On the Ultraviolet Limit of the Pauli-Fierz Hamiltonian in the Lieb-Loss Model

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Abstract

Two decades ago, Lieb and Loss [23] proposed to approximate the ground state energy of a free, nonrelativistic electron coupled to the quantized radiation field by the infimum $E_{\alpha, \Lambda}$ of all expectation values $\langle \phi_{el} \otimes \psi_{ph} | H_{\alpha, \Lambda} | \phi_{el} \otimes \psi_{ph} \rangle$, where $H_{\alpha, \Lambda}$ is the corresponding Hamiltonian with fine structure constant $\alpha > 0$ and ultraviolet cutoff $\Lambda < \infty$, and $\phi_{el}$ and $\psi_{ph}$ are normalized electron and photon wave functions, respectively. Lieb and Loss showed that $c_{\alpha}^{1/2} \Lambda^{3/2} \leq E_{\alpha, \Lambda} \leq c^{-1} \alpha^{2/7} \Lambda^{12/7}$ for some constant $c > 0$. In the present paper we prove the existence of a constant $C < \infty$, such that

$$\left| \frac{E_{\alpha, \Lambda}}{F[1] \alpha^{2/7} \Lambda^{12/7}} - 1 \right| \leq C \alpha^{4/105} \Lambda^{-4/105}$$

holds true, where $F[1] > 0$ is an explicit universal number. This result shows that Lieb and Loss’ upper bound is actually sharp and gives the asymptotics of $E_{\alpha, \Lambda}$ uniformly in the limit $\alpha \to 0$ and in the ultraviolet limit $\Lambda \to \infty$.

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I Introduction and Result

Soon after the discovery of quantum mechanics almost a century ago by Heisenberg and Schrödinger, the quantization of the radiation field was formulated by Born, Heisenberg, and Jordan and by Dirac \[11, 13\], and about seventy years ago quantum electrodynamics (QED) was formulated by Feynman, Schwinger, Tomonaga, and Dyson \[14, 15, 23, 28\], laying the foundation to answer the question whether light rays consisted of particles or waves that was open for several centuries. Besides being conceptually satisfying, QED is one of the most successful theories with quantitative predictions that match experimental data by more than eight decimals.

In spite of its success for applications, however, QED is still lacking essential parts of its mathematical foundation to this very day. Namely, all known formulations require unphysical regularizations at large, ultraviolet, and/or small, infrared, photon energies. While considerable progress has been made in the past three decades on the construction of the infrared limit, i.e., the construction of a theory without regularization at small photon energies \[6, 7, 18, 9, 5\], the construction of the ultraviolet limit is wide open. This difficult problem has been tackled from several angles, e.g., by replacing the fully interacting model by effective mean-field theories of various kinds \[20, 16, 17\].

One approach among these is a simplifying variational model proposed by Lieb and Loss in 1999 \[23\]. Their starting point is the Pauli-Fierz Hamiltonian

$$ H_{\alpha, \Lambda} = \frac{1}{2} \left( i \nabla_x - \alpha^{1/2} \vec{A}\Lambda(x) \right)^2 + H_{ph} \tag{I.1} $$

of a nonrelativistic spinless particle (modelling the electron), minimally coupled to the quantized radiation field. Here \(i \nabla_x\) is the (particle) momentum operator and \(\vec{A}\Lambda(x) = \int_{|k| \leq \Lambda} \left( e^{-ik \cdot x} a^*(k) + e^{ik \cdot x} a(k) \right) \frac{\epsilon(k) \, dk}{(2\pi)^{3/2} |k|^{1/2}}\) is the magnetic vector potential in Coulomb gauge and cut off for momenta larger than \(\Lambda\) in magnitude. Moreover, \(H_{ph} = \int |k| a^*(k) a(k) \, dk\) is the energy of the radiation field, and \(\alpha \approx 1/137\) is the (dimensionless) fine structure constant. The Hamiltonian \(H_{\alpha, \Lambda}\) is an unbounded, self-adjoint operator on the domain \(\text{dom}[H_{0,0}] \subseteq \mathcal{H}_{el} \otimes \mathcal{F}_{ph}\) of the noninteracting Hamiltonian \(H_{0,0} = \frac{1}{2} (-\Delta) \otimes 1_{ph} + 1_{el} \otimes H_{ph}\), see \[22, 21\], where \(\mathcal{H}_{el} = L^2(\mathbb{R}^3)\) is the space of square-integrable functions on \(\mathbb{R}^3\), and \(\mathcal{F}_{ph}\) is the boson Fock space over the space \(L^2(\mathbb{R}^3 \times \mathbb{Z}_2)\) of square-integrable, purely transversal vector fields, see Section II for a precise definition.

Note that \(H_{\alpha, \Lambda} \geq 0\) as a quadratic form. The (nonnegative) ground state of the energy of the system is characterized by the Rayleigh-Ritz variational principle as the infimum of all energy expectation values of the system,

$$ E_{gs}(\alpha, \Lambda) := \inf \left\{ \langle \Psi | H_{\alpha, \Lambda} \Psi \rangle \left| \Psi \in \mathcal{H}_{el} \otimes \mathcal{F}_{ph}, \| \Psi \| = 1 \right. \} . \tag{I.2} $$

1
Lieb and Loss proposed [23] to restrict the variation in (I.2) to wave functions of product form
\[ \Psi = \phi \otimes \psi, \]
with normalized \( \phi \in \mathcal{H}_{el} \) and \( \psi \in \mathcal{F}_{ph} \), to obtain a new approximation and upper bound \( E_{LL}(\alpha, \Lambda) \geq E_{gs}(\alpha, \Lambda) \) to the ground state energy, i.e.,
\[
E_{LL}(\alpha, \Lambda) := \inf \left\{ E_{\alpha,\Lambda}(\phi,\psi) \left| \begin{array}{c}
\phi \in \mathcal{H}_{el}, \psi \in \mathcal{F}_{ph}, \\
\| \phi \| = \| \psi \| = 1
\end{array} \right. \right\}, \tag{I.3}
\]
\[
E_{\alpha,\Lambda}(\phi,\psi) := \langle \phi \otimes \psi | H_{\alpha,\Lambda}(\phi \otimes \psi) \rangle. \tag{I.4}
\]
Note that upper bounds on the ground state energy are of particular interest here because the ultraviolet problem is about the understanding of the divergence of \( E_{gs}(\alpha, \Lambda) \to \infty \), as \( \Lambda \to \infty \). We henceforth refer to Eqs. (I.3)-(I.4) as the Lieb-Loss Model.

In Theorem 1.1 in [23] Lieb and Loss proved the existence of two universal constants \( C_1, C_2 \in \mathbb{R}^+ \) such that
\[
C_1 \alpha^{1/2} \Lambda^{3/2} \leq E_{LL}(\alpha, \Lambda) \leq C_2 \alpha^{2/7} \Lambda^{12/7}. \tag{I.5}
\]
This is the first of a series of results of Lieb and Loss in [23], extending their model to \( N \geq 2 \) fermions or bosons, taking the electron spin into account by studying the Pauli operator, and replacing the nonrelativistic kinetic energy by a pseudorelativistic one. Note that the Lieb-Loss model does not take the renormalization of the electron mass into account, and the actual value of \( E_{LL}(\alpha, \Lambda) \) is of limited quantitative use in physics. The significance of Eq. (I.5), however, lies in the fact that the formal perturbation expansion of the ground state about the photon vacuum yields \( E_{gs}(\alpha, \Lambda) \sim C\alpha \Lambda^2 \). In contrast, Eq. (I.5) says that this grossly overestimates the ground state energy; it is a warning sign that perturbation theory may not be adequate to construct the ultraviolet limit.

The main result of this paper is to derive the asymptotics of \( E_{LL}(\alpha, \Lambda), \) as \( \Lambda \to \infty \) or \( \alpha \to 0 \). We obtain an exact characterization of the ground state and ground state energy of the Lieb-Loss Model for any given \( \alpha > 0 \) and \( \Lambda \geq 1 \), in terms of an auxiliary classical functional. To formulate this precisely, we introduce
\[
\mathcal{F}_\beta(\phi) := \frac{1}{2} \| \vec{\nabla} \phi \|_2^2 + \| \phi \|_1, \tag{I.6}
\]
for all \( \phi \in Y := H^1(\mathbb{R}^3) \cap L^1(\mathbb{R}^3) \), where \( \| f \|_p := (\int \| f(x) \|^p d^3x)^{1/p} \) denotes the usual \( L^p \)-norm, here and henceforth. It is not hard to see that
\[
F[\beta] := \inf \left\{ \mathcal{F}_\beta(\phi) \left| \begin{array}{c}
\phi \in Y, \\
\| \phi \|_2 = 1
\end{array} \right. \right\} \tag{I.7}
\]
satisfies the scaling relation
\[
F[\beta] = \beta^{4/7} F[1], \tag{I.8}
\]
2
and in [19] the second author shows that the infimum in (1.7) is actually attained and strictly positive, in particular,

\[ F[1] > 0 . \]  

(I.9)

Our main result is estimate (1.10) below, showing that the upper bound on \( E_{\text{LL}}(\alpha, \Lambda) \) in (1.5) is actually tight.

**Theorem I.1.** There exists a universal constant \( C < \infty \) such that for all \( \alpha > 0 \) and \( \Lambda \geq 1 \), the estimate

\[
-C \alpha^{\frac{4}{105}} \Lambda^{-\frac{4}{105}} \leq E_{\text{LL}}(\alpha, \Lambda) \leq C \alpha^{\frac{4}{105}} \Lambda^{-\frac{4}{105}}
\]

holds true.

We briefly sketch the derivation of (1.10). The intermediate steps yield further insight on the minimizer of the Lieb-Loss model. The latter is described in detail in Section III.3.

(1) For technical reasons we introduce an infrared cutoff \( \sigma > 0 \). The case \( \sigma = 0 \) can be dealt with by a continuity argument in the limit \( \sigma \to 0 \) using standard relative bounds on \( \tilde{A}_\sigma \). We do not give details of the argument but refer the reader to [6].

(2) We first analyze the functional \( E_{\alpha, \Lambda} \). A direct computation yields

\[
E_{\alpha, \Lambda}(\phi, \psi) = \frac{1}{2} \| \nabla \phi \|_2^2 + \left\langle \psi \left| \mathbb{H}(|\phi|^2, \text{Im} \{\bar{\phi} \nabla \phi\}) \phi \right\rangle_F ,
\]

where \( \langle \cdot | \cdot \rangle_F \) denotes the scalar product on the photon Fock space \( \mathcal{F}_{\text{ph}} \) and \( \mathbb{H}[\rho, \bar{v}] \) is for \( \rho : \mathbb{R}^3 \to \mathbb{R}^+ \) and \( \bar{v} : \mathbb{R}^3 \to \mathbb{R}^3 \) given as

\[
\mathbb{H}[\rho, \bar{v}] := H_{\text{ph}} + \frac{\alpha}{2} \int \rho(x) \bar{A}_{\alpha, \Lambda}(x) d^3x + \sqrt{\alpha} \int \bar{v}(x) \cdot \tilde{A}_{\alpha, \Lambda}(x) d^3x.
\]

(I.12)

In Theorem [IV.4] in Section IV.1 we demonstrate that, by a suitably chosen Weyl transformation \( W_\phi \), the term linear in the fields, i.e., proportional to \( \bar{v} = \text{Im} \{\bar{\phi} \nabla \phi\} \), can be eliminated up to an additive constant in the transformed Hamiltonian. The minimization of the energy functional consequently enforces the reality of the wavefunction \( \phi \). More precisely,

\[
E_{\alpha, \Lambda}(\phi, \psi) \geq E_{\alpha, \Lambda}(|\phi|, W_\phi \psi).
\]

(I.13)
Defining
\[ \hat{\mathcal{E}}_{\alpha,\Lambda}(\phi) := \inf \left\{ \mathcal{E}_{\alpha,\Lambda}(\phi, \psi) \mid \psi \in \mathcal{F}_{\text{ph}}, \|\psi\| = 1 \right\}, \]  
we therefore have that
\[ \hat{\mathcal{E}}_{\alpha,\Lambda}(\phi) \geq \hat{\mathcal{E}}_{\alpha,\Lambda}(|\phi|). \]  
(I.15)

(3) Eq. (I.15) guarantees that we can assume without loss of generality that \( \phi = |\phi| \geq 0 \), and in this case
\[ \mathcal{E}_{\alpha,\Lambda}(\phi, \psi) = \frac{1}{2} \|\vec{\nabla} \phi\|^2 + \left\langle \psi \left( H_{\text{ph}} + \frac{\alpha}{2} \int |\phi(x)|^2 \bar{A}_\Lambda^2(x) \, d^3x \right) \psi \right\rangle_{\mathcal{F}}. \]  
(I.16)

In Theorem IV.5 in Section IV.2 we give an alternative proof for the observation of Lieb and Loss that
\[ \inf \left\{ \left\langle \psi \left( H_{\text{ph}} + \frac{\alpha}{2} \int |\phi(x)|^2 \bar{A}_\Lambda^2(x) \, d^3x \right) \psi \right\rangle_{\mathcal{F}} \mid \psi \in \mathcal{F}_{\text{ph}}, \|\psi\| = 1 \right\} = \frac{1}{2} \text{Tr} \left\{ \sqrt{-\Delta_x + 2\Theta_{\phi,\alpha} - \sqrt{-\Delta_x}} \right\}, \]  
(I.17)

where \( \Theta_{\phi,\alpha} := \alpha(2\pi)^{-3} P_C \chi_{\sigma,\Lambda}(\hat{\phi}^*(\hat{\phi}^*)) \chi_{\sigma,\Lambda} P_C, \chi_{\sigma,\Lambda} := 1[\sigma \leq -\Delta_x \leq \Lambda^2], \) and \( P_C := 1 \left( \bar{\nabla}_x \cdot \right) = 0 \) is the projection onto divergence-free vector fields, i.e., vector fields in Coulomb gauge. Inserting this into (I.14)-(I.15), we arrive at
\[ \hat{\mathcal{E}}_{\alpha,\Lambda}(\phi) = \frac{1}{2} \|\vec{\nabla} \phi\|^2 + \frac{1}{2} X(2\Theta_{\phi,\alpha}), \]  
(I.18)

for \( \phi = |\phi| \geq 0 \), where
\[ X(A) := \text{Tr} \left( \sqrt{|k|^2 + A} - |k| \right) \quad \text{and} \quad \tag{I.19} \]
\[ \Theta_{\phi,\alpha} := \frac{\alpha}{(2\pi)^3} P_C \chi_{\sigma,\Lambda} \phi(x)^2 \chi_{\sigma,\Lambda} P_C, \]  
(I.20)

with \( \phi(x) \equiv \phi(i\nabla_x) \) denoting the corresponding Fourier multiplier (with respect to the momentum representation).

