Ubiquity of bound states for the strongly coupled polaron

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Abstract

We study the spectrum of the Fröhlich Hamiltonian for the polaron at fixed total momentum. We prove the existence of excited eigenvalues between the ground state energy and the essential spectrum at strong coupling. In fact, our main result shows that the number of excited energy bands diverges in the strong coupling limit. To prove this we derive upper bounds for the min-max values of the corresponding fiber Hamiltonians and compare them with the bottom of the essential spectrum, a lower bound on which was recently obtained in [1]. The upper bounds are given in terms of the ground state energy band shifted by momentum-independent excitation energies determined by an effective Hamiltonian of Bogoliubov-type.

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1 Introduction and Main Result

In this article we study the energy-momentum spectrum of the strongly coupled Fröhlich polaron. The Fröhlich polaron is a translation invariant model for a charged particle interacting with a polar crystal that is described by a continuous non-relativistic quantum field. A particular feature of this model is the assumption that the excitations of the quantum field have a constant dispersion.

The energy-momentum spectrum is defined as the energy spectrum as a function of the conserved total momentum. For the Fröhlich polaron, the essential part of the energy spectrum does not depend on the momentum. For all momenta $P$, it is given by the interval $[E_\alpha(0) + \alpha^{-2}, \infty)$ where $E_\alpha(0)$ is the ground state energy at $P = 0$ and $\alpha > 0$ denotes the coupling constant [9, 20]. Moreover, for a certain range of momenta around zero the ground state energy lies strictly below the essential spectrum [7, 18, 19, 22, 27]. These observations naturally pose the question if further bound states exist between the ground state energy and the bottom of the essential spectrum. The aim of this work is to prove that such bound states do exist for large enough values of $\alpha$. In fact, our result shows that the number of energy bands below the essential spectrum diverges in the limit of strong coupling. To our knowledge, this is the first result about the existence of excited bound states for the polaron. In numerical investigations of the problem [16], they have so far not been seen, which may be due to the necessary restriction to relatively small $\alpha$.

From a technical point of view, our analysis can be viewed as an extension of [18] where we gave an upper bound on the ground state energy as a function of the total momentum. A crucial ingredient in our proof is the lower bound on the absolute ground state energy $E_\alpha(0)$ recently obtained in [1], which implies a corresponding lower bound on the edge of the essential spectrum.
The Hilbert space of the polaron is
\[ \mathcal{H} = L^2(\mathbb{R}^3, dx) \otimes \mathcal{F} \] (1.1)
with \( \mathcal{F} \) the bosonic Fock space over \( L^2(\mathbb{R}^3) \), and the Fröhlich Hamiltonian reads
\[ H_\alpha = -\Delta_x + \alpha^{-2}N + \alpha^{-1}\phi(h_x), \] (1.2)
where \(-\Delta_x = (-i\nabla_x)^2\), with \( x \in \mathbb{R}^3 \) and \(-i\nabla_x \) the position and momentum of the electron, and \( N = \int a_y^\dagger a_y \, dy \) the number operator on Fock space. The interaction between the electron and the quantum field is described by the linear field operator
\[ \phi(h_x) = a^\dagger(h_x) + a(h_x) = \int h_x(y) (a_y^\dagger + a_y) \, dy \] (1.3)
with \( x \)-dependent form factor
\[ h_x(y) = -\frac{1}{2\pi^2|x-y|^2}. \] (1.4)
The creation and annihilation operators satisfy the bosonic canonical commutation relations
\[ [a(f), a^\dagger(g)] = \langle f|g\rangle_{L^2}, \quad [a(f), a(g)] = 0 \] (1.5)
and we shall adopt the usual notation \( a(f) = \int dy f(y) a_y \).

After setting \( \hbar = 1 \) and \( m_e = 1/2 \) (the mass of the electron) the polaron model depends on a single dimensionless parameter \( \alpha > 0 \). By rescaling all lengths by a factor \( 1/\alpha \), the operator \( \alpha^2 H_\alpha \) is unitarily equivalent to the Hamiltonian \( H_\alpha^{\text{Pol}} = -\Delta_x + N + \sqrt{\alpha}\phi(h_x) \) which is more common in the physics literature. Let us further note that (1.2) is to be understood in the sense of quadratic forms, since \( h_x \notin L^2(\mathbb{R}^3) \). Since \((1 + |\cdot|)^{-1}h_x \in L^2(\mathbb{R}^3)\) the quadratic form is bounded from below [14, 15].

An important property of the Fröhlich Hamiltonian is that it commutes with the total momentum operator, \( [H_\alpha, -i\nabla_x + P_f] = 0 \), where
\[ P_f = \int dy a_y^\dagger (-\nabla_y) a_y \] (1.6)
denotes the momentum operator of the phonons. It follows that the total momentum and the energy are simultaneously diagonalizable, which is best implemented by the Lee–Low–Pines [11] transformation \( S : \mathcal{H} \to \mathcal{F}, S = F \circ e^{iP_f x} \) where \( F \) indicates the Fourier transformation w.r.t. the electron coordinate. A straightforward computation reveals that \( S(-i\nabla_x + P_f)S^\dagger = \int_{\mathbb{R}^3} P \, dP \) and \( SH_\alpha S^\dagger = \int_{\mathbb{R}^3} H_\alpha(P) \, dP \) with fiber Hamiltonians
\[ H_\alpha(P) = (P_f - P)^2 + \alpha^{-2}N + \alpha^{-1}\phi(h_0). \] (1.7)
The operator $H_\alpha(P)$ acts on the Fock space $\mathcal{F}$ and describes the system at total momentum $P \in \mathbb{R}^3$. Using this fiber decomposition we can introduce the energy-momentum spectrum

$$\Sigma_\alpha := \{(E,P) \in \mathbb{R} \times \mathbb{R}^3 \mid E \in \sigma(H_\alpha(P))\}.$$  

(1.8)

By rotation invariance of the Hamiltonian, we have $(E,P) \in \Sigma_\alpha \Leftrightarrow (E,RP) \in \Sigma_\alpha$ for every $R \in O(3)$. The function $P \mapsto E_\alpha(P) := \inf \sigma(H_\alpha(P))$ is called the energy-momentum relation or ground state energy band. It has a unique global minimum at $P = 0$ [9, 22], thus in particular $E_\alpha(0) = \inf \sigma(H_\alpha)$. It is known that $E_\alpha(P)$ is strictly increasing below the essential spectrum [22] and that the set $\{P : E_\alpha(P) < \inf \sigma_{\text{ess}}(H_\alpha(P))\}$ is non-empty [7, 18, 19, 22, 27]. Moreover, by a Perron–Frobenius type argument the ground state of $H_\alpha$, if it exists, is non-degenerate [19]. In this work we are interested in the existence of other discrete eigenvalues in $\Sigma_\alpha$. As already mentioned, the essential spectrum of $H_\alpha(P)$ is known to be $P$-independent and continuous. For regular polaron models (for instance the Fröhlich Hamiltonian with UV cutoff) the precise location of the essential spectrum has been studied via the HVZ theorem in [20] (see also [7]). This can be extended to the Fröhlich Hamiltonian via a suitable approximation argument [8]. Combining both results, one can prove the following statement [9].

**Lemma 1.1.** For every $\alpha > 0$ and $P \in \mathbb{R}^3$ the essential spectrum of $H_\alpha(P)$ is given by

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

(1.9)

Before we continue with the main result, let us define the critical momentum (at strong-coupling)

$$P_c(\alpha) := \sqrt{2M_{LP}\alpha}$$

(1.10)

where $M_{LP} = \frac{2}{3}||\nabla \phi||_2^2$ is the ($\alpha$-independent) semi-classical effective mass [6, 10] (the classical field $\phi$ is defined in (2.5)). The momentum $P_c(\alpha)$ separates the ground state energy band $P \mapsto E_\alpha(P)$ for large $\alpha$ into two different regimes. On one side, there is the quasi-particle regime $|P| \lesssim P_c(\alpha)$ where $E_\alpha(P)$ is approximately a quadratic function of $P$ and on the other side, the radiation regime $|P| \gtrsim P_c(\alpha)$ where $E_\alpha(P)$ is expected to coincide with the bottom of the essential spectrum; see Figure 1.1 for a sketch of $E_\alpha(P)$. This picture has been mathematically substantiated in recent works [1, 2, 18].

In the present work we shall focus on the quasi-particle regime. Our main result states that the number of energy bands below the essential spectrum diverges in the limit $\alpha \to \infty$.

**Theorem 1.2.** Let $g : [0, \infty) \to [0, \infty)$ be a function with $\lim_{x \to \infty} g(x) = 0$. For all $|P| \leq g(\alpha)P_c(\alpha)$, we have $|\sigma_{\text{disc}}(H_\alpha(P))| \to \infty$ as $\alpha \to \infty$, where $\sigma_{\text{disc}}(H_\alpha(P))$ is the discrete spectrum of $H_\alpha(P)$.

We are not aware of any previous result about the existence of excited bound states or energy bands for the polaron. A complementary result, however, was recently obtained in
[24], proving the absence of excited eigenvalues at $P = 0$ for sufficiently weak coupling. (In a similarly fashion [3] showed that for sufficiently weak coupling and small momentum, there are at most two eigenvalues below the essential spectrum). This suggests, somewhat analogous to the case of Schrödinger operators with a binding potential, that the number of eigenvalues below the essential spectrum is an increasing function of the coupling constant.

To prove Theorem 1.2 we derive upper bounds for the min-max values of $H_\alpha(P)$ and show that for large $\alpha$ they lie strictly below the essential spectrum. By the min-max principle, this implies that the min-max values correspond to eigenvalues of $H_\alpha(P)$. To compare the upper bounds for the min-max values with $\inf \sigma_{\text{ess}}(H_\alpha(P))$, we will use Lemma 1.1 and a recently obtained two-term lower bound for $E_\alpha(0)$ [1]. More concretely, our upper bounds are given in terms of the ground state energy band at large coupling shifted by momentum-independent excitation energies. For $|P| \lesssim P_c(\alpha)$ and $\alpha \to \infty$, the ground state energy band is a quadratic function whose coefficients are determined by the semi-classical approximation [2, 18]. While the leading term in $E_\alpha(P)$ is of order one, the excitation energies are proportional to $\alpha^{-2}$, hence they are comparable to the energy of a free phonon which characterizes the bottom of the essential spectrum. In fact the excitation energies correspond to excitations of the quantum field around its classical value and they are explicitly determined by the eigenvalues of a quadratic Bogoliubov-type Hamiltonian.

A qualitative picture of the bounds for the min-max values is shown in Figure 1.1. The precise statement and its proof require a certain amount of preparations. In the next section we recall the semi-classical theory of the polaron and define the Bogoliubov Hamiltonian that describes the fluctuations of the quantum field. In Section 2.3 we state the upper bounds for the min-max values, which are then used to prove Theorem 1.2. The more technical part concerning the derivation of the upper bounds is postponed to Section 3.

Figure 1.1: Schematic plot of the ground state energy band $P \mapsto E_\alpha(P)$ (lowest curve) and upper bounds for the excited energy bands (dashed curves). The horizontal line represents the bottom of the essential spectrum and the vertical lines indicate the critical momentum $P_c(\alpha) = \sqrt{2/M_{\text{LV}}} \alpha$ that separates the parabolic quasi-particle regime from the flat radiation regime. In the limit $\alpha \to \infty$ the eigenvalues accumulate at the edge of the essential spectrum for all $|P| \ll P_c(\alpha)$. 

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2 Upper Bounds for the Min-Max Values

2.1 Pekar functionals and Bogoliubov Hamiltonian

The semi-classical theory of the polaron [21] arises naturally in the context of strong coupling and corresponds to minimizing the Fröhlich Hamiltonian over product states of the form
\[ \Psi_{u,v} = u \otimes e^{a(\alpha)v - a(\alpha)} \Omega, \]
where \( u \in H^1(\mathbb{R}^3) \) is a normalized electron wave function, \( \Omega = (1, 0, 0, \ldots) \) the Fock space vacuum and \( e^{a(\alpha)v - a(\alpha)} \Omega \) the coherent state associated with the classical field \( v \in L^2(\mathbb{R}^3) \). A simple computation leads to the Pekar energy
\[ G(u, v) = \frac{\langle \Psi_{u,v} | H_\alpha | \Psi_{u,v} \rangle_{\mathcal{H}}}{\langle \Psi_{u,v} | \Psi_{u,v} \rangle_{\mathcal{H}}} = \langle u | (-\Delta + V^v) u \rangle_{L^2} + \| v \|_{L^2}^2 \]  
where the polarization potential is given by
\[ V^v(x) = 2 \text{Re} \langle v | h_x \rangle_{L^2} = -\text{Re} \int \frac{v(y)}{\pi^2 |x - y|^2} dy. \]  
Minimizing over the field variable one obtains the Pekar functional for the electron
\[ E = \inf_{v \in L^2} G(u, v) = \int |\nabla u(x)|^2 dx - \frac{1}{4\pi} \iint \frac{|u(x)|^2 |u(y)|^2}{|x - y|} dxdy, \]  
which is known [13] to admit a unique rotation invariant minimizer \( \psi \geq 0 \) (the minimizer is unique up to translations and multiplication by a constant phase). Alternatively, one can minimize \( G \) w.r.t. the electron wave function first. This leads to the Pekar functional for the classical field
\[ F(v) = \inf_{\| u \|_{L^2} = 1} G(u, v) = \inf \sigma(-\Delta + V^v) + \| v \|_{L^2}^2 \]  
where \( \inf \sigma(-\Delta + V^v) \) is the ground state energy of the Schrödinger operator \(-\Delta + V^v\) acting on \( L^2(\mathbb{R}^3) \). The unique rotation invariant minimizer of \( F(v) \) is given by
\[ \varphi(z) = -\langle \psi | h_z \psi \rangle_{L^2} = \int \frac{|\psi(y)|^2}{2\pi^2 |z - y|^2} dy. \]  
Note that \( \psi \) and \( \varphi \) are both real-valued (in fact positive) functions.

The semi-classical ground state energy is called the Pekar energy
\[ e^{\text{Pek}} = \mathcal{E}(\psi) = \mathcal{F}(\varphi), \quad e^{\text{Pek}} \leq 0, \]  
and by the variational principle \( \inf \sigma(H_\alpha) \leq e^{\text{Pek}} \). The mathematical validity of Pekar’s ansatz was verified by Donsker and Varadhan [4] who proved that \( \lim_{\alpha \to \infty} \inf \sigma(H_\alpha) = e^{\text{Pek}} \) and by Lieb and Thomas [14] who quantified the error by showing that \( \inf \sigma(H_\alpha) \geq e^{\text{Pek}} + O(\alpha^{-1/5}) \).
For the potential $V^\varphi$ we consider the Schrödinger operator for the electron

$$h^\text{Pek} = -\Delta + V^\varphi - \lambda^\text{Pek}, \quad \lambda^\text{Pek} = \inf \sigma(-\Delta + V^\varphi),$$

with $\psi > 0$ the unique ground state of $h^\text{Pek}$ and $\lambda^\text{Pek} = e^\text{Pek} - \|\varphi\|_{L^2}^2$. It follows from general arguments for Schrödinger operators that $h^\text{Pek}$ has a finite spectral gap above zero and thus the reduced resolvent

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

(2.8)
defines a bounded operator ($P_\psi$ denotes the orthogonal projection onto $\text{Span}\{\psi\}$). Note that $R$ has a real-valued kernel.

Next we introduce the operator $H^\text{Pek}: L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ with (real-valued) integral kernel

$$H^\text{Pek}(y, z) = \delta(y - z) - 4\langle \psi | h(y) R h(z) \psi \rangle_{L^2},$$

(2.9)

which arises as the Hessian of the energy functional (2.4) at its minimizer $\varphi$ (see [5, 6, 18]). The following lemma was proved in [18, Lemma 2.1].

**Lemma 2.1.** The operator $H^\text{Pek}$ satisfies the following properties.

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

(ii) $\text{Ker} H^\text{Pek} = \text{Span}\{\partial_i \varphi : i = 1, 2, 3\}$ with $\varphi \in H^1(\mathbb{R}^3)$ defined in (2.5)

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

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

Let $\Pi_0$ and $\Pi_1$ be the orthogonal projections defined by

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

(2.10)

The decomposition $L^2(\mathbb{R}^3) = \text{Ran} (\Pi_0) \oplus \text{Ran} (\Pi_1)$ implies the factorization

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

(2.11)

Through the isomorphisms

$$\mathcal{F}_0 \cong \text{Span}\{(a^\dagger (\partial_1 \varphi))^j_1 (a^\dagger (\partial_2 \varphi))^j_2 (a^\dagger (\partial_3 \varphi))^j_3 \Omega \mid (j_1, j_2, j_3) \in \mathbb{N}_0^3 \} \subset \mathcal{F}$$

(2.12a)

$$\mathcal{F}_1 \cong \text{Ker}(a(\partial_1 \varphi)) \cap \text{Ker}(a(\partial_2 \varphi)) \cap \text{Ker}(a(\partial_3 \varphi)) \subset \mathcal{F}$$

(2.12b)

one can view $\mathcal{F}_0$ and $\mathcal{F}_1$ also as subspaces of $\mathcal{F}$.

