02}| \leq C \int dy H(y)(\sqrt{K}|y| + \alpha|y|^3)n_{\delta,\eta}(y) + C_\delta \alpha^{-10}, \]  

(3.78)

and hence we are in a position to apply Corollary 3.5. This implies for all \(K, \alpha\) large

\[ |N_{02}| \leq C(\sqrt{K}\alpha^{-4(1-\delta)} + \alpha^{-6(1-\delta)+1}) + C_\delta \alpha^{-10} \leq C_\delta \sqrt{K}\alpha^{-4(1-\delta)}. \]  

(3.79)

Term \(N_1\). We start by inserting (2.22) for \(G_K^1\) in expression (3.61b). Since the Weyl operator commutes with \(u_\alpha\), \(R\) and \(P_\psi = |\psi\rangle\langle\psi|\), we can apply (3.10a) to obtain

\[ W(\alpha w_{P,y})G_K^1 = u_\alpha R(\phi(h_{K,x}) + 2\alpha\langle h_{K,x} | \text{Re}(w_{P,y}^1)\rangle_{L^2})P_\psi W(\alpha w_{P,y})G_K^0, \]  

(3.80)

where we used that \(h_{K,x}\) is real-valued. Note that \(\langle h_{K,x} | \text{Re}(w_{P,y}^1)\rangle_{L^2}\) 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 (3.67), we can thus write

\[ N_1 = -\frac{2}{\alpha} \int dy \text{Re} \langle R_{1,y} \psi \otimes (Y_K^{\leq} + Y_K^{\geq}) | W(\alpha w_{P,y})G_K^0 \rangle_{x\bar{e}} = N_1^{\leq} + N_1^{\geq}, \]  

(3.81)

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

\[ R_{1,y}^1 = P_\psi \phi(h_{K,x}) Ru_\alpha T_{-y} P_\psi e^{-A_{P,y}}, \]  

(3.82a)

\[ R_{1,y}^2 = 2\alpha P_\psi \langle h_{K,x} | \text{Re}(w_{P,y}^1)\rangle_{L^2} Ru_\alpha T_{-y} P_\psi e^{-A_{P,y}}. \]  

(3.82b)
Using Lemma 3.8 in combination with \( \|\nabla P_\psi\|_{op} + \|\nabla R^{1/2}\|_{op} < \infty \), see Lemmas 3.6 and 3.7, we can bound the first operator, for any \( \Psi \in \mathcal{H} \), by

\[
\|R_{1,y}^1\Psi\|_{\mathcal{H}} \leq C\|N\| (N + 1)^{1/2} u_\alpha T_{-y} P_\psi e^{-A_{P,\psi} \Psi} \leq C\|u_\alpha T_{-y} P_\psi\|_{op} (N + 1)^{1/2} \|\Psi\|_{\mathcal{H}}.
\] (3.83)

To estimate the second operator, we write out the inner product, use Cauchy–Schwarz twice, apply Corollary 3.9 (with \( A = 1 \), \( X = R \) and \( Y = P_\psi \)) and use (3.32a),

\[
\|R_{1,y}^2\Psi\|_{\mathcal{H}}^2 = 4\alpha^2 \int dz \text{Re}(w_{P,y}^1(z)) P_\psi h_{K_\alpha}(z) R u_\alpha T_{-y} P_\psi e^{-A_{P,\psi} \Psi} \leq 4\alpha^2 \int du |w_{P,y}^1(u)|^2 \int dz \|P_\psi h_{K_\alpha}(z) R\|_{op}^2 \|u_\alpha T_{-y} P_\psi e^{-A_{P,\psi} \Psi}\|_{\mathcal{H}}^2 \\
\leq C\alpha^2 \|w_{P,y}^1\|_{L^2}^2 \|u_\alpha T_{-y} P_\psi e^{-A_{P,\psi} \Psi}\|_{\mathcal{H}}^2 \\
\leq C\alpha^2 (y^4 + \alpha^{-4}) \|u_\alpha T_{-y} P_\psi\|_{op}^2 \|\Psi\|_{\mathcal{H}}^2.
\] (3.84)

Combining the above estimates we arrive at

\[
\|R_{1,y}\Psi\|_{\mathcal{H}} \leq C\|u_\alpha T_{-y} P_\psi\|_{op} (1 + \alpha y^2) (N + 1)^{1/2} \|\Psi\|_{\mathcal{H}}.
\] (3.85)

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

\[
\| \cdot \|_{L^1} \leq \int dy |y|^{\alpha} \left( \int dx \psi(x+y)^2 u_\alpha(x) \right)^{1/2} \leq C_\alpha \alpha^{3+n} \text{ for all } n \in \mathbb{N}_0.
\] (3.86)

With this at hand we can estimate the part containing the tail. Invoking Corollary 3.12

\[
|A_{1,\psi}^\gamma| \leq \frac{C}{\alpha} \|N\| (N + 1)^{1/2} Y_{\mathcal{K}} \int dy f_\alpha(y) (1 + \alpha y^2) \leq C_\delta \alpha^{-5}.
\] (3.87)

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

\[
\|R_{1,y}^1 \psi \|_{\mathcal{H}} \leq \frac{2}{\alpha} \int dy |e^{\kappa \mathcal{H}_{\mathcal{K}} (e^{-A_{P,\psi} R_{1,y} \psi} \otimes Y_{\mathcal{K}})}|_{\mathcal{H}} \|e^{-\kappa \mathcal{H}_{\mathcal{K}} \mathcal{W}(\alpha w_{P,y}) \Omega}\|_{\mathcal{H}} \\
\leq \frac{2}{\alpha} \int dy |e^{\kappa \mathcal{H}_{\mathcal{K}} (e^{-A_{P,\psi} R_{1,y} \psi} \otimes Y_{\mathcal{K}})}|_{\mathcal{H}} \|n_{\delta_\alpha}(y)\|_{\mathcal{H}}.
\] (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 3.13 and (3.85), together with (3.55a), to get

\[
\|e^{\kappa \mathcal{H}_{\mathcal{K}} (e^{-A_{P,\psi} R_{1,y} \psi} \otimes Y_{\mathcal{K}})}\|_{\mathcal{H}} \leq \sqrt{2} \|R_{1,y} \psi \otimes Y_{\mathcal{K}}\|_{\mathcal{H}} \leq C f_\alpha(y) (1 + \alpha y^2).
\] (3.89)
With Corollary 3.5, (3.86) and \( \|f_\alpha\|_{L^\infty} \leq 1 \), this leads to
\[
|N_1^\leq| \leq \frac{C}{\alpha} \int dy f_\alpha(y)(1 + \alpha y^2) n_{\delta,y}(y) \leq C \alpha^{-1-3(1-\delta)}. \tag{3.90}
\]

**Term \( N_2 \).** The strategy for estimating this term is similar to the one for \( N_1 \). Proceeding as described before (3.81), one obtains
\[
N_2 = \frac{1}{\alpha^2} \int dy \langle R_{2,y} \psi \otimes (\Upsilon_K^\leq + \Upsilon_K^\geq) | W(\alpha w_{P,y}) G_K^0 \rangle_{\mathcal{K}} = N_2^\leq + N_2^\geq \tag{3.91}
\]
with \( R_{2,y} = R_{2,y}^1 + R_{2,y}^2 \) and
\[
R_{2,y}^1 = \frac{1}{\alpha} \int dy \langle P_\psi \phi(h_{K,y}) Re^{-A_{P,y}} u_{\alpha} T_{-y} u_{\alpha} R\phi(h_{K,y}) P_\psi, \] \[
R_{2,y}^2 = 2 \alpha P_\psi (h_{K,y}) | Re(w_{P,y}) | Re^{-A_{P,y}} u_{\alpha} T_{-y} u_{\alpha} R\phi(h_{K,y}) P_\psi. \tag{3.92a-b}
\]

It follows in close analogy as for \( R_{1,y} \) in (3.82a)–(3.82b) that given any \( \Psi \in \mathcal{K} \),
\[
\|R_{2,y} \psi\|_{\mathcal{K}} \leq C \|u_{\alpha} T_{-y} u_{\alpha}\|_{op}(1 + \alpha y^2) \|(N + 1) \Psi\|_{\mathcal{K}}, \tag{3.93}
\]
and since \( \|u_{\alpha} T_{-y} u_{\alpha}\|_{op} \leq 1 (|y| \leq 4\alpha) \), we can use Corollary 3.12 to estimate
\[
|N_2^\geq| \leq \frac{C}{\alpha^2} \|(N + 1) \Upsilon_K^\geq\|_{x} \int dy 1(|y| \leq 4\alpha)(1 + \alpha y^2) \leq C \delta \alpha^{-6}. \tag{3.94}
\]

To bound the first term in (3.91) we proceed similarly as for \( N_{01} \),
\[
|N_2^\leq| \leq \alpha^{-2} \int dy \|e^{\mathcal{K} U_{K}}(R_{2,y} \psi \otimes \Upsilon_K^\leq)\|_{x} \|e^{-\mathcal{K} W(\alpha \bar{w}_{P,y}) \Omega}\|_{x}
\leq \frac{\sqrt{2}}{\alpha^2} \int dy \|R_{2,y} \psi \otimes \Upsilon_K^\leq\|_{\mathcal{K}} n_{\delta,y}(y) \leq \frac{C}{\alpha^2} \int dy 1(|y| \leq 4\alpha)(1 + \alpha y^2) n_{\delta,y}(y). \tag{3.95}
\]

The last integral is estimated again via Corollary 3.5, and thus \( |N_2^\leq| \leq C \alpha^{-5+3\delta} \).

Collecting all relevant estimates and choosing \( \delta > 0 \) small enough completes the proof of the proposition. \( \square \)

### 3.6 Energy contribution \( \mathcal{E} \)

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

**Proposition 3.16.** Let \( \mathcal{N}_1 = d\Gamma(\Pi_1) \) and choose \( c > 0 \). For every \( \varepsilon > 0 \) there is a constant \( C_\varepsilon > 0 \) (we omit the dependence on \( c \)) such that
\[
\left| \mathcal{E} - \frac{1}{\alpha^2} \left( \left\langle \Upsilon_K \mathcal{N}_1 \Upsilon_K \right\rangle_x - \frac{3}{2} \right) \mathcal{N} \right| \leq C_\varepsilon \sqrt{K} \alpha^{-6+\varepsilon} \tag{3.96}
\]
for all $|P|/\alpha \leq c$ and $K, \alpha$ large enough.

Proof. Since $G^0_K = \psi \otimes \Upsilon_K$, $\hbar^{0\psi} \psi = 0$ and $N \Upsilon_K = N_1 \Upsilon_K$, one has

$$
\mathcal{E} = \int dy \langle G^0_K | (\alpha^{-2} N_1 + \alpha^{-1} \phi(h. + \varphi_P)) T_y e^{A_{P,y}} W(\alpha w_{P,y}) | G^0_K \rangle \mathcal{F} = \mathcal{E}_1 + \mathcal{E}_2, \quad (3.97)
$$

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

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

$$
\mathcal{E}_1 = \frac{1}{\alpha^2} \int dy H(y) \langle \Upsilon_K | N_1 W(\alpha w_{P,y}) \Upsilon_K \rangle \mathcal{F} + \frac{1}{\alpha^2} \int dy H(y) \langle \Upsilon_K | N_1 (e^{A_{P,y}} - 1) W(\alpha w_{P,y}) \Upsilon_K \rangle \mathcal{F} = \mathcal{E}_{11} + \mathcal{E}_{12}. \quad (3.98)
$$

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

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

and since $e^{a^{\dagger} (\alpha w_{P,y}^0)}$ commutes with $\mathbb{U}_K N_1 \mathbb{U}_K^\dagger$ and $e^{a^{\dagger} (\alpha \bar{w}_{P,y}^1)} \Upsilon_K = \Upsilon_K$ (we use $\mathbb{U}_K a^{\dagger} (f^0) \mathbb{U}_K^\dagger = a^{\dagger} (f^0)$ for $f^0 \in \text{Ran}(\Pi_0)$), this leads to

$$
\mathcal{E}_{11} = \frac{1}{\alpha^2} \int dy H(y) n_{0,1}(y) \langle \Omega | \mathbb{U}_K N_1 \mathbb{U}_K^\dagger e^{a^{\dagger} (\alpha \bar{w}_{P,y}^1)} \Omega \rangle \mathcal{F}. \quad (3.100)
$$

Because $\mathbb{U}_K N_1 \mathbb{U}_K^\dagger$ 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 non-vanishing contribution,

$$
\mathcal{E}_{11} = \frac{1}{\alpha^2} \int dy H(y) n_{0,1}(y) \langle \Upsilon_K | N_1 \Upsilon_K \rangle \mathcal{F} + \frac{1}{2\alpha^2} \int dy H(y) n_{0,1}(y) \langle \Upsilon_K | N_1 \mathbb{U}_K^\dagger a^{\dagger} (\alpha \bar{w}_{P,y}^1) a^{\dagger} (\alpha \bar{w}_{P,y}^1) \Upsilon_K \rangle \mathcal{F} = \mathcal{E}_{111} + \mathcal{E}_{112}. \quad (3.101)
$$

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

$$
\mathcal{E}_{111} = \frac{1}{\alpha^2} \int dy H(y) e^{-\lambda_0 \alpha^{-2} y^2} \langle \Upsilon_K | N_1 \Upsilon_K \rangle \mathcal{F} + \frac{1}{\alpha^2} \int dy H(y) (n_{0,1}(y) - e^{-\lambda_0 \alpha^{-2} y^2}) \langle \Upsilon_K | N_1 \Upsilon_K \rangle \mathcal{F} = \mathcal{E}_{111}^{\text{lo}} + \mathcal{E}_{111}^{\text{err}}. \quad (3.102)
$$