(4) In Section V we introduce the infima
\[ E^{(L)}_{\text{LL}}(\alpha, \Lambda) := \inf \left\{ \hat{\mathcal{E}}_{\alpha,\Lambda}(\phi_L) \mid \phi_L \in Y_L \right\}, \]  
(L.21)
\[ F^{(L)}[\beta] := \inf \left\{ \mathcal{F}_{\beta}(\phi_L) \mid \phi_L \in Y_L \right\}, \]  
(L.22)
of the Lieb-Loss functional \( E_{LL}(\alpha, \Lambda) (\phi_L) \) and the auxiliary functional \( F_\beta(\phi_L) \) under variation only over compactly supported functions \( \phi_L \in Y_L := H^1(B(0, L)) \) and compare these infima to \( E_{LL}(\alpha, \Lambda) \) and \( F[\beta] \) by means of the IMS localization formula. More specifically, we prove in Theorem [V.1] that

\[
E^{(L)}_{LL}(\alpha, \Lambda) - C L^{-2} \leq E_{LL}(\alpha, \Lambda) \leq E^{(L)}_{LL}(\alpha, \Lambda), \tag{I.23}
\]

\[
F^{(L)}[\beta] - C L^{-2} \leq F[\beta] \leq F^{(L)}[\beta], \tag{I.24}
\]

for some universal constant \( C < \infty \) and all \( L > 0 \). Consequently, the leading orders of \( E_{LL}(\alpha, \Lambda) \) and \( F[\beta] \), respectively, are determined by their behavior on compactly supported functions.

(5) The fourth step carried out in Sections [VI] and [VII] is to find upper and lower bounds for all compactly supported \( \phi = |\phi| \in Y_L := H^1(B(0, L)) \) on \( X(\Theta_{\phi_L, \alpha}) \). In Theorem [VI.1] we prove the existence of a universal constant \( C < \infty \) such that, for all \( 0 < \varepsilon \leq 1, L \geq 1/\Lambda \), and \( \phi \in Y_L \),

\[
\frac{1}{2} X(2\Theta_{\phi, \alpha}) - \sqrt{\frac{4\alpha}{9\pi}} \Lambda^3 \|\phi_L\|_1 \leq C(\varepsilon \alpha^{1/2} \Lambda^3 + \alpha^{1/2} \sigma^{1/2} \Lambda^{5/2}) \|\phi_L\|_1 + C \varepsilon^{-2} \Lambda^{7/2} \|\nabla \phi_L\|_2. \tag{I.25}
\]

This is complemented by the lower bound in Theorem [VII.2] which asserts that, there exists a universal constant \( C < \infty \) such that, for all \( L \geq 1/\Lambda \) and \( \phi \in Y_L \),

\[
\frac{1}{2} X(2\Theta_{\phi, \alpha}) - \sqrt{\frac{4\alpha}{9\pi}} \Lambda^3 \|\phi_L\|_1 \geq -C \alpha^{1/2} \Lambda^{7/2} L \|\phi_L\|_1^{\frac{1}{2}}. \tag{I.26}
\]

(6) Estimates (I.25) and (I.26) suggest to compare the functional \( \hat{E}_{\alpha, \Lambda}(\phi) = \frac{1}{2} \|\nabla \phi\|_2 + \frac{1}{2} X(2\Theta_{\phi, \alpha}) \) to \( F_{\beta(\alpha, \Lambda)}(\phi) = \frac{1}{2} \|\nabla \phi\|_2 + \beta(\alpha, \Lambda) \|\phi\|_1 \) with \( \beta(\alpha, \Lambda) := \sqrt{\frac{4\alpha}{9\pi}} \Lambda^3 \) which is done in Section [VIII] Indeed, this leads us to introduce the family of auxiliary functionals \( (F_\beta)_{\beta > 0} \), defined on \( Y := H^1(\mathbb{R}^3) \cap L^1(\mathbb{R}^3) \subset H^1(\mathbb{R}^3) \) as

\[
F_\beta(\phi) := \frac{1}{2} \|\nabla \phi\|_2^2 + \beta \|\phi\|_1, \tag{I.27}
\]

and their infima

\[
F[\beta] := \inf \{ F_\beta(\phi) \mid \phi \in Y, \|\phi\|_2 = 1 \}. \tag{I.28}
\]
This family of functionals is analyzed by direct methods of the calculus of variations in detail by the second author in a separate paper [19], and here we describe its properties only briefly.

- For fixed $\beta > 0$, the functional $F_\beta$ possesses a minimizer, which is unique up to translations, nonnegative, spherically symmetric and decreasing. In particular, its infimum $F[\beta]$ is attained and hence a strictly positive minimum.

- For all $\beta > 0$ both energy and minimizer are uniquely determined by their scaling behaviour in $\beta$ and universal constants corresponding to the case $\beta = 1$. In particular, $F[1] > 0$ is a universal positive number and $F[\beta] = \beta^{4/7} F_1$.

- The Euler-Lagrange equation, which corresponds to the inhomogeneous Helmholtz equation $(-\Delta - \mu^2)\phi + \beta = 0$, yields an explicit characterization of this minimizer in terms of the zeroth Bessel function $j_0$ of the first kind.

In Section [VIII] we use the information on the auxiliary functional and especially the scaling relation $F[\beta] = \beta^{4/7} F_1$ to finally derive (I.10), formulated again as (VIII.3) in Theorem [VIII.1]. In order to simultaneously control the errors on the right side of (I.25) and the localization error of order $O(L^{-2})$ we choose $\varepsilon := \alpha^{4/105} \Lambda^{-4/105}$ and $L := \alpha^{17/105} \Lambda^{-88/105}$ and arrive at the upper bound in (I.10). Similarly, we choose $L := \alpha^{9/49} \Lambda^{-40/49}$ to obtain the lower bound in (I.10) from (I.26) and the localization estimate.

Note that both estimates suggest that the length scale $\ell(\Lambda)$ of the particle in the ground state of the Lieb-Loss model is of order $\ell(\Lambda) \approx \alpha^{\tau - 1} \Lambda^\tau$, with $\tau = \frac{6}{7} \approx 0.86$.

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II  The Lieb-Loss Model

The Lieb-Loss model is a variational model for the study of the ground state energy of a system containing a single nonrelativistic spinless particle which is minimally coupled to the quantized radiation field. The dynamics of such a quantum system is generated by the Pauli-Fierz Hamiltonian

$$H_{\sigma,\Lambda} := \frac{1}{2} \left( i\nabla + \sqrt{\alpha \vec{A}_{\sigma,\Lambda}(\vec{x})} \right)^2 + H_{ph}, \quad (\text{II.1})$$

which we define here as a quadratic form on $H^1(\mathbb{R}^3) \otimes D(N_{ph}^{1/2})$, where $H^1(\mathbb{R}^3) \subseteq L^2(\mathbb{R}^3)$ is the Sobolev space of square-integrable functions whose gradient is square-integrable, as well, and $D(N_{ph}^{1/2}) \subseteq \mathcal{F}_ph$ denotes the subspace of finite photon number expectation value of the photon Fock space $\mathcal{F}_ph$. The latter is the boson Fock space over the one-photon Hilbert space $\mathcal{h}$, i.e., it is the orthogonal sum $\mathcal{F}_ph = \bigoplus_{n=0}^{\infty} \mathcal{F}_ph^{(n)}$ of $n$-photon sectors, where $\mathcal{F}_ph^{(0)} := \mathbb{C} \times \Omega$ is the one-dimensional vacuum sector spanned by the normalized vacuum vector $\Omega$, and for $n \geq 1$, the $n$-photon sector $\mathcal{F}_ph^{(n)} := S_n[\mathcal{h}_{pol}] \subseteq \mathcal{h}_{pol}$, is the subspace of the $n$-fold tensor product of $\mathcal{h}_{pol}$ of totally symmetric vectors.

The one-photon Hilbert space $\mathcal{h}_{pol} := L^2(S_{\sigma,\Lambda} \times \mathbb{Z}_2)$ is the space of square-integrable, divergence-free vector fields $\vec{k} \mapsto \vec{\epsilon}(\vec{k}, \pm) f(k, \pm) + \vec{\epsilon}(\vec{k}, -) f(k, -)$ supported in the momentum shell $S_{\sigma,\Lambda} := \{ \vec{k} \in \mathbb{R}^3 : \sigma \leq |\vec{k}| < \Lambda \} \subseteq \mathbb{R}^3$ which excludes momenta of magnitude below the infrared cutoff $\sigma \geq 0$ and above the ultraviolet cutoff $1 \leq \Lambda < \infty$. The two transversal polarizations are parametrized by the polarization vectors $\vec{\epsilon}(\vec{k}, \pm) \perp \vec{k}$ that are chosen so as to form an orthonormal frame $(\vec{k}/|\vec{k}|, \vec{\epsilon}(\vec{k}, +), \vec{\epsilon}(\vec{k}, -))$ in $\mathbb{C} \otimes \mathbb{R}^3$, for all $\vec{k} \in S_{\sigma,\Lambda} \setminus \{ \vec{0} \}$. Of course, the map $k \rightarrow \vec{\epsilon}(k)$ is assumed to be measurable and, for convenience, chosen to be real, $\vec{\epsilon}(k, \pm) \in \mathbb{R}^3$, almost everywhere in $\mathbb{R}^3 \times \mathbb{Z}_2$.

In (II.1) the field Hamiltonian

$$H_{ph} = d\Gamma(|k|) = \int |k| a^*(k) a(k) \, dk \quad (\text{II.2})$$

represents the energy of the radiation field, and

$$\vec{A}_{\sigma,\Lambda}(\vec{x}) = (2\pi)^{-\frac{3}{2}} \int |k| \frac{\vec{\epsilon}(k)}{|k|^\frac{3}{2}} \left( a^*(k) e^{-i\vec{k} \cdot \vec{x}} + a(k) e^{i\vec{k} \cdot \vec{x}} \right) \, dk \quad (\text{II.3})$$

is the quantized vector potential (in Coulomb gauge). In (II.2), (II.3), we denote elements of $S_{\sigma,\Lambda} \times \mathbb{Z}_2 \ni (\vec{k}, \tau)$ by $k := (\vec{k}, \tau)$ and then further $-k := (-\vec{k}, \tau), \quad |k| := |\vec{k}|$, $\int F(k) \, dk := \sum_{\tau \in \pm} \int_{|\vec{k}| < \Lambda} F(\vec{k}, \tau) \, d^3k$. Furthermore, we use creation and annihilation operators $a^*(k)$ and $a(k)$, for $k \in S_{\sigma,\Lambda} \times \mathbb{Z}_2$, in (II.2) and
These are operator-valued distributions constituting a Fock representation of the canonical commutation relations (CCR) on $F_{\text{ph}}$, i.e.,

$$[a(k_1), a(k_2)] = [a^*(k_1), a^*(k_2)] = 0,$$  \hspace{1cm} (II.4)

$$[a(k_1), a^*(k_2)] = \delta(k_1 - k_2), \quad a(k_1)\Omega = 0,$$  \hspace{1cm} (II.5)

for all $k_1, k_2 \in S_{\sigma,\Lambda} \times \mathbb{Z}_2$ (integrated over $k_1$ and $k_2$ against test functions). Finally, the photon number operator entering the definition of the domain $D(N_{\text{ph}}^{1/2})$ is given by $N_{\text{ph}} := \int a^*(k)a(k)\,dk$.

The Lieb-Loss model is defined by the Lieb-Loss (energy) functional $E_{\alpha,\sigma,\Lambda} : H^1(\mathbb{R}^3) \times D(N_{\text{ph}}^{1/2}) \to \mathbb{R}$ which results from varying only over products $\phi \otimes \psi$ of normalized wave functions of the particle $\phi \in L^2(\mathbb{R}^3)$ and the photon state $\psi \in F_{\text{ph}}$ in the Rayleigh-Ritz principle, i.e.,

$$E_{\alpha,\sigma,\Lambda}(\phi, \psi) := \langle \phi \otimes \psi \mid H_{\alpha,\sigma,\Lambda}(\phi \otimes \psi) \rangle.$$  \hspace{1cm} (II.6)

Note that, given a fixed $\phi \in H^1(\mathbb{R}^3)$ and varying only over $\psi \in D(N_{\text{ph}}^{1/2})$, the Lieb-Loss functional $\psi \mapsto E_{\psi}(\phi, \psi)$ becomes the expectation value in $\psi$ of a Hamiltonian that is quadratic in the boson fields. More specifically, a simple computation shows that

$$E_{\alpha,\sigma,\Lambda}(\phi, \psi) = \frac{1}{2}\|\nabla\phi\|_2^2 + \left\langle \psi \mid H(\|\phi\|^2, \text{Im}\{\nabla\phi\}) \mid \phi \otimes \psi \right\rangle,$$  \hspace{1cm} (II.7)

where $\langle \cdot \mid \cdot \rangle_3$ denotes the scalar product on the photon Fock space $F_{\text{ph}}$ and, for fixed $\rho : \mathbb{R}^3 \to \mathbb{R}^+$ and $\vec{v} : \mathbb{R}^3 \to \mathbb{R}^3$, the quadratic Hamiltonian $H[\rho, \vec{v}]$ is given as

$$H[\rho, \vec{v}] := H_{\text{ph}} + \frac{\alpha}{2} \int \rho(x) \bar{\Lambda}_{\sigma,\Lambda}(x) \,d^3x + \sqrt{\alpha} \int \vec{v}(x) \cdot \bar{\Lambda}_{\sigma,\Lambda}(x) \,d^3x.$$  \hspace{1cm} (II.8)

As we show below it turns out that the minimal values of the Lieb-Loss functional is attained for positive wave functions. To exhibit this we define $r := |\phi| \in H^1(\mathbb{R}^3; \mathbb{R}_0^+)$ and choose $\gamma \in H^1(\mathbb{R}^3; \mathbb{R})$, for a given $\phi \in H^1(\mathbb{R}^3; \mathbb{C})$, so that

$$\phi = re^{i\gamma}, \quad |\phi|^2 = r^2, \quad \text{Im}\{\nabla\phi\} = r^2\nabla\gamma,$$  \hspace{1cm} (II.9)

and thus

$$E_{\alpha,\sigma,\Lambda}(r e^{i\gamma}, \psi) = \frac{1}{2}\|\nabla r\|_2^2 + \frac{1}{2}\|r\nabla\gamma\|_2^2 + \left\langle \psi \mid H(r^2, r^2\nabla\gamma) \mid \psi \right\rangle.$$  \hspace{1cm} (II.11)
Although convenient, the explicit parametrization of Coulomb gauge by polarization vectors $\vec{\epsilon}(\vec{k}, \pm)$ tends to obscure the picture by introducing a seeming dependence of the model on the choice of $\vec{\epsilon}(\vec{k}, \pm)$, which, however, should be physically meaningless. For this reason we choose the one-photon space to be the Hilbert space

$$h := P_C \left[ L^2(S_{\sigma,\Lambda}; \mathbb{C} \otimes \mathbb{R}^3) \right]$$

$$= \left\{ \ f \in L^2(S_{\sigma,\Lambda}; \mathbb{C} \otimes \mathbb{R}^3) \ \bigg| \ \forall \vec{k} \in S_{\sigma,\Lambda} : \ \vec{k} \perp f(\vec{k}) \right\}$$

of divergence-free, square-integrable vector fields, where $P_C \in \mathcal{B}[L^2(S_{\sigma,\Lambda}; \mathbb{C} \otimes \mathbb{R}^3)]$ is the orthogonal projection acting as $[P_C f](\vec{k}) := P_{\vec{k}}^+ f(\vec{k})$, with $P_{\vec{k}} : \mathbb{R}^3 \to \mathbb{R}^3$ being the projection in $\mathbb{R}^3$ onto the unit vector $\vec{k}/\|\vec{k}\| \in \mathbb{S}^2$. Note that for any arbitrary, but fixed, choice of polarization vectors basis $\{\vec{\epsilon}(\vec{k}, +), \vec{\epsilon}(\vec{k}, -)\}_{\vec{k} \in S_{\sigma,\Lambda}}$ described above, the map

$$\Xi : h_{pol} \to h, \quad [\Xi f](\vec{k}) := \vec{\epsilon}(\vec{k}, +) f(\vec{k}, +) + \vec{\epsilon}(\vec{k}, -) f(\vec{k}, -)$$

is unitary, with $[\Xi^{-1} f](\vec{k}, \pm) = [\Xi^* f](\vec{k}, \pm) = \vec{\epsilon}(\vec{k}, \pm) \cdot f(\vec{k})$, and allows us to switch between the photon representations, if necessary.