The Bogoliubov Hamiltonian describing the fluctuations of the quantum field acts non-trivially only in $\mathcal{F}_1$. For a simple notation, however, we define it directly as an operator on
the full Fock space \( \mathcal{F} \). Moreover, for technical reasons, we need to introduce the Bogoliubov Hamiltonian \( \mathbb{H}_K \) with a momentum cutoff \( K \in (0, \infty] \). More concretely we set

\[
\mathbb{H}_K = 1_{\mathcal{F}_0} \otimes \hat{\mathbb{H}}_K
\]  

(2.13)

with the non-trivial part \( \hat{\mathbb{H}}_K : \mathcal{F}_1 \to \mathcal{F}_1 \) defined by

\[
\hat{\mathbb{H}}_K = N_1 - \langle \psi | \phi(h_{K,x}^1)R\phi(h_{K,x}^1)\psi \rangle_{L^2} \quad \text{with} \quad N_1 = \int dydz \Pi_1(y, z)a_y^\dagger a_z^\dagger.
\]  

(2.14)

where \( N_1 \) corresponds to the number operator in \( \mathcal{F}_1 \) and the new form factor is defined by\(^1\)

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

(2.15)

Note that the second term in \( \mathbb{H}_K \) defines the quadratic operator

\[
\langle \psi | \phi(h_{K,x}^1)R\phi(h_{K,x}^1)\psi \rangle_{L^2} = \int dydz \langle \psi | (h_{K,x}^1(y)R(h_{K,x}^1)(z))\psi \rangle_{L^2} (a_y^\dagger + a_y)(a_z^\dagger + a_z).
\]  

(2.16)

In Lemma 2.3 below we shall show that \( \mathbb{H}_K \) is bounded from below and diagonalizable by a unitary Bogoliubov transformation. For the precise statement, we need to introduce the operator \( H_{\text{Pek}}(K) \), \( K \in (0, \infty] \), defined by

\[
H_{\text{Pek}}(K) | \text{Ran}(\Pi_0) = 0, \quad H_{\text{Pek}}(K) | \text{Ran}(\Pi_1) = \Pi_1 - 4T_K
\]  

(2.17)

where the \( \Pi_i \) are given by (2.10) (note that they do not depend on \( K \)) and \( T_K \) is defined by the integral kernel

\[
T_K(y, z) = \langle \psi | h_{K,x}^1(y)Rh_{K,x}(z)\psi \rangle_{L^2}.
\]  

(2.18)

Since \( H_{\text{Pek}}\Pi_1 = \Pi_1 - 4T_{\infty} \) it follows that \( H_{\text{Pek}} = H_{\text{Pek}}^{\infty} \). With \( \Theta_K = (H_{\text{Pek}}^{\infty})^{1/4} \) we further consider \( A_K, B_K : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3) \) given by

\[
A_K | \text{Ran}(\Pi_0) = \Pi_0, \quad B_K | \text{Ran}(\Pi_0) = 0, \quad A_K | \text{Ran}(\Pi_1) = \frac{\Theta_{K}^{-1} + \Theta_K}{2}, \quad B_K | \text{Ran}(\Pi_1) = \frac{\Theta_{K}^{-1} - \Theta_K}{2}.
\]  

(2.19a, b)

The next lemma, whose proof is given in Section 4, collects useful properties of these operators.

\(^{1}\)Our definition of \( \mathbb{H}_K \) is different from the Bogoliubov Hamiltonian used in [12, 17] to describe the effective dynamics of the polaron. On the one hand, we have the cutoff \( K \), which is needed for technical reasons in the proof. On the other hand, more importantly, there is the additional restriction to \( \mathcal{F}_1 \), which is related to the fact that we study the spectrum of the fiber Hamiltonian \( H_\alpha(P) \).
Lemma 2.2. For $K_0$ large enough and $K \in (K_0, \infty]$ let $H_{Pek}^K : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ be defined by (2.17). There exist constants $\beta \in (0, 1)$ and $C > 0$ such that for all $K \in (K_0, \infty]$

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

(ii) $(B_K)^2 \leq C(1 - H_{Pek}^K)$

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

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

(v) $|\sigma_{\text{disc}}(H_{Pek}^K) \cap [0, 1]| = \infty$ with only accumulation point at one.

Let $(\lambda_K^{(n)})_{n \in \mathbb{N}} \subset (0, 1)$ be the non-zero eigenvalues of $H_{Pek}^K$ below one (numbered increasingly counting multiplicity) and denote the corresponding normalized eigenfunctions $u_K^{(n)} \in \text{Ran}(\Pi_1)$. Then

(vi) $|\lambda_K^{(n)} - \lambda_\infty^{(n)}| \leq CK^{-1/2}$ for all $n \in \mathbb{N}, K \geq K_0$

(vii) $\|\nabla u_K^{(n)}\|_{L^2} \leq C\sqrt{K}(1 - \lambda_K^{(n)})^{-1/2}$ for all $n \in \mathbb{N}, K \geq K_0$.

Next we introduce the transformation

$$U_K a(f) U_K^\dagger = a(A_K f) + a^\dagger(B_K \overline{f})$$

for all $f \in L^2(\mathbb{R}^3)$ (2.20)

which, for $K$ large enough, defines a unitary operator $U_K : \mathcal{F} \to \mathcal{F}$. This follows from the Shale–Stinespring condition (see [23, 25, 26]) because $A_K$ is bounded and $B_K$ is Hilbert–Schmidt by Lemma 2.2. Note that $U_K$ acts as the identity in the first component in $\mathcal{F} = \mathcal{F}_0 \otimes \mathcal{F}_1$ and does not mix the two components.

Lemma 2.3. For $K \in (K_0, \infty]$ with $K_0$ large enough and $U_K$ defined by (2.20), we have

$$U_K \mathbb{H}_K U_K^\dagger = d\Gamma((H_{Pek}^K)^{1/2}) + \frac{1}{2} \text{Tr}_{L^2}((H_{Pek}^K)^{1/2} - 1) + \frac{3}{2}$$ (2.21a)

$$\inf \sigma(\mathbb{H}_K) = \frac{1}{2} \text{Tr}_{L^2}((H_{Pek}^K)^{1/2} - 1) + \frac{3}{2}$$ (2.21b)

The proof is obtained by an explicit computation; for details we refer to [18, Lemma 2.3]. From Lemma 2.2, we have $\inf \sigma(\mathbb{H}_K) > -\infty$. Note that by (2.13) the statement holds trivially also as an identity for operators on $\mathcal{F}_1$ if we replace $\mathbb{H}_K$ by $\mathbb{H}_K$ (and $U_K$ and $H_{Pek}^K$ by their restrictions to $\mathcal{F}_1$ and $\text{Ran}(\Pi_1)$).

From now on we shall always assume $K \geq K_0$ with $K_0$ large enough such that Lemmas 2.2 and 2.3 are applicable.
2.2 Excitation spectrum of the Bogoliubov Hamiltonian

To introduce the Bogoliubov spectrum we consider the operator $\tilde{H}_K : \mathcal{F}_1 \to \mathcal{F}_1$ for $K \in (K_0, \infty)$. We are interested in the excitation spectrum of $\tilde{H}_K$ below $\inf \sigma(\tilde{H}_K) + 1$. This part of the spectrum is purely discrete since it is given by the free bosonic excitation spectrum of particles with energies determined by the non-zero eigenvalues of $H^P_{ek}$. More concretely, one can write the excitation spectrum below one as

$$\sigma(\tilde{H}_K - \inf \sigma(\tilde{H}_K)) \cap [0, 1) = \bigcup_{n=0}^{\infty} \{ \Lambda^{(n)}_K \}$$

(2.22)

with the sequence of eigenvalues (counting multiplicities)

$$0 = \Lambda^{(0)}_K < \Lambda^{(1)}_K \leq \Lambda^{(2)}_K \leq \ldots < 1, \quad \Lambda^{(n)}_K = \sum_{j \in J^{(n)}_K} (\lambda^{(j)}_K)^{1/2}$$

(2.23)

where $J^{(n)}_K$ are suitable (finite) integer sets and $0 < \lambda^{(1)}_K \leq \lambda^{(2)}_K \leq \ldots < 1$ the sequence of non-zero eigenvalues of $H^P_{ek}$ below one, cf. Lemma 2.2. We shall write $\Lambda^{(n)}_K = \Lambda^{(n)}_\infty$ for $K = \infty$. The eigenvalues $(\Lambda^{(n)}_K)_{n \in \mathbb{N}_0}$ only accumulate at one and they satisfy

$$\Lambda^{(n)}_K \leq (\lambda^{(n)}_K)^{1/2} \quad \forall n \in \mathbb{N}.$$  

(2.24)

Generally $J^{(n)}_K$ is a subset of integers drawn from $\{1, \ldots, n\}$ with repetitions allowed. Since $\lambda^{(1)}_K \geq \beta > 0$ (with $\beta$ the constant from Lemma 2.2), the length of $J^{(n)}_K$ is bounded by

$$|J^{(n)}_K| \leq m \quad \text{with} \quad m := \left\lceil 1/\sqrt{\beta} \right\rceil = \min \{ j \in \mathbb{N} : j \geq 1/\sqrt{\beta} \}.$$  

(2.25)

We emphasize that $m$ does not depend on $K$ and $n$.

2.3 Upper bounds for the min–max values and proof of Theorem 1.2

We define the min-max values of $H_\alpha(P)$ by

$$\mu_n(H_\alpha(P)) = \inf_{V_{n+1} \subset \mathcal{Q}} \sup \left\{ \langle \Psi | H_\alpha(P) \Psi \rangle_x \mid \Psi \in V_{n+1}, \| \Psi \|_x = 1 \right\}, \quad n \in \mathbb{N}_0,$$  

(2.26)

where the infimum is taken over all $(n + 1)$-dimensional subspaces $V_{n+1} \subset \mathcal{Q}(H_\alpha(P))$ with $\mathcal{Q}(H_\alpha(P)) = \mathcal{Q}(P^2 + \mathbb{N})$ the form domain of $H_\alpha(P)$.

---

2For instance

$J^{(0)}_K = \emptyset$, $J^{(1)}_K = \{1\}$ and $J^{(2)}_K = \begin{cases} \{2\} & \text{if } \lambda^{(2)}_K < 2\lambda^{(1)}_K \smallskip \\ \{1, 1\} & \text{if } \lambda^{(2)}_K > 2\lambda^{(1)}_K. \end{cases}$
Theorem 2.4. Let $M^{LP} = \frac{2}{3}\|\nabla \varphi\|_{L^2}^2$ with $\varphi$ defined in (2.5), $e_{\text{Pek}}$ the Pekar energy (2.6) and $H_{\text{Pek}}$ defined by (2.9). Moreover let $(\Lambda^{(n)})_{n \in \mathbb{N}_0}$ be the sequence of eigenvalues introduced in (2.23) for $K = \infty$. For all $\varepsilon > 0$ and $n \in \mathbb{N}_0$ there exist constants $C(n, \varepsilon) > 0$ and $\alpha(n) \geq 1$ such that

$$\mu_n(H_\alpha(P)) \leq e_{\text{Pek}} + \frac{1}{\alpha^2} \left( \text{Tr}_{L^2}(\sqrt{H_{\text{Pek}}} - 1) + \Lambda^{(n)} \right) + \frac{P^2}{2\alpha^4 M^{LP}} + C(n, \varepsilon)\alpha^{-\frac{2}{3} + \varepsilon} \quad (2.27)$$

for all $P \in \mathbb{R}^3$ and $\alpha \geq \alpha(n)$.

Remark 2.1. For $n = 0$, since $E_\alpha(P) = \mu_0(H_\alpha(P))$ and $\Lambda^{(n)} = 0$, this coincides with [18, Theorem 2.1]. A compatible lower bound on $\mu_0(H_\alpha(P))$ was obtained in [2].

Remark 2.2. We expect that the min-max values $\mu_n(H_\alpha(P))$ are in fact asymptotically described, as $\alpha \to \infty$, by the r.h.s. in (2.27). In other words, that the excited energy bands are given by the ground state energy band $P \mapsto E_\alpha(P)$ shifted by the momentum-independent excitation energies $\Lambda^{(n)}$. The derivation of a compatible lower bound, however, seems out of reach with current methods.

Using Theorem 2.4 in combination with Lemma 1.1 and the lower bound for $E_\alpha(0)$ obtained in [1], we can prove our main result.

Proof of Theorem 1.2. By the min-max theorem the inequality $\mu_n(H_\alpha(P)) < \inf \sigma_{\text{ess}}(H_\alpha(P))$ implies that $\mu_n(H_\alpha(P))$ corresponds to the $(n + 1)$th discrete energy eigenvalue of $H_\alpha(P)$ when counted with multiplicity starting from the lowest eigenvalue.

The main result in [1] is the following lower bound for the ground state energy of (1.2)

$$\inf \sigma(H_\alpha) \geq e_{\text{Pek}} + \frac{1}{2\alpha^2} \text{Tr}_{L^2}(\sqrt{H_{\text{Pek}}} - 1) - \frac{1}{\alpha^{2+s}} \quad (2.28)$$

for all $0 < s < \frac{1}{30}$ and $\alpha \geq \alpha(s)$ for some constant $\alpha(s)$. Since $E_\alpha(0) = \inf \sigma(H_\alpha)$, we can combine (2.27) for $\varepsilon = \frac{7}{15}$ and (2.28) for $s = \frac{1}{30}$ to

$$\mu_n(H_\alpha(P)) \leq E_\alpha(0) + \frac{1}{\alpha^2} \Lambda^{(n)} + \frac{P^2}{2\alpha^4 M^{LP}} + C(n)\frac{1}{\alpha^{2+1/30}} \quad (2.29)$$

for all $\alpha \geq \alpha(n)$. Invoking Lemma 1.1 and (2.24) leads to

$$\mu_n(H_\alpha(P)) - \inf \sigma_{\text{ess}}(H_\alpha(P)) \leq \frac{1}{\alpha^2} \left( (\lambda^{(n)}_\infty)^{1/2} - 1 + \frac{P^2}{2\alpha^4 M^{LP}} + C(n)\frac{1}{\alpha^{1/30}} \right) \quad (2.30)$$

and thus by the min-max theorem

$$|\sigma_{\text{disc}}(H_\alpha(P))| \geq \sup \left\{ n + 1 \in \mathbb{N} : \frac{P^2}{2\alpha^4 M^{LP}} + C(n)\frac{1}{\alpha^{1/30}} < 1 - (\lambda^{(n)}_\infty)^{1/2} \right\}. \quad (2.31)$$
Since \( \lambda^{(n)} \xrightarrow{n \to \infty} 1 \) but \( \lambda^{(n)} < 1 \) for all \( n \in \mathbb{N} \) by Lemma 2.2, the r.h.s. of (\*) is always larger than some small \( \delta(n) > 0 \). On the l.h.s. the second term is smaller than \( \delta(n)/4 \) for \( \alpha \geq \alpha(n) \) with \( \alpha(n) \) sufficiently large. For \( |P| \leq g(\alpha)\sqrt{2M^{Lp}} \alpha \) with \( g(\alpha) \xrightarrow{\alpha \to \infty} 0 \), also the first term is smaller than \( \delta(n)/4 \) for \( \alpha \geq \alpha(n) \) with \( \alpha(n) \) large enough. This implies the statement of Theorem 1.2. \( \square \)

In the next section we prove Theorem 2.4. To this end we first introduce a suitable family of trial subspaces and state the corresponding variational estimates in Proposition 2.5. The proof of Theorem 2.4 is obtained as a corollary of Proposition 2.5.

### 2.4 Variational estimates and proof of Theorem 2.4

To estimate the min-max values, we need to introduce a suitable family of trial subspaces. We first define the linear operator \( \mathcal{S}_P : \mathcal{F} \to \mathcal{F} \), for \( P \in \mathbb{R}^3 \), given by

\[
\Gamma \mapsto \mathcal{S}_P \Gamma = \int dx \, e^{i(P - P) x} \, e^{i(\alpha(\varphi_P - a(\alpha \varphi_P))}(\mathcal{G}^0(x) - \frac{1}{\alpha^2} \mathcal{G}^1(x))) \Gamma,
\]

where

\[
\varphi_P = \varphi + \xi_P \quad \text{with} \quad \xi_P = \frac{i}{\alpha^2 M^{Lp}} (P \nabla) \varphi, \quad M^{Lp} = \frac{2}{3} ||\nabla \varphi||_{L^2}^2,
\]

and

\[
\mathcal{G}^0(x) = \psi(x), \quad \mathcal{G}^1(x) = u_\alpha(x) (R \phi(h_{K,1}^1 \psi)(x)
\]

with form factor \( h_{K,1}^1 \) defined in (2.15), and \( u_\alpha : \mathbb{R}^3 \to [0,1] \) a radial function satisfying

\[
u_\alpha(x) = \begin{cases} 1 & \forall \ |x| \leq \alpha \\ 0 & \forall \ |x| \geq 2\alpha \end{cases} \quad \text{and} \quad ||\nabla u_\alpha||_{L^\infty} + ||\Delta u_\alpha||_{L^\infty} \leq C \alpha^{-1}
\]

for some constant \( C > 0 \). For completeness, we recall that \( \psi > 0 \) and \( \varphi > 0 \) are the unique rotation invariant minimizers of the Pekar functionals (2.3) and (2.4), respectively. The operator \( \mathcal{S}_P \) depends of course also on \( \alpha, K \) and \( u_\alpha \), but we omit this in our notation.

**Remark 2.3.** Note that \( \mathcal{G}(x) \Gamma \) are elements of \( L^2(\mathbb{R}^3, \mathcal{F}) \) and

\[
(R \phi(h_{K,1}^1 \psi)(x) = \int dz dy \, R(x, y) h_{K,1}^1(z) \psi(y) \, (a^\dagger_z + a_z)
\]

defines an \( x \)-dependent Fock space operator. Via \( L^2(\mathbb{R}^3, \mathcal{F}) \cong \mathcal{H} \), we can view these states also as elements in \( \mathcal{H} \). In this case we shall use the notation

\[
\mathcal{G}^0 = \psi \otimes \Gamma, \quad \mathcal{G}^1 = u_\alpha R \phi(h_{K,1}^1) \psi \otimes \Gamma.
\]

(2.37)
Proposition 2.5.

Let $\Gamma$ sequence of integer sets defined by (2.23). Since $H_{\text{Pek}}$ corresponds to non-zero eigenvalues below one are denoted by $\alpha_{K}^{(n)} \in \text{Ran}(\Pi_{1})$, $n \in \mathbb{N}$, cf. Lemma 2.2. We define

$$
\Gamma_{K}^{(n)} = \bigcup_{K} \gamma_{K}^{(n)} \text{ with } \gamma_{K}^{(n)} = \prod_{j \in K^{(n)}} a^{\dagger}(u_{K}^{(j)})\Omega, \quad n \in \mathbb{N}_{0}
$$

(2.38)

where $\Omega \in \mathcal{F}$ is the Fock space vacuum, $U_{K}$ the unitary operator (2.20) and $(J_{K}^{(n)})_{n \in \mathbb{N}_{0}}$ the sequence of integer sets defined by (2.23). Since $J_{K}^{(0)} = \emptyset$, $\gamma_{K}^{(0)} = \Omega$. For $n \geq 1$, we have $|J_{K}^{(n)}| \leq m$ and $u_{K}^{(n)} \in \text{Ran}(\Pi_{1})$, and thus

$$
\gamma_{K}^{(n)} \in \mathcal{F}_{1}^{(\leq m)} \forall n, K \text{ with } \mathcal{F}_{1}^{(\leq m)} := \mathcal{F}_{1} \cap \mathcal{F}^{(\leq m)} \subset \mathcal{F},
$$

(2.39)

where $\mathcal{F}_{1} \subset \mathcal{F}$ was introduced in (2.11) and $\mathcal{F}^{(\leq m)}$ denotes the truncated Fock space

$$
\mathcal{F}^{(\leq m)} = \bigoplus_{j=0}^{m} \mathcal{F}^{(j)}, \quad \mathcal{F}^{(j)} = L^{2}(\mathbb{R}^{3}) \otimes \mathbb{C}^{j}.
$$

(2.40)

Let us now consider the linear subspace

$$
\mathcal{V}_{K}^{(n+1)} = \text{Span}\{\Gamma_{K}^{(0)}, \ldots, \Gamma_{K}^{(n)}\} \subset \mathcal{F}_{1}.
$$

(2.41)

With $\langle \Gamma_{K}^{(i)}|\Gamma_{K}^{(j)}\rangle_{\mathcal{F}} = \delta_{ij}$ it follows from Lemma 2.3 that

$$
\sup \left\{ \langle \Gamma||\mathcal{H}_{K}\Gamma\rangle_{\mathcal{F}} \ | \ |\Gamma||_{\mathcal{F}} = 1 \right\} = \inf \sigma(\mathcal{H}_{K}) + \Lambda_{K}^{(n)}.
$$

(2.42)

The next proposition provides a variational bound on the energy for states of the form $\Psi_{P} = S_{P}\Gamma$ with $S_{P}$ defined in (2.32) and $\Gamma \in \mathcal{V}_{K}^{(n+1)}$.