In $\mathcal{E}_{111}^{\text{lo}}$ we use $|H(y) - 1| \leq C y^2$ and Corollary 3.12 to replace $H(y)$ by unity at the cost of an error of order $\alpha^{-7}$. In the term where $H(y)$ is replaced by unity, we perform the Gaussian integral and use Proposition 3.15 and again Corollary 3.12. This leads to

$$
\left| \mathcal{E}_{111}^{\text{lo}} - \mathcal{N} \frac{1}{\alpha^2} \langle \Upsilon_K | N_1 \Upsilon_K \rangle \mathcal{F} \right| \leq C_{\varepsilon} \sqrt{K} \alpha^{-6 + \varepsilon}. \quad (3.103)
$$
The error in (3.102) is bounded with the help of Lemma 3.4,

\[ |\mathcal{E}_{111}| \leq \frac{C}{\alpha^2} \int dy \, H(y)|n_{0,1}(y) - e^{-\lambda \alpha^2 y^2}| \leq C \alpha^{-6}. \tag{3.104} \]

In \( \mathcal{E}_{112} \) we use the Cauchy–Schwarz inequality, Corollary 3.12 and Lemma 3.3, to obtain

\[ \left| \langle \Upsilon_K | N_1 U_K^\dagger a^\dagger (\alpha \tilde{w}_{P,y}) a^\dagger (\alpha \tilde{w}_{P,y}) \Omega \rangle \right| \]

\[ \leq \| N_1 \Upsilon_K \|_\mathcal{F} \| a^\dagger (\alpha \tilde{w}_{P,y}) a^\dagger (\alpha \tilde{w}_{P,y}) \Omega \|_\mathcal{F} \leq 2 \alpha^2 \| \tilde{w}_{P,y} \|_{L^2} \leq C \alpha^2 (y^4 + \alpha^{-4}). \tag{3.105} \]

With \( \| \cdot \|_{L^1} \leq C_n \) we can now apply Corollary 3.5 to obtain

\[ |\mathcal{E}_{112}| \leq C \int dy \, H(y)(y^4 + \alpha^{-4})n_{0,1}(y) \leq C \alpha^{-7}. \tag{3.106} \]

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

\[ |\mathcal{E}_{12}| \leq \frac{1}{\alpha^2} \int dy \, H(y)\| e^{\delta N} U_K (e^{-A_{P,y}} - 1) N_1 \Upsilon_K^\varsigma \|_\mathcal{F} n_{\delta,\eta}(y) + \frac{2}{\alpha^2} \| N_1 \Upsilon_K^\varsigma \|_\mathcal{F} \int dy \, H(y). \tag{3.107} \]

While the second term is bounded via (3.55b) by \( C_\delta \alpha^{-12} \), in the first term we apply Lemma 3.13 and use the functional calculus for self-adjoint operators,

\[ \| e^{\delta N} U_K (e^{-A_{P,y}} - 1) N_1 \Upsilon_K^\varsigma \|_\mathcal{F} \leq \sqrt{2}\| (e^{-A_{P,y}} - 1) N_1 \Upsilon_K^\varsigma \|_\mathcal{F} \]

\[ \leq \sqrt{2} \| (P_f y + g_P(y)) N_1 \Upsilon_K^\varsigma \|_\mathcal{F}. \tag{3.108} \]

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

\[ \| (P_f y + g_P(y)) N_1 \Upsilon_K^\varsigma \|_\mathcal{F} \leq (\alpha^\delta + 1) \| (P_f y + g_P(y)) \Upsilon_K \|_\mathcal{F} \leq C \alpha^\delta (\sqrt{K}|y| + \alpha|y|^3), \tag{3.109} \]

where we used \( 1 \leq \alpha^\delta \), Lemma 3.14 and (3.77) in the second step. We conclude via Corollary 3.5 that

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

**Term \( \mathcal{E}_2 \).** Here we start with

\[ \mathcal{E}_2 = \alpha^{-1} \int dy \, \langle \Upsilon_K | L_{1,y} W(\alpha w_{P,y}) \Upsilon_K \rangle_\mathcal{F} \]

\[ + \alpha^{-1} \int dy \, \langle \Upsilon_K | L_{1,y} (e^{A_{P,y}} - 1) W(\alpha w_{P,y}) \Upsilon_K \rangle_\mathcal{F} = \mathcal{E}_{21} + \mathcal{E}_{22}, \tag{3.111} \]

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where

\[ L_{1,y} = \langle \psi | (h + \varphi P) T_y \psi \rangle_{L^2} = \phi(l_y) + \pi(j_y) \]  \hfill (3.112)

with

\[ l_y = H(y) \varphi + \langle \psi | h T_y \psi \rangle_{L^2}, \quad j_y = H(y) \xi_P, \]  \hfill (3.113)

and \( \xi_P \) defined in (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 3.17.** For \( k = 0, 1 \) and for all \( n \in \mathbb{N}_0 \),

\[
\sup_y \| \nabla^k l_y \|_{L^2} < \infty, \quad \int |y|^n \| \nabla^k l_y \|_{L^2} \, dy < \infty. \]  \hfill (3.114)

Note that, by Lemma 3.6, \( j_y \) clearly has these properties as well. We proceed by writing

\[
E_{21}^{0} = E_{21}^{0} + E_{21}^{P} \]

with

\[
E_{21}^{0} = \alpha^{-1} \int dy \langle \Upsilon_K | \phi(l_y) W(\alpha w_{P,y}) \Upsilon_K \rangle_x \]  \hfill (3.115a)

\[
E_{21}^{P} = \alpha^{-1} \int dy \langle \Upsilon_K | \pi(j_y) W(\alpha w_{P,y}) \Upsilon_K \rangle_x, \]  \hfill (3.115b)

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

\[
E_{21}^{0} = \int \langle l_y^0 | \tilde{w}_{P,y} \rangle_{L^2} n_{0,1}(y) \, dy \]

\[
= \int \left( \langle l_y^0 | w_{P,y}^0 \rangle_{L^2} + \langle l_y^1 | \text{Re}(w_{P,y}^1) \rangle_{L^2} + i \langle l_y^1 | \Theta_K^{-2} \text{Im}(w_{P,y}^1) \rangle_{L^2} \right) n_{0,1}(y) \, dy \]  \hfill (3.116)

where we used that \( l_y \) is real-valued. Note that \( l_{-y}(-z) = l_y(z) \). As discussed in Remark 3.1, \( n_{0,1}(y) \) is even, and using the arguments therein one can conclude that \( \Theta_K^{-2} \text{Im}(w_{P,y}^1) \) and \( \text{Im}(w_{P,y}^0) \) are odd functions on \( \mathbb{R}^6 \) since \( (y, z) \mapsto \text{Im}(w_{P,y})(z) \) is odd on this space, and hence

\[
\int \langle l_y^0 | \text{Im}(w_{P,y}^0) \rangle_{L^2} n_{0,1}(y) \, dy = \int \langle l_y^1 | \Theta_K^{-2} \text{Im}(w_{P,y}^1) \rangle_{L^2} n_{0,1}(y) \, dy = 0. \]  \hfill (3.117)

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

\[
v(y) := \langle l_y^0 | w_{0,y} \rangle_{L^2} \]  \hfill (3.118)

we finally have

\[
E_{21}^{0} = \int \langle l_y^0 + l_y^1 | \text{Re}(w_{P,y}^0) + \text{Re}(w_{P,y}^1) \rangle_{L^2} n_{0,1}(y) \, dy = \int v(y) n_{0,1}(y) \, dy. \]  \hfill (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 $\varphi(z) = -\langle \psi| h.(z) \psi \rangle_{L^2}$ and $\nabla_z h(x - z) = -\nabla_x h(x - z)$ we have by integration by parts

$$\nabla \varphi = -2\langle \nabla \psi| h.\psi \rangle_{L^2}. \quad (3.120)$$

Thus

$$l_y = -\frac{1}{2} y \nabla \varphi + \varphi(H(y) - 1) + \langle \psi| h.(T_y \psi - \psi - y \nabla \psi) \rangle_{L^2}. \quad (3.121)$$

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

$$||T_y \psi - \psi - y \nabla \psi||_{L^\infty} \leq Cy^2. \quad (3.122)$$

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

$$x \mapsto (h.(z) \nabla^k \psi)(x) \in L^1(\mathbb{R}^3, dx) \quad \text{and} \quad z \mapsto ||h.(z) \nabla^k \psi||_{L^1} \in L^2(\mathbb{R}^3, dz). \quad (3.123)$$

The first statement follows easily from Lemma 3.6; to show the second one, use

$$\int d\sigma \frac{1}{|u - z|^2|v - z|^2} = \frac{1}{\pi^3|u - v|} \quad (3.124)$$

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

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

Now let

$$b_y(z) := w_{0,y}(z) - y \nabla \varphi(z) = \int_0^1 ds \int_0^s dt (y \nabla)^2 \varphi(z - ty) \quad (3.126)$$

and note that $||b_y||_{L^2}^2 \leq \frac{4}{3} y^4 ||\Delta \varphi||_{L^2}^2$ which is finite since $\Delta \varphi \in L^2$. This equation, together with (3.125), implies

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

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

$$\int dy \ v(y) n_{0,1}(y) = \int dy \ v(y)e^{-\alpha^2 \lambda y^2} + \int dy \ |y|^{-2} v(y)y^2(n_{0,1}(y) - e^{-\alpha^2 \lambda y^2}) \quad (3.128)$$
and use Lemma 3.4 for $g = | \cdot |^{-2} |v|$ to bound

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

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

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

which finally gives the estimate

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

using Proposition 3.15.

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

$$\mathcal{E}_{21}^P = \frac{1}{\alpha^2 M L^P} \int \langle iP \nabla \varphi | w_0^{P,y} \rangle_{L^2} H(y) n_{0,1}(y) dy. \quad (3.132)$$

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

$$\frac{1}{3} w_0^{P,y}(z) = -\frac{(\varphi \ast \nabla \varphi)(y)}{\| \nabla \varphi \|_{L^2}^2} \nabla \varphi(z) + \frac{i P}{\alpha^2 M L^P} \left( \| \nabla \varphi \|_{L^2}^2 - (\nabla \varphi \ast \nabla \varphi)(y) \right) \frac{\nabla \varphi(z)}{\| \nabla \varphi \|_{L^2}^2}. \quad (3.133)$$

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

$$\int \langle \nabla \varphi | \text{Re}(w_0^{P,y}) \rangle_{L^2} n_{0,1}(y) H(y) dy = 0, \quad (3.134)$$

and, taking rotational invariance of $\varphi$ into account, we arrive at

$$\mathcal{E}_{21}^P = \frac{P^2}{\alpha^4 (M L^P)^2} \int \left( \| \nabla \varphi \|_{L^2}^2 - (\nabla \varphi \ast \nabla \varphi)(y) \right) n_{0,1}(y) H(y) dy. \quad (3.135)$$

Further note that $\| \nabla \varphi \|_{L^2}^2 - (\nabla \varphi \ast \nabla \varphi)(y) \leq C y^2$ and thus, by Lemma 3.6 and Corollary 3.5, one obtains

$$|\mathcal{E}_{21}^P| \leq C \frac{P^2}{\alpha^5} \leq C \frac{1}{\alpha^7}. \quad (3.136)$$

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

In order to estimate the term $\mathcal{E}_{22}$, we proceed as before by splitting $\Upsilon_K = \Upsilon_{K>1} + \Upsilon_{K<1}$. Using
(3.44) we can estimate

\[
\left| \alpha^{-1} \int \mathrm{d}y \, \langle \mathcal{Y}_k^> (\phi(l_y)+\pi(j_y)) (e^{A_{P,y}}-1) W(\alpha w_{P,y}) Y_K \rangle_x \right| \\
\leq C \alpha^{-1} \int \mathrm{d}y \, (l_y^2 + j_y^2)(N + 1)^{1/2} Y_K^< \|_x \leq C_\delta \alpha^{-11}
\]  

(3.137)

where we used Corollary 3.12 and Lemmas 3.6 and 3.17. The term involving \( Y_K^< \), we split again into two contributions,

\[
E_{22}^0 = \alpha^{-1} \int \mathrm{d}y \, \langle \mathcal{Y}_k^< (\phi(l_y)) (e^{A_{P,y}}-1) W(\alpha w_{P,y}) Y_K \rangle_x
\]  

(3.138a)

\[
E_{22}^P = \alpha^{-1} \int \mathrm{d}y \, \langle \mathcal{Y}_k^< (\pi(j_y)) (e^{A_{P,y}}-1) W(\alpha w_{P,y}) Y_K \rangle_x.
\]  

(3.138b)

To bound the first one we proceed as in (3.107), i.e. use Lemma 3.13 and the fact that \( \phi(l_y) \) changes the number of phonons at most by one. This leads to

\[
|E_{22}^0| \leq \alpha^{-1} \int \mathrm{d}y \, \|e^{N U_K} (e^{-A_{P,y}}-1) \phi(l_y) Y_K^< \|_x n_{\delta,\eta}(y) \\
\leq \sqrt{2} \alpha^{-1} \int \mathrm{d}y \, \| (e^{-A_{P,y}}-1) \phi(l_y) Y_K^< \|_x n_{\delta,\eta}(y).
\]  

(3.139)

Furthermore, we have

\[
\| (e^{-A_{P,y}}-1) \phi(l_y) Y_K^< \|_x \leq \| A_{P,y} \phi(l_y) Y_K^< \|_x \leq \| \phi(l_y) A_{P,y} Y_K^< \|_x + \| [A_{P,y}, \phi(l_y)] Y_K^< \|_x \\
\leq C \alpha^{\delta/2} (\| l_y^2 \|_{L^2} \| A_{P,y} Y_K \|_x + \| y \nabla l_y \|_{L^2})
\]  