Accordingly, the photon Fock space we use is $\mathcal{F}_{ph} := \mathcal{F}_{b}[h]$ the bosonic Fock space over divergence-free vector fields. On $\mathcal{F}_{ph}$ we have a Fock representation of the CCR of the form

$$[a(\vec{k}_1, \nu_1), a(\vec{k}_2, \nu_2)] = [a^*(\vec{k}_1, \nu_1), a^*(\vec{k}_2, \nu_2)] = 0,$$

$$[a(\vec{k}_1, \nu_1), a^*(\vec{k}_2, \nu_2)] = \delta(\vec{k}_1 - \vec{k}_2) \left( P_{\vec{k}_1}^+ \right)_{\nu_1, \nu_2} : a(k_1)\Omega = 0,$$

for all $\vec{k}_1, \vec{k}_2 \in S_{\sigma,\Lambda}$ and $\nu_1, \nu_2 \in \mathbb{Z}_3$, as operator-valued distributions, or

$$[a(f), a(g)] = [a^*(f), a^*(g)] = 0,$$

$$[a(f), a^*(g)] = \langle f \mid P_C g \rangle, \quad a(f)\Omega = 0,$$

for all $f, g \in h$, where we write

$$a^*(f) := \sum_{\nu=1}^{3} \int f_{\nu}(\vec{k}) a^*(\vec{k}, \nu) \, d^3k, \quad a(f) := \sum_{\nu=1}^{3} \int f_{\nu}(\vec{k}) a(\vec{k}, \nu) \, d^3k.$$
for all $f = (f_1, f_2, f_3) \in \mathfrak{h}$. In this representation the operator $\vec{A}_{\sigma, \Lambda}(x)$ of the magnetic vector potential becomes $\vec{A}(x) = (A_1(x), A_2(x), A_3(x))$, with

$$A_{\mu}(x) = a^*(m_{\mu}(x)) + a(m_{\mu}(x)) = \sum_{\nu=1}^{3} \int \left\{ m_{\mu, \nu}(x, \vec{k}) a^*(\vec{k}, \nu) + \overline{m_{\mu, \nu}(x, \vec{k}) a(\vec{k}, \nu)} \right\} d^3k ,$$

$$m_{\mu, \nu}(x, \vec{k}) := \frac{1}{(2\pi)^{3/2} |\vec{k}|^{1/2}} \left( P_{\perp}^\perp \right)_{\mu, \nu} e^{-ik \cdot x},$$

and the Hamiltonian $\mathbb{H}(r^2, r^2 \vec{\nabla} \gamma)$ in (II.11) turns into

$$\mathbb{H}(r^2, r^2 \vec{\nabla} \gamma) =$$

$$H_{ph} + \frac{\alpha}{2} \int (r(x) \vec{A}(x))^2 d^3x + \sqrt{\alpha} \int (r(x) \vec{\nabla} \gamma(x)) \cdot (r(x) \vec{A}(x)) d^3x .$$

Note that the dependence of $\vec{A}(x)$ on the cutoff parameters $0 < \sigma \leq 1$ and $1 \leq \Lambda < \infty$ is not displayed anymore.
III  Bogolubov Transformations

Next, we analyze the infimum of \( \psi \mapsto \langle \psi \mid \mathbb{H}[^{I/2}\bar{\gamma}] \psi \rangle \), as \( \psi \in \mathcal{D}(\mathcal{N}_{\text{ph}}^{I/2}) \) varies over normalized states, by means of Bogolubov transformations. For a suitable definition of these in the present context, the choice of the antilinear involution \( J : \mathfrak{h} \to \mathfrak{h} \) defined by

\[
[Jf](\bar{k}) := f(-\bar{k})
\]  

(III.1)

plays a key role. Before using \( J \), we recall a few facts about antiunitary maps and generalized creation and annihilation operators.

III.1  Antiunitary Maps and Generalized Field Operators

For a general complex Hilbert space \( \mathfrak{h} \) the Riesz map \( R : \mathfrak{h} \to \mathfrak{h}^* \), \( \psi \mapsto \langle \psi \rangle \) is a canonical isomorphism from \( \mathfrak{h} \) onto its dual \( \mathfrak{h}^* = \mathcal{B}[\mathfrak{h}; \mathbb{C}] \). Moreover, \( R \) is \textit{antiunitary}, i.e., it obeys \( \langle R(f)|R(g) \rangle_{\mathfrak{h}^*} = \langle g|f \rangle_{\mathfrak{h}} \). Note that \( R \) is not the only antiunitary map from \( \mathfrak{h} \) to \( \mathfrak{h}^* \), for if \( u : \mathfrak{h} \to \mathfrak{h} \) and \( v : \mathfrak{h}^* \to \mathfrak{h}^* \) are unitary operators on \( \mathfrak{h} \) and \( \mathfrak{h}^* \), respectively, then \( R \circ u : \mathfrak{h} \to \mathfrak{h}^* \) and \( v \circ R : \mathfrak{h} \to \mathfrak{h}^* \) are antiunitary, too. Conversely, any antiunitary from \( \mathfrak{h} \) to \( \mathfrak{h}^* \) is of this form.

In the present paper we prefer to work with an \textit{antiunitary} \( J \) which additionally constitutes an \textit{antilinear involution} or \textit{real structure}. Given a general complex Hilbert space \( \mathfrak{h} \) these are antiunitary bijections \( J : \mathfrak{h} \to \mathfrak{h} \), which obey

\[
J^2 = 1_{\mathfrak{h}} \quad \text{and} \quad \forall f, g \in \mathfrak{h} : \langle J(f)|J(g) \rangle_{\mathfrak{h}} = \langle g|f \rangle_{\mathfrak{h}}. \quad (\text{III.2})
\]

Given an \textit{antiunitary involution} \( J : \mathfrak{h} \to \mathfrak{h} \) we can define the maximal \( J \)-invariant subspace

\[
\mathfrak{h}_{\mathbb{R}} = \{ f \in \mathfrak{h} \mid Jf = f \} \subsetneq \mathfrak{h}, \quad (\text{III.3})
\]

which is a \( \mathbb{R} \)-linear subspace of \( \mathfrak{h} \). Writing \( f \in \mathfrak{h} \) as \( f = f_1 + if_2 \), with \( f_1 := \frac{1}{2}(f + Jf) \in \mathfrak{h} \) and \( f_2 := \frac{1}{2i}(f - Jf) \in \mathfrak{h} \), we obtain a direct sum decomposition \( \mathfrak{h} = \mathfrak{h}_{\mathbb{R}} \oplus i\mathfrak{h}_{\mathbb{R}} \). Similar to antiunitary operators \( \mathfrak{h} \to \mathfrak{h}^* \), antiunitary involutions \( \mathfrak{h} \to \mathfrak{h} \) are not unique. This gives us freedom to make a suitable choice for the problem to solve, namely, (III.1) in the present case.

To define Bogolubov transformations it is convenient to use \textit{generalized creation and annihilation operators} which were first introduced by Araki and Shi- raishi in [2, 3] to describe the second quantization of one-body Hamiltonians. Bogolubov transformations are also discussed in detail in [27, 8]. Given an antiunitary involution \( J : \mathfrak{h} \to \mathfrak{h} \), the generalized creation and annihilation (field) operators \( A_J^+, A_J : \mathfrak{h} \oplus \mathfrak{h} \to \mathcal{B}[\mathcal{D}(N^{I/2}); \mathfrak{h}] \) are defined by

\[
A_J^+(f \oplus Jg) := a^*(f) + a(g) \quad \text{and} \quad A_J(f \oplus Jg) := a(f) + a^*(g), \quad (\text{III.4})
\]

11
for any \( f, g \in h \). Note that
\[
A_J(F) = A_J'(JF), \quad \text{with} \quad J := \begin{pmatrix} 0 & J \\ J & 0 \end{pmatrix}
\]
(III.5)

being an antiunitary involution on \( h \oplus h \). The vectors in \( h \oplus h \) which are invariant under \( J \) are of the form \( y \oplus Jy \), with \( y \in h \). They form a real subspace
\[
(h \oplus h)_J := \left\{ G \in h \oplus h \mid G = JG \right\} = \left\{ y \oplus Jy \mid y \in h \right\} = q[h],
\]
(III.6)

where \( q : h \rightarrow (h \oplus h)_J \) is the real-linear map
\[
q := \begin{pmatrix} 1 \\ J \end{pmatrix}, \quad \text{with adjoint} \quad q^* : (h \oplus h)_J \rightarrow h, \quad q^* = (1, J).
\]
(III.7)

One advantage of the generalized formalism consists in encoding all orderings in the second quantization of operators, so that we need not worry about imposing normal-ordering. The price for this is the slightly modified form of the canonical commutation relations (CCR), the generalized field operators obey, namely,
\[
[A_J(F), A_J'(F')] = \langle F \mid SF' \rangle,
\]
(III.8)

where \( S \) is a natural symplectic form on \( h \oplus h \) given by
\[
S := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\]
(III.9)

### III.2 Second Quantization and Bogolubov Transformations

Next, we introduce the second quantization of one-photon operators. Let \( J : h \rightarrow h \) be an antiunitary involution and \( \{F_i\}_{i=1}^{\infty} \subseteq h \oplus h \) an orthonormal basis. For \( T = T^* \in B[h \oplus h] \) and \( y \in h \), we define their second quantization \( d\Gamma_J[T, y] \in B[D(N_{ph}); \mathfrak{F}_{ph}] \) by
\[
d\Gamma_J[T, y] := \sum_{i,j=1}^{\infty} \langle F_i \mid TF_j \rangle A_J^*(F_i) A_J(F_j) + \sum_{i=1}^{\infty} \left\{ \langle F_i \mid q(y) \rangle A_J^*(F_i) + \langle F_i \mid q(y) \rangle A_J(F_i) \right\}.
\]
(III.10)

Note that the definition [III.10] of \( d\Gamma_J[T, y] \) is independent of the choice of the orthonormal basis \( \{F_i\}_{i=1}^{\infty} \subseteq h \oplus h \). Moreover, \( d\Gamma_J[T, y] \) is self-adjoint on \( D(N_{ph}) \) and \( d\Gamma_J[T, y] \) is semibounded, provided \( T \geq 0 \). Finally, \( [a(f), a(g)] = 0 \) and
\[ [a^*(f), a^*(g)] = 0 \text{ imply that } d\Gamma_J[\begin{pmatrix} a & b \\ c & d \end{pmatrix}, y] = d\Gamma_J[\begin{pmatrix} a & b^* \\ c & d \end{pmatrix}, y], \text{ and we can and will henceforth always assume that} \]
\[
b^* = JbJ, \text{ for } T = T^* = \begin{pmatrix} a & b \\ b^* & a \end{pmatrix} = \begin{pmatrix} a & b \\ Jb & J^*a \end{pmatrix}. \tag{III.11}
\]

A second advantage of the generalized creation and annihilation operators is that their use eases the definition of Bogolubov transformations. We recall that Bogolubov transformations are unitary transformations \( \hat{U} \) on Fock space \( \mathcal{F}_{ph} \) which preserve (III.7) and are linear in the field operators, i.e., they act as
\[
\hat{U} a^*(f) \hat{U}^* := a^*(Uf) + a(JVf) + \langle \eta | f \rangle, \tag{III.12}
\]
for all \( f \in \mathcal{H} \), where \( U \) and \( V \) are linear operators on \( \mathcal{H} \) and \( \eta \in \mathcal{H} \). The Bogolubov transformations form a group which is the semidirect product of the group of homogenous Bogolubov transformations and the group of Weyl transformations. That is, every Bogolubov transformation \( \hat{U} \) can be written as a composition
\[
\hat{U} = U_B \hat{W}_\eta = \hat{W}_\mu U_B \tag{III.13}
\]
of a homogeneous Bogolubov transformation \( U_B \) and a Weyl transformation \( \hat{W}_\eta \) or a composition of a Weyl transformation \( \hat{W}_\mu \) and \( U_B \), but with \( \mu \neq \eta \), in general.