**Proposition 2.5.** Let $M^{\text{LP}} = \frac{2}{3}||\nabla \varphi||_{L^{2}}^{2}$ with $\varphi$ defined in (2.5), $e_{\text{Pek}}$ the Pekar energy (2.6) and $H_{\text{Pek}}^{K}$ defined by (2.9). For all $\varepsilon > 0$ and $n \in \mathbb{N}_{0}$ there exist constants $C(n, \varepsilon) > 0$ and $\alpha(n) \geq 1$ such that

$$
\left| \frac{\langle S_{P}\Gamma|H_{\alpha}(P)S_{P}\Gamma\rangle_{\mathcal{F}}}{\langle S_{P}\Gamma|S_{P}\Gamma\rangle_{\mathcal{F}}} - \left( e_{\text{Pek}} + \frac{1}{\alpha^{2}} \left( \langle \Gamma||\mathcal{H}_{K}\Gamma\rangle_{\mathcal{F}} - \frac{2}{3} \right) + \frac{P^{2}}{2\alpha^{4}M^{\text{LP}}} \right) \right| \leq C(n, \varepsilon)\alpha^{\varepsilon} \left( K^{-1/2}\alpha^{-2} + K^{1/2}\alpha^{-3} \right)
$$

(2.43)

for all normalized $\Gamma \in \mathcal{V}_{K}^{(n+1)}$, $|P| \leq \sqrt{2M^{\text{LP}}\alpha}$, $K_{0} \leq K \leq \alpha$ and $\alpha \geq \alpha(n)$.

To use Proposition 2.5 to estimate the min-max values, we have to show that the subspace $S_{P}\mathcal{V}_{K}^{(n+1)}$ has dimension $n+1$. That this holds for large enough $\alpha$ is the content of the following lemma, whose proof is given in Section 4.
Lemma 2.6. For every \( n \in \mathbb{N} \) there exists a constant \( \alpha(n) \geq 1 \) such that

\[
\dim(\mathcal{S}_P \mathcal{V}_K^{(n+1)}) = n + 1
\]

for all \( |P| \leq \sqrt{2M_L} \alpha \), \( K_0 \leq K \leq \alpha \) and \( \alpha \geq \alpha(n) \).

We can now combine Proposition 2.5 and Lemmas 2.2 and 2.6 to prove Theorem 2.4.

Proof of Theorem 2.4. For \( |P| > \sqrt{2M_L} \alpha \), we use \( \mu_n(H_\alpha(P)) \leq \sigma_{\text{ess}}(H_\alpha(P)) \leq \mu_n(H_\alpha(0)) + \alpha^{-2} \) by definition of the min-max values and Lemma 1.1. Hence it is sufficient to consider \( |P| \leq \sqrt{2M_L} \alpha \).

With the aid of Lemma 2.6 we can choose \( \mathcal{V}_{n+1} = \mathcal{S}_P \mathcal{V}_K^{(n+1)} \) in (2.26). Applying Proposition 2.5 together with (2.42), we obtain

\[
\mu_n(H_\alpha(P)) \leq e^{P_\text{ek}} + \frac{1}{\alpha^2} \left( \inf \sigma(\mathbb{H}_K) + \Lambda_K^{(n)} - \frac{3}{2} \right)
\]

\[
+ \frac{P^2}{2\alpha^4M_L} + C(n, \varepsilon) \alpha^\varepsilon \left( K^{-1/2} \alpha^{-2} + \sqrt{K} \alpha^{-3} \right)
\]

for all \( |P| \leq \sqrt{2M_L} \alpha \), \( K_0 \leq K \leq \alpha \) and \( \alpha \geq \alpha(n) \). Next we use \( \inf \sigma(\mathbb{H}_K) - \inf \sigma(K) \leq CK^{-1/2} \) (see [18, Section 3.9]) and \( |\Lambda_K^{(n)} - \Lambda^{(n)}| \leq CK^{-1/2} \). The second inequality is a consequence of (2.23) together with the uniform bound (2.25) and \( |(\Lambda_K^{(n)})^{1/2} - (\Lambda^{(n)})^{1/2}| \leq CK^{-1/2} \). The latter is obtained from Lemma 2.2 (vi) and \( \Lambda_K^{(n)} \geq \beta > 0 \). The proof of Theorem 2.4 now follows by using (2.21b) for \( K = \infty \), and choosing \( K = \alpha \) in the term quantifying the error.

The remainder of the paper is dedicated to the proof of Proposition 2.5. After reviewing some general relations, we start in Section 3.1 with a suitable formula for the expectation value of \( H_\alpha(P) \) in states of the form \( \mathcal{S}_P \Gamma \). Sections 3.2 – 3.4 collect further preparations for the proof of Proposition 2.5. Some of the statements in Sections 3.2 and 3.3 were already used in [18]; for the reader’s convenience we provide the statements and refer to the proofs in [18]. In Sections 3.6 – 3.9 we derive estimates for the norm of our trial states and for the different terms in the energy formula that was obtained in Section 3.1. A heuristic sketch of this part of the proof is given in Section 3.5. Some of the terms can be estimated similarly as the corresponding ones in [18]; for these terms some details will be skipped. The main contributions, however, require substantial modifications and thus we present them in more detail. The results from Sections 3.6 – 3.9 are combined in Section 3.10 to complete the proof of Proposition 2.5. All remaining proofs of auxiliary lemmas are postponed until Section 4.

Throughout the remainder we will abbreviate constants by the letter \( C \) (and \( c \)) and write \( C(\tau) \) or \( C_\tau \) 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 Proof of Proposition 2.5

We recall the definition of the field operators

\[ \phi(f) = a^\dagger(f) + a(f), \quad \pi(f) = \phi(if) \]  

and the Weyl operator

\[ W(f) = e^{-i\pi(f)} = e^{a^\dagger(f) - a(f)} = e^{a^\dagger(f)}e^{-a(f)}e^{-\frac{1}{2}\|f\|_2^2}. \]  

The Weyl operator is unitary and satisfies

\[ W^\dagger(f) = W(-f), \quad W(f)W(g) = W(f + g)e^{i\text{Im}(gf)}_2. \]  

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

\[ W(g)^\dagger a^\dagger(f)W(g) = a^\dagger(f) + \langle gf \rangle_2, \quad W(g)^\dagger a(f)W(g) = a(f) + \langle gf \rangle_2, \]  

and thus

\[ W(g)^\dagger \phi(f)W(g) = \phi(f) + 2\text{Re} \langle f|g \rangle_2, \]  

\[ W(g)^\dagger N W(g) = N + \phi(g) + \|g\|_2^2, \]  

\[ W(g)^\dagger P_f W(g) = P_f - a^\dagger(i\nabla g) - a(i\nabla g) - \langle g|\nabla g \rangle_2. \]  

3.1 The total energy

The proof of Proposition 2.5 starts with a convenient formula for the expectation value of the fiber Hamiltonian \( H_\alpha(P) \) in a state \( \Psi_P = S_P \Gamma \) for general \( \Gamma \in F \). The precise statement requires some more notation.

We introduce the \( y \)-dependent \( L^2(\mathbb{R}^3) \)-function

\[ w_{P,y} = (1 - e^{-y\nabla})\varphi_P \]  

with \( \varphi_P \) defined in (2.33), and the \( y \)-dependent Fock space operator

\[ A_{P,y} = iP_f y + ig_P(y), \quad g_P(y) = -\frac{2}{M_LF} \int_0^1 ds \langle \varphi|e^{-sy\nabla}(y\nabla)^3(P\nabla)\varphi \rangle_2. \]  

Since \( g_P(y) \) is real-valued, it satisfies \( (A_{P,y})^\dagger = -A_{P,y} \).

We further introduce the Hamiltonian (acting on \( L^2(\mathbb{R}^3) \otimes F \))

\[ \tilde{H}_\alpha = h^\text{Pek} + \alpha^{-2}N + \alpha^{-1}\phi(h_x + \varphi_P) \]  

\[ (3.8a) \]
with \( h_{\text{Pek}} \) defined in (2.7), and the shift operator (that will exclusively act on the electron coordinate \( x \))

\[
T_y : L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3), \quad (T_y f)(x) = f(x + y) \quad \text{for all} \quad f \in L^2(\mathbb{R}^3).
\] (3.9)

**Lemma 3.1.** For every \( P \in \mathbb{R}^3 \) and \( \Gamma \in V^{(n+1)}_K \) we have

\[
\langle S_P \Gamma | H_\alpha(P) S_P \Gamma \rangle_\mathcal{F} = \left( c_{\text{Pek}} + \frac{P^2}{2\alpha^4 M^{L_P}} \right) \|S_P \Gamma\|_\mathcal{F}^2 + \mathcal{E}^\Gamma + \mathcal{G}^\Gamma + \mathcal{K}^\Gamma 
\]

(3.10)

where

\[
\mathcal{E}^\Gamma = \int dy \langle \mathcal{G}^0_{\Gamma} | \tilde{H}_{\alpha,P} T_y e^{A_P y} W(\alpha w_{P,y}) \mathcal{G}^0_{\Gamma} \rangle_\mathcal{F}
\]

(3.11a)

\[
\mathcal{G}^\Gamma = -\frac{2}{\alpha} \int dy \Re \langle \mathcal{G}^1_{\Gamma} | \tilde{H}_{\alpha,P} T_y e^{A_P y} W(\alpha w_{P,y}) \mathcal{G}^1_{\Gamma} \rangle_\mathcal{F}
\]

(3.11b)

\[
\mathcal{K}^\Gamma = \frac{1}{\alpha^2} \int dy \langle \mathcal{G}^1_{\Gamma} | \tilde{H}_{\alpha,P} T_y e^{A_P y} W(\alpha w_{P,y}) \mathcal{G}^1_{\Gamma} \rangle_\mathcal{F}
\]

(3.11c)

with \( \mathcal{G}^i_{\Gamma} \) defined in (2.37).

We omit the proof since it follows verbatim the proof of [18, Lemma 3.1].

### 3.2 The Gaussian lemma

With (2.10), (3.6) and \( \Theta_K = (H_{\text{Pek}}^K)^{1/4} \) we introduce

\[
w^0_{P,y} := \Pi_0 w_{P,y} \in \text{Ker} H_{\text{Pek}}
\]

(3.12a)

\[
w^1_{P,y} := \Pi_1 w_{P,y} \in (\text{Ker} H_{\text{Pek}})^\perp
\]

(3.12b)

\[
\tilde{w}^1_{P,y} := \Theta_K \Re(w^1_{P,y}) + i\Theta_K^{-1} \Im(w^1_{P,y})
\]

(3.12c)

\[
\tilde{w}_{P,y} := w^0_{P,y} + \tilde{w}^1_{P,y}.
\]

(3.12d)

**Remark 3.1.** For later use, let us note some symmetries of the above functions. As explained in [18, Remark 3.1] \((y, z) \mapsto \Re(w^i_{P,y})(z), i = 0, 1, \) are even as functions on \( \mathbb{R}^6 \), while \( \Im(w^i_{P,y})(z), i = 0, 1, \) are odd on the same space. Moreover, it follows by rotation invariance of \( \varphi \) that \( \Re(w^0_{P,-y})(z) = -\Re(w^0_{P,y})(z) \) for all \( y, z \in \mathbb{R}^3 \). (Note that \( \Re(w^i_{P,y}) = w^i_{0,y} \)).

The following lemma is proved in [18, Lemma 3.3].

**Lemma 3.2.** Let \( \lambda = \frac{1}{6} \|\nabla \varphi\|_{L^2}^2 \) and \( K_0 > 0 \) large enough. For every \( c > 0 \) there exists a constant \( C > 0 \) such that

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

(3.13a)

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

(3.13b)
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

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

where we omit the dependence on $\alpha$, $P$ and $K$. By Remark 3.1, it follows that $n_{\delta, \eta}(y)$ is even as a function of $y$. 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 $y$. This is a crucial ingredient in our proofs and the content of the next lemma.

**Lemma 3.3.** Let $\eta_0 > 0$, $c > 0$, $\lambda = \frac{1}{6}\|\nabla \varphi\|_{L^2}^2$ and $n_{\delta, \eta}$ defined in (3.14). For every $n \in \mathbb{N}_0$ there exist constants $d, C(n) > 0$ such that

$$\int |y|^n g(y) n_{\delta, \eta}(y) - e^{-\eta \lambda \alpha^{2(1-\delta)} y^2} dy \leq C(n) \frac{\|g\|_{L^\infty}}{\alpha^{(4+n)(1-\delta) + \delta}} + e^{-\alpha^{-2\delta + 1}} \|\cdot n\|_{L^1}$$

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 $K, \alpha$ large enough.

For the proof see [18, Lemma 3.3]. As a direct consequence that will be useful to estimate error terms, we find

**Corollary 3.4.** Given the same assumptions as in Lemma 3.3, for every $n \in \mathbb{N}_0$ there exist constants $d, C(n) > 0$ such that

$$\int |y|^n g(y) n_{\delta, \eta}(y) dy \leq C(n) \frac{\|g\|_{L^\infty}}{\alpha^{(3+n)(1-\delta)}} + e^{-\alpha^{-2\delta + 1}} \|\cdot n\|_{L^1}$$

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 $K, \alpha$ large enough.

**Proof of Corollary 3.4.** Since

$$\int dy |y|^n e^{-\eta \lambda \alpha^{2(1-\delta)} y^2} = (\eta \lambda \alpha^{2(1-\delta)} - \frac{3+n}{2}) \int dy |y|^n e^{-y^2} = C(n) \alpha^{-(3+n)(1-\delta)},$$

the statement follows immediately from Lemma 3.3. \(\square\)

### 3.3 Further preliminaries

In this section we summarize further helpful results. The proofs of Lemmas 3.5–3.10, Corollary 3.8 and Lemma 3.12 can be found in [18, Section 3].
3.3.1 Estimates involving the Pekar minimizers

**Lemma 3.5.** Let $\psi > 0$ be the unique rotation invariant minimizer of the Pekar functional (2.3), and let

$$H(x) := \langle \psi | T_x \psi \rangle_{L^2} = (\psi \ast \psi)(x).$$  \hspace{1cm} (3.18)

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

$$|H(x) - 1| \leq Cx^2.$$ \hspace{1cm} (3.19)

The next lemma contains bounds for the potential $V^\varphi$ and the resolvent $R$ introduced in (2.2), (2.5) and (2.8).

**Lemma 3.6.** There is a constant $C > 0$ such that

$$(V^\varphi)^2 \leq C(1 - \Delta), \quad \pm V^\varphi \leq \frac{1}{2}(-\Delta) + C \quad \text{and} \quad ||\nabla R^{1/2}||_{op} \leq C.$$ \hspace{1cm} (3.20)

### 3.3.2 The commutator method

In our proof we are faced with bounding field operators like $\phi(h_x)$. The standard estimates for creation and annihilation operators,

$$||a(f)\Psi||_{\mathcal{H}} \leq ||f||_{L^2}||N^{1/2}\Psi||_{\mathcal{H}} , \quad ||a^\dagger(f)\Psi||_{\mathcal{H}} \leq ||f||_{L^2}||N + 1||^{1/2}\Psi||_{\mathcal{H}}, \quad \Psi \in \mathcal{H},$$ \hspace{1cm} (3.21)

are not sufficient since $h_0(y)$ is not square-integrable. For this purpose we shall use the following lemma, which is a version of the commutator method by Lieb and Yamazaki [15].

**Lemma 3.7.** Let $h_K$, for $K \in (1, \infty)$ as defined in (2.15), let $A$ denote a bounded operator in $L^2(\mathbb{R}^3)$ (acting on the field variable) and $a^\dagger \in \{a, a^\dagger\}$. 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

$$||Xa^\dagger(Ah_{K,+,y})Y\Psi||_{\mathcal{H}} \leq CD_0||(N + 1)^{1/2}\Psi||_{\mathcal{H}}$$  \hspace{1cm} (3.22a)

$$||Xa^\dagger(\Lambda_{\Lambda,+,y} - Ah_{K,+,y})Y\Psi||_{\mathcal{H}} \leq \frac{CD_0}{\sqrt{K}}||(N + 1)^{1/2}\Psi||_{\mathcal{H}}$$  \hspace{1cm} (3.22b)

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

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

$$(Ah_{K,x})(z) = \int du \, A(z, u)h_{K,x}(u).$$ \hspace{1cm} (3.23)

A simple but useful corollary is given by
Corollary 3.8. Under the same conditions as in Lemma 3.7, with the additional assumption that $Y$ is a rank-one operator, there exists a constant $C > 0$ such that

\[
\int dz \|X(\mathcal{A}h_{K,+y})(z)Y\|_\text{op}^2 \leq CD_0^2 \quad (3.24a)
\]

\[
\int dz \|X((\mathcal{A}h_{K,+y})(z) - (\mathcal{A}h_{\Lambda,+y})(z))Y\|_\text{op}^2 \leq \frac{CD_0^2}{K} \quad (3.24b)
\]

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

3.3.3 Transformation properties of $U_K$

The next lemma collects relations for the Bogoliubov transformation $U_K$ defined in (2.20). Its proof follows directly from this definition and the fact that $\Theta_K = (H^K_{\text{Pek}})^{1/4}$ is real-valued.