(3.140)

where we used \([iP_{f,y}, \phi(f)] = \pi(y \nabla f)\) and \( Y_K^< = 1 (N \leq \alpha^\delta) Y_K \). Note that in order to estimate the remaining expression, it is not sufficient to directly apply Corollary 3.5. To obtain a better bound, we first replace \( n_{\delta,\eta}(y) \) by \( e^{-\eta \lambda^2 (1-\delta)y^2} \) and then, for the part containing the Gaussian, we use that \( \| l_y^2 \|_{L^2} \) and \( \| \nabla l_y \|_{L^2} \) provide additional factors of \( |y| \), as is shown below. More precisely, with Lemma 3.17 and the aid of Lemmas 3.4 and 3.14, we bound

\[
\alpha^{\delta-1} \int \mathrm{d}y \, \| l_y^2 \|_{L^2} \| A_{P,y} Y_K \|_x n_{\delta,\eta}(y) \leq C \alpha^{\delta-1} \int \mathrm{d}y \, \| l_y^2 \|_{L^2} (\sqrt{K}|y| + \alpha |y|^3) n_{\delta,\eta}(y) \\
\leq C \alpha^{\delta-1} \int \mathrm{d}y \, \| l_y^2 \|_{L^2} (\sqrt{K}|y| + \alpha |y|^3) e^{-\eta \lambda^2 (1-\delta)y^2} + C \sqrt{K} \alpha^{-6+\eta \delta}. \]

(3.141)

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

\[
|l_y(z)| \leq \frac{1}{2} |y \nabla \varphi(z)| + f(z) y^2.
\]  

(3.142)
Hence, by integration
\[
\alpha^{\delta/2-1} \int dy \|y\| L^2 \left( \sqrt{K} |y| + \alpha |y|^3 \right) e^{-\lambda \eta a^{2(1-\delta)} y^2} \leq C \sqrt{K} \alpha^{-6+11/2\delta}.
\] (3.143)

With regard to the second term in (3.140),
\[
\alpha^{\delta/2-1} \int dy |y| \|\nabla l_y\| L^2 n_{\delta,\eta}(y)
\] (3.144)
we proceed in a similar way, using that
\[
\|\nabla l_y\| L^2 \leq C (|y| + y^2).
\] (3.145)

In fact, since \( \nabla \varphi(z) = -\langle \psi | h(z) \nabla \psi \rangle \), we have the identity
\[
\nabla l_y(z) = H(y) \nabla \varphi(z) + \langle \nabla \psi | h(z) T_y \psi \rangle_{L^2} + \langle \psi | h(z) \nabla T_y \psi \rangle_{L^2} + \langle \psi | h(z) (T_y - 1) \nabla \psi \rangle_{L^2}.
\] (3.146)

Again using that \( \psi \) has bounded derivatives, we have
\[
\|(T_y - 1) \psi\|_{L^\infty} + \|(T_y - 1) \nabla \psi\|_{L^\infty} \leq C |y|,
\] (3.147)
and the desired inequality now follows from \( |H(y) - 1| \leq Cy^2 \) and (3.123). Given (3.114), we can use Lemma 3.4 to replace \( n_{\delta,\eta}(y) \) in (3.144) with \( e^{-\lambda \eta a^{2(1-\delta)} y^2} \) at the energy penalty \( C \alpha^{-6+9\delta/2} \), and then use (3.145) to bound the remaining integral involving the Gaussian factor, which yields an error of the same order. Altogether, this gives the estimate
\[
|E_{22}^0| \leq C \sqrt{K} \alpha^{-6+11/2\delta}.
\] (3.148)

For the term \( E_{22}^P \) we proceed in exactly the same way as in (3.139):
\[
|E_{22}^P| \leq \sqrt{2} \alpha^{-1} \int dy \| (e^{-A_{P,y}} - 1) \pi(j_y) \|_{L^2} n_{\delta,\eta}(y)
\leq C \alpha^{\delta/2-1} \int dy \| j_y \|_{L^2} \| A_{P,y} \gamma_K \|_{L^2} n_{\delta,\eta}(y) + C \alpha^{\delta/2-1} \int dy \| y \nabla j_y \|_{L^2} n_{\delta,\eta}(y)
\leq C \alpha^{\delta/2-1} \frac{|P|}{\alpha^2} \int dy \| H(y) (\sqrt{K} |y| + \alpha |y|^3) n_{\delta,\eta}(y)
+ C \alpha^{\delta/2-1} \frac{|P|}{\alpha^2} \int dy \| H(y) n_{\delta,\eta}(y)
\leq C \alpha^{-6+11/2} \sqrt{K}
\] (3.149)

where the last estimate follows from Corollary 3.5 and the assumption \( |P| \leq c \alpha \).

Combining the relevant estimates, that is (3.103), (3.104), (3.106) and (3.110) for \( E_1 \) as
well as (3.131), (3.136), (3.137), (3.148) and (3.149) for $E_2$, we arrive at the statement of Proposition 3.16, thus providing an appropriate bound for $E$.

Proof of Lemma 3.17. Since $H$ has the desired properties, we need to show them for

$$
I_{1y}(1) = \langle \psi | h.T_y \psi \rangle_{L^2}.
$$

(3.150)

To this end we introduce

$$
S = \{ f \in L^p(\mathbb{R}^3, (1 + |y|^n)dy) \quad \forall 1 \leq p \leq \infty, \quad \forall n \geq 0 \}
$$

(3.151)

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

$$
S(y) := \iint dudv \frac{f_1(u)f_2(v)f_3(u+y)f_4(v+y)}{|u-v|} \in S.
$$

(3.152)

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

$$
\int dy |y|^n S(y) \leq C \|f_4\|_{L^\infty} (\|u\| \|f_1\|_{L^r} \|f_2\|_{L^r} \|f_3\|_{L^1} + \|f_1\|_{L^r} \|f_2\|_{L^r} \|n f_3\|_{L^1})
$$

(3.153)

from which (3.152) follows. Moreover,

$$
f \in S \Rightarrow \sqrt{|f|} \in S.
$$

(3.154)

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

$$
\int |y|^n \sqrt{|f|} dy \leq \sqrt{\|f\|_{L^\infty}} \int_{|y| \leq 1} |y|^n dy + \frac{1}{2} \int |y|^{n+m} |f| dy + \frac{1}{2} \int_{|y| > 1} |y|^{n-m} dy < \infty
$$

(3.155)

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

$$
\|I^{(1)}_{1y}\|_{L^2}^2 = \frac{1}{4\pi} \iint dudv \frac{\psi(u)\psi(v)\psi(u+y)\psi(v+y)}{|u-v|}.
$$

(3.156)

The statement now follows easily from (3.152) and Lemma 3.6. Arguing again via (3.154), for $k = 1$ it suffices to show the statement for

$$
\|\nabla I^{(1)}_{1y}\|_{L^2}^2 = \|\langle \nabla \psi | h.T_y \psi \rangle_{L^2} + \langle \psi | h.\nabla T_y \psi \rangle_{L^2}\|_{L^2}^2
$$

$$
\leq 2\|\langle \nabla \psi | h.T_y \psi \rangle_{L^2}\|_{L^2}^2 + 2\|\langle \psi | h.\nabla T_y \psi \rangle_{L^2}\|_{L^2}^2
$$

(3.157)

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

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we find
\[
\|\langle \nabla \psi | h.T_y \psi \rangle_{L^2}\|^2 \leq C \int \int dudv \frac{|\nabla \psi(u)||\nabla \psi(v)\psi(v + y)\psi(u+y)|}{|u - v|}, \tag{3.158a}
\]
\[
\|\langle \psi | h.T_y \psi \rangle_{L^2}\|^2 \leq C \int \int dudv \frac{|\nabla \psi(u+y)||\nabla \psi(v+y)\psi(v)\psi(u)|}{|u - v|}. \tag{3.158b}
\]
We arrive at the desired conclusion by Lemma 3.6 and (3.152).

3.7 Energy contribution $G$

This energy contribution, defined in (3.8b), is evaluated by the following proposition.

**Proposition 3.18.** Let $\mathbb{H}_K$ as in (2.4), $N_1 = d\Gamma(\Pi_1)$ and choose $c > 0$. For every $\varepsilon > 0$ there exists a constant $C_\varepsilon > 0$ (we omit the dependence on $c$) such that
\[
\left| G - \mathcal{N} \frac{1}{\alpha^2} \langle \chi_K | (\mathbb{H}_K - N_1) \chi_K \rangle \right| \leq C_\varepsilon \alpha^\varepsilon (\sqrt{K}\alpha^{-6} + K^{-1/2}\alpha^{-5}) \tag{3.159}
\]
for all $|P|/\alpha \leq c$ and all $K, \alpha$ large enough.

**Proof.** Using $h^{Pk}G^0_K = 0$ and $NG^0_K = N_1G^1_K$ we can decompose $G$ into two terms
\[
G = -\frac{2}{\alpha} \int dy \text{Re} \langle G^0_K | (\alpha^{-2}N_1 + \alpha^{-1}\phi(h + \varphi_P))T_ye^{A_P}W(\alpha w_P)G^1_K \rangle_{\mathcal{H}}.
\]
We proceed for each one separately.

**Term $G_1$.** With the aid of (3.67), (3.80) and $(T_ye^{A_P})^\dagger = T_{-y}e^{-A_P}$, one finds
\[
G_1 = -\frac{2}{\alpha^3} \int dy \text{Re} \langle R_{3,y} \psi \otimes (Y_K^< + Y_K^>) | W(\alpha w_P)G^0_K \rangle_{\mathcal{H}} = G_{1^<} + G_{1^>} \tag{3.161}
\]
where we introduced the operator $R_{3,y} = R_{3,y}^1 + R_{3,y}^2$ with
\[
R_{3,y}^1 = \text{Re}(h_{K,.})Ru_{T_y}T_{-y}P e^{-A_P}N_1, \tag{3.162a}
\]
\[
R_{3,y}^2 = 2\alpha P_{\psi} h_{K,.} \text{Re}(w_{P,y}^1)_{L^2} Ru_{T_y}T_{-y}P e^{-A_P}N_1. \tag{3.162b}
\]
Proceeding similarly as for $R_{1,y}^1$ and $R_{2,y}^2$ in (3.82a)-(3.82b), one further verifies
\[
\|R_{3,y} \Psi\|_{\mathcal{H}} \leq C \|u_{T_y}T_{-y}P \psi\|_{\text{op}} (1 + \alpha y^2) \|(N + 1)^{3/2} \Psi\|_{\mathcal{H}}. \tag{3.163}
\]
Recalling the definition $f_\alpha (y) = \|u_{T_y}T_{-y}P \psi\|_{\text{op}}$ and (3.86), we can use Corollary 3.12 to find
\[
|G_{1^>}| \leq \frac{C}{\alpha^3} \|(N + 1)^{3/2} \chi_K\|_{\mathcal{H}} \int dy f_\alpha (y)(1 + \alpha y^2) \leq C_\delta \alpha^{-7}. \tag{3.164}
\]
In the first term we proceed with (3.74) and Lemma 3.13 to obtain

\[ |G_1^-| \leq \frac{2}{\alpha^3} \int \, dy \, ||e^{\kappa N}\mathcal{U}_K(R_{3,y}\psi \otimes \Upsilon_K)||_{\mathcal{F}} \, ||e^{-\kappa N}W(\alpha \bar{w}_P y)\Omega||_{\mathcal{F}} \]

\[ \leq \frac{2\sqrt{2}}{\alpha^3} \int \, dy \, ||R_{3,y}\psi \otimes \Upsilon_K||_{\mathcal{F}} \, n_{\delta,\eta}(y) \leq \frac{C}{\alpha^3} \int \, dy \, f_\alpha(y)(1 + \alpha y^2) \, n_{\delta,\eta}(y), \]  \hspace{1cm} (3.165)

which brings us again into a position to apply Corollary 3.5. Hence

\[ |G_1^-| \leq C\alpha^{-6+3\delta}. \]  \hspace{1cm} (3.166)

**Term \( \mathcal{G}_2 \).** Here we have

\[ \mathcal{G}_2 = -\frac{2}{\alpha^2} \int \, dy \, \text{Re} \left\langle G_K^0 | \phi(h, \varphi_P)T_y W(\alpha \bar{w}_P y)G_K^1 \right\rangle_{\mathcal{F}} \]

\[ -\frac{2}{\alpha^2} \int \, dy \, \text{Re} \left\langle G_K^0 | \phi(h, \varphi_P)T_y (e^{A_P,y} - 1)W(\alpha \bar{w}_P y)G_K^1 \right\rangle_{\mathcal{F}} = \mathcal{G}_{21} + \mathcal{G}_{22}. \]  \hspace{1cm} (3.167)

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

\[ \mathcal{G}_{21} = -\frac{2}{\alpha^2} \int \, dy \, \text{Re} \left\langle \psi \otimes \Omega | a(h, \varphi_P)T_y W(\alpha \bar{w}_P y)u_\alpha R a_\dagger(h_{K,0}^1) \psi \otimes \Omega \right\rangle_{\mathcal{F}}, \]  \hspace{1cm} (3.168)

where \( \_ \) is defined in (3.52a). Next we write \( W(\alpha \bar{w}_P y) = n_{0,1}(y)e^{a(\alpha \bar{w}_P y)}e^{-a(\alpha \bar{w}_P y)} \) 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

\[ \mathcal{G}_{21} = -\frac{2}{\alpha^2} \int \, dy \, n_{0,1}(y) \, \text{Re} \left\langle \psi \otimes \Omega | a(h, \varphi_P)T_y u_\alpha R a_\dagger(h_{K,0}^1) \psi \otimes \Omega \right\rangle_{\mathcal{F}} \]  \hspace{1cm} (3.169a)

\[ + 2 \int \, dy \, n_{0,1}(y) \, \text{Re} \left\langle \psi \otimes \Omega | \langle h, \varphi_P | \bar{w}_P y \rangle L^2 T_y u_\alpha R \langle \bar{w}_P y | h_{K,0}^1 \rangle L^2 \psi \otimes \Omega \right\rangle_{\mathcal{F}}. \]  \hspace{1cm} (3.169b)