Homogeneous Bogolubov transformations \( U_B \) are the special case \( \eta = 0 \) of (III.12). In terms of the generalized field operators they assume the form
\[
U_B A_j^*(F) U_B^* := A_j^*(BF), \quad B \equiv B(U, V) := \begin{pmatrix} U & JV \\ V & JU \end{pmatrix}, \tag{III.14}
\]
where the form of \( B \) is determined by (III.5), i.e., \( JB = BJ \), and (III.12). Note that this makes explicit use of the antunitary involution \( J : \mathcal{H} \rightarrow \mathcal{H} \). The homogeneous Bogolubov transformation \( U_B \) is unitary iff it leaves the CCR invariant and preserves the norm of the vacuum vector \( \Omega \in \mathcal{F}_{ph} \), which is equivalent to
\[
B^* S B = S, \quad B S B^* = S, \quad \text{and} \quad Tr(V^* V) < \infty. \tag{III.15}
\]
The second identity in (III.15) is actually a consequence of the first, as the latter implies the invertibility of \( B \), and then the second identity follows from the uniqueness of the inverse. The requirement that \( V \) be a Hilbert-Schmidt operator is known as the Shale-Stinespring condition. A simple computation shows that the second quantization \( d\Gamma_J[T, y] \) of \( T \) and \( y \) transforms under a homogeneous Bogolubov transformation \( U_B \) with \( B \equiv B(U, V) \) as
\[
U_B d\Gamma_J[T, y] U_B^* = d\Gamma_J[BTB^*, Jq^*Bq(y)]. \tag{III.16}
\]

13
Weyl transformations \( \mathbb{W}_\eta \) are the special case \( U = 1_h \) and \( V = 0 \) of (III.12). They act on the generalized field operators as
\[
\mathbb{W}_\eta A^*_j(F) \mathbb{W}_\eta^* := A^*_j(F) + \langle q(\eta) | F \rangle.
\] (III.17)

The unitarity of \( \mathbb{W}_\eta \) is equivalent to the requirement \( \eta \in \mathfrak{h} \). Another simple computation shows that the second quantization \( \mathbb{d}_\mathcal{J} J \) of \( T \) and \( y \) transforms under a Weyl transformation \( \mathbb{W}_\eta \) as
\[
\mathbb{W}_\eta \mathbb{d}_\mathcal{J} J \left[ T, y \right] \mathbb{W}_\eta^* = \mathbb{d}_\mathcal{J} J \left[ T, y + \frac{1}{2} q^* T q(\eta) \right] + \langle \eta | q^* T q(\eta) \rangle + 4 \text{Re} \langle \eta | y \rangle.
\] (III.18)

### III.3 The Lieb-Loss Model in Terms of Second Quantization

We turn to the analysis of the Lieb-Loss model. Note that \( \mathbb{d}_\mathcal{J} J \left[ T, y \right] \) depends on the choice of the antiunitary involution \( \mathcal{J} : \mathfrak{h} \to \mathfrak{h} \). For the analysis of the Lieb-Loss model it is of key importance to choose the antiunitary involution \( \mathcal{J} : \mathfrak{h} \to \mathfrak{h} \) as
\[
\forall f \in \mathfrak{h}, \vec{k} \in S_{\sigma,\Lambda} : \quad [Jf](\vec{k}) := f(-\vec{k})
\] (III.19)
because with this choice the operator \( T : \mathfrak{h}_\mathbb{R} \oplus \mathfrak{h}_\mathbb{R} \to \mathfrak{h}_\mathbb{R} \oplus \mathfrak{h}_\mathbb{R} \) leaves the real subspace \( \mathfrak{h}_\mathbb{R} \oplus \mathfrak{h}_\mathbb{R} \) of \( \mathfrak{h} \oplus \mathfrak{h} \) invariant, and the vector \( y \in \mathfrak{h}_\mathbb{R} \) is contained in the real subspace \( \mathfrak{h}_\mathbb{R} \subseteq \mathfrak{h} \) of \( \mathcal{J} \)-invariant vectors, as is discussed below.

We identify \( H(r^2, r^2 \vec{\nabla} \gamma) \) with \( \mathbb{d}_\mathcal{J} J \left[ T_{r,\alpha}, y_{r,\gamma,\alpha} \right] \), for suitably chosen \( T_{r,\alpha} \) and \( y_{r,\gamma,\alpha} \). We state the result in form of Lemma III.1 below.

**Lemma III.1.** Let \( J : \mathfrak{h} \to \mathfrak{h} \) be defined by (III.19) and \( r, \gamma \in H^1(\mathbb{R}^3) \). Then the Lieb-Loss functional (II.11) is given by
\[
\mathcal{E}_{\alpha,\sigma,\Lambda}(r e^{i \gamma}, \psi) = \frac{1}{2} \| \vec{\nabla} r \|_2^2 + \frac{1}{2} \| r \vec{\nabla} \gamma \|_2^2 + \frac{1}{2} \left\langle \psi \right| \mathbb{d}_\mathcal{J} J \left[ T_{r,\alpha}, y_{r,\gamma,\alpha} \right] \psi \right\rangle, \tag{III.20}
\]
where
\[
T_{r,\alpha} := |k|^{-1/2} \left( 2|k|^2 + \Theta_{r,\alpha} \Theta_{r,\alpha}^* \right) |k|^{-1/2}, \tag{III.21}
\]
with \(|k|\) denoting the multiplication operator \([|k| f](\vec{k}) := |k| f(\vec{k}) \) (Fourier multiplier), \( \Theta_{r,\alpha} \) being a nonnegative, \( J \)-invariant, self-adjoint Hilbert-Schmidt operator, \( \Theta_{r,\alpha} = \Theta_{r,\alpha}^* = \Theta_{r,\alpha}^T = J \Theta_{r,\alpha} J \geq 0 \) given by
\[
\Theta_{r,\alpha} = \Phi_{r,\alpha}^* \Phi_{r,\alpha}, \quad \Phi_{r,\alpha} = (\hat{r}*) P_C \chi_{\sigma,\Lambda}, \tag{III.22}
\]
\[
\Phi_{r,\alpha}(\vec{p}, \mu; \vec{k}, \nu) := \alpha^{1/2} (2\pi)^{-3/2} \hat{r}(\vec{p} - \vec{k}) \left( F_{\vec{k}}^+ \right)_{\mu,\nu} \chi_{\sigma,\Lambda}(\vec{k}), \tag{III.23}
\]
where \([\chi_{\sigma, \Lambda} f](\vec{k}) := 1[\sigma \leq |\vec{k}| < \Lambda] f(\vec{k})\) is a multiplication operator, and \(\hat{\ast}\) is the convolution operator \([\hat{\ast} f](\vec{k}) = \int \hat{\ast}(\vec{k} - \vec{k}') f(\vec{k}') d^3k'\), where \(\hat{\ast} \equiv \mathcal{F}[\cdot]\) denotes the Fourier transform \(\mathcal{F}[v](\vec{k}) := (2\pi)^{-3/2} \int e^{-i\vec{k} \cdot \vec{r}} v(\vec{r}) d^3r\) of \(v\), normalized as to preserve the \(L^2\)-scalar product.
Furthermore, \(y_{r, \gamma, \alpha} = J[y_{r, \gamma, \alpha}] \in \mathfrak{h}\) is given by
\[
y_{r, \gamma, \alpha} = |k|^{-1/2} \Phi^*_{r, \alpha} \mathcal{F}[r \nabla \gamma] \iff
y_{r, \gamma, \alpha}(\vec{k}, \nu) := \sum_{\mu=1}^3 |\vec{k}|^{-1/2} \Phi^*_{r, \alpha}(\vec{k}, \nu; \vec{p}, \mu) \mathcal{F}[r \nabla \gamma](\vec{p}) d^3p .
\] (III.24)

**Proof.** We first observe that
\[
\frac{\alpha}{2} \int (r(x) \hat{h}(x))^2 d^3x = \sum_{\mu=1}^3 \int \frac{\alpha}{2} \left[ a^*(r(x) m_{\mu}(x)) + a(r(x) m_{\mu}(x)) \right]^2 d^3x
\]
\[
= \sum_{\mu=1}^3 \frac{\alpha}{2} \int A^*_J \left( q[r(x) m_{\mu}(x)] \right) A_J \left( q[r(x) m_{\mu}(x)] \right) d^3x
\]
\[
= \frac{1}{2} \text{d} \Gamma_J \left[ |k|^{-1/2} \begin{pmatrix} \Theta_{r, \alpha} & \Theta_{r, \alpha} \\ \Theta_{r, \alpha}^{\top} & \Theta_{r, \alpha}^{\top} \end{pmatrix} |k|^{-1/2}, 0 \right] ,
\] (III.25)

where \(\Theta_{r, \alpha} : \mathfrak{h} \to \mathfrak{h}\) is the bounded operator given by the integral kernel
\[
|k|^{-1/2} \Theta_{r, \alpha}(\vec{k}, \nu; \vec{k}', \nu') |k|^{-1/2} := \sum_{\mu=1}^3 \int \alpha r^2(x) m_{\mu, \nu}(x, \vec{k}) m_{\mu, \nu'}(x, \vec{k}') d^3x ,
\] (III.26)

recalling the definition \(m_{\mu, \nu}(x, \vec{k}) := (2\pi)^{-3/2} |\vec{k}|^{-1/2} \chi_{\sigma, \Lambda}(\vec{k}) (P^\perp_k)_{\mu, \nu} e^{-i\vec{k} \cdot \vec{r}}\) from (II.20). As \(J(e^{i\vec{k} \cdot \vec{r}} e_\nu) = e^{i\vec{k} \cdot \vec{r}} e_\nu\) we have that \(J[r(x) m_{\mu}(x)] = r(x) m_{\mu}(x)\) and hence
\[
\Theta_{r, \alpha} = J \Theta_{r, \alpha} = \Theta_{r, \alpha} J = J \Theta_{r, \alpha} J .
\] (III.27)

Moreover, using the Plancherel theorem, we have that
\[
\Theta_{r, \alpha} = \Phi^*_{r, \alpha} \Phi_{r, \alpha} ,
\] (III.28)

where \(\Phi_{r, \alpha} = \alpha^{1/2} (2\pi)^{-3/2} (\hat{\ast} P_{\sigma, \Lambda} |\vec{k}|^{-1/2})\) is defined by the integral kernel
\[
\Phi_{r, \alpha}(\vec{p}, \mu; \vec{k}, \nu) := \frac{\alpha^{1/2}}{(2\pi)^{3/2}} \hat{\ast} (\vec{p} - \vec{k}) (P^\perp_k)_{\mu, \nu} \chi_{\sigma, \Lambda}(\vec{k}) ,
\] (III.29)
i.e., $\hat{r}$ is the convolution operator $[\hat{r} * f](\vec{k}) = \int \hat{r}(\vec{k} - \vec{k'}) f(\vec{k'}) d^3k'$, convolving $f$ with the Fourier transform

$$\mathcal{F}[r](\vec{k}) \equiv \hat{r} (\vec{k}) := \int e^{-i\vec{k} \cdot \vec{r}} r(x) \frac{d^3x}{(2\pi)^{3/2}} \quad (\text{III.30})$$

of $r$, normalized as to preserve the $L^2$-scalar product.

Similarly, we obtain

$$\alpha^{1/2} \int r^2(x) \vec{\nabla}_y r(x) \cdot \vec{A}(x) \, d^3x$$

$$= \sum_{\mu=1}^3 \int \alpha^{1/2} \left\{ a^* \left( r^2(x) \partial_\mu y(x) m_\mu(x) \right) + a \left( r^2(x) \partial_\mu y(x) m_\mu(x) \right) \right\} \, d^3x$$

$$= \sum_{\mu=1}^3 \int \frac{\alpha^{1/2}}{2} \left\{ A_\mu^* \left( q \left[ r^2(x) \partial_\mu y(x) m_\mu(x) \right] \right) + A_\mu \left( q \left[ r^2(x) \vec{\nabla} y(x) \cdot \vec{m}(x) \right] \right) \right\} \, d^3x$$

$$= \frac{1}{2} d\Gamma_j[0, y_{r,\gamma,\alpha}], \quad (\text{III.31})$$

where $y_{r,\gamma,\alpha} \in \mathfrak{h}$ is given as

$$y_{r,\gamma,\alpha}(\vec{k}, \nu) := \sum_{\mu=1}^3 \int r^2(x) \partial_\mu y(x) \alpha^{1/2} m_{\mu,\nu}(x, \vec{k}) \, d^3x. \quad (\text{III.32})$$

Note that $Jm_\mu(x) = m_\mu(x)$ implies $y_{r,\gamma,\alpha} = J[y_{r,\gamma,\alpha}] \in \mathfrak{h}_R$ and the Plancherel theorem yields $y_{r,\gamma,\alpha} = |k|^{-1/2} \Phi_{r,\alpha}^* \mathcal{F}[\gamma \vec{\nabla} y]$, i.e.,

$$y_{r,\gamma,\alpha}(\vec{k}, \nu) := \sum_{\mu=1}^3 \int |\vec{k}|^{-1/2} \Phi_{r,\alpha}^* (\vec{k}, \nu; \vec{p}, \mu) \mathcal{F}[r \partial_\mu y] (\vec{p}) \, d^3p. \quad (\text{III.33})$$

□
IV Minimization over Photon States

IV.1 Weyl Transformations and Positivity of the Electron Wave Function

In this section we show that the optimal electron wave function is nonnegative. More precisely, given any normalized complex-valued electron wave function $\phi \in H^1(\mathbb{R}^3)$, we show that the Lieb-Loss functional for the electron wave function $|\phi| \in H^1(\mathbb{R}^3)$ yields a lower value, if minimized over all photon states. This is done by a suitable Weyl transformation that eliminates the term in the Hamiltonian which is linear in the field operators. The proper choice (III.19) of the antiunitary $J$ is of key importance for the construction of this Weyl transformation. Equally important is the observation, that the energy shift induced by this Weyl transformation is balanced by the term \( \frac{1}{2} \| r \nabla \gamma \|_2^2 \) that vanishes for real $\phi$.

We start with a preparatory lemma.