Lemma 3.9. Let $f \in L^2(\mathbb{R}^3)$, $f^0 = \Pi_0 f$, $f^1 = \Pi_1 f$ with $\Pi_i$ defined in (2.10) and set

\[
\begin{align*}
\hat{f} & := f^0 + \Theta_K^{-1} \text{Re}(f^1) + i\Theta_K \text{Im}(f^1) \\
\tilde{f} & := f^0 + \Theta_K \text{Re}(f^1) + i\Theta_K^{-1} \text{Im}(f^1).
\end{align*}
\]

(3.25a)

(3.25b)

The unitary operator $U_K$ defined in (2.20) satisfies the relations

\[
\begin{align*}
U_K a(f) U_K^\dagger & = a(f^0) + a(A_K f^1) + a^\dagger (B_K f^\dagger) \\
U_K^\dagger a(f) U_K & = a(f^0) + a(A_K f^1) - a^\dagger (B_K f^\dagger) \\
U_K \phi(f) U_K^\dagger & = \phi(\hat{f}), \quad U_K \pi(f) U_K^\dagger = \pi(\tilde{f}) \\
U_K W(f) U_K^\dagger & = W(\tilde{f}).
\end{align*}
\]

(3.26a)

(3.26b)

(3.26c)

(3.26d)

Note that (3.25b) is consistent with the notation introduced in (3.12d). The following statements provide helpful bounds on the number operator when transformed with the Bogoliubov transformation.

Lemma 3.10. There exists a constant $b > 0$ such that

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

(3.27)

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

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

Corollary 3.11. Let $\mathcal{V}_K^{(n+1)} \subset \mathcal{F}_1$ as in (2.41) and $m \in \mathbb{N}$ defined by (2.25). Further set $\Gamma^> := \mathbb{1}(N > \alpha^\delta) \Gamma$ for $\delta > 0$. There exist constants $b, C(\delta, j) > 0$ such that

\[
\langle \Gamma | (N + 1)^j \Gamma \rangle_\mathcal{F} \leq b^j j^j (m + 1)^j
\]

(3.28a)
\[
\langle \Gamma^\uparrow |(N+1)^j \Gamma^\uparrow \rangle_{\mathcal{F}} \leq C(\delta, j) \alpha^{-20}.
\]
for all normalized $\Gamma \in \mathcal{V}_K^{(n+1)}$ and all $n, j \in \mathbb{N}_0$ and $K \in (K_0, \infty)$ with $K_0$ large enough.

**Proof.** The first bound follows from Lemma 3.10 together with (2.25). The second one is obtained from
\[
\langle \Gamma^\uparrow |(N+1)^j \Gamma^\uparrow \rangle_{\mathcal{F}} \leq \|N^k(N+1)^j \Gamma^\uparrow\|_{\mathcal{F}} \|N^{-k} \Gamma^\uparrow\|_{\mathcal{F}} \\
\leq \|(N+1)^{j+k} \Gamma\|_{\mathcal{F}} \alpha^{-k\delta} \leq (2(j+k)b(m+1))^{j+k} \alpha^{-k\delta}
\]
with $k \geq 20/\delta$.

**Lemma 3.12.** For $\delta > 0$ and $\kappa = 1/(16e\alpha^3)$ with $b > 0$ the constant from Lemma 3.10, the operator inequality
\[
\mathbb{1}(N \leq 2\alpha^3) \mathbb{U}_K \exp(2\kappa N) \mathbb{U}_K \mathbb{1}(N \leq 2\alpha^3) \leq 2
\]
holds for all $K \geq K_0$ and $\alpha$ large enough.

The reason for introducing the cutoff $K$ in $\mathbb{H}_K$ is the following lemma, whose proof is given in Section 4. The statement is a generalization of [18, Lemma 3.13] to excited eigenstates of the Bogoliubov Hamiltonian.

**Lemma 3.13.** For every $n \in \mathbb{N}_0$ there exist constants $C(n), K(n) > 0$ such that
\[
\|P \Gamma\|_{\mathcal{F}} \leq C(n)\sqrt{K}
\]
for all normalized $\Gamma \in \mathcal{V}_K^{(n+1)}$ and $K \geq K(n)$.

### 3.4 Replacing the Weyl operator by the weight function

The next two lemmas will be useful in order to replace the Weyl operator $W(\alpha \hat{w}_{P,y})$ (when multiplied with different operators) by the weight function (3.14). The proofs are given in Section 4. For the precise statements, recall the notation $\mathcal{G}_0^0 = \psi \otimes \gamma \in L^2(\mathbb{R}^3) \otimes \mathcal{F}$ and definitions (3.12d), (3.14) and (2.39).

**Lemma 3.14.** Let $X, Y : L^2(\mathbb{R}^3) \otimes \mathcal{F}_1 \to L^2(\mathbb{R}^3) \otimes \mathcal{F}_1$ be densely defined operators whose Fock space components are at most quadratic in creation and annihilation operators.\(^3\) Moreover let $p_{\alpha}(y) = 1 + (\alpha |y|)^{4m+8}$ with $m$ defined in (2.25). There exists a constant $C > 0$ such that
\[
\left| \langle \mathcal{G}_0^0 | XW(\alpha \hat{w}_{P,y}) Y \mathcal{G}_0^0 \rangle_{\mathcal{F}} - \langle \mathcal{G}_0^0 | XY \mathcal{G}_0^0 \rangle_{\mathcal{F}} p_{\alpha}(y) n_{0,1}(y) \right| \\
\leq C\alpha^{-1} \|X\|_{\mathcal{F}} \|Y\|_{\mathcal{F}} \|\mathcal{G}_0^0\|_{\mathcal{F}} \|p_{\alpha}(y) n_{0,1}(y)\|_{\mathcal{F}} \forall y \in \mathbb{R}^3
\]
\(^3\)Meaning $X(L^2(\mathbb{R}^3) \otimes \mathcal{F}_1^{(n)}) \subset L^2(\mathbb{R}^3) \otimes \bigoplus_{m=\max(0,n-2)}^{n+2} \mathcal{F}_1^{(m)} \forall n \in \mathbb{N}_0$, with $\mathcal{F}_1^{(m)} = \mathcal{F}_1 \cap \mathcal{F}^{(m)}$, cf. (2.40).
for all such operators $X,Y$ and all $\gamma,\xi \in \mathcal{F}^{(\leq m)}$, $|P| \leq \sqrt{2M^{\text{LP}}\alpha}$, $K \geq K_0$ and $\alpha \geq 1$.

**Lemma 3.15.** Let $c,\delta > 0$ and $\kappa = 1/(16eb \delta^3)$ with $b > 0$ the constant from Lemma 3.10. Moreover let $p_\alpha(y) = 1 + (\alpha |y|)^{4m+8}$ with $m$ defined in (2.25). There exist constants $\eta,C > 0$ and $\alpha_0 \geq 1$ such that

$$
\|e^{-\kappa N}w_\alpha T_y W(\alpha w_{P,y})\gamma\|_F \leq C p_\alpha(y) n_{\delta,y}(y) \quad \forall y \in \mathbb{R}^3
$$

(3.33)

for all normalized $\gamma \in \mathcal{F}^{(\leq m)}$, $|P| \leq \sqrt{2M^{\text{LP}}\alpha}$ and $\alpha \geq \alpha_0$.

### 3.5 Sketch of the remaining part of the proof

With Lemma 3.1, the task is to show that $(\mathcal{E}^\Gamma + \mathcal{G}^\Gamma + \mathcal{K}^\Gamma)/\|S_P \Gamma\|_F^2$ for $\Gamma \in \mathcal{V}^{(n+1)}_K$ coincides, up to small errors, with the energy contribution of order $\alpha^{-2}$ in (2.43). Since this part of the proof is somewhat technical, we explain in this section the heuristic ideas behind the different steps. The main point is that the integrands in (3.11a) – (3.11c) are all localized around $y = 0$ at the length scale of order $\alpha^{-1}$. In a first step, this allows us to replace $e^{\Lambda_P y}$ by the identity, and keeping only the terms that will contribute to the energy of order $\alpha^{-2}$, this gives

$$
\mathcal{E}^\Gamma = \frac{1}{\alpha^2} \int dy \langle \mathcal{G}_T^0 | N_1 T_y W(\alpha w_{P,y}) \mathcal{G}_T^0 \rangle_F
$$

(3.34a)

$$
+ \frac{1}{\alpha} \int dy \langle \mathcal{G}_T^0 | \phi(h + \varphi) T_y W(\alpha w_{P,y}) \mathcal{G}_T^0 \rangle_F + \text{Errors}
$$

(3.34b)

$$
\mathcal{G}^\Gamma = -\frac{2}{\alpha^2} \int dy \text{Re} \langle \mathcal{G}_T^0 | \phi(h^1) T_y W(\alpha w_{P,y}) \mathcal{G}_T^1 \rangle_F + \text{Errors}
$$

(3.34c)

$$
\mathcal{K}^\Gamma = \frac{1}{\alpha^2} \int dy \langle \mathcal{G}_T^1 | \mathcal{H} \mathcal{K}_T \gamma \rangle_F W(\alpha w_{P,y}) \mathcal{G}_T^1 \rangle_F + \text{Errors}.
$$

(3.34d)

In the first, third and fourth term, we use the transformation property (2.20), e.g.

$$
\langle \mathcal{G}_T^0 | N_1 T_y W(\alpha w_{P,y}) \mathcal{G}_T^0 \rangle_F = \langle \mathcal{G}_T^0 | U_K N_1 U_K^\dagger T_y W(\alpha \tilde{w}_{P,y}) \mathcal{G}_T^0 \rangle_F,
$$

(3.35)

where we introduced $\gamma = U_K \Gamma$. Since in the relevant regime, that is for $|y| = O(\alpha^{-1})$, we have $\tilde{w}_{P,y} \approx y \nabla \varphi \in \text{Ran}(\Pi_0)$, the Weyl operator $W(\alpha \tilde{w}_{P,y})$ can be effectively replaced by the Gaussian factor $e^{-\lambda \alpha^2 y^2}$ (recall that $\mathcal{G}_T^0$ is the vacuum in $\mathcal{F}_0$). Technically we first apply Lemma 3.14 to replace the Weyl operator by the weight function $n_{0,1}(y)$, and then Lemma 3.3 to replace the weight function by $e^{-\lambda \alpha^2 y^2}$. For that purpose, we need to show that the functions that multiply $n_{0,1}(y)$ are indeed bounded and integrable as needed in Lemma 3.3 (e.g. in (3.34a), we have $g(y) = \langle \psi | T_y \psi \rangle_{\mathcal{L}^2} \langle \gamma | U_K N_1 U_K^\dagger \gamma \rangle_F$, which satisfies these properties by Lemmas 3.5 and 3.10). In the leading order terms, we proceed by approximating $T_y \approx 1$, $h \approx h_K$, and $u_\alpha \approx 1$. Ignoring all errors resulting from these steps, this will lead to

$$
(3.34a) + (3.34c) + (3.34d) \approx \frac{1}{\alpha^2} \langle \Gamma | \mathcal{H}_K \Gamma \rangle_F \int dy e^{-\lambda \alpha^2 y^2},
$$

(3.36)
and similarly we show that the last factor is approximately given by the norm $\|S_F\|_F \approx (\frac{\pi}{\lambda \alpha})^{3/2}$. This explains the first part of the energy of order $\alpha^{-2}$ in (2.43).

To compute (3.34b), we use the CCR, the fact that $G_0$ coincides with the vacuum in $F_0$, together with $(y, z) \mapsto \tilde{w}_{P,y}(z)$ being symmetric and $w_{P,y}^0 \approx y \nabla \varphi$ for $|y| = O(\alpha^{-1})$. A careful analysis will show that

\[
(3.34b) \approx \int dy \langle \psi \otimes \gamma | \langle h_\gamma | (y \nabla \varphi)_{\xi}^2 (y \nabla)^2 (\alpha \tilde{w}_{P,y}) \psi \otimes \gamma \rangle_{\mathcal{H}}.
\]

where we can replace again the Weyl operator by $e^{-\lambda \alpha^2 y^2}$, and using integration by parts and (2.5), one finds that

\[
(3.34b) \approx -\frac{1}{2} \int dy e^{-\lambda \alpha^2 y^2} \|y \nabla \varphi\|_2^2 = -\frac{3}{2\alpha^2} \int dy e^{-\lambda \alpha^2 y^2}.
\]

This explains the energy contribution $-\frac{3}{2\alpha^2}$ in (2.43).

### 3.6 Norm of the trial state

In this section we derive an estimate for the inner product between two trial states. This gives a bound on the norm and provides the almost orthogonality of different states that is used to prove Lemma 2.6.

**Proposition 3.16.** Let $V_K^{(n+1)}$ be defined as in (2.41). For all $\varepsilon > 0$ and $n \in \mathbb{N}_0$ there exist constants $C(n, \varepsilon) > 0$ and $\alpha_0 \geq 1$ such that

\[
\left| \langle S_F \Gamma | S_F \Xi \rangle_x - \langle \Gamma | \Xi \rangle_x \left( \frac{\pi}{\lambda \alpha^2} \right)^{3/2} \right| \leq C(n, \varepsilon) \sqrt{K} \alpha^{-4+\varepsilon}
\]

for all normalized $\Gamma, \Xi \in V_K^{(n+1)}$, $|P| \leq \sqrt{2MLP} \alpha$, $K \geq K_0$ and $\alpha \geq \alpha_0$.

**Proof.** Let $N := \langle S_F \Gamma | S_F \Xi \rangle_x$. Following the argument of [18, Proof of Lemma 3.1], one verifies that $N = N_0 + N_{1a} + N_{1b} + N_2$ with

\[
N_0 = \int dy \langle \mathcal{G}_T^0 | T_y e^{A_{P,y}} W(\alpha w_{P,y}) \mathcal{G}_\Xi^0 \rangle_{\mathcal{H}} \tag{3.40a}
\]

\[
N_{1a} = \frac{1}{\alpha} \int dy \langle \mathcal{G}_T^0 | T_y e^{A_{P,y}} W(\alpha w_{P,y}) \mathcal{G}_\Xi^0 \rangle_{\mathcal{H}} \tag{3.40b}
\]

\[
N_{1b} = -\frac{1}{\alpha} \int dy \langle T_y e^{A_{P,y}} W(\alpha w_{P,y}) \mathcal{G}_T^1 | \mathcal{G}_\Xi^0 \rangle_{\mathcal{H}} \tag{3.40c}
\]

\[
N_2 = \frac{1}{\alpha^2} \int dy \langle T_y e^{A_{P,y}} W(\alpha w_{P,y}) \mathcal{G}_T^1 | \mathcal{G}_\Xi^1 \rangle_{\mathcal{H}} \tag{3.40d}
\]

with $A_{P,y}$ defined in (3.7) and $T_y$ denoting the shift operator (3.9).

**Term $N_0$.** This part contains the contribution $\langle \Gamma | \Xi \rangle_x \left( \frac{\pi}{\lambda \alpha^2} \right)^{3/2}$. With $H$ defined in (3.18), let
us write
\[ \mathcal{N}_0 = \int dy \, H(y) \langle \Gamma | W(\alpha w_{P,y}) \Xi \rangle_x \]
\[ + \int dy \, H(y) \langle \Gamma | (e^{A_{F,y}} - 1) W(\alpha w_{P,y}) \Xi \rangle_x = \mathcal{N}_{01} + \mathcal{N}_{02}. \]  
(3.41)

In the first term we insert \( \Gamma = \mathbb{U}_K^\dagger \gamma, \Xi = \mathbb{U}_K^\dagger \xi \) with \( \gamma, \xi \in \mathcal{F}_1^{(\leq m)} \), and apply (3.26d) to transform the Weyl operator with the Bogoliubov transformation. This gives
\[ \mathbb{U}_K W(\alpha w_{p,y}) \mathbb{U}_K^\dagger = W(\alpha \tilde{w}_{p,y}) \]  
(3.42)

with \( \tilde{w}_{p,y} \) defined in (3.12d). Applying Lemma 3.14 for \( X = Y = 1 \) leads to the bound
\[ \left| \mathcal{N}_{01} - \langle \gamma | \xi \rangle_x \right| \leq \alpha^{-1} \int dy \, H(y) n_{0,1}(y). \]  
(3.43)

Since \( \|H\|_{L^1} + \|H\|_{L^\infty} \leq C \), cf. Lemma 3.5, we can apply Lemma 3.3 in order to replace the weight function \( n_{0,1}(y) \) in the term containing \( \langle \gamma | \xi \rangle_x \) by the Gaussian \( e^{-\lambda^2 y^2} \). More precisely
\[ \left| \int dy \, H(y) n_{0,1}(y) - \int dy \, H(y) e^{-\lambda^2 y^2} \right| \leq C \alpha^{-4} \]  
(3.44)

for all \( |P| \leq c \alpha \) and \( K, \alpha \) large enough. Next we use \( |H(y) - 1| \leq Cy^2 \) to obtain
\[ \left| \int dy \, H(y) n_{0,1}(y) - \left( \frac{\pi}{\lambda \alpha^2} \right)^{3/2} \right| \leq C \alpha^{-4}. \]  
(3.45)

For the remainder term in (3.43), we recall \( p_{\alpha}(y) = 1 + (\alpha |y|)^{4m+8} \) and apply Corollary 3.4. This leads to
\[ \left| \mathcal{N}_{01} - \langle \gamma | \xi \rangle_x \left( \frac{\pi}{\lambda \alpha^2} \right)^{3/2} \right| \leq C \alpha^{-4}. \]  
(3.46)

To treat \( \mathcal{N}_{02} \) it is convenient to decompose the state \( \Gamma \) into a part with bounded particle number and a remainder. To this end, we choose \( \delta > 0 \) small (but fixed w.r.t. \( \alpha \)) and write
\[ \Gamma = \Gamma^- + \Gamma^+ = \mathbb{1}(N \leq \alpha^\delta) \Gamma + \mathbb{1}(N > \alpha^\delta) \Gamma. \]  
(3.47)

Inserting this into \( \mathcal{N}_{02} \) and using unitarity of \( e^{A_{F,y}} \) and \( \|H\|_{L^1} \leq C \), we can estimate
\[ |\mathcal{N}_{02}| \leq \int dy \, H(y) \langle \Gamma^- | (e^{A_{F,y}} - 1) W(\alpha w_{P,y}) \Xi \rangle_x + C \|\Gamma^+\|_{L^1}. \]  
(3.48)

By Corollary 3.11 for \( j = 0, \|\Gamma^+\|_{L^1} \leq C_\delta \alpha^{-10} \). In the remaining expression we use \( \Xi = \mathbb{U}_K^\dagger \xi \)
and (3.42),
\[
\langle \Gamma^\leq |(e^{A_{P,y}} - 1)W(\alpha w_{P,y})\Xi \rangle_x = \langle \Gamma^\leq |(e^{A_{P,y}} - 1)U_K W(\alpha \tilde{w}_{P,y})\xi \rangle_x,
\]
and then insert the identity
\[
1 = e^{\kappa N}e^{-\kappa N} \quad \text{with} \quad \kappa = \frac{1}{16eb\alpha^\delta}
\]
on the left of the Weyl operator (here \(b > 0\) is the constant from Lemma 3.10). With Cauchy–Schwarz, this leads to
\[
\|e^{\kappa N}U_K(e^{-A_{P,y}} - 1)\Gamma^\leq\|_x \leq \sqrt{2}\|e^{-\kappa N}W(\alpha \tilde{w}_{P,y})\xi\|_x.
\]
In the second factor we can employ Lemma 3.15,
\[
\|e^{-\kappa N}W(\alpha \tilde{w}_{P,y})\xi\|_x \leq C_p \alpha(y) n_{\delta,\eta}(y) \quad \forall y \in \mathbb{R}^3
\]
for some \(\alpha\)-independent \(\eta > 0\) and \(\alpha\) large enough. To estimate the first factor in (3.51), we apply Lemma 3.12 (note that \((e^{A_{P,y}} - 1)\Gamma^\leq \in \text{Ran}(1(N \leq \alpha^\delta))\)) to obtain
\[
\|e^{\kappa N}U_K(e^{-A_{P,y}} - 1)\Gamma^\leq\|_x \leq \sqrt{2}\|e^{-A_{P,y}} - 1)\Gamma\|_x.
\]
On the right side we proceed with the functional calculus for self-adjoint operators
\[
\|(e^{-A_{P,y}} - 1)\Gamma\|_x \leq \|A_{P,y}\|_x \leq |y| \|P_f\|_x + |g_P(y)| \leq C(C(n)\sqrt{K}|y| + \alpha|y|^3),
\]
where we applied Lemma 3.13 in the second step and also used
\[
|g_P(y)| \leq C\alpha|y|^3,
\]
which is inferred from (3.7) using \(\|\Delta \varphi\|_{L^2} < \infty\). Returning to (3.51) we have shown that
\[
|\mathcal{N}_0^\leq| \leq C \int dy H(y)(C(n)\sqrt{K}|y| + \alpha|y|^3)p_\alpha(y) n_{\delta,\eta}(y) + C_\delta^\alpha^{-10},
\]
and hence we are in a position to apply Corollary 3.4. This implies for all \(K, \alpha\) large
\[
|\mathcal{N}_0^\leq| \leq C(n)\sqrt{K}\alpha^{-4+(12+4m)\delta} + C_\delta\alpha^{-10},
\]
where we used that \(\|\cdot \|^2 H\|_{L^1} + \|H\|_{L^\infty} \leq C(n)\). Note that the largest error comes from the term \(C(n)\sqrt{K} \int H(y)|\alpha| |\alpha(y)||^{4m+8}n_{\delta,\eta}(y)\), which explains the factor \(\alpha^{-4+(12+4m)\delta}\).