In the first line we write \( h + \varphi_P = h_0^0 + h_1 + \varphi + i\xi_P, \) with \( h_i^\dagger = (\Pi_i h_i), \) and use that

\[ \left\langle \psi \otimes \Omega | a(h_0^0 + i\xi_P)T_y u_\alpha R a_\dagger(h_{K,0}^1) \psi \otimes \Omega \right\rangle_{\mathcal{F}} = 0 \]  \hspace{1cm} (3.170)

since \( h_{K,x}^0 + i\xi_P \in \text{Ran}(\Pi_0) \) whereas \( h_{K,x}^1 \in \text{Ran}(\Pi_1) \). Finally we can replace \( a \) and \( a_\dagger \) by \( \phi, \) and then transform back with \( \mathbb{U}_K, \) using (3.53c), in order to obtain

\[ (3.169a) = -\frac{2}{\alpha^2} \int \, dy \, n_{0,1}(y) \, \text{Re} \left\langle \psi \otimes \Upsilon_K | \phi(h_1 + \varphi)T_y u_\alpha R \phi(h_{K,0}^1) \psi \otimes \Upsilon_K \right\rangle_{\mathcal{F}}. \]  \hspace{1cm} (3.171)
To summarize, we have shown that

$$G_{21} = -\frac{2}{\alpha^2} \int dy \text{Re} (G^0_K |L_{2,y} G^0_K \rangle \rangle n_{0,1}(y) + \int dy \ell_2(y)n_{0,1}(y) = G_{211} + G_{212} \quad (3.172)$$

with

$$L_{2,y} = P_\psi \phi(h^1_y + \varphi)T_y u_\alpha R(\phi(h^1_{K,-})P_\psi \quad (3.173a)$$

$$\ell_2(y) = 2 \text{Re} \langle \psi |(h_y + \varphi)\bar{P}_y |L^2 T_y u_\alpha R(\bar{w}_{P,y}) |h^1_{K,-}) L^2 |\psi \rangle \quad (3.173b)$$

In the first term we add and subtract the Gaussian,

$$G_{211} = -\frac{2}{\alpha^2} \int dy \text{Re} (G^0_K |L_{2,y} G^0_K \rangle \rangle e^{-\lambda \alpha^2 y^2} - \frac{2}{\alpha^2} \int dy \text{Re} (G^0_K |L_{2,y} G^0_K \rangle \rangle (n_{0,1}(y) - e^{-\lambda \alpha^2 y^2}) = G^{lo}_{211} + G^{err}_{211}, \quad (3.174)$$

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

$$G^{lo}_{211} = -\frac{2}{\alpha^2} \text{Re} (G^0_K |\phi(h^1_{K,-} + \varphi)R(\phi(h^1_{K,-})G^0_K \rangle \rangle \int dy e^{-\lambda \alpha^2 y^2} - \frac{2}{\alpha^2} \text{Re} (G^0_K |\phi(h^1_{K,-} + \varphi)(u_\alpha - 1)R(\phi(h^1_{K,-})G^0_K \rangle \rangle \int dy e^{-\lambda \alpha^2 y^2} - \frac{2}{\alpha^2} \int dy \text{Re} (G^0_K |\phi(h^1_{K,-} + \varphi)(T_y - 1)u_\alpha R(\phi(h^1_{K,-})G^0_K \rangle \rangle e^{-\lambda \alpha^2 y^2} - \frac{2}{\alpha^2} \int dy \text{Re} (G^0_K |\phi(h^1_y - h^1_{K,-})T_y u_\alpha R(\phi(h^1_{K,-})G^0_K \rangle \rangle e^{-\lambda \alpha^2 y^2}$$

$$= \sum_{n=1}^{\frac{4}{\alpha^2}} G^{lo,n}_{211} \quad (3.175)$$

Since $P_\psi \phi(\varphi)R = 0$, we have $G^{lo,1}_{211} = \frac{2}{\alpha^2} \langle T_K \mid (H - N_1)T_K \rangle \langle \frac{\pi}{\alpha^2} \rangle^{3/2}$, cf. (2.4), and hence we can use Proposition 3.15 to conclude that

$$\left| G^{lo,1}_{211} - N \frac{2}{\alpha^2} \langle T_K \mid (H - N_1)T_K \rangle \right| \leq C_\epsilon \sqrt{K} \alpha^{-6+\epsilon} \quad (3.176)$$

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

$$|G^{lo,2}_{211}| + |G^{lo,3}_{211}| + |G^{lo,4}_{211}| \leq C \left( \sqrt{K} \alpha^{-6} + K^{-1/2} \alpha^{-5} \right) \quad (3.177)$$

In the last term, we recall $h.(y) = h_{K,-}(y)$, and apply Lemma 3.8 in combination with $\|R^{1/2}u_\alpha T_{-y} \nabla\|_{op} \leq C$. This gives

$$|G^{lo,4}_{211}| \leq \frac{2}{\alpha^2} \int dy e^{-\lambda \alpha^2 y^2} \|R^{1/2}u_\alpha T_{-y} \phi(h^1_y - h^1_{K,-})P_\psi G^0_K\|_{\infty} \|R^{1/2}P_\psi G^0_K\|_{\infty} \quad (3.178)$$
≤ Cα^{-5}K^{-1/2}. \tag{3.178}

Next we write $T_y - 1 = \int_0^1 ds T_{sy}(y \nabla)$ in the third term to obtain an additional $|y|$, $|G_{211}^{\text{lo.3}}| \leq \frac{2}{\alpha^2} \left( \int \mathrm{d}y \ |y| e^{-\alpha^2 y^2} \right) \| \nabla u_\alpha R^{1/2} \|_{op} \| \phi(h_{K_1}^1 + \varphi)G_0^0 \|_{\infty} \| R^{1/2} \phi(h_{K_1}^1)G_0^0 \|_{\infty}$
\leq C\alpha^{-6} \sqrt{K}, \tag{3.179}

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

$$|G_{211}^{\text{lo.2}}| \leq \frac{C}{\alpha^2} \|(u_\alpha - 1)\psi\|_{L^2} \| \phi(h_{K_1}^1 + \varphi)R\phi(h_{K_1}^1)G_0^0 \|_{\infty} \leq C\sqrt{K}e^{-\alpha/C}. \tag{3.180}$$

This proves (3.177).

To bound the remaining contributions in $G_{err}^{\text{lo.3}}$ and $G_{212}$, we shall use

$$|\langle G_0^0 \rangle_{\text{L}_2 \psi} | \leq C f_{2,\alpha}(y) \tag{3.181a}$$

$$|\ell_2(y)| \leq C f_{2,\alpha}(y)(y^2 + \alpha^{-2})(|y| + |y|^3 + \alpha^{-2}) \tag{3.181b}$$

where

$$f_{2,\alpha}(y) = \|u_\alpha T_{-y} P_\psi\|_{op} + \|\nabla u_\alpha T_{-y} P_\psi\|_{op}. \tag{3.182}$$

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

$$\|f_{2,\alpha}\|_{L^\infty} \leq C \quad \text{and} \quad \| \cdot \|^n f_{2,\alpha} \|_{L^1} \leq C_n \alpha^{3+n} \quad \text{for all } n \in \mathbb{N}_0. \tag{3.183}$$

To verify (3.181a) and (3.181b), use $u_\alpha T_{-y} \phi(h.) = \phi(h_{-y})u_\alpha T_{-y}$ and Cauchy–Schwarz to bound

$$|\langle G_0^0 \rangle_{\text{L}_2 \psi} | \leq \| R^{1/2} \phi(h_{-y}^1 + \varphi)u_\alpha T_{-y} P_\psi G_0^0 \|_{\infty} \| R^{1/2} \phi(h_{K_1}^1)P_\psi G_0^0 \|_{\infty}. \tag{3.184}$$

Now we can use (3.44) and Lemma 3.8 to obtain (3.181a). To estimate $\ell_2(y)$, defined in (3.173b), we proceed with

$$|\ell_2(y)| \leq 2|\langle \psi | T_y u_\alpha \langle h_{-y} \rangle \psi \rangle_{L^2} R(|\bar{w}_{P,y} h_{K_1}^1 \rangle_{L^2} \psi)_{L^2}| \leq 2|\langle \psi | T_y u_\alpha \langle \psi \rangle \bar{w}_{P,y} \psi \rangle_{L^2} R(|\bar{w}_{P,y} h_{K_1}^1 \rangle_{L^2} \psi)_{L^2} | + 2|\langle \psi | T_y u_\alpha \langle \varphi \psi \rangle \bar{w}_{P,y} \psi \rangle_{L^2} R(|\bar{w}_{P,y} h_{K_1}^1 \rangle_{L^2} \psi)_{L^2} | \tag{3.185a}$$

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,

\[
|(3.185a)| \leq 2 \int du \, |\tilde{w}_{P,y}(u)| \|P_y T_y u_\alpha h_{-y}(u)\|_{\text{op}} \int dz \, |\tilde{w}_{P,y}(z)| \|R^{1/2} h_{\mathcal{K}}(z)\psi\|
\]

\[
\leq 2 \|\tilde{w}_{P,y}\|_{L^2} \|\tilde{w}_{P,y}\|_{L^2} \left( \int du \|P_y T_y u_\alpha h_{-y}(u)\|_{\text{op}} \int dz \|R^{1/2} h_{\mathcal{K}}(z)\psi\|^2_{L^2} \right)^{1/2}
\]

\[
\leq C f_2(y) (|y| + y^3 + \alpha^{-2})(y^2 + \alpha^{-2}),
\]

(3.186)

where the last step follows from Lemma 3.3 and Corollary 3.9 together with $h_{\mathcal{K}} = h_{\mathcal{K}}^0 + \Theta^{-1}_{\mathcal{K}} h_{\mathcal{K}}$. Since the second line is estimated similarly, we arrive at (3.181b). With (3.181a) at hand we can apply Lemma 3.4 and (3.183) to get

\[
|G_{211}| \leq \frac{2}{\alpha^2} \int dy \left| \langle C_{\mathcal{K}}^0 | L_{2,y} G_{\mathcal{K}}^0 \rangle_{\mathcal{F}} \right| |n_{0,1}(y)| - e^{-\lambda \alpha^2 y^2} \leq C \alpha^{-6},
\]

(3.187)

and further, using (3.181b) and Corollary 3.5, we obtain

\[
|G_{212}| \leq C \int dy \left| \ell_2(y) \right| n_{0,1}(y) \leq C \alpha^{-6}.
\]

(3.188)

This completes the analysis of $G_{21}$. Next we introduce $R_{4,y} = R_{4,y}^1 + R_{4,y}^2$ with

\[
R_{4,y}^1 = P_y \phi(h_{\mathcal{K}}^c) R_{\mathcal{F}}^1 (e^{-A_{P,y}} - 1) R_{\mathcal{F}}^2 \phi(h_{-y} + \varphi_P) u_\alpha T_{-y} P_y
\]

(3.189a)

\[
R_{4,y}^2 = 2\alpha P_y \langle h_{\mathcal{K}}^c | \Re(w_{P,y}) \rangle_{L^2} R_{\mathcal{F}}^1 (e^{-A_{P,y}} - 1) R_{\mathcal{F}}^2 \phi(h_{-y} + \varphi_P) u_\alpha T_{-y} P_y.
\]

(3.189b)

Inserting (3.67) and (3.80) into (3.167) it follows that

\[
G_{22} = -\frac{2}{\alpha^2} \int dy \, \Re \left( R_{4,y} \Psi \otimes (Y_K^c + Y_K^c) | W(\alpha w_{P,y}) G_{\mathcal{K}}^0 \rangle_{\mathcal{F}} \right) = G_{22}^c + G_{22}^\circ.
\]

(3.190)

With the aid of Lemma 3.8 we obtain

\[
\|R_{4,y} \Psi\|_{\mathcal{F}} \leq C \|(e^{-A_{P,y}} - 1)(N + 1)^{1/2} R_{\mathcal{F}}^1 \phi(h_{-y} + \varphi_P) u_\alpha T_{-y} P_y \Psi\|_{\mathcal{F}},
\]

(3.191)

and proceeding similarly as in (3.84), we find

\[
\|R_{4,y} \Psi\|_{\mathcal{F}} \leq C \alpha(y^2 + \alpha^{-2}) \|(e^{-A_{P,y}} - 1) R_{\mathcal{F}}^1 \phi(h_{-y} + \varphi_P) u_\alpha T_{-y} P_y \Psi\|_{\mathcal{F}}.
\]

(3.192)

For $\Psi = \psi \otimes Y_K^c$, a second application of Lemma 3.8 (after using unitarity of $e^{-A_{P,y}}$) together with $\|\varphi_P\|^2_{L^2} \leq C$ for $|P|/\alpha \leq c$ and Corollary 3.12 is sufficient to find

\[
\|R_{4,y} \Psi \otimes Y_K^c\|_{\mathcal{F}} \leq C \left( \|u_\alpha T_{-y} P_y\|_{\text{op}} + \|\nabla u_\alpha T_{-y} P_y\|_{\text{op}} \right) (1 + \alpha y^2) \|(N + 1) Y_K^c\|_{\mathcal{F}}
\]

\[
\leq C \delta \alpha^{-10} f_{2,\alpha}(y)(1 + \alpha y^2)
\]