**Lemma IV.1.** Let $\kappa \in B[\mathcal{H}]$ be a bounded operator and $\delta \in \mathbb{R}^+$. Then

$$
\kappa \left( \delta^2 + \kappa^* \kappa \right)^{-1} \kappa^* \leq 1. \tag{IV.1}
$$

**Proof.** Note that, if $\kappa$ is invertible, the assertion follows trivially from the operator monotonicity of $A \mapsto A^{-1}$, namely,

$$
\kappa \left( \delta^2 + \kappa^* \kappa \right)^{-1} \kappa^* \leq \kappa \left( \kappa^* \kappa \right)^{-1} \kappa^* = \kappa \kappa^{-1} \left( \kappa^* \right)^{-1} \kappa^* = 1. \tag{IV.2}
$$

If $\kappa$ is, however, not invertible then we define the bounded operator $A \in B[\mathcal{H} \oplus \mathcal{H}]$ by

$$
A := \begin{pmatrix} \delta & \kappa^* \\ \kappa & -\delta \end{pmatrix} = A^*, \tag{IV.3}
$$

and observe that

$$
A^2 = \begin{pmatrix} \delta^2 + \kappa^* \kappa & 0 \\ 0 & \delta^2 + \kappa \kappa^* \end{pmatrix} =: M \geq \delta^2 \cdot 1 \tag{IV.4}
$$

clearly is invertible. Hence

$$
A^2 M^{-1} = M^{-1} A^2 = 1, \tag{IV.5}
$$

and $A$ has a left inverse $M^{-1} A$ and a right inverse $A M^{-1}$. Thus $A$ is invertible and its left and right inverses coincide. In particular,

$$
\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = A M^{-1} A = \begin{pmatrix} (\delta^2 + \kappa^* \kappa)^{-1} \delta^2 + \kappa^* (\delta^2 + \kappa \kappa^*)^{-1} \kappa & \delta (\delta^2 + \kappa^* \kappa)^{-1} \kappa^* - \kappa^* (\delta^2 + \kappa \kappa^*)^{-1} \delta \\ \kappa (\delta^2 + \kappa^* \kappa)^{-1} \delta - \delta (\delta^2 + \kappa \kappa^*)^{-1} \kappa & (\delta^2 + \kappa \kappa^*)^{-1} \delta^2 + \kappa (\delta^2 + \kappa^* \kappa)^{-1} \kappa^* \end{pmatrix}. \tag{IV.6}
$$
Evaluating the lower right corner, we obtain

$$1 = (\delta^2 + \kappa \kappa^*)^{-1} \delta^2 + \kappa (\delta^2 + \kappa^* \kappa)^{-1} \kappa^* \geq \kappa^* (\delta^2 + \kappa^* \kappa)^{-1} \kappa \cdot \tag{IV.7}$$

□

**Lemma IV.2.** Let $J : \mathfrak{h} \to \mathfrak{h}$ be defined by (III.19), $\gamma, \gamma' \in H^1(\mathbb{R}^3)$, and $T_{r,\alpha}, \Theta_{r,\alpha}$, and $y_{r,\gamma,\alpha} \in \mathfrak{h}_{\mathbb{R}}$ as in (III.21)-(III.24). Then there is a unique $\eta_{r,\gamma} \in \mathfrak{h}_{\mathbb{R}}$ such that

$$y_{r,\gamma,\alpha} = \frac{1}{2} q^* T_{r,\alpha} q(\eta_{r,\gamma}) \cdot \tag{IV.8}$$

Moreover, as a quadratic form

$$d\Gamma J [T_{r,\alpha}, y_{r,\gamma,\alpha}] \geq \mathbb{W}_{\eta_{r,\gamma}} d\Gamma J [T_{r,\alpha}, 0] \mathbb{W}_{\eta_{r,\gamma}} - \| r \nabla \gamma \|_2^2 \cdot \tag{IV.9}$$

**Proof.** We first compute that

$$q^* T_{r,\alpha} q = |k|^{-1/2} (1 J) \begin{pmatrix} 2|k|^2 + \Theta_{r,\alpha}^* \Theta_{r,\alpha} & \Theta_{r,\alpha} \\ \Theta_{r,\alpha}^* & \Theta_{r,\alpha} \end{pmatrix} (1 J) |k|^{-1/2}$$

$$= |k|^{-1/2} (2|k|^2 + \Theta_{r,\alpha} + J\Theta_{r,\alpha} + \Theta_{r,\alpha} J + J\Theta_{r,\alpha} J) |k|^{-1/2} \cdot \tag{IV.10}$$

so $\eta_{r,\gamma}$ sought for fulfills

$$2y_{r,\gamma,\alpha} = |k|^{-1/2} (2|k|^2 + \Theta_{r,\alpha} + J\Theta_{r,\alpha} + \Theta_{r,\alpha} J + J\Theta_{r,\alpha} J) |k|^{-1/2} \eta_{r,\gamma} \cdot \tag{IV.11}$$

If $J$ was any general antiunitary map, the determination of $\eta_{r,\gamma}$ from (IV.11) appeared to be fairly complicated, but thanks to our choice (III.19) of $J$ we have that $\Theta_{r,\alpha} = J\Theta_{r,\alpha} = \Theta_{r,\alpha} J = J\Theta_{r,\alpha} J$ and $y_{r,\gamma,\alpha} = J y_{r,\gamma,\alpha}$. Therefore, $y_{r,\gamma,\alpha}$ is an element of $\mathfrak{h}_{\mathbb{R}}$ which is left invariant by $q^* T_{r,\alpha} q = |k|^{-1/2}(2|k|^2 + 4\Theta_{r,\alpha}) |k|^{-1/2}$. Moreover, $q^* T_{r,\alpha} q \geq 2|k| \geq 2\sigma \cdot 1 > 0$ is strictly positive and hence invertible, due to $\Theta_{r,\alpha} \geq 0$. (Here, the infrared cutoff $\sigma > 0$ comes in handy.) It follows that

$$\eta_{r,\gamma} = |k|^{1/2} (|k|^2 + 2\Theta_{r,\alpha})^{-1} |k|^{1/2} y_{r,\gamma,\alpha} \in \mathfrak{h}_{\mathbb{R}} \tag{IV.12}$$

and

$$\left( \eta_{r,\gamma} \mid |k|^{-1/2} (|k|^2 + 2\Theta_{r,\alpha}) |k|^{-1/2} \eta_{r,\gamma} \right)$$

$$\geq \left( |k|^{1/2} y_{r,\gamma,\alpha} \mid (|k|^2 + 2\Theta_{r,\alpha})^{-1} |k|^{1/2} y_{r,\gamma,\alpha} \right)$$

$$\geq \left( F[r \nabla \gamma] \mid \Phi_{r,\alpha} (|k|^2 + 2 \Phi^*_r \Phi_r) -1 \Phi^*_r \Phi_r F[r \nabla \gamma] \right)$$

$$\leq \left( F[r \nabla \gamma] \mid F[r \nabla \gamma] \right) = \| r \nabla \gamma \|_2^2 \cdot \tag{IV.13}$$

estimating $\left( |k|^2 + 2 \Phi^*_r \Phi_r \right)^{-1} \leq (\sigma^2 + 2 \Phi^*_r \Phi_r)^{-1}$ and then using Lemma [IV.1].

We obtain the assertion from here by (III.18). □
As a corollary of Lemma IV.2, we now find the following lower bound on the Lieb-Loss functional defined in (I.4).

**Corollary IV.3.** Let \( \phi \in H^1(\mathbb{R}^3) \) and \( \psi \in \mathcal{F}_{\text{ph}} \) be normalized wave functions. Then there exists a unitary Weyl transformation \( \mathbb{W}_\phi \) such that

\[
\mathcal{E}_{\alpha, \Lambda}(\phi, \psi) \geq \mathcal{E}_{\alpha, \Lambda}(|\phi|, \mathbb{W}_\phi \psi).
\] (IV.14)

As a consequence it follows that the partial minimization of the Lieb-Loss functional

\[
\hat{\mathcal{E}}_{\alpha, \Lambda}(\phi) := \inf \left\{ \mathcal{E}_{\alpha, \Lambda}(\phi, \psi) \mid \psi \in \mathcal{F}_{\text{ph}}, \|\psi\| = 1 \right\},
\] (IV.15)

over photon wave functions [see (I.14)] allows us to restrict the minimization over electron wave functions to nonnegative functions.

**Theorem IV.4.** Let \( \mathcal{J} : \mathfrak{h} \to \mathfrak{h} \) be defined by (III.19) and suppose that \( \phi \in \mathcal{H}_{\text{el}} \) is normalized and \( \phi \in H^1(\mathbb{R}^3) \). Then

\[
\hat{\mathcal{E}}_{\alpha, \Lambda}(\phi) \geq \hat{\mathcal{E}}_{\alpha, \Lambda}(|\phi|) = \frac{1}{2} \left\| \nabla |\phi| \right\|_2^2 + \frac{1}{2} \inf \left\{ \sigma \left( d\Gamma_{\mathcal{J}}[T_{|\phi|, \alpha}, 0] \right) \right\},
\] (IV.16)

where \( \sigma(A) \subseteq \mathbb{R} \) denotes the spectrum of a self-adjoint operator \( A \) and \( T_{|\phi|} \) is as defined in (III.21)-(III.23).

### IV.2 The Ground State Energy of \( T_{|\phi|, \alpha} \)

In this section we show that the infimum of the spectrum of \( \frac{1}{2} d\Gamma_{\mathcal{J}}[T_{|\phi|}, 0] \) equals \( X(\Theta_{|\phi|, \alpha}) \), as defined in (I.19) and (III.21)-(III.23). This fact had already been observed in [23], and we give an alternative and detailed proof here. More specifically, we prove the following theorem in this section.

**Theorem IV.5.** Let \( \mathcal{J} : \mathfrak{h} \to \mathfrak{h} \) be defined by (III.19), suppose that \( \phi = |\phi| \in H^1(\mathbb{R}^3) \), and let \( T_{\phi, \alpha} \) and \( \Theta_{\phi, \alpha} \) be given as in (III.21)-(III.24). Then

\[
\inf \left\{ \sigma \left( d\Gamma_{\mathcal{J}}[T_{\phi, \alpha}, 0] \right) \right\} = \text{Tr} \left( \sqrt{|k|^2 + 2 \Theta_{\phi, \alpha} - |k|} \right).
\] (IV.17)

Inserting (IV.17) into (IV.16), we immediately obtain the following Corollary.

**Corollary IV.6.** Let \( \mathcal{J} : \mathfrak{h} \to \mathfrak{h} \) be defined by (III.19) and suppose that \( \phi = |\phi| \in \mathcal{H}_{\text{el}} \) is normalized and \( \phi \in H^1(\mathbb{R}^3) \). Then

\[
\hat{\mathcal{E}}_{\alpha, \Lambda}(\phi) = \frac{1}{2} \left\| \nabla \phi \right\|_2^2 + \frac{1}{2} \text{Tr} \left( \sqrt{|k|^2 + 2 \Theta_{\phi, \alpha} - |k|} \right).
\] (IV.18)

where \( \Theta_{\phi, \alpha} \) is defined in (III.22)-(III.23).
Proof. [Proof of Theorem IV.5] The first step in our proof rests on an observation made in [H] that, given a nonnegative Hamiltonian $H$ representing an interacting quantum system, it holds true that

$$\inf_{\rho \in qfDM} \{ \text{Tr}(\rho^{1/2} H \rho^{1/2}) \} = \inf_{\rho \in qfDM} \{ \text{Tr}(\rho^{1/2} H \rho^{1/2}) \mid \rho \text{ is pure} \}, \quad (IV.19)$$

where $qfDM$ denotes the set of quasifree density matrices. In other words, for the computation of the Bogolubov-Hartree-Fock energy of the system, one may restrict the variation over all quasifree states to pure states. This statement may be viewed as a generalization of Lieb’s variational principle [24]. In Lemma IV.7 below, the observation from [H] is applied to the Hamiltonian $d\Gamma_J[T_{\phi,\alpha}, 0]$ and yields the statement, that its ground state energy is the lowest vacuum expectation value of all homogeneous Bogolubov transforms of $d\Gamma_J[T_{\phi,\alpha}, 0]$,

$$\inf \{ \sigma(d\Gamma_J[T_{\phi,\alpha}, 0]) \} = \inf \left\{ \langle \Omega | U_B d\Gamma_J[T_{\phi,\alpha}, 0] U_B^* \Omega \rangle \mid B \in \text{Bog}_J[h] \right\}, \quad (IV.20)$$

where $\text{Bog}_J[h]$ is defined in (IV.28).

Next, an application of Lemma IV.8 with $a := 2|k|$, $b := |k|^{-1/2}\Theta_{\phi,\alpha}|k|^{-1/2}$, and $d := 0$ yields the following lower bound on the vacuum expectation values on the right of (IV.20) in terms of $|v|$, where $v \in L^2[h]$ is the lower left matrix entry of $B$ of the Bogolubov transformation $U_B$,

$$\langle \Omega | U_B d\Gamma_J[T_{\phi,\alpha}, 0] U_B^* \Omega \rangle \geq \inf_{v \in L^2[h], v \geq 0} \left\{ \text{Tr} \left[ 2|k|^{1/2} v^2 |k|^{1/2} + \Theta_{\phi,\alpha}^{1/2} |k|^{-1/2}(v - \sqrt{1 + v^2})^2 |k|^{-1/2} \Theta_{\phi,\alpha}^{1/2} \right] \right\}. \quad (IV.21)$$

The infimum on the right side of the lower bound (IV.21) is explicitly computed in Lemma IV.9 below, using $\sigma \cdot 1 \leq a := 2|k| \leq \Lambda \cdot 1$, $b := |k|^{-1/2}\Theta_{\phi,\alpha}|k|^{-1/2} \geq 0$, and $d := 0$ again. Consequently,

$$\inf \left\{ \langle \Omega | U_B d\Gamma_J[T_{\phi,\alpha}, 0] U_B^* \Omega \rangle \mid B \in \text{Bog}_J[h] \right\} \geq \text{Tr} \left[ \sqrt{k^2 + 2\Theta_{\phi,\alpha}} - |k| \right]. \quad (IV.22)$$

We finally define

$$B_\star := \begin{pmatrix} \sqrt{1 + v_\star^2} & -v_\star \\ -v_\star & \sqrt{1 + v_\star^2} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} y_\star^{1/2} + y_\star^{-1/2} & -y_\star^{1/2} + y_\star^{-1/2} \\ -y_\star^{1/2} + y_\star^{-1/2} & y_\star^{1/2} + y_\star^{-1/2} \end{pmatrix}, \quad (IV.23)$$

$$v_\star := \frac{1}{2}(y_\star^{1/2} - y_\star^{-1/2}) \geq 0, \quad y_\star := |k|^{-1/2} \sqrt{k^2 + 2\Theta_{\phi,\alpha}} |k|^{-1/2} \geq 1, \quad (IV.24)$$
in accordance with (IV.52) and (IV.58). Then, by (IV.68), \( \Theta_{\phi,\alpha} \in \mathcal{L}^2[\hbar] \) implies that \( y_s - 1 \in \mathcal{L}^2[\hbar] \) which is equivalent to \( v_s \in \mathcal{L}^2[\hbar] \), thanks to (IV.65), and thus

\[
1 - y_s^{-1} = y_s - 1 - 4v_s^2 \in \mathcal{L}^2[\hbar].
\]