Terms \(\mathcal{N}_{1a}\) and \(\mathcal{N}_{1b}\). We start with \(\mathcal{N}_{1a}\) by inserting (2.37) for \(\mathcal{Q}_1^0, \mathcal{Q}_2^0\) in (3.40b). Since the
Weyl operator commutes with $u_\alpha$, $R$ and $P_\psi = |\psi\rangle\langle\psi|$, we can apply (3.5a) to obtain

$$W(\alpha w_{P,y})q^0_\pi = u_\alpha R(\phi(h_{K,\cdot}) + 2\alpha\langle h_{K,\cdot} | \text{Re}(w_{P,y}) \rangle_{L^2}) P_\psi W(\alpha w_{P,y})q^0_\pi,$$

(3.58)

where we used that $h_{K,x}$ is real-valued. Note that $\langle h_{K,\cdot} | \text{Re}(w_{P,y}) \rangle_{L^2}$ is a $y$-dependent multiplication operator in the electron variable. With $(T_y e^{A_{F,y}})^\dagger = T_{-y} e^{-A_{F,y}}$ and (3.47), we can thus write

$$\mathcal{N}_{1a} = -\frac{2}{\alpha} \int dy \text{Re} \langle R_{1,y} \psi \otimes (\Gamma^< + \Gamma^> \rangle |W(\alpha w_{P,y})q^0_\pi \rangle_{\mathcal{H}} = \mathcal{N}_{1a}^\leq + \mathcal{N}_{1a}^\gtrless,$$

(3.59)

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

$$R_{1,y}^{(1)} = P_\psi (\phi(h_{K,\cdot}) R u_\alpha T_{-y} P_\psi e^{-A_{F,y}},$$

and $R_{1,y}^{(2)} = 2\alpha P_\psi \langle h_{K,\cdot} | \text{Re}(w_{P,y}) \rangle_{L^2} R u_\alpha T_{-y} P_\psi e^{-A_{F,y}}.$

As shown in [18, Eq. (3.85)] this operator satisfies

$$\|R_{1,y} \Psi\|_{\mathcal{H}} \leq C \|\alpha T_{-y} P_\psi\|_{op}(1 + \alpha y^2)\|N + 1\|^{1/2} \Psi\|_{\mathcal{H}}, \quad \Psi \in \mathcal{H},$$

(3.61)

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

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

(3.62)

With this at hand we can estimate the part with the tail by invoking Corollary 3.11

$$|\mathcal{N}_{1a}^\gtrless| \leq \frac{C}{\alpha} \|(N + 1)^{1/2} \Gamma^>\|_\mathcal{H} \int dy f_\alpha(y)(1 + \alpha y^2) \leq C_\delta \alpha^{-5}.$$  

(3.63)

To estimate the first term in (3.59), we proceed similarly as in the bound for $N_{02}$. We insert the identity (3.50), apply Cauchy–Schwarz and employ $\Xi = \bigcup_{K} K \xi$ together with Lemma 3.15. This leads to

$$|\mathcal{N}_{1a}^\leq| \leq \frac{1}{\alpha} \int dy \|e^{N\bigcup_{K}(e^{-A_{F,y}} R_{1,y} \psi \otimes \Gamma^<})\|_{\mathcal{H}} \|e^{-N\bigcup_{K}(\alpha \tilde{w}_{P,y}) \xi}\|_\mathcal{H}$$

$$\leq \frac{1}{\alpha} \int dy \|e^{N\bigcup_{K}(e^{-A_{F,y}} R_{1,y} \psi \otimes \Gamma^<})\|_{\mathcal{H}} \|p_\alpha(y) n_{\delta,\eta}(y)\|.$$

(3.64)

In the remaining norm we use the fact that $e^{-A_{F,y}} R_{1,y}$ changes the number of phonons at most by one, and thus we can apply Lemma 3.12 and (3.61) together with (3.28a), to get

$$\|e^{N\bigcup_{K}(e^{-A_{F,y}} R_{1,y} \psi \otimes \Gamma^<})\|_\mathcal{H} \leq \sqrt{2} \|R_{1,y} \psi \otimes \Gamma^<\|_\mathcal{H} \leq C f_\alpha(y)(1 + \alpha y^2).$$

(3.65)
With Corollary 3.4, (3.62) and \( f_\alpha \|_{L^p} \leq 1 \), this leads to the bound
\[
|N_{1a}^{\lessgtr}| \leq \frac{C}{\alpha} \int dy \, f_\alpha(y)(1 + \alpha y^2) p_\alpha(y) n_{\delta,\eta}(y) \lesssim C\alpha^{-4+(1+4m)\delta}. \tag{3.66}
\]
The term \( N_{1b} \) can be estimated in the same way as \( N_{1a} \), exchanging the roles of \( \Gamma \) and \( \Xi \).

**Term \( N_2 \).** The strategy for this term is similar to the one for \( N_{1a} \). Proceeding as explained before (3.59), one obtains
\[
N_2 = \frac{1}{\alpha^2} \int dy \, \left< R_{2,y} \psi \otimes (\Gamma^{\lessgtr} + \Gamma^{\gtrless}) \right> \left| W(\alpha w_{P,y})\mathcal{G}_\Xi^0 \right|_{\mathcal{H}} = N_2^{\lessgtr} + N_2^{\gtrless} \tag{3.67}
\]
with \( R_{2,y} = R_{2,y}^{(1)} + R_{2,y}^{(2)} \)
\[
R_{2,y}^{(1)} = P_\psi \phi(h_{K,\alpha}^1) Re^{-\Lambda_{P,y}} u_\alpha T_{-y} u_\alpha R\phi(h_{K,\alpha}^1) P_\psi, \tag{3.68a}
\]
\[
R_{2,y}^{(2)} = 2\alpha P_\psi \langle h_{K,\alpha}^1 \rangle Re^{-\Lambda_{P,y}} u_\alpha T_{-y} u_\alpha R\phi(h_{K,\alpha}^1) P_\psi. \tag{3.68b}
\]
It follows in close analogy as for \( R_{1,y} \) in (3.60a)–(3.60b) that
\[
\|R_{2,y} \psi\|_{\mathcal{H}} \leq C \|u_\alpha T_{-y} u_\alpha\|_o (1 + \alpha y^2) \| (N + 1) \psi \|_{\mathcal{H}}, \quad \psi \in \mathcal{H}, \tag{3.69}
\]
and since \( \|u_\alpha T_{-y} u_\alpha\|_o \leq 1 (|y| \leq 4\alpha) \), we can use Corollary 3.11 to estimate
\[
|N_2^{\gtrless}| \leq \frac{C}{\alpha^2} \| (N + 1) \Gamma^{\gtrless} \|_{\mathcal{H}} \int dy \, 1(|y| \leq 4\alpha)(1 + \alpha y^2) \leq C\beta \alpha^{-6}. \tag{3.70}
\]
To bound the first term in (3.67) we proceed similarly as for \( N_{01} \), that is
\[
|N_2^{\lessgtr}| \leq \alpha^{-2} \int dy \, \| e^{\kappa N U_K} (R_{2,y} \psi \otimes \Gamma^{\lessgtr}) \|_{\mathcal{H}} e^{-\kappa N} W(\alpha w_{P,y}) \xi \|_{\mathcal{H}} \\
\leq \frac{C}{\alpha^2} \int dy \, 1(|y| \leq 4\alpha)(1 + \alpha y^2) p_\alpha(y) n_{\delta,\eta}(y) \leq C\alpha^{-5+(12+4m)\delta}, \tag{3.71}
\]
where the last step follows again from Corollary 3.4.

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

### 3.7 Energy contribution \( \mathcal{E}^{\Gamma} \)

In this section we prove an estimate for the energy contribution \( \mathcal{E}^{\Gamma} \) defined in (3.11a).

**Proposition 3.17.** Let \( V_K^{(n+1)} \) be defined as in (2.41) and \( N_1 \) be defined by (2.13). For all \( \varepsilon > 0 \) and \( n \in \mathbb{N}_0 \) there exist constants \( C(n,\varepsilon) > 0 \) and \( \alpha_0 \geq 1 \) such that
\[
\left| \mathcal{E}^{\Gamma} - \frac{1}{\alpha^2} \left( \langle \Gamma | N_1 | \Gamma \rangle \|_{\mathcal{H}} - \frac{3}{2} \right) \right|_{\mathcal{H}} \| S_p \Gamma \|_{\mathcal{H}}^2 \leq C(n,\varepsilon) \sqrt{K} \alpha^{-6+\varepsilon} \tag{3.72}
\]
for all normalized $\Gamma \in \mathcal{V}_K^{(n+1)}$, $|P| \leq \sqrt{2M} \sqrt{\alpha}$, $K \geq K_0$ and $\alpha \geq \alpha_0$.

Proof. Since $\mathcal{G}_\Gamma^0 = \psi \otimes \Gamma$, $h_{\text{Fek}} \psi = 0$ and $\mathcal{N} \Gamma = \mathcal{N}_1 \Gamma$, one finds

$$\mathcal{E}^\Gamma = \int dy \langle \mathcal{G}_\Gamma^0 \mid [(\alpha^{-2} \mathcal{N}_1 + \alpha^{-1} \phi (h + \varphi_P)) T_y e^{A_{p,y}} W(\alpha w_{P,y})] \mathcal{G}_\Gamma^0 \rangle_{\mathcal{X}} = \mathcal{E}_1^\Gamma + \mathcal{E}_2^\Gamma, \quad (3.73)$$

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

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

$$\mathcal{E}_1^\Gamma = \frac{1}{\alpha^2} \int dy \, H(y) \langle \Gamma \mid \mathcal{N}_1 W(\alpha w_{P,y}) \Gamma \rangle_{\mathcal{X}}$$

and

$$+ \frac{1}{\alpha^2} \int dy \, H(y) \langle \Gamma \mid \mathcal{N}_1 (e^{A_{p,y}} - 1) W(\alpha w_{P,y}) \Gamma \rangle_{\mathcal{X}} = \mathcal{E}_{11}^\Gamma + \mathcal{E}_{12}^\Gamma. \quad (3.74)$$

Also recall $\Gamma = \mathcal{U}_K^\dagger \gamma$ for some $\gamma \in \mathcal{F}_1^{(m)}$. With (3.42) and writing

$$\langle \Gamma \mid \mathcal{N}_1 W(\alpha w_{P,y}) \Gamma \rangle_{\mathcal{X}} = \langle \gamma \mid \mathcal{U}_K \mathcal{N}_1 \mathcal{U}_K^\dagger W(\alpha w_{P,y}) \gamma \rangle_{\mathcal{X}} \quad (3.75)$$

we can apply Lemma 3.14 with $X = \mathcal{U}_K \mathcal{N}_1 \mathcal{U}_K^\dagger$ (this is a quadratic operator $\mathcal{F}_1 \rightarrow \mathcal{F}_1$) and $Y = 1$. Since $\| \mathcal{U}_K \mathcal{N}_1 \mathcal{U}_K^\dagger \gamma \| \leq C$ by Lemma 3.10, it follows that

$$\left| \mathcal{E}_{11}^\Gamma - \frac{1}{\alpha^2} \langle \Gamma \mid \mathcal{N}_1 \Gamma \rangle_{\mathcal{X}} \int dy \, H(y) n_{0,1}(y) \right| \leq \frac{1}{\alpha^2} \int dy \, H(y) p_{\alpha}(y) n_{0,1}(y). \quad (3.76)$$

For the error term we find as a direct consequence of Corollary 3.4 that it is bounded by $C \alpha^{-6}$.

The second term on the l.h.s. we call $\mathcal{E}_{111}^\Gamma$ and write it as

$$\mathcal{E}_{111}^\Gamma = \frac{1}{\alpha^2} \langle \Gamma \mid \mathcal{N}_1 \Gamma \rangle_{\mathcal{X}} \int dy \, H(y) e^{-\lambda \alpha^2 y^2}$$

and

$$+ \frac{1}{\alpha^2} \langle \Gamma \mid \mathcal{N}_1 \Gamma \rangle_{\mathcal{X}} \int dy \, H(y) (n_{0,1}(y) - e^{-\lambda \alpha^2 y^2}) = \mathcal{E}_{111}^{\Gamma,\text{lo}} + \mathcal{E}_{111}^{\Gamma,\text{err}}. \quad (3.77)$$

In $\mathcal{E}_{111}^{\Gamma,\text{lo}}$ we use $|H(y) - 1| \leq C y^2$ and Corollary 3.11 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 3.16 for $\| S_P \Gamma \|_{\mathcal{X}}^2$, and again Corollary 3.11. This leads to

$$\left| \mathcal{E}_{111} - \frac{1}{\alpha^2} \langle \Gamma \mid \mathcal{N}_1 \Gamma \rangle_{\mathcal{X}} \| S_P \Gamma \|_{\mathcal{X}}^2 \right| \leq C(n, \varepsilon) \sqrt{k} \alpha^{-6+\varepsilon}. \quad (3.78)$$

The error in (3.77) is bounded with the help of Lemma 3.3,

$$|\mathcal{E}_{111}^{\Gamma,\text{err}}| \leq \frac{C}{\alpha^2} \int dy \, H(y) |n_{0,1}(y) - e^{-\lambda \alpha^2 y^2}| \leq C \alpha^{-6}. \quad (3.79)$$

In order to bound $\mathcal{E}_{12}^\Gamma$ in (3.74), we decompose $\Gamma = \Gamma^< + \Gamma^>$ for some $\delta > 0$ as in (3.47).
and then follow similar steps as described below (3.49). This way we can estimate

$$|\mathcal{E}_{12}^{\Gamma}| \leq \frac{1}{\alpha^2} \int dy \, H(y) \| e^{N_U K (e^{-A_P,y} - 1)} N_1 \Gamma_\prec \|_F \, p_\alpha(y) \, n_{\delta,\eta}(y) + \frac{2}{\alpha^2} \| N_1 \Gamma_\prec \|_F \int dy \, H(y). \quad (3.80)$$

While the second term is bounded via (3.28b) by $C_\delta \alpha^{-12}$, in the first term we apply Lemma 3.12 and use the functional calculus for self-adjoint operators,

$$\| e^{N_U K (e^{-A_P,y} - 1)} N_1 \Gamma_\prec \|_F \leq \sqrt{2} \| (P_f y + g_P(y)) N_1 \Gamma_\prec \|_F. \quad (3.81)$$

Since $P_f$ changes the number of phonons in $F_1$ at most by one, we can proceed by

$$\| (P_f y + g_P(y)) N_1 \Gamma_\prec \|_F \leq (\alpha^\delta + 1) \| (P_f y + g_P(y)) \Gamma_\prec \|_F \leq C \alpha^\delta \| y \|_F \| P_f \Gamma \|_F + \alpha |y|^3 \) \leq C \alpha^\delta \| C(n) \sqrt{K} |y| + \alpha |y|^3 \), \quad (3.82)$$

where we used $1 \leq \alpha^\delta$ and (3.55) in the second step and Lemma 3.13 in the third one. We conclude via Corollary 3.4 that

$$|\mathcal{E}_{12}^{\Gamma}| \leq \frac{C}{\alpha^2} \int dy \, H(y) \| C(n) \sqrt{K} |y| + \alpha |y|^3 \) \| p_\alpha(y) \, n_{\delta,\eta}(y) + C_\delta \alpha^{-12} \leq C_\delta C(n) \sqrt{K} \alpha^{-6+(12+4m)} \delta. \quad (3.83)$$

**Term $\mathcal{E}_2^{\Gamma}$**. Here we start with

$$\mathcal{E}_2^{\Gamma} = \alpha^{-1} \int dy \, \langle \mathcal{G}_{1,y}^{0} | L_{1,y} W(\alpha w_{P,y}) \mathcal{G}_{1,y}^{0} \rangle_F$$

$$+ \alpha^{-1} \int dy \, \langle \mathcal{G}_{1,y}^{0} | L_{1,y} (e^{A_P,y} - 1) W(\alpha w_{P,y}) \mathcal{G}_{1,y}^{0} \rangle_F = \mathcal{E}_{21}^{\Gamma} + \mathcal{E}_{22}^{\Gamma}, \quad (3.84)$$

where

$$L_{1,y} = \langle \psi | \phi(h + \varphi_P) T_y \psi \rangle_{L^2} = \phi(l_y) + \pi(j_y) \quad (3.85)$$

with

$$l_y = H(y) \varphi + \langle \psi | h T_y \psi \rangle_{L^2}, \quad j_y = H(y) \xi_P, \quad (3.86)$$

and $\xi_P$ defined in (2.33). The proof of the following lemma is given in [18, Lemma 3.17].