(3.193)
with \( f_{2,\alpha} \) defined in (3.182). Using this bound in \( G_{22}^\infty \) and recalling Corollary 3.12 and (3.183) we thus obtain
\[
|G_{22}^\infty| \leq C_\delta \alpha^{-6}. \tag{3.194}
\]
In \( G_{22}^\infty \) we proceed by inserting (3.70) and use (3.74) and Lemma 3.13. This gives
\[
|G_{22}^\infty| \leq \frac{2\sqrt{2}}{\alpha^2} \int dy \|R_{1,y}^\psi \otimes Y_K^\infty\|_\infty n_\delta n(y). \tag{3.195}
\]
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 \( G_{K}^{(0)} = \psi \otimes Y_K^\infty \). We start from (3.191) and (3.192) where we insert \( h = h_K + (h - h_K) \) and use the triangle inequality,
\[
\begin{align*}
\|R_{1,y}^1 G_{K}^{(0)}\|_\infty &\leq C\|(e^{-A_{P,y} - 1})(N + 1)^{1/2} R_{z}^1 \phi(h_{K,-y} + \varphi_P) u_\alpha T_{-y} G_{K}^{(0)}\|_\infty \tag{3.196a} \\
&\quad + C\|(e^{-A_{P,y} - 1})(N + 1)^{1/2} R_{z}^1 \phi(h_{-y} - h_{K,-y}) u_\alpha T_{-y} G_{K}^{(0)}\|_\infty, \\
\|R_{1,y}^2 G_{K}^{(0)}\|_\infty &\leq C\alpha(y^2 + \alpha^{-2})\|(e^{-A_{P,y} - 1}) R_{z}^1 \phi(h_{K,-y} + \varphi_P) u_\alpha T_{-y} G_{K}^{(0)}\|_\infty \tag{3.196c} \\
&\quad + C\alpha(y^2 + \alpha^{-2})\|(e^{-A_{P,y} - 1}) R_{z}^1 \phi(h_{-y} - h_{K,-y}) u_\alpha T_{-y} G_{K}^{(0)}\|_\infty. \tag{3.196d}
\end{align*}
\]
For the second and fourth line, we apply Lemma 3.8 a second time (after bringing \((N + 1)^{1/2}\) to the right of \(a\) and \(a^1\) to find
\[
(3.196b) + (3.196d) \leq CK^{-1/2}(1 + \alpha y^2)(\|u_\alpha T_{-y} P_{\psi}\|_{op} + \|\nabla u_\alpha T_{-y} P_{\psi}\|_{op})(N + 1)Y_K^\infty\|_\infty \\
\leq CK^{-1/2}(1 + \alpha y^2) f_{2,\alpha}(y). \tag{3.197}
\]
In the first and third line, we use the functional calculus and write out \( A_{P,y} = iP_{fy} + ig_{P}(y) \),
\[
(3.196a) + (3.196c) \leq C\|(P_{fy})(N + 1)^{1/2} R_{z}^1 \phi(h_{K,-y} + \varphi_P) u_\alpha T_{-y} G_{K}^{(0)}\|_\infty \tag{3.198a} \\
&\quad + C\alpha(y^2 + \alpha^{-2})\|(P_{fy}) R_{z}^1 \phi(h_{K,-y} + \varphi_P) u_\alpha T_{-y} G_{K}^{(0)}\|_\infty \tag{3.198b} \\
&\quad + C\|g_{P}(y)\|(N + 1)^{1/2} R_{z}^1 \phi(h_{K,-y} + \varphi_P) u_\alpha T_{-y} G_{K}^{(0)}\|_\infty \tag{3.198c} \\
&\quad + C\alpha(y^2 + \alpha^{-2})\||g_{P}(y)||R_{z}^1 \phi(h_{K,-y} + \varphi_P) u_\alpha T_{-y} G_{K}^{(0)}\|_\infty. \tag{3.198d}
\]
Now we use \([iP_{fy}, \phi(f)] = \pi(y\nabla f)\) such that we can estimate the first line by
\[
(3.198a) \leq C\|(N + 1)^{1/2} R_{z}^1 \phi(h_{K,-y} + \varphi_P) (P_{fy}) u_\alpha T_{-y} G_{K}^{(0)}\|_\infty \\
+ \|(N + 1)^{1/2} R_{z}^1 \pi(y\nabla h_{K,-y} + y\nabla \varphi_P) u_\alpha T_{-y} G_{K}^{(0)}\|_\infty. \tag{3.199}
\]
To bound the first line, we use again Lemma 3.8, while in the second line we use \((\nabla h_K) = -\nabla(h_{K,}) = -[\nabla, h_{K,}]\) and (3.44) together with \(\|\nabla \varphi_P\|_{L^2} \leq C\) for \(|P|/\alpha \leq c\). Together we
obtain

\[(3.198a) \leq C|y|(\|u_\alpha T_\alpha P_\psi\|_{op} + \|\nabla u_\alpha T_\alpha P_\psi\|_{op}) (\|(N + 1) P_\psi \mathcal{Y}_K\|_\infty + \sqrt{K}\|(N + 1) \mathcal{Y}_K\|_\infty) \]
\[ \leq C\alpha^4|y|f_{2,\alpha}(y)(\|P_\psi \mathcal{Y}_K\|_\infty + \sqrt{K}) \]
\[ \leq C\alpha^4\sqrt{K}|y|f_{2,\alpha}(y), \tag{3.200} \]

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 3.14. In a similar fashion, one shows

\[(3.198b) \leq C\alpha^4\sqrt{K}|y|(1 + \alpha y^2)f_{2,\alpha}(y), \tag{3.201} \]

and, with (3.77), one also verifies

\[(3.198c) + (3.198d) \leq C\alpha^4(\alpha^2|y|^5 + \alpha|y|^3)f_{2,\alpha}(y). \tag{3.202} \]

Collecting the estimates (3.197), (3.200), (3.201) and (3.202) we arrive at

\[\left\| R_{4,y} \psi \otimes \mathcal{Y}_K^< \right\|_{\mathcal{H}} \leq C f_{2,\alpha}(y)\alpha^\delta \left(K^{-\frac{1}{2}}(1 + \alpha y^2) + \alpha^2|y|^{5} + \sqrt{K}(|y| + \alpha|y|^3)\right)\]. \tag{3.203} \]

Now we can apply Corollary 3.5 together with (3.183) to bound the right side of (3.195). The result is

\[|G_{22}^<| \leq C\alpha^{-2+\delta}(K^{-1/2}\alpha^{-3} + \sqrt{K}\alpha^{-4+\delta}). \tag{3.204} \]

In view of the estimates (3.164), (3.166), (3.176), (3.177), (3.187), (3.188), (3.194) and (3.204), the proof of Proposition 3.18 is now complete.

\section{3.8 Energy contribution \(K\)}

Recall that \(K\) was defined in (3.8c).

\textbf{Proposition 3.19.} Let \(\mathbb{H}_K\) as in (2.4), \(N_1 = d\Gamma(\Pi_1)\) and choose \(c > 0\). For every \(\varepsilon > 0\) there exists a constant \(C_\varepsilon > 0\) (we omit the dependence on \(c\)) such that

\[\left| K + \mathcal{N}\frac{1}{\alpha^2}\langle \mathcal{Y}_K|\mathcal{H}_K - N_1\rangle \mathcal{Y}_K \right| \leq C_\varepsilon \alpha^\varepsilon \left(\sqrt{K}\alpha^{-6} + K^{-1/2}\alpha^{-5}\right) \tag{3.205} \]

for all \(|P|/\alpha \leq c\) and all \(K,\alpha\) large enough.

\textbf{Proof.} We split this contribution into three terms

\[K = \frac{1}{\alpha^2} \int dy \langle G^1_K| (h^{Pek} + \alpha^{-2}N + \alpha^{-1}\phi(h + \phi_P)) T_y \psi A_P W(\alpha w_P y) G^1_K \rangle_{\mathcal{H}} \]
\[= K_1 + K_2 + K_3, \tag{3.206} \]
and note that $\mathcal{K}_1$ provides the energy contribution of order $\alpha^{-2}$.

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

$$
\mathcal{K}_1 = \frac{1}{\alpha^2} \int dy \langle G_{K}^1 | h^{\text{Pek}} T_y W(\alpha w_{P,y}) G_{K}^1 \rangle_{\mathcal{F}} + \frac{1}{\alpha^2} \int dy \langle G_{K}^1 | h^{\text{Pek}} T_y (e^{A_{P,y}} - 1) W(\alpha w_{P,y}) G_{K}^1 \rangle_{\mathcal{F}} = \mathcal{K}_{11} + \mathcal{K}_{12}. 
$$

(3.207)

and proceed for the first term similarly as in the computation of $G_2$, see (3.167). This leads to

$$
\mathcal{K}_{11} = \frac{1}{\alpha^2} \int dy \langle G_{K}^0 | \phi(h_{K,.}^1) R u_{\alpha} h^{\text{Pek}} T_y W(\alpha w_{P,y}) u_{\alpha} R\phi(h_{K,.}^1) G_{K}^0 \rangle_{\mathcal{F}}
= \frac{1}{\alpha^2} \int dy \langle \psi \otimes \Omega | a(h_{K,.}^1) R u_{\alpha} h^{\text{Pek}} T_y W(\alpha \bar{w}_{P,y}) u_{\alpha} R\phi(h_{K,.}^1) \psi \otimes \Omega \rangle_{\mathcal{F}}
= \frac{1}{\alpha^2} \int dy \langle G_{K}^0 | L_{3,y} G_{K}^0 \rangle_{\mathcal{F}} n_{0,1}(y) - \int dy \ell_3(y) n_{0,1}(y) = \mathcal{K}_{111} + \mathcal{K}_{112} 
$$

(3.208)

where

$$
L_{3,y} = P_{\psi} \phi(h_{K,.}^1) R u_{\alpha} h^{\text{Pek}} T_y u_{\alpha} R\phi(h_{K,.}^1) P_{\psi} 
$$

(3.209a)

$$
\ell_3(y) = \langle \psi | \langle h_{K,.}^1 | \bar{w}_{P,y}^1 \rangle_{L^2} R u_{\alpha} h^{\text{Pek}} T_y u_{\alpha} R \langle \bar{w}_{P,y}^1 | h_{K,.}^1 \rangle_{L^2} \psi \rangle_{L^2}. 
$$

(3.209b)

We go on with

$$
\mathcal{K}_{111} = \frac{1}{\alpha^2} \int dy \langle G_{K}^0 | L_{3,y} G_{K}^0 \rangle_{\mathcal{F}} e^{-\lambda \alpha^2 y^2} + \frac{1}{\alpha^2} \int dy \langle G_{K}^0 | L_{3,y} G_{K}^0 \rangle_{\mathcal{F}} (n_{0,1}(y) - e^{-\lambda \alpha^2 y^2}) = \mathcal{K}_{111}^\text{lo} + \mathcal{K}_{111}^\text{corr}, 
$$

(3.210)

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

$$
\mathcal{K}_{111}^\text{lo} = \frac{1}{\alpha^2} \langle G_{K}^0 | \phi(h_{K,.}^1) R h^{\text{Pek}} R \phi(h_{K,.}^1) G_{K}^0 \rangle_{\mathcal{F}} \int dy e^{-\lambda \alpha^2 y^2}
+ \frac{1}{\alpha^2} \langle G_{K}^0 | \phi(h_{K,.}^1) R(u_{\alpha} - 1) h^{\text{Pek}} R \phi(h_{K,.}^1) G_{K}^0 \rangle_{\mathcal{F}} \int dy e^{-\lambda \alpha^2 y^2}
+ \frac{1}{\alpha^2} \langle G_{K}^0 | \phi(h_{K,.}^1) R u_{\alpha} h^{\text{Pek}}(u_{\alpha} - 1) R \phi(h_{K,.}^1) G_{K}^0 \rangle_{\mathcal{F}} \int dy e^{-\lambda \alpha^2 y^2}
+ \frac{1}{\alpha^2} \int dy \langle G_{K}^0 | \phi(h_{K,.}^1) R u_{\alpha} h^{\text{Pek}}(T_y - 1) u_{\alpha} R \phi(h_{K,.}^1) G_{K}^0 \rangle_{\mathcal{F}} \int dy e^{-\lambda \alpha^2 y^2}
= \sum_{n=1}^{4} \mathcal{K}_{111}^{\text{lo,n}}. 
$$

(3.211)

Since $R h^{\text{Pek}} R = R$, one finds $\mathcal{K}_{111}^{\text{lo,1}} = -\frac{1}{\alpha^2} \langle \Upsilon_{K} | (\Upsilon_{K} - N_1) \Upsilon_{K} \rangle_{\mathcal{F}} (\frac{\pi}{\lambda \alpha^2})^3$, cf. (2.4), and with the
aid of Proposition 3.15, this gives the leading-order contribution

\[ |K_{111}^{\text{lo},1} + N_1^{-1} \langle \mathcal{Y}_K (\mathbb{H}_K - \mathbb{N}_1) \mathcal{Y}_K \rangle_x | \leq C e^{\sqrt{K} \alpha^{-6+\varepsilon}}. \]  

(3.212)

For the other terms, we shall show that

\[ |K_{111}^{\text{lo},2}| + |K_{111}^{\text{lo},3}| + |K_{111}^{\text{lo},4}| \leq C \sqrt{K} \alpha^{-6}. \]  

(3.213)

In the second term we use \( h_{\text{Pek}} R = Q_{\psi} = 1 - P_{\psi} \) to write

\[ K_{111}^{\text{lo},2} = \alpha^{-2} \langle G_K^0 \phi(h_{K,1}^1) R(u_{a1} - 1)(1 - P_{\psi}) \phi(h_{K,1}^1) G_K^0 \rangle_x \left( \frac{\pi}{\lambda \alpha^2} \right)^{3/2} \]  

(3.214)

which is exponentially small in \( \alpha \), since \( \|(u_{a1} - 1) \psi\|_{L^2} \leq C e^{-\alpha/C} \), and thus with Lemma 3.8 one obtains \( |K_{111}^{\text{lo},2}| \leq C \sqrt{K} \alpha^{-6/C} \). In the next term we use \([h_{\text{Pek}}, u_{a1}] = -[\Delta, u_{a1}]\) and again \( h_{\text{Pek}} R = 1 - P_{\psi} \) to get

\[ K_{111}^{\text{lo},3} = \alpha^{-2} \langle G_K^0 \phi(h_{K,1}^1) R u_{a1} (u_{a1} - 1)(1 - P_{\psi}) \phi(h_{K,1}^1) G_K^0 \rangle_x \left( \frac{\pi}{\lambda \alpha^2} \right)^{3/2} \]  

\[ - \alpha^{-2} \langle G_K^0 \phi(h_{K,1}^1) R[\Delta, u_{a1}] R \phi(h_{K,1}^1) G_K^0 \rangle_x \left( \frac{\pi}{\lambda \alpha^2} \right)^{3/2}. \]  

(3.215)