Moreover, as \(|k|\) and \( \Theta_{\phi,\alpha} \) are \( J \)-invariant, so are \( y_s \) and hence also \( v_s \) and \( \sqrt{1 + v_s^2} \). It follows that \( B_s \in \text{Bog}_j[\hbar] \) is a homogeneous Bogolubov transformation. Finally,

\[
B_s T_{\phi,\alpha} B_s^* = \left( \begin{array}{cc} 2|k| & 0 \\ 0 & 0 \end{array} \right) B_s^* + B_s \left( \begin{array}{cc} |k|^{-1/2} \Theta_{\phi,\alpha} |k|^{-1/2} & |k|^{-1/2} \Theta_{\phi,\alpha} |k|^{-1/2} \\ |k|^{-1/2} \Theta_{\phi,\alpha} |k|^{-1/2} & |k|^{-1/2} \Theta_{\phi,\alpha} |k|^{-1/2} \end{array} \right) B_s^*
\]

(IV.25)

\[
= \frac{1}{2} \left( \begin{array}{cc}
(y_s^{1/2} + y_s^{-1/2}) |k| (y_s^{1/2} + y_s^{-1/2}) & -(y_s^{1/2} + y_s^{-1/2}) |k| (y_s^{1/2} - y_s^{-1/2}) \\
+2y_s^{-1/2} |k|^{-1/2} \Theta_{\phi,\alpha} |k|^{-1/2} y_s^{-1/2} & +2y_s^{-1/2} |k|^{-1/2} \Theta_{\phi,\alpha} |k|^{-1/2} y_s^{-1/2}
\end{array} \right)
\]

so

\[
\langle \Omega | \mathcal{U}_{B_s} d\Gamma_J[T_{\phi,\alpha}, 0] \mathcal{U}_{B_s}^* \Omega \rangle = \langle \Omega | d\Gamma_J[B_s T_{\phi,\alpha} B_s^*, 0] \Omega \rangle
\]

\[
= \frac{1}{2} \text{Tr} \left[ (y_s^{1/2} - y_s^{-1/2}) |k| (y_s^{1/2} - y_s^{-1/2}) + 2y_s^{-1/2} |k|^{-1/2} \Theta_{\phi,\alpha} |k|^{-1/2} y_s^{-1/2} \right]
\]

\[
= \frac{1}{2} \text{Tr} \left[ |k|^{1/2} (y_s + y_s^{-1} - 2)|k|^{1/2} + 2\Theta_{\phi,\alpha}^{1/2} |k|^{-1/2} y_s - 1 |k|^{-1/2} \Theta_{\phi,\alpha}^{1/2} \right]
\]

\[
= \frac{1}{2} \text{Tr} \left[ \sqrt{k^2 + 2\Theta_{\phi,\alpha}} - |k| + |k|^{1/2} (y_s^{-1} - 1)|k|^{1/2} + 2\Theta_{\phi,\alpha} |k|^{-1/2} y_s^{-1} |k|^{-1/2} \right]
\]

\[
= \frac{1}{2} \text{Tr} \left[ \sqrt{k^2 + 2\Theta_{\phi,\alpha}} - |k| - (k^2 + 2\Theta_{\phi,\alpha}) |k|^{-1/2} y_s^{-1} |k|^{-1/2} - |k| \right]
\]

(IV.26)

\[
= \text{Tr} \left[ \sqrt{k^2 + 2\Theta_{\phi,\alpha}} - |k| \right].
\]

The first step in our derivation rests on an observation made in [4] which may be viewed as a generalization of Lieb’s variational principle [24].

**Lemma IV.7.** Let \( J : \hbar \to \hbar \) be an antiunitary involution and \( T = T^* \in \mathcal{B}[\hbar \oplus \hbar] \) be nonnegative, \( T \geq 0 \). Then

\[
\inf \left\{ \sigma (d\Gamma_J[T, 0]) \right\} = \inf \left\{ \langle \Omega | \mathcal{U}_B d\Gamma_J[T, 0] \mathcal{U}_B^* \Omega \rangle \left| B \in \text{Bog}_J[\hbar] \right\}, \quad (IV.27)
\]

where

\[
\text{Bog}_J[\hbar] := \left\{ B = \left( \begin{array}{cc} U & JV \\ V & JU \end{array} \right) \left| B^* S B = S, \quad \text{Tr}(V^* V) < \infty \right. \right\} \quad (IV.28)
\]

21
denotes the set of generators of homogeneous Bogolubov transformations.

Proof. Suppose that $H \geq 0$ is a nonnegative Hamiltonian on $\mathcal{F}_{ph}$ and define its Bogolubov-Hartree-Fock energy by

$$E_{BHF}(H) := \inf \left\{ \text{Tr}\left\{ \rho^{1/2} H \rho^{1/2} \right\} \left| \rho \in \mathcal{D} \mathcal{M}, \rho \text{ is quasifree} \right. \right\},$$

where $\mathcal{D} \mathcal{M} := \left\{ \rho \in B[\mathcal{F}_{ph}] \mid 0 \leq \rho \leq \text{Tr}\{\rho\} = 1 \right\}$ denotes the set of density matrices on $\mathcal{F}_{ph}$. In [4] it is shown that the Bogolubov-Hartree-Fock energy is already obtained by taking the infimum over all pure quasifree states,

$$E_{BHF}(H) = \inf \left\{ \text{Tr}\left\{ \rho^{1/2} H \rho^{1/2} \right\} \left| \rho \in \mathcal{D} \mathcal{M}, \rho \text{ is quasifree and pure} \right. \right\}. \tag{IV.30}$$

Since $d\Gamma_j[T_{\phi}, 0]$ is quadratic in the field operators, its ground state energy agrees with its Bogolubov-Hartree-Fock energy,

$$\inf \left\{ \sigma (d\Gamma_j[T, 0]) \right\} = E_{BHF}(d\Gamma_j[T, 0]). \tag{IV.31}$$

On the other hand, the pure quasifree density matrices $\rho_{\text{pure}} \in \mathcal{D} \mathcal{M}$ are precisely the rank-one orthogonal projections $\rho_{\text{pure}} = |U_B^* W^* \eta \rangle \langle U_B^* W^* \eta |$ onto Bogolubov and Weyl transforms $U_B^* W^* \eta \Omega$ of the vacuum vector $\Omega$, using that, $U_B^* = \cup_{SB \cdot S}$ is a homogeneous Bogolubov transformation, for $B \in \text{Bog}_J[h]$, and $W^* \eta = W_{-\eta}$ is a Weyl transformation, for $\eta \in \mathfrak{h}$. Thus we obtain

$$\inf \left\{ \sigma (d\Gamma_j[T, 0]) \right\}$$

$$= \inf \left\{ \langle \Omega | W^* \eta U_B d\Gamma_j[T, 0] U_B^* W^* \eta \Omega \rangle \left| B \in \text{Bog}_J[h], \eta \in \mathfrak{h} \right. \right\}$$

$$= \inf \left\{ \langle \Omega | \Gamma_j [BTB^*, -\frac{i}{2} q^* BTB^* q \eta] \Omega \rangle + \langle \eta | q^* BTB^* q \eta \rangle \left| B \in \text{Bog}_J[h], \eta \in \mathfrak{h} \right. \right\},$$

using (III.16) and (III.18). Since

$$\langle \Omega | \Gamma_j [BTB^*, -\frac{i}{2} q^* BTB^* q \eta] \Omega \rangle = \langle \Omega | \Gamma_j [BTB^*, 0] \Omega \rangle \tag{IV.33}$$

and

$$\langle \eta | q^* BTB^* q \eta \rangle \geq 0, \tag{IV.34}$$

it follows that the infimum on the right side of (IV.32) is attained for $\eta = 0$. \qed
Lemma IV.8. Let \( j : h \to h \) be an antiunitary involution. Let \( a \in \mathcal{B}[h] \) be a bounded, \( b \in \mathcal{L}^2[h] \) a Hilbert-Schmidt, and \( d \in \mathcal{L}^1(h) \) a trace-class operator such that all three are nonnegative and commute with \( j \), i.e., \( a = jaj \geq 0 \), \( b = jbj \geq 0 \), \( d = jdj \geq 0 \). Furthermore let \( B \in \text{Bog}_j[h] \), with \( \text{Bog}_j[h] \) as defined in (IV.28). Then

\[
T = \begin{pmatrix} a + b & b \\ b & d + b \end{pmatrix} \geq 0, \tag{IV.35}
\]

and

\[
\langle \Omega | \mathbb{U}_B d \Gamma_j[T, 0] \mathbb{U}_B^\dagger \Omega \rangle \geq \inf \left\{ \operatorname{Tr} \left[ a v^2 + b (v - \sqrt{1 + v^2})^2 + d (1 + v^2) \right] \mid v \geq 0, \operatorname{Tr}(v^2) < \infty \right\}. \tag{IV.36}
\]

Proof. First, we note that

if \( \tilde{T} = \begin{pmatrix} \bar{a} & \bar{b}^* \\ \bar{b} & \bar{d} \end{pmatrix} \), then \( \langle \Omega | d \Gamma_j[\tilde{T}, 0] \Omega \rangle = \operatorname{Tr}(\tilde{d}) \). \tag{IV.37}

Next, if \( B \in \text{Bog}_j[h] \) is of the form

\[
B = \begin{pmatrix} u & jv \nu j \\ v & ju \end{pmatrix}, \tag{IV.38}
\]

then a simple computation using that \( j \) commutes with \( a, b, \) and \( d \), shows that

\[
BTB^* = \begin{pmatrix} u(a + b)u^* + ubjv^* & u(a + b)v^* + ubju^* \\ +vbjvu + u(d + b)v^* & +vbjvu^* + u(d + b)v^* \\ v(a + b)u^* + juvb^* & v(a + b)v^* + juvb^* \\ +vbjv^* + ju(d + b)v^* & +vbjv^* + ju(d + b)v^* \end{pmatrix}. \tag{IV.39}
\]

Using (IV.37), this yields

\[
\langle \Omega | d \Gamma_j[B^*TB, 0] \Omega \rangle = \operatorname{Tr} \left[ (a + b)v^* + v^*bju + ju^*jbv + u(d + b)u^* \right] \tag{IV.40}
\]

\[
= \operatorname{Tr} \left[ av^*v + du^*u + 2\operatorname{Re} \operatorname{Tr}[bv^*ju] \right].
\]

From the Cauchy-Schwarz inequality for traces we obtain

\[
|\operatorname{Tr}[bv^*ju]|^2 \leq \operatorname{Tr}[bv^* x^{-1} v] \operatorname{Tr}[bju^* x ju] = \operatorname{Tr}[b v^* x^{-1} v] \operatorname{Tr}[b u^* x ju], \tag{IV.41}
\]

23
for any bounded and invertible positive operator \( x \geq \mu \cdot 1 > 0 \).

Next we remark that, due to (III.15), we have
\[
    u^*u - v^*v = j u u^* j - v v^* = 1, \quad v^* j u = u^* j v, \quad j u v^* = v u^* j.
\]

(IV.42)

For any \( r > 0 \), this implies that
\[
    (r + vv^*) u = r j u + v u^* j v = j u (r + v^* v), \quad (r + vv^*) v = v (r + v^* v),
\]

(IV.43)

which, in turn, gives
\[
    (r + vv^*)^{-1} j u = j u (r + v^* v)^{-1}, \quad (r + vv^*)^{-1} v = v (r + v^* v)^{-1}.
\]

(IV.44)

Writing the square root as an integral over resolvents according to
\[
    A^{-1/2} = \frac{1}{\pi} \int_0^\infty (s + A)^{-1} ds, \quad (IV.44)
\]

yields
\[
    (r + vv^*)^{1/2} j u = j u (r + v^* v)^{1/2}, \quad (r + vv^*)^{1/2} v = v (r + v^* v)^{1/2},
\]

(IV.45)

for all \( r > 0 \). For small \( 0 < \epsilon < 1 \), we define
\[
    x_\epsilon := (1 + vv^*)^{-1/2} (\epsilon + vv^*)^{1/2}
\]

(IV.46)

and observe that, due to (IV.45) and (IV.42), we have
\[
    u^* j x_\epsilon j u = u^* j (1 + vv^*)^{-1/2} (\epsilon + vv^*)^{1/2} j u = u^* u (1 + v^* v)^{-1/2} (\epsilon + v^* v)^{1/2}
\]
\[
    = (1 + v^* v)^{1/2} (\epsilon + v^* v)^{1/2}
\]

(IV.47)

and further
\[
    v^* x_\epsilon^{-1} v = v^* (\epsilon + vv^*)^{-1/2} (1 + vv^*)^{1/2} v = v^* v (\epsilon + v^* v)^{-1/2} (1 + v^* v)^{1/2}
\]
\[
    \leq (v^* v)^{1/2} (1 + v^* v)^{1/2}. \quad (IV.48)
\]

Inserting (IV.47) and (IV.48) into (IV.41) and taking the limit \( \epsilon \to 0 \), we obtain
\[
    \left| \text{Tr}[b v^* j u j] \right| \leq \text{Tr}[b v^* v]^{1/2} (1 + v^* v)^{1/2} \right].
\]

(IV.49)

Using this estimate and (IV.40), we arrive at
\[
    \langle \Omega | d\Gamma [B^* T B, 0] | \Omega \rangle \geq \text{Tr} \left[ a |v|^2 + b (|v| - \sqrt{1 + |v|^2})^2 + d (1 + |v|^2) \right],
\]

(IV.50)

from which the asserted estimate (IV.36) is immediate.
Lemma IV.9. Let $j : h \to h$ be an antiunitary involution. Let $a \in \mathcal{B}[h]$ be a bounded, $b \in \mathcal{L}^2[h]$ a Hilbert-Schmidt, and $d \in \mathcal{L}^1(h)$ a trace-class operator such that $a = jadj \geq \sigma \cdot 1 > 0$, for some $\sigma > 0$, and $b = jbj \geq 0$, $d = jdj \geq 0$, i.e., all three are nonnegative and commute with $j$. Then

$$\inf \left\{ \text{Tr} \left[ a v^2 + b(v - \sqrt{1 + v^2})^2 + d(1 + v^2) \right] \bigg| v \geq 0, \ \text{Tr}(v^2) < \infty \right\} = \frac{1}{2} \text{Tr} \left[ \left( \sqrt{a + d}(a + d + 4b) \sqrt{a + d} \right)^{1/2} - a + d \right].$$

(IV.51)

Proof. It is convenient to parametrize $v$ as

$$v = \frac{1}{2} \left( y^{1/2} - y^{-1/2} \right),$$

(IV.52)

where $y \geq 1$ is a positive operator defined by (IV.52) through functional calculus. Note in passing that $y$ is uniquely determined by $v$ up to $\ker(y - 1)$ and that $y - 1 \in \mathcal{L}^2[h]$, due to Lemma [IV.10](i). Then

$$v^2 = \frac{y}{4} + \frac{y^{-1}}{4} - \frac{1}{2} \quad \text{and} \quad 1 + v^2 = \frac{y}{4} + \frac{y^{-1}}{4} + \frac{1}{2} = \left[ \frac{1}{2} \left( y^{1/2} + y^{-1/2} \right) \right]^2.$$