**Lemma 3.18.** For $k = 0, 1$ and for all $n \in N_0$,

$$\sup_y \| \nabla^k l_y \|_{L^2} < \infty, \quad \int |y|^n \| \nabla^k l_y \|_{L^2} \, dy < \infty. \quad (3.87)$$

Note that, by Lemma 3.5, $j_y$ clearly has these properties as well. In [18, Eqs. (3.125) and
It was also shown that
\[ \|w_{0,y} - y \nabla \varphi\|_{L^2} + \|\frac{1}{2} y \nabla \varphi\|_{L^2} \leq C y^2. \] (3.88)

We proceed by writing \( \mathcal{E}_{21}^\Gamma = \mathcal{E}_{21}^{\Gamma,0} + \mathcal{E}_{21}^{\Gamma,P} \) with

\[ \mathcal{E}_{21}^{\Gamma,0} = \alpha^{-1} \int dy \langle \gamma | \phi(t_0^0) W(\alpha \tilde{w}_{P,y}) \gamma \rangle_x + \alpha^{-1} \int dy \langle \gamma | \phi(t_0^1) W(\alpha \tilde{w}_{P,y}) \gamma \rangle_x \] (3.89a)
\[ \mathcal{E}_{21}^{\Gamma,P} = \alpha^{-1} \int dy \langle \gamma | \pi(j_y) W(\alpha \tilde{w}_{P,y}) \gamma \rangle_x, \] (3.89b)

where we used \( \Gamma = \bigcup_K^\dagger \gamma \) and applied Lemma 3.9 together with \( j_y \in \text{Ran}(\Pi_0) \), cf. (2.33) and (3.86). The three terms are estimated separately.

For the first term, and also for later use, let us note the following identity. For any \( x \mapsto g_x^0 \) with \( g_x^0 \in \text{Ran}(\Pi_0) \) for all \( x \in \mathbb{R}^3 \) and \( \Psi, \Phi \in L^2(\mathbb{R}^3) \otimes \mathcal{F}_1 \), we have

\[ \frac{1}{\alpha} \langle \Psi | \phi(g_0^0) W(\alpha \tilde{w}_{P,y}) \Phi \rangle_{\mathcal{F}_x} = \frac{1}{\alpha} \langle \Psi | a(g_0^0) e^{it(\alpha \tilde{w}_{P,y})} W(\alpha \tilde{w}_{P,y}) \Phi \rangle_{\mathcal{F}_x} e^{-\frac{1}{2} \|\alpha \tilde{w}_{P,y}\|_{L^2}^2}, \]
\[ = \langle \Psi | g_0^0 | w_{P,y}^0 \rangle_{L^2} W(\alpha \tilde{w}_{P,y}) \Phi \rangle_{\mathcal{F}_x} e^{-\frac{1}{2} \|\alpha \tilde{w}_{P,y}\|_{L^2}^2}, \]
\[ = \langle \Psi | g_0^0 | w_{P,y}^0 \rangle_{L^2} W(\alpha \tilde{w}_{P,y}) \Phi \rangle_{\mathcal{F}_x}, \] (3.90)

where we used \( W(\alpha \tilde{w}_{P,y}) = W(\alpha w_{P,y}^0) W(\alpha \tilde{w}_{P,y}) \), \( a(g_0^0) \Psi = a(w_{P,y}^0) \Phi = 0 \) and the canonical commutation relations. Invoking this identity with \( \Psi = \Phi = g_x^0 \) and \( g_x^0 = l_y^0 \) (x-independent), we find \( \langle \gamma | \phi(l_y^0) W(\alpha \tilde{w}_{P,y}) \gamma \rangle_x = \langle l_y^0 | w_{P,y}^0 \rangle_{L^2} \langle \gamma | W(\alpha \tilde{w}_{P,y}) \gamma \rangle_x \), and thus we can apply Lemma 3.14 for \( \mathbf{X} = \langle l_y^0 | w_{P,y}^0 \rangle_{L^2} \) and \( \mathbf{Y} = 1 \) to bound the first term in (3.89a) as

\[ \left| \alpha^{-1} \int dy \langle \gamma | \phi(l_y^0) W(\alpha \tilde{w}_{P,y}) \gamma \rangle_x - \int dy \langle l_y^0 | w_{P,y}^0 \rangle_{L^2} n_{0,1}(y) \right| \leq C \int dy |\langle l_y^0 | w_{P,y}^0 \rangle_{L^2}| p_\alpha(y) n_{0,1}(y). \] (3.91)

Note that \( l_y^i(-z) = l_y^i(z), i = 0, 1 \), which is easily verified for \( l_y(z) \) and preserved by the projections \( \Pi^i \) as their kernels are even functions on \( \mathbb{R}^6 \). As discussed in Remark 3.1, \( n_{0,1}(y) \) is even, and similarly, \( \text{Im}(w_{P,y}) \) is an odd function on \( \mathbb{R}^6 \) since \( (y,z) \mapsto \text{Im}(w_{P,y})(z) \) is odd on this space. Hence we can conclude that

\[ \int dy \langle l_y^0 | \text{Im}(w_{P,y}) \rangle_{L^2} n_{0,1}(y) = 0. \] (3.92)

Moreover, we use \( \langle l_y^0 | \text{Re}(w_{P,y}) \rangle_{L^2} = \langle l_y^0 | w_{0,y}^0 \rangle_{L^2} \) since \( \text{Re}(w_{P,y}) = w_{0,y} \). The function

\[ v(y) := \langle l_y^0 | w_{0,y}^0 \rangle_{L^2} \] (3.93)
satisfies \( v \in L^1 \cap L^\infty \) since \( y \mapsto \|y\|_{L^2} \) does (see [18, Section 3.6]) and \( \|w_{0,y}\|_{L^2} \leq 2\|\varphi\|_{L^2} \). Using (3.88) we can thus estimate

\[
\left| v(y) + \frac{1}{2}\|y\nabla\varphi\|_{L^2}^2 \right| \leq C(|y|^3 + y^4). \tag{3.94}
\]

From this bound and from \( v \in L^1 \cap L^\infty \) it is also easy to deduce that \( \cdot |^{-2}v \in L^1 \cap L^\infty \). Coming back to (3.91) we write

\[
\int dy \ v(y)n_{0,1}(y) = \int dy \ v(y)e^{-\alpha^2\gamma y^2} + \int dy \ y^2|y|^{-2}v(y)(n_{0,1}(y) - e^{-\alpha^2\gamma y^2}) \tag{3.95}
\]

and apply Lemma 3.3 with \( g = \cdot |^{-2}v \) to estimate

\[
\left| \int dy \ y^2|y|^{-2}v(y)(n_{0,1}(y) - e^{-\alpha^2\gamma y^2}) \right| \leq C\alpha^{-6}. \tag{3.96}
\]

Using (3.94), the definition of \( \lambda = \frac{1}{\delta}\|\nabla \varphi\|_{L^2}^2 \) and \( \int y^2e^{-y^2}dy = \frac{\pi}{2}x^{-3/2} \), we further have

\[
\left| \int dy \ v(y)e^{-\alpha^2\gamma y^2} + \frac{3}{2\alpha^2} \left( \frac{\pi}{\lambda\alpha^2} \right)^{3/2} \right| \leq C\alpha^{-6}. \tag{3.97}
\]

In a similar way, we can estimate the error in (3.91) by

\[
\int dy \ |v(y)| \ p_\alpha(y) n_{0,1}(y) \leq C\alpha^{-6}, \tag{3.98}
\]

which concludes the analysis of the first term in \( E_{21}^{\Gamma,0} \).

For the second term, we apply Lemma 3.14 with \( X = \phi(t_y^1) \) and \( Y = 1 \) to find

\[
\alpha^{-1} \int dy \langle \gamma | \phi(t_y^1)W(\alpha\tilde{w}_{P,y})\gamma \rangle_x \leq C \int dy \|\phi(t_y^1)\gamma\|_x (1 + p_\alpha(y)) n_{0,1}(y), \tag{3.99}
\]

where we used that \( \langle \gamma | \phi(t_y^1)\gamma \rangle_x \leq C\|t_y^1\|_{L^2} \). Lemma 3.18 and Eq. (3.88) imply that \( y \mapsto |y|^{-2}\|t_y^1\|_{L^2} \in L^1 \cap L^\infty \). By Corollary 3.4 the expression on the r.h.s. is thus bounded by \( C\alpha^{-6} \).

Collecting all terms and invoking Proposition 3.16 gives the final estimate for (3.89a)

\[
E_{21}^{\Gamma,0} + \frac{3}{2\alpha^2} \|S_{P\Gamma}\|_x^2 \leq C(n, \varepsilon)\sqrt{K}\alpha^{-6+\varepsilon}. \tag{3.100}
\]

For the term \( E_{21}^{\Gamma,P} \) in (3.89b) we recall \( j_y \in \text{Ran}(\Pi_\varphi) \) and thus we can use (3.90) and apply Lemma 3.14 with \( X = \langle j_y | w_{0,y}^0 \rangle_{L^2} \) and \( Y = 1 \). This gives

\[
E_{21}^{\Gamma,P} \leq \int dy |\langle j_y^0 | w_{0,y}^0 \rangle_{L^2}| (1 + p_\alpha(y)) n_{0,1}(y). \tag{3.101}
\]
Using \( \|j_y\|_{L^2} \leq CH(y)|P|\alpha^{-2} \leq CH(y)\alpha^{-1} \) (since \( |P| \leq c\alpha \)) and \( \|w_{P,y}^0\|_{L^2} \leq C(|y| + |y|^3) \) as follows from Lemma 3.2, we obtain \( \mathcal{E}_2^{\Gamma,P} \leq C\alpha^{-6} \).

The term \( \mathcal{E}_2^{\Gamma} \) is estimated similarly as the term \( \mathcal{E}_{22} \) in [18, Section 3.6], with the result

\[
|\mathcal{E}_2^{\Gamma}| \leq C(n,\varepsilon)\sqrt{K}\alpha^{-6+\varepsilon}. \tag{3.102}
\]

Here, the only difference compared to [18] is that we use Lemmas 3.13 and 3.15 in appropriate places; we shall skip the details.

Combining the relevant estimates, we arrive at the statement of Proposition 3.17.

\[\square\]

### 3.8 Energy contribution \( \mathcal{G}^\Gamma \)

The energy contribution \( \mathcal{G}^\Gamma \) defined in (3.11b) is evaluated by the following proposition.

**Proposition 3.19.** Let \( V^{(n+1)}_K \) be defined as in (2.41) and \( H_K \) be defined by (2.13). For all \( \varepsilon > 0 \) and \( n \in \mathbb{N}_0 \) there exist constants \( C(n,\varepsilon) > 0 \) and \( \alpha_0 \geq 1 \) such that

\[
\begin{align*}
\left| \mathcal{G}^\Gamma - \frac{2}{\alpha^2} \langle \mathcal{G}^0\rangle \left( \|H_K - N_1\Gamma\|_F^2 \|S_P\Gamma\|_F^2 \right) \right| &\leq C(n,\varepsilon)\alpha^\varepsilon (\sqrt{K}\alpha^{-6} + K^{-1/2}\alpha^{-5}) \\
\end{align*}
\tag{3.103}
\]

for all normalized \( \Gamma \in V^{(n+1)}_K, |P| \leq \sqrt{2ML^P}\alpha, K \geq K_0 \) and \( \alpha \geq \alpha_0 \).

**Proof.** Using \( h^{\text{Pek}}\mathcal{G}_1^0 = 0 \) and \( N_1\mathcal{G}_1^0 = N_1\mathcal{G}_1^\Gamma \) we can decompose \( \mathcal{G}^\Gamma \) into the two terms

\[
\begin{align*}
\mathcal{G}^\Gamma &= -\frac{2}{\alpha^2} \int dy \text{Re} \langle \mathcal{G}^0\rangle \langle (\alpha^{-2}N_1 + \alpha^{-1}\phi(h. + \varphi_P))T_y e^{A_{P,y}}W(\alpha w_{P,y})\mathcal{G}^1\rangle_{\mathcal{F}} \\
&= \mathcal{G}^\Gamma_1 + \mathcal{G}^\Gamma_2, \\
\end{align*}
\tag{3.104}
\]

where the first term will contribute to the error while the second one provides an energy contribution of order \( \alpha^{-2} \).

Term \( \mathcal{G}^\Gamma_1 \). Using Lemma 3.15 this term can be treated in close analogy to the estimation of \( \mathcal{G}_1 \) in [18, Section 3.7]. This results in

\[
|\mathcal{G}^\Gamma_1| \leq C(\varepsilon)\alpha^{-6+\varepsilon}. \tag{3.105}
\]

Term \( \mathcal{G}^\Gamma_2 \). Here we start by writing

\[
\begin{align*}
\mathcal{G}^\Gamma_2 &= -\frac{2}{\alpha^2} \int dy \text{Re} \langle \mathcal{G}^0\rangle \langle \phi(h. + \varphi_P)T_y W(\alpha w_{P,y})\mathcal{G}^1\rangle_{\mathcal{F}} \\\n&\quad - \frac{2}{\alpha^2} \int dy \text{Re} \langle \mathcal{G}^0\rangle \langle \phi(h. + \varphi_P)T_y (e^{A_{P,y}} - 1)W(\alpha w_{P,y})\mathcal{G}^1\rangle_{\mathcal{F}} = \mathcal{G}^\Gamma_{21} + \mathcal{G}^\Gamma_{22}. \tag{3.106}
\end{align*}
\]

In the first term we insert \( 1 = \mathcal{U}_K^{\Gamma}\mathcal{U}_K \) next to \( \mathcal{G}^0_1 \) and bring \( \mathcal{U}_K^{\Gamma} \) to the right side of the inner
product. With $\mathbb{U}_K \mathcal{G}^0_\Gamma = \psi \otimes \gamma = \mathcal{G}^0_\gamma$ for some $\gamma \in \mathcal{F}_1$, (3.26c) and (3.42) this gives

$$
\mathcal{G}^\Gamma_{21} = -\frac{2}{\alpha^2} \int dy \text{Re} \langle \mathcal{G}^0_\gamma | \phi(h_+ + \varphi P) T_y W(\alpha \tilde{w}_{P,y}) u_\alpha R \phi(h_{K_y}^1) \mathcal{G}^0_\gamma \rangle_{\mathcal{H}}
$$

(3.107)

where the notation $\_\gamma$ is defined in (3.25a). Next we use $h_+ + \varphi P = h_1^1 + \varphi + h_0^0 + \xi P$ to write

$$
\mathcal{G}^\Gamma_{21} = -\frac{2}{\alpha^2} \int dy \text{Re} \langle \mathcal{G}^0_\gamma | \phi(h_1^1 + \varphi) T_y W(\alpha \tilde{w}_{P,y}) u_\alpha R \phi(h_{K_y}^1) \mathcal{G}^0_\gamma \rangle_{\mathcal{H}}
$$

$$
- \frac{2}{\alpha^2} \int dy \text{Re} \langle \mathcal{G}^0_\gamma | \phi(h_0^0 + \xi P) T_y W(\alpha \tilde{w}_{P,y}) u_\alpha R \phi(h_{K_y}^1) \mathcal{G}^0_\gamma \rangle_{\mathcal{H}}
$$

$$
= \mathcal{G}^\Gamma_{211} + \mathcal{G}^\Gamma_{212}.
$$

(3.108)

Since $h_1^1 + \varphi \in \text{Ran}(\Pi_1)$ for every $x \in \mathbb{R}^3$, we can apply Lemma 3.14 in the first term with

$$
X = X_y = P_\psi \phi(h_1^1 + \varphi) T_y u_\alpha R^{1/2}, \quad Y = R^{1/2} \phi(h_{K_y}^1) P_\psi
$$

(3.109)

and thus

$$
\left| \mathcal{G}^\Gamma_{211} + \frac{2}{\alpha^2} \int dy \text{Re} \langle \mathcal{G}^0_\gamma | X_y Y \mathcal{G}^0_\gamma \rangle_{\mathcal{H}} n_{0,1}(y) \right|
$$

$$
\leq \frac{2}{\alpha^3} \int dy n_{0,1}(y) \|X_y^1 \mathcal{G}^0_\gamma\|_{\mathcal{H}} \|Y \mathcal{G}^0_\gamma\|_{\mathcal{H}}.
$$

(3.110)

To estimate the error we use Lemma 3.7 to bound

$$
\|X_y^1 \mathcal{G}^0_\gamma\|_{\mathcal{H}} = \|R^{1/2} \phi(h_{1,y}^1 + \varphi) u_\alpha T_{-y} P_\psi \mathcal{G}^0_\gamma\|_{\mathcal{H}} \leq C f_{2,\alpha}(y) \|(N + 1)^{1/2}\|_{\mathcal{H}}
$$

(3.111a)

$$
\|Y \mathcal{G}^0_\gamma\|_{\mathcal{H}} = \|R^{1/2} \phi(h_{K_y}^1) P_\psi \mathcal{G}^0_\gamma\|_{\mathcal{H}} \leq C \|(N + 1)^{1/2}\|_{\mathcal{H}}
$$

(3.111b)

with $f_{2,\alpha}(y) = \|\nabla u_\alpha T_{-y} P_\psi\|_{o_p} + \|T_{-y} u_\alpha P_\psi\|_{o_p}$. From [18, Eq. (3.183)] we know that

$$
\|f_{2,\alpha}\|_{L^\infty} \leq C, \quad \|n \cdot f_{2,\alpha}\|_{L^1} \leq C(n) \alpha^{2+n} \quad \text{for all } n \in \mathbb{N}_0,
$$

(3.112)

and thus we can apply Corollary 3.4 to estimate the r.h.s. in (3.110), the result being

$$
\left| \mathcal{G}^\Gamma_{211} + \frac{2}{\alpha^2} \int dy \text{Re} \langle \mathcal{G}^0_\gamma | X_y Y \mathcal{G}^0_\gamma \rangle_{\mathcal{H}} n_{0,1}(y) \right| \leq C \alpha^{-6}.
$$