Here the first line is bounded again exponentially in \( \alpha \), whereas in the second line we use \([\Delta, u_{a1}] = 2(\nabla u_{a1}) \nabla + (\Delta u_{a1})\) and \( \|\nabla u_{a1}\|_{L^\infty} + \|\Delta u_{a1}\|_{L^\infty} \leq C \alpha^{-1} \), see (2.20). Together with Lemmas 3.7 and 3.8, this implies \( |K_{111}^{\text{lo},3}| \leq C \alpha^{-6} \). In the last term we employ \( T_y - 1 = \int_0^1 ds \mathcal{T}_{sy}(y \nabla) \), \([h_{\text{Pek}}, u_{a1}] = -[\Delta, u_{a1}]\) and \( h_{\text{Pek}} R = Q_{\psi} \) to find

\[ K_{111}^{\text{lo},4} = \alpha^{-2} \int dy \int_0^1 ds \langle G_K^0 \phi(h_{K,1}^1) Q_{\psi} u_{a1} T_{sy}(y \nabla) u_{a1} R \phi(h_{K,1}^1) G_K^0 \rangle_x e^{-\lambda \alpha^2 y^2} \]  

\[ + \alpha^{-2} \int dy \int_0^1 ds \langle G_K^0 \phi(h_{K,1}^1) R[\Delta, u_{a1}] T_{sy}(y \nabla) u_{a1} R \phi(h_{K,1}^1) G_K^0 \rangle_x e^{-\lambda \alpha^2 y^2}. \]  

(3.216)

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

\[ |K_{111}^{\text{lo},4}| \leq C \alpha^{-6} \|\phi(h_{K,1}^1) G_K^0 \|_x \|\nabla u_{a1} R^{1/2} \|_{op} \|R^{1/2} \phi(h_{K,1}^1) G_K^0 \|_x \]  

\[ + C \alpha^{-6} \|R^{1/2} \phi(h_{K,1}^1) G_K^0 \|_x \|R^{1/2} \Delta, u_{a1} \|_{op} \|\nabla u_{a1} R^{1/2} \|_{op} \|R \phi(h_{K,1}^1) G_K^0 \|_x \]

\[ \leq C (\alpha^{-6} \sqrt{K} + \alpha^{-7}). \]  

(3.217)

This proves (3.213).
To estimate $K_{112}$ and $K^\text{err}_{111}$, we make use of

\begin{align}
\|G_K^0|L_3 y G_K^0\|_{\infty} & \leq C f_{3,\alpha}(y) \quad (3.218a) \\
|\ell_3(y)| & \leq C f_{3,\alpha}(y)(y^4 + \alpha^{-4}) \quad (3.218b)
\end{align}

where

\[ f_{3,\alpha}(y) = \|u_\alpha T_y u_\alpha\|_{op} + \|(\nabla u_\alpha)T_y u_\alpha\|_{op} + \|u_\alpha T_y (\nabla u_\alpha)\|_{op} + \|(\nabla u_\alpha)T_y (\nabla u_\alpha)\|_{op}. \quad (3.219) \]

Recalling that by definition $|\nabla^k u_\alpha(y)| \leq 1(|y| \leq 2\alpha)$ for $k = 0, 1$, it follows that $f_{3,\alpha}(y) \leq 41(|y| \leq 4\alpha)$ and thus

\[ \|f_{3,\alpha}\|_{L^\infty} \leq 4 \quad \text{and} \quad \|\cdot^n f_{3,\alpha}\|_{L^1} \leq C n \alpha^{3+n} \quad \text{for all } n \in \mathbb{N}_0. \quad (3.220) \]

In order to verify (3.218a), use $h^{\text{Pek}} = -\Delta + V^\phi - \lambda^{\text{Pek}}$ to write

\[ R^{\frac{1}{2}} u_\alpha T_y h^{\text{Pek}} u_\alpha R^{\frac{1}{2}} = R^{\frac{1}{2}} u_\alpha \left( (-i\nabla)T_y (-i\nabla) + T_y (V^\phi - \lambda^{\text{Pek}}) \right) u_\alpha R^{\frac{1}{2}} = -R^{\frac{1}{2}} (-i\nabla u_\alpha)T_y (-i\nabla u_\alpha) R^{\frac{1}{2}} + R^{\frac{1}{2}} (-i\nabla) u_\alpha T_y u_\alpha (-i\nabla) R^{\frac{1}{2}} + R^{\frac{1}{2}} (-i\nabla u_\alpha)T_y u_\alpha (-i\nabla) R^{\frac{1}{2}} + R^{\frac{1}{2}} u_\alpha T_y u_\alpha (V^\phi - \lambda^{\text{Pek}}) R^{\frac{1}{2}}. \quad (3.221) \]

Since $\|V^\phi R^{1/2}\|_{op} \leq C(\|R\|_{op} + \|\nabla R^{1/2}\|_{op}) \leq C$, see Lemma 3.7, it thus follows that

\[ \|R^{\frac{1}{2}} u_\alpha T_y h^{\text{Pek}} u_\alpha R^{\frac{1}{2}}\|_{op} \leq C f_{3,\alpha}(y). \quad (3.222) \]

With this at hand one applies Lemma 3.8 to conclude the bound stated in (3.218a). For $\ell_3(y)$ we proceed similarly as in (3.186), that is

\[ |\ell_3(y)| \leq \|R^{1/2} u_\alpha h^{\text{Pek}} T_y u_\alpha R^{1/2}\|_{op} R^{1/2}\langle \tilde{w}_{P,y} h_{K,z} \rangle_{L^2}\|\psi\|_{L^2} \leq f_{3,\alpha}(y) \|\tilde{w}_{P,y}\|_{L^2}^2 \int dz \|P_y h_{K,z} \|_{L^2}^2 \leq C f_{3,\alpha}(y)(y^4 + \alpha^{-4}). \quad (3.223) \]

Now we can apply Lemma 3.4 and (3.220) to estimate

\[ |K_{111}^\text{err}| \leq \frac{C}{\alpha^2} \int dy f_{3,\alpha}(y) |n_{0,1}(y) - e^{-\lambda \alpha^2 y^2}| \leq C \alpha^{-6}, \quad (3.224) \]

and further invoke Corollary 3.5 to obtain

\[ |K_{112}| \leq \int dy f_{3,\alpha}(y)(|y|^4 + \alpha^{-4}) n_{0,1}(y) \leq C \alpha^{-7}. \quad (3.225) \]
Next we come to $K_{12}$ which we rewrite with the aid of (3.67) and (3.80) as

$$K_{12} = \frac{1}{\alpha^2} \int dy \langle R_{5,y} \psi \otimes (\mathcal{Y}_K^- + \mathcal{Y}_K^+) \rangle |W(\alpha w_{P,y})G_K^0\rangle_{x^*} = K_{12}^- + K_{12}^+ \quad (3.226)$$

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

$$R_{5,y}^1 = P_\psi \phi(h_{K,.}^1) R_u \alpha e^{-A_{P,y}} - 1)T_{-y} h^{\text{pek}} u \alpha R \phi(h_{K,.}^1) P_\psi \quad (3.227a)$$

$$R_{5,y}^2 = 2\alpha P_\psi \langle h_{K,.} | \text{Re}(w_{P,y}^1) \rangle \psi \phi(h_{K,.}^1) P_\psi \quad (3.227b)$$

Utilizing Lemma 3.8 and (3.32a), we have

$$\|R_{5,y} \psi\|_{x^*} \leq C \|(e^{-A_{P,y}} - 1)(N + 1)^{1/2} R_{y}^{1/2} u \alpha T_{-y} h^{\text{pek}} u \alpha R \phi(h_{K,.}^1) P_\psi \psi\|_{x^*}, \quad (3.228)$$

and following the same steps as in (3.84),

$$\|R_{5,y}^2 \psi\| \leq C(\alpha(y^2 + \alpha^{-2}) \|(e^{-A_{P,y}} - 1)R^2_{y} u \alpha T_{-y} h^{\text{pek}} u \alpha R \phi(h_{K,.}^1) P_\psi \psi\|_{x^*}. \quad (3.229)$$

After using unitarity of $e^{-A_{P,y}}$ and (3.220), we can apply Lemma 3.8 another time to obtain

$$\|R_{5,y} \psi \otimes \mathcal{Y}_K^+\|_{x^*} \leq C f_{3,\alpha}(-y)(1 + \alpha y^2) \|(N + 1)\mathcal{Y}_K^+\|_{x^*}. \quad (3.230)$$

Thus we can estimate the tail with the aid of Corollary 3.12 and (3.220),

$$|K_{12}^+| \leq \frac{C}{\alpha^2} \|(N + 1)\mathcal{Y}_K^-\|_{x} \int dy f_{3,\alpha}(-y)(1 + \alpha y^2) \leq C \alpha^{-6}. \quad (3.231)$$

Then we use (3.63), (3.74) and apply Lemma 3.13 to get

$$|K_{12}^-| \leq \frac{1}{\alpha^2} \int dy \|U \mathcal{Y}_K^- \mathcal{Y}_K^+\|_{x^*} \|e^{-\kappa N} W(\alpha \bar{w}_{P,y}) \Omega\|_{x}$$

$$\leq \frac{\sqrt{2}}{\alpha^2} \int dy \|R_{5,y} \psi \otimes \mathcal{Y}_K^-\|_{x^*} n_{\eta}(y). \quad (3.232)$$

To bound the norm in the integral, we proceed in close analogy to the steps following (3.195). We abbreviate again $G_K^{0,-} = \psi \otimes \mathcal{Y}_K^-$ and start from (3.228) and (3.229). With (3.220), the functional calculus and $A_{P,y} = i P_f y + ig_P(y)$, one finds

$$\|R_{5,y} \psi \otimes \mathcal{Y}_K^-\|_{x^*} \leq C f_{3,\alpha}(-y) \|(e^{-A_{P,y}} - 1)(N + 1)^{1/2} R_{y}^{1/2} \phi(h_{K,.}^1) G_K^{0,-}\|_{x^*}$$

$$+ \alpha(y^2 + \alpha^{-2}) f_{3,\alpha}(-y) \|(e^{-A_{P,y}} - 1)R^2_{y} \phi(h_{K,.}^1) G_K^{0,-}\|_{x^*}$$

$$\leq C f_{3,\alpha}(-y) \|(y P_f)(N + 1)^{1/2} R_{y}^{1/2} \phi(h_{K,.}^1) G_K^{0,-}\|_{x^*} \quad (3.233a)$$

$$+ f_{3,\alpha}(-y) \|g_P(y)(N + 1)^{1/2} R_{y}^{1/2} \phi(h_{K,.}^1) G_K^{0,-}\|_{x^*} \quad (3.233b)$$
In the first and third line, we employ the commutator $[iP_y, \phi] = \partial_y \phi$, to obtain

$$+ f_{3, a}(-y)(\alpha y^2 + \alpha^{-1})|(P_f y)R^\frac{1}{2} \phi(h_{K, \cdot})G^0_K \|_x$$

$$+ f_{3, a}(-y)(\alpha y^2 + \alpha^{-1})|yP_f(y)||R^\frac{1}{2} \phi(h_{K, \cdot})G^0_K \|_x).$$

(3.233c)

(3.233d)

In the second and fourth line, we use $|g_P(y)| \leq C\alpha|y|^3$ and Lemma 3.8,

$$(3.233b) + (3.233d) \leq C(\alpha^2|y|^5 + \alpha|y|^3)f_{3, a}(-y)||y(N + 1)Y^\leq_K \|_x$$

$$\leq C(\alpha^2|y|^5 + \alpha|y|^3)f_{3, a}(-y).$$

(3.234)

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

$$(3.233a) + (3.233c) \leq C(f_{3, a}(-y)||y(N + 1)\frac{1}{2}R^\frac{1}{2} \phi(h_{K, \cdot})\phi(yP_f)G^0_K \|_x$$

$$+ f_{3, a}(-y)||y(N + 1)\frac{1}{2}R^\frac{1}{2} \pi(y\nabla h_{K, \cdot})G^0_K \|_x$$

$$+ f_{3, a}(-y)(\alpha y^2 + \alpha^{-1})||R^\frac{1}{2} \phi(h_{K, \cdot})\phi(yP_f)G^0_K \|_x$$

$$+ f_{3, a}(-y)(\alpha y^2 + \alpha^{-1})||R^\frac{1}{2} \pi(y\nabla h_{K, \cdot})G^0_K \|_x).$$

(3.235a)

(3.235b)

(3.235c)

(3.235d)

After another application of Lemma 3.8, we can use (3.67) and then Lemma 3.14 for the terms involving $P_f$,

$$(3.235a) + (3.235c) \leq C f_{3, a}(-y)(\alpha y^2 + 1)|y||(N + 1)P_fY^\leq_K \|_x$$

$$\leq C f_{3, a}(-y)(\alpha|y|^3 + |y|)\alpha^\delta \sqrt{K},$$

(3.236)

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

$$(3.235b) + (3.235d) \leq C f_{3, a}(-y)|y|(\alpha y^2 + 1)||h_{K, 0}\|_{L^2}||(N + 1)Y^\leq_K \|_x$$

$$\leq C f_{3, a}(-y)(\alpha|y|^3 + |y|)\sqrt{K}.$$ 

(3.237)

Collecting all estimates we have thus shown that

$$\|R_{5, y}\psi \otimes Y^\leq_K \|_x \leq C f_{3, a}(-y)\alpha^\delta \left(\alpha^2|y|^5 + \sqrt{K}(\alpha|y|^3 + |y|)\right).$$

(3.238)

Using this bound in (3.232) we can invoke Corollary 3.5 together with (3.220) in order to obtain

$$|K_{12}^\leq| \leq C\sqrt{K}a^{-6+\delta}.$$ 

(3.239)

Term $K_2$. Using (3.67) and (3.80), one finds

$$K_2 = \frac{1}{\alpha^4} \int d\eta \langle R_{6, y}\psi \otimes (Y^\leq_K + Y^\geq_K)W(\alpha w_{P, y})G^0_K \|_x \rangle = K_2^\leq + K_2^\geq,$$ 