(IV.53)

Hence we have that

$$\sqrt{1 + v^2} = \frac{1}{2} \left( y^{1/2} + y^{-1/2} \right) \quad \text{and} \quad (v - \sqrt{1 + v^2})^2 = y^{-1}.$$

(IV.54)

Inserting the parametrization (IV.52) into the trace in (IV.51), we obtain

$$\text{Tr} \left[ a v^2 + b(v - \sqrt{1 + v^2})^2 + d(1 + v^2) \right] = \frac{1}{4} G(y),$$

(IV.55)

with

$$G(y) := \text{Tr} \left[ m^2 y + (m^2 + 4b) y^{-1} + 2(d - a) \right],$$

(IV.56)

$m := \sqrt{a + d} \geq \sigma^{1/2} > 0$, and $y - 1 \in \mathcal{L}^2[h]$. Obviously, $y \mapsto G(y)$ is convex. We define $y_* \geq 1$ by

$$y_* := m^{-1} \left( m^2 y + (m^2 + 4b) \right) m^{1/2} m^{-1}$$

(IV.57)

and observe that $y_* - 1 \in \mathcal{L}^2[h]$, by Lemma [IV.10](ii), and that $y_*, m^2 y_* = m^2 + 4b$ which is equivalent to

$$y_*^{-1} (m^2 + 4b) y_*^{-1} = m^2.$$  

(IV.58)
The latter is the formal condition for stationarity of $y \mapsto G(y)$. We refrain from turning this formal into a mathematically rigorous condition by establishing differentiability of $G$ in a suitable sense. Instead, we simply check by computation that $y_\ast$ is the minimizer of $G$. Namely, we have that

$$G(y) - G(y_\ast) := \text{Tr} \left[ m^2 (y - y_\ast) + (m^2 + 4b) (y^{-1} - y_\ast^{-1}) \right], \quad (IV.59)$$

and the second resolvent equation gives

$$y^{-1} - y_\ast^{-1} = -y_\ast^{-1} (y - y_\ast) y_\ast^{-1} + y_\ast^{-1} (y - y_\ast) y^{-1} (y - y_\ast) y_\ast^{-1}. \quad (IV.60)$$

Thus from (IV.58) derives

$$G(y) - G(y_\ast) = \text{Tr} \left[ \left( m^2 - y_\ast^{-1} (m^2 + 4b) y_\ast^{-1} \right) (y - y_\ast) \right. \left. + y^{-1/2} (y - y_\ast) y_\ast^{-1} (m^2 + 4b) y_\ast^{-1} (y - y_\ast) y^{-1/2} \right]$$

$$= \text{Tr} \left[ y^{-1/2} (y - y_\ast) y_\ast^{-1} (m^2 + 4b) y_\ast^{-1} (y - y_\ast) y^{-1/2} \right] \geq 0. \quad (IV.61)$$

Finally,

$$G(y_\ast) = \text{Tr} \left[ m^2 y_\ast + (m^2 + 4b) y_\ast^{-1} + 2(d - a) \right]$$

$$= 2 \text{Tr} \left[ m y_\ast m + d - a \right] = 2 \text{Tr} \left[ (m (m^2 + 4b) m)^{1/2} + d - a \right]$$

$$= 2 \text{Tr} \left[ \left( \sqrt{a + d} (a + d + 4b) \sqrt{a + d} \right)^{1/2} - a + d \right], \quad (IV.62)$$

arriving at (IV.51).

**Lemma IV.10.** Let $h$ be a Hilbert space and $m, b, y \in \mathcal{B}[h]$ be positive bounded operators such that $b \in \mathcal{L}^2[h]$ is Hilbert-Schmidt, $y \geq 1$, and $m \geq \sigma^{1/2} \cdot 1$, for some $\sigma > 0$. Then the following assertions hold true.

(i) Define $v := \frac{1}{2} (y^{1/2} - y^{-1/2}) > 0$. Then $v \in \mathcal{L}^2[h]$ is Hilbert-Schmidt if, and only if, $y - 1 \in \mathcal{L}^2[h]$ is Hilbert-Schmidt.

(ii) Define $y := m^{-1} \left[ m (m^2 + 4b) m \right]^{1/2} m^{-1}$. Then $y \geq 1$ and $y - 1 \in \mathcal{L}^2[h]$ is Hilbert-Schmidt.

**Proof.**

(i): First $0 < y^{-1/2} \leq 1$ and thus $1 \leq y^{1/2} = y^{-1/2} + 2v \leq 1 + 2 \|v\|_{\text{op}}$, which implies that

$$1 \leq y \leq \left( 1 + 2 \|v\|_{\mathcal{B}[h]} \right)^2 \cdot 1. \quad (IV.63)$$
Secondly note that

\[ v^2 = y^4 + y^{-1} - \frac{1}{2} = \frac{1}{4y}(y - 1)^2, \quad \text{(IV.64)} \]

and taking (IV.63) into account, we arrive at (i) because

\[ \text{Tr}[v^2] \leq \text{Tr}[(y - 1)^2] \leq 4(1 + 2\|v\|_{B^2})^2 \text{Tr}[v^2]. \quad \text{(IV.65)} \]

(ii): For \( y = m^{-1}\left[m(m^2 + 4b)m\right]^{1/2}m^{-1} \) we trivially have \( y \geq 1 \) since \( b \geq 0 \) and the square root is operator monotone. Moreover, using

\[ A^{-1/2} = \frac{1}{\pi} \int_0^\infty (s + A)^{-1} \frac{ds}{s^{1/2}}, \quad \text{(IV.66)} \]

the second resolvent equation, and \( R_s := (s + m^4)^{-1} \leq (s + \sigma^2)^{-1} \), we have that

\[
\begin{align*}
    y-1 &= m^{-1}\left[m^4 + 4mbm\right]^{1/2} - m^2 \right] m^{-1} \\
    &= \frac{1}{\pi} \int_0^\infty m^{-1} \left\{ \frac{m^4 + 4mbm}{s + m^4 + 4mbm} - \frac{m^4}{s + m^4} \right\} m^{-1} \frac{ds}{s^{1/2}} \\
    &= \frac{1}{\pi} \int_0^\infty m^{-1} \left\{ (s + m^4)^{-1} - (s + m^4 + 4mbm)^{-1} \right\} m^{-1} s^{1/2} ds \\
    &= \frac{4}{\pi} \int_0^\infty \left\{ R_s b R_s - 4R_s bm (s + m^4 + 4mbm)^{-1} mb R_s \right\} s^{1/2} ds \\
    &\leq \frac{4}{\pi} \int_0^\infty \left\{ R_s b R_s \right\} s^{1/2} ds. \quad \text{(IV.67)}
\end{align*}
\]

Consequently,

\[
\begin{align*}
    \text{Tr}[(y - 1)^2] \\
    \leq \frac{16}{\pi^2} \int_0^\infty \int_0^\infty \text{Tr}\left[ \sqrt{R_s} \sqrt{R_t} b^2 \sqrt{R_t} R_s \sqrt{R_t} b \sqrt{R_t} \sqrt{R_s} \sqrt{s} \sqrt{t} ds dt \right] \\
    \leq \frac{16}{\pi^2} \int_0^\infty \int_0^\infty \text{Tr}\left[ \sqrt{R_s} \sqrt{R_t} b^2 \sqrt{R_t} \sqrt{R_s} \sqrt{s} ds \sqrt{t dt} \right] \frac{s + \sigma^2}{t + \sigma^2} \\
    \leq \frac{16}{\pi^2} \left( \int_0^\infty \frac{\sqrt{s} ds}{(s + \sigma^2)^2} \right)^2 \text{Tr}[b^2] = \frac{16}{\pi^2 \sigma^2} \left( \int_0^\infty \frac{\sqrt{r} ds}{(r + 1)^4} \right)^2 \text{Tr}[b^2] < \infty. \quad \text{(IV.68)}
\end{align*}
\]

\[ \square \]
V Localization Estimates

In this section we turn to the analysis of the effective energy functional

\[ \hat{E}_{\alpha, \Lambda}(\phi) = \frac{1}{2} \| \nabla \phi \|^2 + \frac{1}{2} X(2\Theta_{\phi, \alpha}), \]  

(V.1)

where \( \phi = |\phi| \in \mathcal{H}_{el} \) is normalized and \( \phi \in H^1(\mathbb{R}^3) \), \( \Theta_{\phi, \alpha} \) is defined in (III.22)-(III.23), and

\[ X(A) := \text{Tr} \left( \sqrt{|k|^2 + A} - |k| \right), \]  

(V.2)

for positive operators \( A \geq 0 \). Recall that, according to Theorem IV.4 and Corollary IV.6, the Lieb-Loss energy defined in Eqs. (I.3)-(I.4) is given by

\[ E_{LL}(\alpha, \Lambda) = \inf \{ \hat{E}_{\alpha, \Lambda}(\phi) \mid |\phi| = |\phi| \in H^1(\mathbb{R}^3), \| \phi \|^2 = 1 \}. \]  

(V.3)

Ultimately, we compare \( \hat{E}_{\alpha, \Lambda} \) and its infimum \( E_{LL}(\alpha, \Lambda) \) to \( F_{\beta(\alpha, \Lambda)} \) and its infimum \( F[\beta(\alpha, \Lambda)] \), respectively, where

\[ F_{\beta}(\phi) := \frac{1}{2} \| \nabla \phi \|^2 + \beta \| \phi \|_1, \]  

(V.4)

\[ F[\beta] := \inf \{ F_{\beta}(\phi) \mid \phi = |\phi| \in H^1(\mathbb{R}^3) \cap L^1(\mathbb{R}^3), \| \phi \|^2 = 1 \}, \]  

(V.5)

\[ \beta(\alpha, \Lambda) := \sqrt{\frac{4\alpha}{9\pi}} \Lambda^3. \]  

(V.6)

In the present section we demonstrate that the minimization in (V.3) may be restricted to functions supported in the ball \( B(0, L) = \{ x \in \mathbb{R}^3 : |x| < L \} \) of radius \( L < \infty \), provided \( L \gg 1 \) is sufficiently large. That is, we prove in Theorem V.1 below that

\[ E^{(L)}_{LL}(\alpha, \Lambda) := \inf \{ \hat{E}_{\alpha, \Lambda}(\phi) \mid \phi = |\phi| \in Y_L, \| \phi \|^2 = 1 \}, \]  

(V.7)

approximates \( E_{LL}(\alpha, \Lambda) \), as \( L \to \infty \), by showing that the error made by this restriction is of order \( L^{-2} \), as suggested by the IMS localization formula. Here,

\[ Y_L := H^1(B(0, L)) \subseteq H^1(\mathbb{R}^3) \cap L^1(\mathbb{R}^3) \subseteq H^1(\mathbb{R}^3) =: Y, \]  

(V.8)

and we correspondingly approximate \( F[\beta] \) by

\[ F^{(L)}[\beta] := \inf \{ F_{\beta}(\phi) \mid \phi = |\phi| \in Y_L, \| \phi \|^2 = 1 \}. \]  

(V.9)
Theorem V.1. There exists a universal constant $C < \infty$ such that, for all $\alpha, \beta, L > 0$, $\sigma \geq 0$, and $\Lambda \geq 1$,
\[
E_{LL}(\alpha, \Lambda)^{(L)} - \frac{C}{L^2} \leq E_{LL}(\alpha, \Lambda) \leq E_{LL}(\alpha, \Lambda),
\]
\[
F(\beta) - \frac{C}{L^2} \leq F[\beta] \leq F(\beta),
\]
with $E_{LL}(\alpha, \Lambda), F(\alpha, \Lambda), E^{(L)}_{LL}(\alpha, \Lambda),$ and $F^{(L)}(\alpha, \Lambda)$ as in (V.3), (V.5), (V.7), and (V.9), respectively.

Proof. The inequalities $E_{LL}(\alpha, \Lambda) \leq E_{LL}(\alpha, \Lambda)^{(L)}$ and $F[\beta] \leq F^{(L)}[\beta]$ are trivial consequences of the inclusions $Y_L \subseteq Y$ and $Y_L \subseteq H^1(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$, respectively.

For the derivation of the lower bound (V.10) on $E_{LL}(\alpha, \Lambda)$, we pick a smooth and compactly supported function $\eta \in C^\infty_0(\mathbb{R}^3; \mathbb{R}^+)$, chosen such that $\text{supp}(\eta) \subseteq B(0, 1)$ and $\|\eta\|_2 = 1$. Then we define $\eta_{L,z}(x) := L^{-\frac{3}{2}} \eta[L^{-1}(x - z)]$, for all $L > 0$, and we observe that $\|\eta_{L,z}\|_2 = 1$ and $\int \eta_{L,z}^2(x) \, d^3z = 1$. We further set $\rho_L(z) := \|\eta_{L,z}\|_2^2$, $\phi_{L,z}(x) := \left\{ \begin{array}{ll} \eta_{L,z}(x) \phi(x) / \rho_L(z) & \text{if } \rho_L(z) > 0, \\ 0 & \text{if } \rho_L(z) = 0, \end{array} \right.$ (V.13)
and observe that $\rho_L$ is a probability density on $\mathbb{R}^3$. A variant of the IMS localization formula [12] now yields
\[
\|\nabla \phi\|_2^2 = \int \|\nabla (\eta_{L,z} \phi)\|_2^2 d^3z - \int |\nabla \eta_{L,z}|^2 d^3z
\]
\[
= \int \|\nabla \phi_{L,z}\|_2^2 \rho_L(z) \, d^3z - \frac{\|\nabla \eta\|_2^2}{L^2}.
\]
(V.14)

Note that
\[
\Phi^*_{\phi,\alpha} \Phi_{\phi,\alpha} = \int \left\{ \Phi^*_{\phi_{L,z,\alpha}} \Phi_{\phi_{L,z,\alpha}} \right\} \rho_L(z) \, d^3z,
\]
and since $A \mapsto X(A)$ is concave according to Lemma (V.3) (ii), we obtain
\[
X(\Phi^*_{\phi,\alpha} \Phi_{\phi,\alpha}) \geq \int X(\Phi^*_{\phi_{L,z,\alpha}} \Phi_{\phi_{L,z,\alpha}}) \rho_L(z) \, d^3z.
\]
(V.16)
Consequently

\[
\hat{E}_{\alpha,\Lambda}(\phi) \geq \int \hat{E}_{\alpha,\Lambda}(\phi_{L,z}) \rho_L(z) \, d^3z \geq \int E_{LL}^{(L)}(\alpha, \Lambda) \rho_L(z) \, d^3z = E_{LL}^{(L)}(\alpha, \Lambda) - \frac{\|\nabla \eta\|_2^2}{L^2}.
\]

Taking the infimum over \( \phi \in H^1(\mathbb{R}^3) \) concludes the proof of the first inequality in (V.10). The proof of the first inequality in (V.11) is similar.