(3.113)

In the remaining term we use $\gamma = \mathbb{U}_K \Gamma$ such that

$$
\langle \mathcal{G}^0_\gamma | X_y Y \mathcal{G}^0_\gamma \rangle_{\mathcal{H}} = \langle \mathcal{G}^0_\Gamma | \phi(h_1^1 + \varphi) T_y u_\alpha R \phi(h_{K_y}^1) \mathcal{G}^0_\Gamma \rangle_{\mathcal{H}}.
$$

(3.114)
By the same argument as in the computation of \( G_{211} \) in [18, Eqs. (3.172)–(3.187)], one finds

\[
\left| G_{211}^\Gamma - \frac{1}{\alpha^2} \langle \Gamma | (\mathbb{H}_K - N_1) \Gamma \rangle_x \| S_P \Gamma \|^2_x \right| \leq C(n, \varepsilon) \alpha^6 \left( \sqrt{K} \alpha^{-6} + K^{-1/2} \alpha^{-5} \right).
\] (3.115)

To estimate \( G_{212}^\Gamma \) we first note that \( h^0 + \xi_P \in \text{Ran}(\Pi_0) \) (hence \( h^0 + \xi_P = h^0 + \xi_P \), cf. (3.25a)). From (3.90) for \( g^0_x = h^0 + \xi_P \), \( \Psi = P_\psi \mathcal{G}^0 \) and \( \Phi = T_y u_\alpha R \phi(h_K^1) \mathcal{G}^0 \gamma \) it follows that

\[
G_{212}^\Gamma = -\frac{2}{\alpha} \int dy \text{Re} \langle \mathcal{G}^0_\gamma | (h^0 + \xi_P | w^0_{P,y} \rangle L^2 T_y W(\alpha \hat{\omega}_{P,y} u_\alpha R \phi(h_K^1) \mathcal{G}^0_{\gamma}) \rangle_x.
\] (3.116)

Thus we can apply Lemma 3.14 with

\[
X = X_y = P_\psi \langle h^0 + \xi_P | w^0_{P,y} \rangle L^2 T_y u_\alpha R^{1/2}, \quad Y = R^{1/2} \phi(h_K^1) P_\psi,
\] (3.117)

to obtain

\[
\left| G_{212}^\Gamma + \frac{2}{\alpha} \int dy \text{Re} \langle \mathcal{G}^0_\gamma | (h^0 + \xi_P | w^0_{P,y} \rangle L^2 T_y W(\alpha \hat{\omega}_{P,y} u_\alpha R \phi(h_K^1) \mathcal{G}^0_{\gamma}) \rangle_x \right| n_0,1(y)
\]

\[
\leq \frac{C}{\alpha^2} \int dy \| X_y^\dagger \mathcal{G}^0_\gamma \|_x \| Y \mathcal{G}^0_\gamma \|_x p_\alpha(y) n_0,1(y).
\] (3.118)

To bound the norm

\[
\| X_y^\dagger \mathcal{G}^0_\gamma \|_x = \| R^{1/2} \langle w^0_{P,y} | h^0_y + \xi_P \rangle L^2 T_y u_\alpha T_y P_\psi \|_{op}
\] (3.119)

we write out the inner product, use the triangle inequality and Cauchy–Schwarz and then apply Corollary 3.8,

\[
\| X_y^\dagger \mathcal{G}^0_\gamma \|_x \leq \int dz |w^0_{P,y}(z)| \left( \| R^{1/2} h^0_{-y}(z) u_\alpha T_y P_\psi \|_{op} + |\xi_P(x)| \| R^{1/2} u_\alpha T_y P_\psi \|_{op} \right)
\]

\[
\leq \| w^0_{P,y} \|_{L^2} \left( \int dz \| R^{1/2} h^0_{-y}(z) u_\alpha T_y P_\psi \|_{op}^2 \right)^{1/2} + \| \xi_P \|_2 \| R^{1/2} u_\alpha T_y P_\psi \|_{op}
\]

\[
\leq C \| w^0_{P,y} \|_{L^2} (1 + \| \xi_P \|_2) f_{2,\alpha}(y)
\] (3.120)

with \( f_{2,\alpha}(y) \) as defined before (3.112). Using \( \| \xi_P \|_{L^2} \leq C\alpha^{-1} \) and invoking Lemma 3.2 thus gives \( \| X_y^\dagger \mathcal{G}^0_\gamma \|_x \leq C(|y| + |y|^3) f_{2,\alpha}(y) \). Using in addition (3.111b) and (3.112), we can thus bound the error in (3.118) by means of Corollary 3.4. This leads to

\[
\left| G_{212}^\Gamma + \frac{2}{\alpha} \int dy \text{Re} \langle \mathcal{G}^0_\gamma | X_y Y \mathcal{G}^0_\gamma \rangle_x \right| n_0,1(y) \leq \frac{C}{\alpha^6}.
\] (3.121)

The remaining term on the l.h.s. only contributes to the error. To see this, we replace the weight function by the Gaussian, i.e. we use (3.120), (3.111b) and (3.112) in order to be able
to apply Lemma 3.3
\[
\left| \frac{2}{\alpha} \int dy \, \text{Re} \langle \gamma | X(y) Y \gamma \rangle_{\mathcal{H}} (n_{0,1}(y) - e^{-\lambda y^2}) \right| \lesssim \frac{C}{\alpha^6}. \tag{3.122}
\]

Then we write \( X_y = X_y^{(1)} + X_y^{(2)} + X_y^{(3)} \) with
\[
X_y^{(1)} = P_y \langle h^0_{K,-} | w_{P_y}^0 \rangle_{L^2} u_\alpha R^{1/2} \tag{3.123a}
\]
\[
X_y^{(2)} = P_y \langle h^0_0 - h^0_{K,-} + \xi_P | w_{P_y}^0 \rangle_{L^2} T_y u_\alpha R^{1/2} \tag{3.123b}
\]
\[
X_y^{(3)} = P_y \langle h^0_{K,-} | w_{P_y}^0 \rangle_{L^2} (T_y - 1) u_\alpha R^{1/2}. \tag{3.123c}
\]

The contribution from \( X_y^{(1)} \) is zero since \( n_{0,1}(y) \) is an even function whereas \( \text{Re}(w_{P,y}^0)(z) = -\text{Re}(w_{P,y}^0)(z) \), cf. Remark 3.1, and thus
\[
\text{Re}(\gamma | X_y^{(1)} Y \gamma \rangle_{\mathcal{H}} = \text{Re}(\gamma | P_y \langle h^0_{K,-} | \text{Re}(w_{P,y}^0) \rangle_{L^2} u_\alpha R^{1/2} Y \gamma \rangle_{\mathcal{H}}
\]
\[
= - \text{Re}(\gamma | P_y \langle h^0_0 | w_{P,y}^0 \rangle_{L^2} u_\alpha R^{1/2} Y \gamma \rangle_{\mathcal{H}}
\]
\[
= - \text{Re}(\gamma | X_y^{(1)} Y \gamma \rangle_{\mathcal{H}}. \tag{3.124}
\]

where we used that the part involving \( \text{Im}(w_{P,y}^0) \) vanishes because of the real part in front of the inner product. For the second term we proceed with Cauchy–Schwarz and (3.111b)
\[
\left| \frac{2}{\alpha} \int dy \, \text{Re} \langle \gamma | X_y^{(2)} Y \gamma \rangle_{\mathcal{H}} e^{-\lambda y^2} \right| \lesssim \frac{C}{\alpha^5} \int dy \frac{||Y||_\mathcal{H} ||(X_y^{(2)})^\dagger \gamma||_{\mathcal{H}} e^{-\lambda y^2}} \tag{3.125}
\]

and bound the remaining norm similarly as in (3.120) by
\[
||x^{(2)}||_\mathcal{H} \leq \|R^{1/2} \langle w_{P,y}^0 | h^0_{K,-} - h^0_{K,-} + \xi_P \rangle_{L^2} T_y \|_{o_p}
\]
\[
\leq C \|w_{P,y}^0\|_{L^2} (K^{-1/2} + ||\xi_P||_2 f_{2,y}(y) \leq C (|y| + |y|^3) (K^{-1/2} + \alpha^{-1}) \tag{3.126}
\]

where we used \( f_{2,y}(y) \leq C \) and \( ||\xi_P||_{L^2} \leq C \alpha^{-1} \). Thus by Corollary 3.4
\[
\left| \frac{2}{\alpha} \int dy \, \text{Re} \langle \gamma | X_y^{(2)} Y \gamma \rangle_{\mathcal{H}} e^{-\lambda y^2} \right| \leq C \alpha^{-5} (K^{-1/2} + \alpha^{-1}). \tag{3.127}
\]

In the last term we insert \( T_y - 1 = \int_0^1 ds T_{sy}(y \nabla) \), such that
\[
\left| \text{Re} \langle \gamma | X_y^{(3)} Y \gamma \rangle_{\mathcal{H}} \right|
\]
\[
\leq \int_0^1 ds \left| \text{Re} \langle \gamma | P_y \langle h^0_{K,-} | w_{P,y}^0 \rangle_{L^2} T_{sy}(y \nabla) u_\alpha R^{1/2} Y \gamma \rangle_{\mathcal{H}} \right|
\]
\[
\leq C \sqrt{K} |y| \|w_{P,y}^0\|_{L^2} \|\nabla u_\alpha R^{1/2}\|_{o_p} \|Y \gamma \|_{\mathcal{H}} \leq C \sqrt{K} (y^2 + y^4) \tag{3.128}
\]

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where we used $\|h_{K,\gamma}\|_{L^2} \leq C\sqrt{K}$, $\|\nabla u_{\gamma} R^{1/2}\|_{op} \leq C$ and (3.111b). Again by Corollary 3.4

$$\left| \frac{2}{\alpha} \int \text{Re} \langle \mathcal{F}_y^{(3)} X_y \mathcal{Y}_y \rangle_{\mathcal{F}} \epsilon^{-\lambda^2 y^2} \right| \leq C\sqrt{K} \alpha^{-6}. \quad (3.129)$$

Combining all estimates, we arrive at the final bound for (3.116)

$$\mathcal{G}_{212}^\Gamma \leq C(K^{1/2}\alpha^{-6} + K^{-1/2}\alpha^{-5}). \quad (3.130)$$

The estimation for the remaining term $\mathcal{G}_{22}^\Gamma$ in (3.106) is somewhat lengthy, but works analogous, with some obvious modifications, to the bound for $\mathcal{G}_{22}$ in [18, Section 3.7]. We leave out the details and only state the result

$$|\mathcal{G}_{22}^\Gamma| \leq C(n, \varepsilon)\alpha^\varepsilon (K^{-1/2}\alpha^{-5} + \sqrt{K} \alpha^{-6}). \quad (3.131)$$

In view of (3.105), (3.115), (3.130) and (3.131), the proof of Proposition 3.19 is now complete.

3.9 Energy contribution $\mathcal{K}^\Gamma$

Recall (3.11c) for the definition of $\mathcal{K}^\Gamma$.

**Proposition 3.20.** Let $\mathcal{V}_K^{(n+1)}$ be defined as in (2.41) and $\mathbb{H}_K$ be defined by (2.13). For all $\varepsilon > 0$ and $n \in \mathbb{N}_0$ there exist constants $C(n, \varepsilon) > 0$ and $\alpha_0 \geq 1$ such that

$$\left| \mathcal{K}^\Gamma + \frac{1}{\alpha^2} \langle \Gamma| (\mathbb{H}_K - \mathbb{N}_1) \Gamma \rangle_{\mathcal{F}} \|S \Gamma\|_{\mathcal{F}} \right| \leq C(n, \varepsilon)\alpha^\varepsilon (\sqrt{K} \alpha^{-6} + K^{-1/2}\alpha^{-5}) \quad (3.132)$$

for all normalized $\Gamma \in \mathcal{V}_K^{(n+1)}$, $|P| \leq \sqrt{2MLP}\alpha$, $K \geq K_0$ and $\alpha \geq \alpha_0$.

**Proof.** We split this contribution into three terms

$$\mathcal{K}^\Gamma = \frac{1}{\alpha^2} \int dy \langle \mathcal{F}_y^{(1)}| (h_{\text{Pek}} + \alpha^{-2}\mathbb{N} + \alpha^{-1}\phi(h, \varphi_P)) T_y e^{A_P(y)} W(\alpha w_{P,y}) \mathcal{F}_y^{(1)} \rangle_{\mathcal{F}}$$

$$= \mathcal{K}^\Gamma_1 + \mathcal{K}^\Gamma_2 + \mathcal{K}^\Gamma_3 \quad (3.133)$$

and note that $\mathcal{K}^\Gamma_1$ provides the energy contribution of order $\alpha^{-2}$.

**Term $\mathcal{K}^\Gamma_1$.** We start again by separating the main term as follows,

$$\mathcal{K}^\Gamma_1 = \frac{1}{\alpha^2} \int dy \langle \mathcal{F}_y^{(1)}| h_{\text{Pek}} T_y W(\alpha w_{P,y}) \mathcal{F}_y^{(1)} \rangle_{\mathcal{F}}$$

$$+ \frac{1}{\alpha^2} \int dy \langle \mathcal{F}_y^{(1)}| h_{\text{Pek}} T_y (e^{A_P(y)} - 1) W(\alpha w_{P,y}) \mathcal{F}_y^{(1)} \rangle_{\mathcal{F}} = \mathcal{K}^\Gamma_{11} + \mathcal{K}^\Gamma_{12}. \quad (3.134)$$
Inserting $\mathcal{G}_1 = u_\alpha R \phi(h_{K,\gamma}) P_\gamma \mathbb{U}_K \gamma$ for $\gamma \in \mathcal{F}_1^{(m)}$ we can write the first term as

$$\kappa_{11}^\Gamma = \frac{1}{\alpha^2} \int dy \langle \mathcal{G}_0^\Gamma | X_y W(\alpha \bar{w}_P \psi \bar{u}) \mathcal{Y} \mathcal{G}_0^\Gamma \rangle_{\mathcal{H}} \tag{3.135}$$

where

$$X_y = P_\gamma \phi(h_{K,\gamma}) R u_\alpha h_{Pek} T_y u_\alpha R^{1/2}, \quad Y = R^{1/2} \phi(h_{K,\gamma}) P_\psi. \tag{3.136}$$

An application of Lemma 3.14 leads to

$$\left| \kappa_{11}^\Gamma - \frac{1}{\alpha^2} \int dy \langle \mathcal{G}_0^\Gamma | X_y \mathcal{Y} \mathcal{G}_0^\Gamma \rangle_{\mathcal{H}} n_{0,1}(y) \right| \leq \frac{C}{\alpha^3} \int dy \| X_y \mathcal{G}_0^\Gamma \|_{\mathcal{H}} \| Y \mathcal{G}_0^\Gamma \|_{\mathcal{H}} p_\alpha(y) n_{0,1}(y). \tag{3.137}$$

Using [18, Eq. (3.222)] and Lemma 3.7, one further verifies that

$$\| X_y \mathcal{G}_0^\Gamma \|_{\mathcal{H}} \leq C f_{3,\alpha}(y) \| (N + 1)^{1/2} \gamma \|_{\mathcal{F}}, \quad \| Y \mathcal{G}_0^\Gamma \|_{\mathcal{H}} \leq C \| (N + 1)^{1/2} \gamma \|_{\mathcal{F}} \tag{3.138}$$

where

$$f_{3,\alpha}(y) = \| u_\alpha T_y u_\alpha \|_{op} + \| (\nabla u_\alpha) T_y u_\alpha \|_{op} + \| u_\alpha T_y (\nabla u_\alpha) \|_{op} + \| (\nabla u_\alpha) T_y (\nabla u_\alpha) \|_{op} \tag{3.139}$$

satisfies (see [18, Eq. (3.220)])

$$\| f_{3,\alpha} \|_{L^\infty} \leq 4 \quad \text{and} \quad \| \cdot \|^n_{f_{3,\alpha}} \|_{L^1} \leq C(n) \alpha^{3+n} \quad \text{for all} \ n \in \mathbb{N}_0. \tag{3.140}$$

With the aid of Corollary 3.4 we can thus bound the error in (3.137) to obtain

$$\left| \kappa_{11}^\Gamma - \frac{1}{\alpha^2} \int dy \langle \mathcal{G}_0^\Gamma | X_y \mathcal{Y} \mathcal{G}_0^\Gamma \rangle_{\mathcal{H}} n_{0,1}(y) \right| \leq \frac{C}{\alpha^6}. \tag{3.141}$$

In the inner product we transform again with the Bogoliubov transformation $\mathbb{U}_K$,

$$\langle \mathcal{G}_0^\Gamma | X_y \mathcal{Y} \mathcal{G}_0^\Gamma \rangle_{\mathcal{H}} = \langle \mathcal{G}_0^\Gamma | P_\psi \phi(h_{K,\gamma}) R u_\alpha h_{Pek} T_y u_\alpha R \phi(h_{K,\gamma}) P_\psi \mathcal{G}_0^\Gamma \rangle_{\mathcal{H}}. \tag{3.142}$$

In the estimation of the remaining expression, we can follow closely the argument from [18, Eqs. (3.210)–(3.225)]. We state the result without further details,

$$\left| \kappa_{11}^\Gamma + \frac{1}{\alpha^2} \langle (\mathbb{U}_K - N_1) \Gamma \rangle_{\mathcal{F}} \| S_F \Gamma \|_{\mathcal{F}}^2 \right| \leq C(n, \varepsilon) \sqrt{K \alpha^{-6+\varepsilon}}. \tag{3.143}$$

Using Lemma 3.15, the term $\kappa_{12}^\Gamma$ is estimated following the same steps from the bound of

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that at one. Moreover, it follows from Ker compact, and thus the spectrum of $H$ if and only if $\text{Supp} p \in \text{infinite dimensional subspace, the spectrum}$

$\sigma$ in view of Lemma 3.1 this completes the proof of Proposition 2.5.

Combining Propositions 3.17, 3.19 and 3.20, we have for all normalized $\Gamma \in V_K^{(n+1)}$ that

$$\left| \mathcal{E}^\Gamma + \mathcal{G}^\Gamma + \mathcal{K}^\Gamma \right| \leq \frac{\langle H ||K \Gamma \rangle_{H_x}^2}{\alpha^2} + \frac{3}{2\alpha^2} \leq C(n, \varepsilon) \alpha^\varepsilon \left( \frac{K^{-1/2} \alpha^{-5} + \sqrt{K} \alpha^{-6}}{\| S \Gamma \|^2_{H_x}} \right)$$

(3.146)

for all $|P| \leq \sqrt{2M_{\Gamma \Gamma}} \alpha$, $K \geq K_0$ and $\alpha \geq \alpha_0$. Applying Proposition 3.16 for $K \leq \alpha$ and $\alpha \geq \alpha(n)$ with $\alpha(n)$ large enough, we further obtain $\| S \Gamma \|^2_{H_x} \geq C \alpha^{-3}$ for some constant $C > 0$. Hence the right side in (3.146) is bounded by $C(n, \varepsilon) \alpha^\varepsilon (K^{-1/2} \alpha^{-2} + K^{1/2} \alpha^{-3})$. In view of Lemma 3.1 this completes the proof of Proposition 2.5.