(3.240)
with the operator $R_{6,y} = R_{6,y}^1 + R_{6,y}^2$ and
\begin{align}
R_{6,y}^1 &= P\phi(h^{1}_{K_\cdot})Ru_{\alpha}NT_{-y}e^{-A_{P_y}u_\alpha R\phi(h^{1}_{K_\cdot})P_\psi} \\
R_{6,y}^2 &= 2\alpha P\psi(h^{1}_{K_\cdot})Ru_{\alpha}NT_{-y}e^{-A_{P_y}}u_\alpha R(\text{Re}(w_{P_y}^L|h^{1}_{K_\cdot})L^2 P_\psi).
\end{align}

(3.241a) (3.241b)

With Lemma 3.8 and (3.32a) it is not difficult to verify
\[
\|R_{6,y}P\|_{\mathcal{K}} \leq C\|u_\alpha T_{-y}u_\alpha\|_{op}(1 + \alpha y^2)(N + 1)^2\|\mathcal{K}\|_{\mathcal{K}},
\]

(3.242)

and since $\|u_\alpha T_{-y}u_\alpha\|_{op} \leq 1(|y| \leq 4\alpha)$, we can use Corollary 3.12 to estimate the part with the tail by
\[
|\mathcal{K}_{2}^\leq| \leq \frac{C}{\alpha^4}\|\mathcal{K}\|_{\mathcal{K}}\int dy 1(|y| \leq 4\alpha)(1 + \alpha y^2) \leq C_\delta \alpha^{-8}.
\]

(3.243)

It now follows from Corollary 3.5 that
\[
|\mathcal{K}_{2}^\leq| \leq C\alpha^{-7}.
\]

(3.245)

Term $\mathcal{K}_3$. This term is similarly estimated as the previous one. With the aid of (3.67) and (3.80), we have
\[
\mathcal{K}_3 = \frac{1}{\alpha^3}\int dy \langle R_{7,y}P\| \otimes (\mathcal{Y}_{K}^\leq + \mathcal{Y}_{K}^\geq)\|_{\mathcal{K}_\cdot}W(\alpha w_{P_y}^L G_{K_{\cdot}}^{0})\|_{\mathcal{K}} = \mathcal{K}_3^\leq + \mathcal{K}_3^\geq
\]

(3.246)

with the operator $R_{7,y} = R_{7,y}^1 + R_{7,y}^2$ and
\begin{align}
R_{7,y}^1 &= P\phi(h^{1}_{K_\cdot})Ru_{\alpha}e^{-A_{P_y}y_{-y}}\phi(h + \varphi_{y})u_\alpha R\phi(h^{1}_{K_\cdot})P_\psi \\
R_{7,y}^2 &= 2\alpha P\psi(h^{1}_{K_\cdot})Ru_{\alpha}e^{-A_{P_y}y_{-y}}\phi(h + \varphi_{y})u_\alpha R\phi(h^{1}_{K_\cdot})P_\psi.
\end{align}

(3.247a) (3.247b)

Utilizing again Lemma 3.8 and (3.32a), one shows that
\[
\|R_{7,y}P\|_{\mathcal{K}} \leq C f_{3,\alpha}(-y)(1 + \alpha y^2)(N + 1)^{3/2}\|\mathcal{K}\|_{\mathcal{K}}
\]

(3.248)

with $f_{3,\alpha}$ defined in (3.219). Invoking Corollary 3.12 and (3.220) we thus find
\[
|\mathcal{K}_3^\geq| \leq \frac{C}{\alpha^3}\|\mathcal{K}\|_{\mathcal{K}}\int dy f_{3,\alpha}(-y)(1 + \alpha y^2) \leq C_\delta \alpha^{-7}.
\]

(3.249)
Similarly as in (3.232), we also obtain
\[ |\mathcal{K}_3^\leq| \leq \frac{\sqrt{2}}{\alpha^3} \int dy \| R_{7,y} \psi \otimes \mathcal{Y}_{K} \|_{\mathcal{F}} n_{\delta,y}(y) \leq \frac{C}{\alpha^3} \int dy f_{3,\alpha}(1 + \alpha y^2) n_{\delta,y}(y). \]  
(3.250)

By Corollary 3.5 and (3.219) it follows that
\[ |\mathcal{K}_3^\leq| \leq C \alpha^{-6+3\delta}. \]  
(3.251)

This completes the analysis of \( \mathcal{K} \). The proof of Proposition 3.19 follows from combining (3.212), (3.213), (3.224), (3.225), (3.231), (3.239), (3.243), (3.245), (3.249) and (3.251).

3.9 Concluding the proof of Proposition 2.4

Combining Propositions 3.16, 3.18 and 3.19, we arrive at
\[ \left| \mathcal{E} + \mathcal{G} + \mathcal{K} \mathcal{N} - \inf_{\sigma} (H_\mathcal{K}) \right| \leq C \varepsilon \left( \frac{K^{-1/2} \alpha^{-5} + \sqrt{K} \alpha^{-6}}{N} \right). \]  
(3.252)

Now for \( K \leq \tilde{c} \alpha \) we know from Proposition 3.15 that \( N \geq C \alpha^3 \) for some \( C > 0 \), such that the right side is bounded by \( C \varepsilon \mathcal{F} \mathcal{N} \alpha^3 \). It remains to show that one can replace \( \alpha^{-2} \inf \sigma(\mathcal{H}_\mathcal{K}) \) by \( \alpha^{-2} \inf \sigma(\mathcal{H}_\infty) \) at the cost of an additional error. To this end, recall that \( \inf \sigma(\mathcal{H}_\mathcal{K}) = \langle \mathcal{Y}_\mathcal{K} | \mathcal{H}_\mathcal{K} \mathcal{Y}_\mathcal{K} \rangle_{\mathcal{F}} \) and use the variational principle to find
\[ \langle \mathcal{Y}_\mathcal{K} | (\mathcal{H}_\mathcal{K} - \mathcal{H}_\infty) \mathcal{Y}_\mathcal{K} \rangle_{\mathcal{F}} \leq \inf \sigma(\mathcal{H}_\mathcal{K}) - \inf \sigma(\mathcal{H}_\infty) \leq \langle \mathcal{Y}_\infty | (\mathcal{H}_\mathcal{K} - \mathcal{H}_\infty) \mathcal{Y}_\infty \rangle_{\mathcal{F}}. \]  
(3.253)

Writing
\[ \mathcal{H}_\mathcal{K} - \mathcal{H}_\infty = \langle \psi | \phi(h_{K_x}^1 - h_1^1) R \phi(h_{K_x}^1), \psi \rangle_{L^2} - \langle \psi | \phi(h_1^1) R \phi(h_1^1 - h_{K_x}^1), \psi \rangle_{L^2}, \]  
(3.254)

and using Lemma 3.8, we can infer that for any \( \Psi \in \mathcal{F} \)
\[ \left| \langle \mathcal{Y}_\mathcal{K} | (\mathcal{H}_\mathcal{K} - \mathcal{H}_\infty) \mathcal{Y}_\mathcal{K} \rangle_{\mathcal{F}} \right| \leq C K^{-1/2} \langle \Psi | (N_1 + 1) \Psi \rangle_{\mathcal{F}}. \]  
(3.255)

By Corollary 3.12 we know that \( \langle \mathcal{Y}_\mathcal{K} | (N_1 + 1) \mathcal{Y}_\mathcal{K} \rangle_{\mathcal{F}} \leq C \) for all \( K \in (K_0, \infty] \) with \( K_0 \) large enough, and thus \( \inf \sigma(\mathcal{H}_\mathcal{K}) - \inf \sigma(\mathcal{H}_\infty) \leq C K^{-1/2} \). In view of (3.252) and Lemma 3.1 this completes the proof of Proposition 2.4.

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 \( H^\text{Pek} \geq 0 \) follows from (1.19) whereas
$H_{\text{Pek}} \leq 1$ is a consequence of

$$
\langle v | (1 - H_{\text{Pek}}) v \rangle_{L^2} = 4 \left\| \int dy \, v(y) R^{1/2} h.(y) \psi \right\|_{L^2}^2.
$$

(4.1)

(ii) That \( \text{Span}\{\partial_i \varphi : i = 1, 2, 3\} \subseteq \text{Ker} H_{\text{Pek}} \) follows from translation invariance of the energy functional \( \mathcal{F} \). To show equality we argue that there is a \( \tau > 0 \) such that \( \langle v | H_{\text{Pek}} v \rangle_{L^2} \geq \tau \|v\|_{L^2}^2 \) for all \( v \in L^2(\mathbb{R}^3) \) with \( \langle v | \nabla \varphi \rangle_{L^2} = 0 \) (note that this also implies (iii)). For that purpose we quote [11, Lemma 2.7] stating that there exists a constant \( \tau > 0 \) such that

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

(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 [29]; see [11] for a detailed derivation). Combined with (1.19) this implies

$$
\langle v | H_{\text{Pek}} v \rangle_{L^2} \geq \tau \lim_{\varepsilon \to 0} \inf_{y \in \mathbb{R}^3} f_v(y, \varepsilon),
$$

(4.3a)

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

(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

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

(4.4)

it follows that \( \lim_{n \to \infty} f_v(y^*(\varepsilon_n), \varepsilon_n) = \infty \), 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 \( f_v(y^*(\varepsilon), \varepsilon) = \|v\|_{L^2}^2 \)). With this we can estimate

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

(4.5)

To bound the right side, write

$$
\eta(\varepsilon)(z) = \int_0^1 ds \, (y^*(\varepsilon) \nabla) \varphi(z - sy^*(\varepsilon))
$$

(4.6)

and use, by dominated convergence, that

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

(4.7)
Combining the last statement with \(|y^*(\varepsilon)| \to 0 \text{ as } \varepsilon \to 0\) and \(\langle v|\nabla \varphi \rangle_{L^2} = 0\) we conclude that

\[
\lim_{\varepsilon \to 0} f_\varepsilon(y^*(\varepsilon), \varepsilon) \geq \|v\|_{L^2}^2.
\]  
(4.8)

This completes the proof of items (ii) and (iii). Property (iv) follows from \(H_{\text{pek}}^K \leq (H_{\text{pek}}^K)^{1/2}\) and \(\text{Tr}_{L^2}(1 - H_{\text{pek}}^K) < \infty\), see Lemma 2.2 for \(K = \infty\). \(\square\)

**Proof of Lemma 2.2.** (i) The bound \(H_{\text{pek}}^K \upharpoonright \text{Ran}(\Pi_1) \leq 1\) follows analogously to (4.1) and \(H_{\text{pek}}^K \upharpoonright \text{Ran}(\Pi_0) = 0\) holds by definition. The lower bound on \(\text{Ran}(\Pi_1)\) is a consequence of \((H_{\text{pek}}^K - \tau) \upharpoonright \text{Ran}(\Pi_1) \geq 0\) for some \(\tau > 0\), see Lemma 1.1, in combination with

\[
\pm (H_{\text{pek}}^K - H_{\text{pek}}^K) \leq CK^{-1/2}.
\]  
(4.9)

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

\[
\langle v|(H_{\text{pek}}^K - H_{\text{pek}}^K)v\rangle_{L^2} = 4 \int \text{d}y \text{ Re} \langle \psi|(h_K.(y) - \cdot h.)(y)R(\Pi_v h_K.)(y)\psi \rangle_{L^2} \\
+ 4 \int \text{d}y \text{ Re} \langle \psi|(\Pi_v h.)(y)R(h_K.(y) - \cdot h.)(y)\psi \rangle_{L^2}.
\]  
(4.10)

With Cauchy–Schwarz it follows that

\[
|\langle v|(H_{\text{pek}}^K - H_{\text{pek}}^K)v\rangle_{L^2}| \leq 4K^{1/2} \int \text{d}y \|R^{1/2}(h_K.(y) - \cdot h.)(y)P_\psi\|^2_{\text{op}} \\
+ 4K^{-1/2} \int \text{d}y \left(\|R^{1/2}(\Pi_v h_K.)(y)P_\psi\|^2_{\text{op}} + \|R^{1/2}(\Pi_v h.)(y)P_\psi\|^2_{\text{op}}\right),
\]  
(4.11)

and from Corollary 3.9, we obtain

\[
|\langle v|(H_{\text{pek}}^K - H_{\text{pek}}^K)v\rangle_{L^2}| \leq CK^{-1/2}.
\]  
(4.12)

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

(iii) Here we use \(\text{Tr}_{\text{Ran}(\Pi_0)}(1 - H_{\text{pek}}^K) = 3\), write

\[
\text{Tr}_{\text{Ran}(\Pi_1)}(1 - H_{\text{pek}}^K) = \int \text{d}y \langle \psi|h_{\text{pek}}^K.\rangle(y)Rh_{\text{pek}}^K.\rangle(y)\psi \rangle_{L^2} = \int \text{d}y \|R^{1/2}h_{\text{pek}}^K.\rangle(y)P_\psi\|^2_{\text{op}}
\]  
(4.13)

and apply Corollary 3.9.

(iv) Since \(1 - H_{\text{pek}}^K = \Pi_0 + \Pi_1(1 - H_{\text{pek}}^K)\Pi_1 = \Pi_0 + 4T_K\), cf. (2.7a) and (2.7b), we can write

\[
\text{Tr}_{L^2}((-i\nabla)(1 - H_{\text{pek}}^K)(-i\nabla)) = \text{Tr}_{L^2}(\nabla \Pi_0 \nabla) + 4\text{Tr}_{L^2}(\nabla T_K \nabla).
\]  
(4.14)
Using the explicit form of $\Pi_0$, one shows that the first term is given by

$$\text{Tr}_{L^2}(\nabla \Pi_0 \nabla) = \frac{3}{3} \sum_{j=1}^{\infty} \text{Tr}_{L^2}(\nabla |\nabla_j \varphi \rangle \langle \nabla_j \varphi | \nabla) \leq \frac{3}{3} \| \Delta \varphi \|^2_{L^2},$$  \hspace{1cm} (4.15)

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

$$\text{Tr}_{L^2}(\nabla T_K \nabla) = \int dy \langle \psi | [\nabla, h_K^1(y)] R(\nabla, h_K^1(y)) \rangle \psi \rangle_{L^2}. \hspace{1cm} (4.16)$$

Using the Cauchy–Schwarz inequality and $\| \nabla \psi \|_{L^2} + \| R^{1/2} \|_{op} + \| R^{1/2} \nabla \|_{op} < \infty$, see Lemmas 3.6 and 3.7, we can estimate the last expression by

$$\int dy \| R^{1/2} [\nabla, h_K^1(y)] \psi \|_{L^2}^2 \leq C \int dy (\| h_K^1(y) \psi \|_{L^2}^2 + \| h_K^1(y) \nabla \psi \|_{L^2}^2) \leq C \int dy \| h_K^1(y) \psi \|_{L^2}^2 \leq C \| h_K^1 \|_{L^2}^2 = C K. \hspace{1cm} (4.17)$$

This completes the proof of the lemma.

Proof of Lemma 2.3. We recall that $H_K^{\text{Pek}} \upharpoonright \text{Ran}(\Pi_0) = 0$ and $T_K = \frac{1}{4} (H_K^{\text{Pek}} - \Pi_1)$, and set $S_K = \frac{1}{2} (\Pi_1 + H_K^{\text{Pek}})$. For $(u_n)_{n \in \mathbb{N}}$ an orthonormal basis of $\text{Ran}(\Pi_1)$, we further set $a_n = a(u_n)$ and use this to write the Bogoliubov Hamiltonian as

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

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

$$\mathbb{U}_K \mathbb{H}_K \mathbb{U}_K^\dagger = \sum_{n,m=1}^{\infty} \left( \langle u_n| (A_K S_K A_K + B_K S_K B_K + 4 A_K T_K B_K) u_m \rangle_{L^2} a_n^\dagger a_m^\dagger \\
+ \langle u_n| (A_K S_K B_K + A_K T_K A_K + B_K T_K B_K) \overline{u_m} \rangle_{L^2} a_n^\dagger a_m^\dagger + \text{h.c.} \right) \\
+ \text{Tr}_{\text{Ran}(\Pi_1)}(T_K + B_K S_K B_K + 2 A_K T_K B_K). \hspace{1cm} (4.19)$$

The statement of the lemma now follows from

$$\Pi_1(A_K S_K A_K + B_K S_K B_K + 4 A_K T_K B_K) \Pi_1 = \sqrt{H_K^{\text{Pek}}}, \hspace{1cm} (4.20a)$$

$$\Pi_1(A_K S_K B_K + A_K T_K A_K + B_K T_K B_K) \Pi_1 = 0 \hspace{1cm} (4.20b)$$

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

$\square$
Proof of Lemma 3.3. To bound $\|w_{P,y}^1\|_{L^2}^2$ we expand
\[
w_{P,y}^1 = \Pi_1(1 - e^{-y\nabla})(\varphi + i\xi_P) = \int_0^1 ds_1 \int_0^{s_1} ds_2 \Pi_1 e^{-s_2 y\nabla} (y\nabla)^2 \varphi + \frac{i}{\alpha^2 ML} \int_0^1 ds \Pi_1 e^{-s y\nabla} (y\nabla)(P\nabla)\varphi,
\]
(4.21)
where we used $\Pi_1(y\nabla)\varphi = 0$. Thus, since $\Delta \varphi \in L^2$, we easily arrive at
\[
\|w_{P,y}^1\|_{L^2}^2 \leq C \left( y^4 + \alpha^{-4} y^2 P^2 \right)
\]
(4.22)
for some constant $C > 0$, and with $|P| \leq \alpha c$ we obtain the stated estimated. The bound for $\|\tilde{w}_{P,y}^1\|_{L^2}^2$ follows from
\[
\|\tilde{w}_{P,y}^1\|_{L^2}^2 = \|\Theta K \text{Re}(w_{P,y}^1)\|_{L^2}^2 + \|\Theta K^{-1} \text{Im}(w_{P,y}^1)\|_{L^2}^2 \leq C \|w_{P,y}^1\|_{L^2}^2,
\]
(4.23)
where we used that $\Theta K$ is real-valued and satisfies
\[
0 < \beta \leq \Theta_K^2 \leq 1
\]
(4.24)
when restricted to $\text{Ran}(\Pi_1)$; see Lemma 2.2. To bound $\|w_{P,y}^0\|_{L^2}^2$ we use
\[
\|w_{P,y}^0\|_{L^2}^2 = \|w_{0,y}^0\|_{L^2}^2 + \|\Pi_0(1 - e^{-y\nabla})\xi_P\|_{L^2}^2,
\]
(4.25)
since $\varphi, \xi_P$ and $\Pi_0$ are all real-valued. Expanding $1 - e^{-y\nabla}$ as in (4.21), it is easy to conclude that $\|\Pi_0(1 - e^{-y\nabla})\xi_P\|_{L^2}^2 \leq CP^2 y^2 \alpha^{-4}$. Using the explicit form of $\Pi_0$ and $\langle \nabla \varphi | \varphi \rangle_{L^2} = 0$, we can write
\[
\|w_{0,y}^0\|_{L^2}^2 = \frac{3}{\|\nabla \varphi\|_{L^2}^2} \sum_{i=1}^3 |\langle \nabla_i \varphi | e^{-y\nabla} \varphi \rangle_{L^2}|^2.
\]
(4.26)
Using the Fourier representation and rotation invariance, we have
\[
|\langle \nabla_i \varphi | e^{-y\nabla} \varphi \rangle_{L^2}| = \left| \int p_i |\hat{\varphi}(p)|^2 \sin(py) \, dy \right|.
\]
(4.27)
By the elementary inequality $|\sin z - z| \leq C z^3$, the formula $\|(y\nabla)\varphi\|_{L^2}^2 = 2\lambda y^2$ and the finiteness of $\|\Delta \varphi\|_{L^2}$, we conclude that
\[
\|w_{P,y}^0\|_{L^2}^2 - 2\lambda y^2 \leq C \left( y^4 + y^6 + \alpha^{-4} y^2 P^2 \right).
\]
(4.28)
To prove the last bound, we use
\[
\|\tilde{w}_{P,y}\|_{L^2}^2 = \|w_{P,y}^0\|_{L^2}^2 + \|\Theta K \text{Re}(w_{P,y}^1)\|_{L^2}^2 + \|\Theta K^{-1} \text{Im}(w_{P,y}^1)\|_{L^2}^2,
\]
(4.29)
and hence with (4.24),
\[
\beta \|\tilde{w}_{P,y}\|_{L^2}^2 \leq \|\tilde{w}_{P,y}\|_{L^2}^2 - \|w_{P,y}\|_{L^2}^2 \leq \beta^{-1} \|w_{P,y}\|_{L^2}^2.
\]
(4.30)

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

**Proof of Lemma 3.4.** From Lemma 3.3, we have
\[
\|\tilde{w}_{P,y}\|_{L^2}^2 - 2\lambda y^2 \leq C(\alpha^{-2}y^2 + y^4 + y^6) \leq C\frac{y^2}{\alpha} \quad \text{for all } \frac{|P|}{\alpha} \leq c, \ y^2 \leq \alpha^{-1}.
\]
(4.31)

Hence there is a constant \(\mu > 0\) such that for all \(y^2 \leq \alpha^{-1}\) the weight function (3.33) satisfies
\[
\begin{align*}
n_{\delta,\eta}(y) & \leq \exp(-\lambda \eta \alpha^{2(1-\delta)} - \mu \alpha^{-2\delta+1}y^2) \quad (4.32a) \\
n_{\delta,\eta}(y) & \geq \exp(-\lambda \eta \alpha^{2(1-\delta)} + \mu \alpha^{-2\delta+1}y^2). \quad (4.32b)
\end{align*}
\]

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
\[
\int dy f_n(y)Z(y) = \int_{B_\alpha} dy f_n(y)Z(y) + \int_{B_\alpha^c} dy f_n(y)Z(y)
\]
(4.33)

with \(B_\alpha = \{y \in \mathbb{R}^3 : y^2 \leq \alpha^{-1}\}\). The bounds (4.32a) and (4.32b) imply that
\[
|Z(y)| \leq e^{-\lambda \eta \alpha^{2(1-\delta)}} \left(e^{\mu \alpha^{-2\delta+1}y^2} - 1\right) \quad \forall y \in B_\alpha
\]
(4.34)

and thus by \(|e^z - 1| \leq z e^z\) for \(z > 0\), we obtain
\[
\int_{B_\alpha} dy f_n(y)Z(y) \leq \mu \alpha^{-2\delta+1} \int dy f_n(y)y^2 e^{-(\lambda \eta - \mu \alpha^{-1})\alpha^{2(1-\delta)}y^2}.
\]
(4.35)

The last expression is further bounded by
\[
\int dy f_n(y)y^2 e^{-(\lambda \eta - \mu \alpha^{-1})\alpha^{2(1-\delta)}y^2} \leq \|g\|_{L^{\infty}} \int dy |y|^{n+2} e^{-(\eta \alpha^{-1} - \mu \alpha^{-1})\alpha^{2(1-\delta)}y^2}
\]
\[
= \frac{C_n \|g\|_{L^{\infty}}}{\alpha^{4(n+1)(1-\delta)}/2}
\]
(4.36)

and since the resulting expression is uniformly bounded in \(\eta \geq \eta_0\) and \(\alpha\) large, we get
\[
\int_{B_\alpha} dy f_n(y)Z(y) \leq C_n \frac{\|g\|_{L^{\infty}}}{\alpha^{(4+n)(1-\delta)+\delta}}.
\]
(4.37)

To bound the second term in (4.33), we estimate
\[
\int_{B_\alpha^c} dy f_n(y)Z(y) \leq \int_{B_\alpha^c} dy f_n(y)n_{\delta,\eta}(y) + e^{-\lambda \eta \alpha^{-2\delta+1}} \int dy f_n(y).
\]
(4.38)
To see that the first summand is exponentially small as well, we use (4.29), (4.24) and $\text{Re}(w^i_{P,y}) = \Pi_i \text{Re}(w_{P,y}) = \Pi_i \text{Re}(w_{0,y})$ for $i = 0, 1,$

$$\|w_{P,y}\|_{L^2}^2 \geq \|\text{Re}(w^0_{P,y})\|_{L^2}^2 + \beta \|\text{Re}(w^1_{P,y})\|_{L^2}^2 \geq \beta \|\text{Re}(w_{0,y})\|_{L^2}^2 = \beta \|(1 - e^{-y\nabla})\varphi\|_{L^2}^2,$$

and hence

$$n_{\delta,\eta}(y) \leq \exp\left(-\eta\beta\alpha^{2(1-\delta)}q(y)\right) \quad \text{with} \quad q(y) = \frac{1}{2} \|(1 - e^{-y\nabla})\varphi\|_{L^2}^2. \hspace{1cm} (4.40)$$

Since $\varphi$ 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

$$q(y) = \| \varphi \|_{L^2}^2 - (\varphi * \varphi)(y). \hspace{1cm} (4.41)$$

Recall that, as shown in [32], the electronic Pekar minimizer $\psi$ is radial and non-increasing and hence $\varphi$, cf. (1.14), is radial and non-increasing as well, as convolutions of radial non-increasing functions are themselves radial non-increasing functions. Consequently, $q(y)$ is radial and monotone non-decreasing, and thus $q(y) \geq q(y')$ for all $y \in B^c_\alpha$, $y' \in B_\alpha$. On the other hand, by a simple computation, using the regularity of $\varphi$, one finds that $q(y) \geq C_0 y^2$ for some $C_0 > 0$ and all $|y|$ small enough, and thus $q(y) \geq C_0 \alpha^{-1}$ for all $y \in B^c_\alpha$ and $\alpha$ large. Therefore

$$\int_{B^c_\alpha^c} dy \, f_n(y) n_{\delta,\eta}(y) \leq \int_{B^c_\alpha^c} dy \, f_n(y) e^{-\eta\beta\alpha^{2(1-\delta)}q(y)}$$

$$\leq e^{-C_0\eta\beta\alpha^{2(1-\delta)-1}} \int dy \, f_n(y) \leq e^{-d\alpha^{-2+1}} \int dy \, f_n(y) \hspace{1cm} (4.42)$$

for some $d > 0$, which completes the proof of the lemma. \hspace{1cm} $\Box$

**Proof of Lemma 3.14.** Let $p = -i\nabla$. By a straightforward computation using the transformation property (2.11), we arrive at

$$\text{Tr}_{L^2}[B_K p B_K] = \sum_n a^\dagger(A_K a_n) a^\dagger(B_K p a_n) \Omega + \text{Tr}_{L^2}(B_K p B_K)\Omega \hspace{1cm} (4.43)$$

for some orthonormal basis $(a_n)_{n \in \mathbb{N}}$ of $L^2(\mathbb{R}^3)$. That $B_K p B_K$ is trace-class can be seen via

$$\text{Tr}_{L^2}[B_K p B_K] \leq \|B_K\|_{\text{HS}} \|pB_K\|_{\text{HS}} \leq C K, \hspace{1cm} (4.44)$$

where the second step follows from Lemma 2.2, implying $\|B_K\|_{\text{HS}} \leq C$, and

$$\|pB_K\|_{\text{HS}}^2 = \text{Tr}_{L^2}(pB_K pB_K) \leq \text{Tr}_{L^2}(p(1 - H^\text{Pek}_K) p) \leq C K. \hspace{1cm} (4.45)$$

By rotation invariance $\text{Tr}_{L^2}(B_K p B_K) = 0$. The first term in (4.43), on the other hand, is seen
to be a two-particle wave function $\Phi_K$ given by

$$\Phi_K(x, y) = \frac{1}{\sqrt{2}} (A_K p B_K + B_K p A_K)(x, y).$$

Thus

$$\langle \Upsilon_K | (P_f)^2 \Upsilon_K \rangle_F = \frac{1}{2} \| A_K p B_K + B_K p A_K \|_{HS}^2 \leq 2 \| A_K \|_{op}^2 \| p B_K \|_{HS}^2 \leq CK, \quad (4.47)$$

where we invoked again (4.45).

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