### 3.10 Finishing the proof of Proposition 2.5

Proof of Proposition 2.5 follows from combining (3.143), (3.144) and (3.145).

### 4 Proofs of Auxiliary Lemmas

**Proof of Lemma 2.2.** For the proof of Items (i) – (iv) see [18, Lemma 2.2].

To show (v), first note that because of (iii) the operator $1 - H_{K}^{\text{Pek}} \geq 0$ is trace-class, hence compact, and thus the spectrum of $H_{K}^{\text{Pek}}$ below one is purely discrete and possibly accumulates at one. Moreover, it follows from $\text{Ker}(R^{1/2}) = \text{Span}\{\psi\}$, $\psi > 0$ and

$$\langle v \rangle (1 - H_{K}^{\text{Pek}}v \rangle L^2 = 4 \left\| R^{1/2} \int dy \psi \langle y \rangle \langle \psi \rangle \right\|_{L^2}^2$$

(4.1)

that $v \in \text{Ker}(1 - H_{K}^{\text{Pek}})$ if and only if $\int dy \psi \langle y \rangle \langle \psi \rangle = 0$ for all $x \in \mathbb{R}^3$. This is the case if and only if $\text{Supp}(\hat{\psi}) \subset [K, \infty)$. Since $\{v \in L^2(\mathbb{R}^3) : \text{Supp}(\hat{\psi}) \subset [0, K]\}$ corresponds to an infinite dimensional subspace, the spectrum $\sigma(H_{K}^{\text{Pek}}) \cap (0, 1)$ consists in fact of infinitely many eigenvalues (of finite multiplicity) with accumulation point at one.

The bound $|\lambda_{K}^{(n)} - \lambda_{K}^{(n)}| \leq CK^{-1/2}$, $n \in \mathbb{N}_0$, follows from the min-max principle in combination with $\langle \psi (H_{K}^{\text{Pek}} - H_{K}^{\text{Pek}}v \rangle L^2 \leq CK^{-1/2}$ for $v \in \text{Ran}(\Pi_{1})$. The latter has been shown in [18, Proof of Lemma 2.2].

To show (vi), we write $\langle 1 - \lambda_{K}^{(n)} \rangle^{1/2} u_{K}^{(n)} = (1 - H_{K}^{\text{Pek}})^{1/2} u_{K}^{(n)}$ and use (iv) to obtain

$$\langle 1 - \lambda_{K}^{(n)} \rangle \| \nabla u_{K}^{(n)} \|_{L^2}^2 \leq \| (-i\nabla)(1 - H_{K}^{\text{Pek}})^{1/2} \|_{\text{op}}^2 \leq \| (-i\nabla)(1 - H_{K}^{\text{Pek}})^{1/2} \|_{\text{hs}}^2 \leq CK.$$  

(4.2)
Proof of Lemma 2.6. We argue by contradiction and assume that \( \{S_P \Gamma^{(j)}_K\}_{j=0}^n \) are linearly dependent, meaning that there is a set of complex coefficients \( (c_j)_{j=0}^n \) with \( \max_{0 \leq j \leq n} |c_j| > 0 \) such that

\[
0 = \sum_{j=0}^n c_j S_P \Gamma^{(j)}_K. \tag{4.3}
\]

By Proposition 3.16 together with \( K \leq \alpha \) and \( \langle \Gamma^{(i)}_K | \Gamma^{(j)}_K \rangle_x = \delta_{ij} \), we have

\[
\left| \langle S_P \Gamma^{(i)}_K | S_P \Gamma^{(j)}_K \rangle_x - \delta_{ij} \left( \frac{\pi}{\lambda \alpha^2} \right)^{3/2} \right| \leq C(n, \varepsilon) \alpha^{-\frac{7}{2}+\varepsilon}. \tag{4.4}
\]

After taking the inner product of (4.3) with \( S_P \Gamma^{(\ell)}_K \) where \( \ell \) is such that \( |c_{\ell}| \geq |c_j| \) for all \( 1 \leq j \leq n \), and dividing by \( |c_{\ell}| \), we find

\[
\| S_P \Gamma^{(\ell)}_K \|^2_x \leq \sum_{j=0}^n \left| \langle S_P \Gamma^{(i)}_K | S_P \Gamma^{(j)}_K \rangle_x \right|. \tag{4.5}
\]

Invoking (4.4) it follows that

\[
\left( \frac{\pi}{\lambda \alpha^2} \right)^{3/2} - C(n, \varepsilon) \alpha^{-\frac{7}{2}+\varepsilon} \leq C(n, \varepsilon) n \alpha^{-\frac{7}{2}+\varepsilon}, \tag{4.6}
\]

which, for \( \varepsilon < \frac{1}{2} \) and \( \alpha \geq \alpha(n) \) with \( \alpha(n) \) large enough, is a contradiction. Hence, the set \( \{S_P \Gamma^{(j)}_K\}_{j=0}^n \) is linearly independent and its linear span has dimension \( n + 1 \). \qed

Proof of Lemma 3.13. Let \( p := -i \nabla \) and \( \lambda^{(n)}_K \), \( n \in \mathbb{N}_0 \), as in (2.38). As explained in Section 2.2, the tuple \( \lambda^{(n)}_K \) has maximal length \( |J^{(n)}_K| \leq m \) and consists of numbers from \( \{1, \ldots, n\} \), thus we can write \( J^{(n)}_K = \{j_1, \ldots, j_m\} \) with \( m \leq m \) and \( 1 \leq j_\ell \leq n \) for all \( 1 \leq \ell \leq m \). From [18, Lemma 3.14] we know that

\[
\| P_f \bar{u}_K \Omega \|_x \leq C \sqrt{K}. \tag{4.7}
\]

By unitarity of \( U_K \), we can thus estimate

\[
\| P_f \Gamma^{(n)}_K \|_x = \| (U_K P_f U_K^\dag) a^\dag(u_{j_1}^{(j_1)}) \ldots a^\dag(u_{j_m}^{(j_m)}) \Omega \|_x \leq \| a^\dag(u_{j_1}^{(j_1)}) \ldots a^\dag(u_{j_m}^{(j_m)}) (U_K P_f U_K^\dag) \Omega \|_x + \| U_K P_f U_K^\dag a^\dag(u_{j_1}^{(j_1)}) \ldots a^\dag(u_{j_m}^{(j_m)}) \|_x \leq C_m \sqrt{K} + \| [U_K P_f U_K^\dag, a^\dag(u_{j_1}^{(j_1)}) \ldots a^\dag(u_{j_m}^{(j_m)})] \Omega \|_x. \tag{4.8}
\]

where we used (3.21), \( \| u^{(j_i)}_K \|_{L^2} = 1 \), \( U_K P_f U_K^\dag \Omega \in \mathcal{F}^{(\leq2)} \) and (4.7). In the second term we use
Lemma 2.2. To bound the first summand, recall that $u_K$.

We proceed with bounding the first part of the commutator with $C$ and $r$, where $g_K$ is a suitable ONB of $L^2(\mathbb{R}^d)$. The first term is zero by rotational invariance (see also the proof of [18, Lemma 3.14]). With this we evaluate the commutator applied to the vacuum state as

$$[U_K P_j U_K^\dagger, a^\dagger(u_K^{(j_1)}) \ldots a^\dagger(u_K^{(j_m)})]\Omega = \mathcal{C}_1 + \mathcal{C}_2$$

(4.10)

with

$$\mathcal{C}_1 = \sum_{k,l} \left\langle g_k | (A_K p A_K + B_K p B_K) g_l \right\rangle_{L^2} \left[ a^\dagger(g_k) a(g_l), a^\dagger(u_K^{(j_1)}) \ldots a^\dagger(u_K^{(j_m)}) \right] \Omega$$

$$= \sum_{\ell=1}^m \left( \prod_{k=1}^m a^\dagger(u_K^{(j_k)}) \right) a^\dagger((A_K p A_K + B_K p B_K) u_K^{(j_\ell)}) \Omega,$$

(4.11)

and $\mathcal{C}_2 = 0$ for $m \in \{0, 1\}$ while

$$\mathcal{C}_2 = \sum_{k,l} \left\langle g_k | B_K p A_K g_l \right\rangle_{L^2} \left[ a(g_k) a(g_l), a^\dagger(u_K^{(j_1)}) \ldots a^\dagger(u_K^{(j_m)}) \right] \Omega$$

$$= \sum_{\ell=1}^m a(A_K p B_K u_K^{(j_\ell)}) \left( \prod_{k=1}^m a^\dagger(u_K^{(j_k)}) \right) \Omega \quad \text{for } m \geq 2.$$  

(4.12)

We proceed with bounding the first part of the commutator

$$\|\mathcal{C}_1\|_F \leq C_m \sum_{\ell=1}^m \left( \|A_K p A_K u_K^{(j_\ell)}\|_{L^2} + \|B_K p B_K u_K^{(j_\ell)}\|_{L^2} \right),$$

(4.13)

where the second summand is bounded by $\|B_K p B_K\|_{op} \leq \|B_K\|_{HS} \|p B_K\|_{HS} \leq C K^{1/2}$, cf. Lemma 2.2. To bound the first summand, recall that $u_K^{(j_\ell)}$ is a normalized eigenfunction of $H_K^{\text{Pek}}$ with eigenvalue $1 > \lambda_K^{(j_\ell)} \geq \beta$, hence also an eigenfunction of $A_K$ whose eigenvalue is uniformly bounded in $K$ and $j_\ell$, see (2.19b). By Lemma 2.2 we obtain

$$\|A_K p A_K u_K^{(j_\ell)}\|_{L^2} \leq C \|p A_K u_K^{(j_\ell)}\|_{L^2} \leq C \|p u_K^{(j_\ell)}\|_{L^2} \leq C \sqrt{K} (1 - \lambda_K^{(j_\ell)})^{-1/2}. $$

(4.14)

With $\lambda_K^{(j_n)} \leq \lambda_K^{(n)}$ as $j_\ell \leq n$, we can combine the bounds to

$$\|\mathcal{C}_1\|_F \leq C \sqrt{K} (1 - \lambda_K^{(n)})^{-1/2}. $$

(4.15)
We proceed (for $m \geq 2$) with
\[
\|e_2\|_F \leq \sum_{\ell=1}^{m} \|a(A_K b K u^{(i)}_K) \left( \prod_{k=1, k \neq \ell}^{m} a^{(i)}(u^{(i)}_K) \right) \Omega \|_F \\
\leq C_m \sum_{\ell=1}^{m} \|A_K b K u^{(i)}_K \|_{L^2} \leq C_m \|b K\|_{HS} \leq C_m \sqrt{K},
\]
and thus, in combination with (4.8), we have
\[
\|P_f \Gamma^{(n)}_K\|_F \leq C \sqrt{K} (1 - \lambda_K^{(n)})^{-1/2}.
\]
for all $n \in \mathbb{N}_0$ and $K \geq K_0$.

Next let $\Gamma = \sum_{j=0}^{n} c_j \Gamma^{(j)}_K$ with $\sum_{j=0}^{n} |c_j|^2 = 1$, and use (4.17) to estimate
\[
\|P_f \Gamma\|_F^2 \leq C \sqrt{K} \sum_{j=0}^{n} |c_j|(1 - \lambda_K^{(j)})^{-1/2} \leq C \sqrt{K} \sqrt{n} + 1(1 - \lambda_K^{(n)})^{-1/2}
\]
where we used $\lambda_K^{(j)} \leq \lambda_K^{(n)}$ for $j \leq n$ and $\sum_{j=0}^{n} |c_j| \leq \sqrt{n + 1}$. The last factor is bounded by
\[
\frac{1}{1 - \lambda_K^{(n)}} \leq \frac{1}{1 - \lambda_{\infty}^{(n)}} \left( 1 + \frac{\lambda_{\infty}^{(n)} - \lambda_K^{(n)}}{1 - \lambda_K^{(n)}} \right)^{-1} \leq \frac{2}{1 - \lambda_{\infty}^{(n)}}
\]
for all $n \in \mathbb{N}_0$ and $K \geq K(n)$ for large enough $K(n)$, where we used Lemma 2.2 (vii). This completes the proof of the lemma. \hfill \Box

**Proof of Lemma 3.14.** With (3.14) and (3.12a) – (3.12d), we have
\[
\langle \varphi_\gamma^0 | X W(\alpha w_{P_y}) Y \varphi_\xi^0 \rangle_F = \langle \varphi_\gamma^0 | X e^{(-a(\alpha w_{P_y}) e^{(-a(\alpha w_{P_y})) Y \varphi_\xi^0} \rangle_F \rangle_{n_0,1}(y) \\
= \langle \varphi_\gamma^0 | Y \varphi_\xi^0 \rangle_F \rangle_{n_0,1}(y) + \langle \varphi_\gamma^0 | X (e^{(-a(\alpha w_{P_y}) e^{(-a(\alpha w_{P_y})) - 1}) Y \varphi_\xi^0 \rangle_F \rangle_{n_0,1}(y)
\]
since $X^\dagger \varphi_\gamma^0$ and $Y \varphi_\xi^0$ correspond to the vacuum in the $F_0$ component. To estimate the error, we write
\[
\langle \varphi_\gamma^0 | X (e^{(-a(\alpha w_{P_y}) e^{(-a(\alpha w_{P_y})) - 1}) Y \varphi_\xi^0 \rangle_F \\
= \langle e^{(-a(\alpha w_{P_y})} X^\dagger \varphi_\gamma^0 | (e^{(-a(\alpha w_{P_y}) - 1}) Y \varphi_\xi^0 \rangle_F + \langle (e^{(-a(\alpha w_{P_y})} - 1) X^\dagger \varphi_\gamma^0 | Y \varphi_\xi^0 \rangle_F,
\]
truncate the Taylor expansion of the exponential series at order $m + 2$ (all other terms vanish since $X^\dagger \varphi_\gamma^0, Y \varphi_\xi^0 \in L^2(\mathbb{R}^3) \otimes F_1^{(\leq m+2)})$, and apply Cauchy–Schwarz. We show the details for the first term (the second term works the same way)
\[
|\langle e^{(-a(\alpha w_{P_y})} X^\dagger \varphi_\gamma^0 | (e^{(-a(\alpha w_{P_y}) - 1) Y \varphi_\xi^0 \rangle_F|
\]
Next we use (3.21) together with \( \|a(\alpha \hat{w}_{P,y})\|_{L^2} \leq C \alpha^{-1}(1 + \alpha^2 y^2) \), cf. Lemma 3.2, to obtain

\[
(4.22) \leq \sum_{k=0}^{m+2} \sum_{\ell=1}^{m+2} (C \alpha^{-1})^{k+\ell} (1 + \alpha^2 y^2)^{k+\ell} \|N^{k/2} X \nabla_y^0 \|_F \|N^{\ell/2} Y \nabla_\xi^0 \|_F \leq \alpha^{-1} \sum_{k=0}^{m+2} \sum_{\ell=1}^{m+2} \frac{C^{k+\ell} (m+2)^{k+\ell}}{\ell!} (1 + \alpha \|y\|)^{2(k+\ell)} \|X \nabla_y^0 \|_F \|Y \nabla_\xi^0 \|_F \leq C \alpha^{-1} p_\alpha(y) \|X \nabla_y^0 \|_F \|Y \nabla_\xi^0 \|_F
\]

with \( p_\alpha(y) = 1 + (\alpha \|y\|)^{4m+8} \), where we used \( \alpha \geq 1 \).

**Proof of Lemma 3.15.** Using (3.2) and \( e^{-\kappa N} a^\dagger(f)e^{\kappa N} = a^\dagger(e^{-\kappa} f) \) one finds

\[
e^{-\kappa N} W(\alpha \hat{w}_{P,y}) e^{\kappa N} = e^{\dagger(\alpha e^{-\kappa} \hat{w}_{P,y})} e^{-a(\alpha e^{-\kappa} \hat{w}_{P,y})} e^{-a(2\alpha \sinh(\kappa) \hat{w}_{P,y})} e^{-\frac{1}{2} \alpha^2 \|\hat{w}_{P,y}\|_{L^2}^2} = W(\alpha e^{-\kappa} \hat{w}_{P,y}) e^{-a(2\alpha \sinh(\kappa) \hat{w}_{P,y})} \exp \left( \frac{\alpha^2(e^{-2\kappa}-1)}{2} \|\hat{w}_{P,y}\|_{L^2}^2 \right),
\]

and thus

\[
\| e^{-\kappa N} W(\alpha \hat{w}_{P,y}) \gamma \|_F = \| e^{-a(2\alpha \sinh(\kappa) \hat{w}_{P,y})} e^{-\kappa N} \gamma \|_F \exp \left( \frac{\alpha^2(e^{-2\kappa}-1)}{2} \|\hat{w}_{P,y}\|_{L^2}^2 \right).
\]

For \( \kappa = 1/(16e^{b\alpha^\delta}) \) we can find an \( \alpha \)-independent constant \( \eta > 0 \) such that for \( \alpha \) large enough

\[
\exp \left( \frac{\alpha^2(e^{-2\kappa}-1)}{2} \|\hat{w}_{P,y}\|_{L^2}^2 \right) \leq \exp \left( -\frac{\eta \alpha^{2(1-b)}}{2} \|\hat{w}_{P,y}\|_{L^2}^2 \right) = n_{\delta,\eta}(y).
\]

For normalized \( \gamma \in F(\leq m) \), and since \( \|\hat{w}_{P,y}\|_{L^2} \leq C(\|y\| + \|y\|^3) \), cf. Lemma 3.2, we can further estimate

\[
\| e^{-a(2\alpha \sinh(\kappa) \hat{w}_{P,y})} e^{-\kappa N} \gamma \|_F \leq \sum_{k=0}^{m} \frac{2^k k!}{k!} \sinh(\kappa)^k \alpha^k \|\hat{w}_{P,y}\|_{L^2}^k \leq \sum_{k=0}^{m} \frac{C^{k} k! \sinh(\kappa)^k \alpha^k \|\hat{w}_{P,y}\|_{L^2}^k}{k!} \leq C p_\alpha(y)
\]

where we used \( \alpha \geq 1 \) in the last step.

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