For the proof of Theorem [V.1], we supply various properties of \( X(A) \) in the following two lemmata. To formulate these it is convenient to denote

\[
K_A := \sqrt{k^2 + A},
\]

so that

\[
X(A) = \text{Tr}[K_A - K_0].
\]

Since on \( \mathfrak{h} \), the multiplication operator \( \sigma \cdot 1 \leq |k| \leq \Lambda \cdot 1 \) is bounded and bounded invertible, we observe that

\[
\sigma \cdot 1 \leq K_0 \leq K_A \leq (\Lambda + \|A\|_{B(\mathfrak{h})}) \cdot 1.
\]

**Lemma V.2.** Let \( A = A^* \geq 0 \) be a bounded self-adjoint operator on \( \mathfrak{h} \) such that \((k^2 + A)^{\frac{1}{2}} - |k| \) is trace class. Then

\[
\text{Tr}[(k^2 + A)^{\frac{1}{2}} - |k|] = \text{Tr}[A^{\frac{1}{2}} \left\{(k^2 + A)^{\frac{1}{2}} + |k| \right\}^{-1} A^{\frac{1}{2}}].
\]

**Proof.** Using (V.18)-(V.20), we have that

\[
\text{Tr}[K_A - K_0]
\]

\[
= \frac{1}{2} \text{Tr}\left[\left\{K_A - K_0\right\}\left\{K_A + K_0\right\}\left(K_A + K_0\right)^{-1}\right]
\]

\[
+ \frac{1}{2} \text{Tr}\left[\left\{K_A - K_0\right\}\left(K_A + K_0\right)^{-1}\left\{K_A + K_0\right\}\right]
\]

\[
= \text{Tr}\left[\left\{K_A^2 - K_0^2\right\}\left(K_A + K_0\right)^{-1}\right]
\]

\[
= \text{Tr}\left[A^{\frac{1}{2}} \left\{K_A + K_0\right\}^{-1} A^{\frac{1}{2}}\right],
\]

where the finiteness of the left side of (V.22) implies finiteness of all following lines. \(\square\)
**Lemma V.3.** Let $A = A^*, B = B^* \geq 0$ be two bounded self-adjoint operators on $\mathfrak{h}$ such that $K_A - K_0$ and $K_B - K_0$ are trace class. Then

(i) \[ X(A) \leq X(A + B) \leq X(A) + X(B), \quad \text{(V.23)} \]

(ii) \[ A \mapsto X(A) \text{ is concave}. \quad \text{(V.24)} \]

**Proof.** Since $A, B \geq 0$ we may use the operator monotonicity of the square root and the inverse to infer that $A \mapsto K_A$ and $A \mapsto K_A^{-1}$ are monotone and thus

\[ X(A) = \operatorname{Tr}[K_A - K_0] \leq \operatorname{Tr}[K_{A+B} - K_0] = X(A + B), \quad \text{(V.25)} \]

and

\[ X(A + B) = \operatorname{Tr}\left[(A + B) \left\{ K_{A+B} + K_0 \right\}^{-1} \right] \leq \operatorname{Tr}\left[A \left\{ K_A + K_0 \right\}^{-1} \right] + \operatorname{Tr}\left[B \left\{ K_B + K_0 \right\}^{-1} \right] = X(A) + X(B), \quad \text{(V.26)} \]

additionally using Lemma V.2. This yields (V.23).

As for (V.24), we note that

\[ X\left(\frac{1}{2}A + \frac{1}{2}B\right) - \frac{1}{2}X(A) - \frac{1}{2}X(B) = \operatorname{Tr}[P - Q], \quad \text{(V.27)} \]

where

\[ P := K_{A+B} \quad \text{and} \quad Q := \frac{1}{2}K_A + \frac{1}{2}K_B. \quad \text{(V.28)} \]

Now,

\[
\operatorname{Tr}[P - Q] = \frac{1}{2} \operatorname{Tr}[\left(\frac{1}{2}A + \frac{1}{2}B\right) \left(k^2 + \frac{1}{2}A + \frac{1}{2}B - \frac{1}{2}K_A K_B - \frac{1}{2}K_B K_A\right) \leq 0, \quad \text{(V.29)}
\]

which yields midpoint concavity of $A \mapsto X(A)$, i.e.,

\[ X\left(\frac{1}{2}A + \frac{1}{2}B\right) \geq \frac{1}{2}X(A) + \frac{1}{2}X(B). \quad \text{(V.30)} \]

Finally, midpoint concavity and continuity of $A \mapsto X(A)$ implies general concavity and hence (V.24).
VI  Upper Bound on $X(2\Theta_{\phi,\alpha})$

We proceed to deriving an upper bound on $E_{L\Lambda}^{(L)}(\alpha, \Lambda)$ defined in \((V.7)\) in terms of $F^{(L)}(\alpha, \Lambda)$ given in \((V.9)\). Our derivation uses two essential tools:

(i) The functional calculus for self-adjoint operators described in [1], which yields a good control on projections onto different momentum shells emerging from the decomposition $\chi_{\sigma,(1+\varepsilon)\Lambda} = \chi_{\sigma,\Lambda} + \chi_{\Lambda,(1+\varepsilon)\Lambda}$, where $\varepsilon > 0$ and we recall that $\chi_{\sigma,\Lambda} = 1[\sigma \leq |k| < \Lambda]$. We show that the contribution of $\chi_{\Lambda,(1+\varepsilon)\Lambda}$ is negligible, provided $\varepsilon > 0$ is chosen sufficiently small.

(ii) Inequalities for Schatten-$p$-norms of operators of the type “$f(x)g(-i\nabla)$”, for $1 \leq p \leq 2$, in order to estimate the error terms emerging from (i). More specifically, Birman and Solomyak have shown [10, 26] that, for any $1 \leq p \leq 2$, there exists a universal constant $C_{BS}(p) < \infty$ such that

$$\|f(x)g(-i\nabla)\|_{L^p(h_0)} \leq C_{BS}(p) \|f\|_{2;p} \|g\|_{2;p}, \quad (VI.1)$$

provided $\|f\|_{2;p}, \|g\|_{2;p} < \infty$, where

$$\|f\|_{2;p} := \left( \sum_{\beta \in \mathbb{Z}^3} \|f \cdot 1_{Q+\beta}\|_2^p \right)^{1/p} \quad (VI.2)$$

and $Q = [-\frac{1}{2}, \frac{1}{2}]^3 \subseteq \mathbb{R}^3$ is the unit cube centered at the origin.

**Theorem VI.1.** There exists a universal constant $C < \infty$ such that, for all $\alpha, L > 0$, all $0 \leq \sigma \leq 1 \leq \Lambda < \infty$, all $0 < \varepsilon \leq 1$ and all $\phi = |\phi| \in Y_L$, the estimate

$$\frac{1}{2} X(2\Theta_{\phi,\alpha}) \leq \sqrt{\frac{4\alpha}{9\pi}} \left[ \left( \Lambda^3 - \sigma^3 \right) + 54\varepsilon \Lambda^3 + 5\sigma^{3/2} \Lambda^{3/2} \right] \|\phi\|_1 + \frac{C \alpha^{1/2}(L \Lambda + 1)^2}{\varepsilon^{2} L^{3/2} \Lambda} \|\nabla \phi\|_2. \quad (VI.3)$$

holds true.

**Proof.** We first apply Lemma \((\ref{V.2})\) and the operator monotonicity of $A \mapsto \sqrt{A}$ and $A \mapsto A^{-1}$ and observe that

$$X(A) = \text{Tr} \left[ \sqrt{A} \left( \sqrt{k^2 + A} + |k| \right)^{-1} \sqrt{A} \right] \leq \text{Tr} \left[ \sqrt{A} \right]. \quad (VI.4)$$

Secondly, we note that $(\hat{\phi}^*)^*(\hat{\phi}^*) = \mathcal{F} \phi^2 \mathcal{F}^*$, where $\mathcal{F}$ is (componentwise) Fourier transformation. As is customary, we denote by $\phi(x) := \mathcal{F} \phi \mathcal{F}^* \geq 0$ the corresponding nonnegative multiplication operator, indicating the change from momentum to position space by explicitly keeping the argument “$x$” for the spatial
variable. Using (VI.4), the decomposition \( 1 = \chi_{0,\sigma} + \chi_{\sigma,\Lambda} + \chi_{\Lambda,(1+\varepsilon)\Lambda} + \chi_{(1+\varepsilon)\Lambda} \), where \( \chi_{r} := 1 - \chi_{r} \), and the triangle inequality for the trace norm, we obtain

\[
X(2\Theta_{\phi,\alpha}) = X(2\Phi^{*}_{\phi,\alpha} \Phi_{\phi,\alpha}) \leq \text{Tr} \left[ \sqrt{2\Phi^{*}_{\phi,\alpha} \Phi_{\phi,\alpha}} ^{2} \right] = \sqrt{2} \| \Phi_{\phi,\alpha} \|_{\mathcal{L}^{1}[b]} \]

\[
= \frac{(2\alpha)^{1/2}}{(2\pi)^{3/2}} \| \phi(x) \chi_{\sigma,\Lambda} P_{C} \|_{\mathcal{L}^{1}[b]} \]

\[
\leq \frac{(2\alpha)^{1/2}}{(2\pi)^{3/2}} \left( \| \chi_{\sigma,\Lambda} \phi(x) \chi_{\sigma,\Lambda} P_{C} \|_{\mathcal{L}^{1}[b]} + 3X_{1} + 3X_{2} + 3X_{3} \right),
\]

where

\[
\| P_{C} \chi_{\sigma,\Lambda} \phi(x) \chi_{\sigma,\Lambda} P_{C} \|_{\mathcal{L}^{1}[b]} = \| \sqrt{\phi(x)} \chi_{\sigma,\Lambda} P_{C} \|_{\mathcal{L}^{2}[b]} \]

\[
= 2 \left( \text{Vol}[B(0, \Lambda)] - \text{Vol}[B(0, \sigma)] \right) \left( \int \phi(x) d^{3}x \right) = \frac{8\pi}{3} (\Lambda^{3} - \sigma^{3}) \| \phi \|_{1}
\]

is the main term. Note that the factor 2 takes into account that \( P_{C} \) is an orthogonal projection of rank 2 on \( \mathbb{C} \otimes \mathbb{R}^{3} \). Moreover, we denote by \( \text{Vol}[M] := \int 1_{M}(k) d^{3}x \) the three-dimensional Lebesgue measure of a measurable set \( M \subseteq \mathbb{R}^{3} \) in (VI.6) and henceforth. Furthermore,

\[
X_{1} := \| \chi_{0,\sigma} \phi(x) \chi_{\sigma,\Lambda} \|_{\mathcal{L}^{1}[b_{0}]},
\]

\[
X_{2} := \| \chi_{\Lambda,(1+\varepsilon)\Lambda} \phi(x) \chi_{\sigma,\Lambda} \|_{\mathcal{L}^{1}[b_{0}]},
\]

\[
X_{3} := \| \chi_{(1+\varepsilon)\Lambda} \phi(x) \chi_{\sigma,\Lambda} \|_{\mathcal{L}^{1}[b_{0}]}
\]

are error terms we proceed to estimate next. Before we remark that the Hilbert space in (VI.7)-(VI.9) is the space \( h_{0} := L^{2}(\mathbb{R}^{3}) \) of complex-valued (scalar) square-integrable functions, as opposed to the one-photon Hilbert space \( h \) of square-integrable divergence-free vector fields used before. The factors 3 on the right side of (VI.5) account for the three components of the latter.

Using the trace inequality \( \| AB \|_{\mathcal{L}^{1}[b_{0}]} \leq \| A \|_{\mathcal{L}^{2}[b_{0}]} \| B \|_{\mathcal{L}^{2}[b_{0}]} \) and \((1+\varepsilon)^{3} - 1 \leq 3\varepsilon(1+\varepsilon)^{2} \leq 12\varepsilon\), we obtain

\[
X_{1} \leq \| \chi_{0,\sigma} \sqrt{\phi(x)} \|_{\mathcal{L}^{2}[b_{0}]} \| \sqrt{\phi(x)} \chi_{0,\Lambda} \|_{\mathcal{L}^{2}[b_{0}]} \leq \frac{12\pi}{3} \Lambda^{3/2} \sigma^{3/2} \| \phi \|_{1},
\]

\[
X_{2} \leq \| \chi_{\Lambda,(1+\varepsilon)\Lambda} \sqrt{\phi(x)} \|_{\mathcal{L}^{2}[b_{0}]} \| \sqrt{\phi(x)} \chi_{0,\Lambda} \|_{\mathcal{L}^{2}[b_{0}]} \leq \frac{144\pi}{3} \varepsilon \Lambda^{3} \| \phi \|_{1},
\]

(VI.10)

(VI.11)
similarly to (VI.6).

To estimate $X_3$ we pick a smooth function $\tilde{g} \in C^\infty(\mathbb{R}; [0, 1])$ such that $\tilde{g} \equiv 1$ on $\mathbb{R}_{\leq 0}$, $\tilde{g}' \leq 0$, and $\tilde{g} \equiv 0$ on $[1, \infty)$. We then define a smooth function of compact support by

$$g_\varepsilon(\lambda) := \tilde{g}(\varepsilon^{-1}(\lambda - 1)) \tilde{g}(\varepsilon^{-1}(-\lambda - 1)).$$  \hspace{1cm} (VI.12)

Note that, for $\varepsilon < 1$ and suitable constants $C_1, C_2, \ldots < \infty$, we have

$$\text{supp}(g_\varepsilon) \subseteq (-2, 2), \quad \|g_\varepsilon\|_\infty = 1$$ \hspace{1cm} (VI.13)

$$\text{supp}(g_\varepsilon^{(k)}) \subseteq (-1 - \varepsilon, 1) \cup (1, 1 + \varepsilon), \quad \|g_\varepsilon^{(k)}\|_\infty \leq C_k \varepsilon^{-k},$$ \hspace{1cm} (VI.14)

for all $k \in \mathbb{N}$. We use the functional calculus developed by Amrein, Boutet de Monvel, and Georgescu in [1, Thm. 6.1.4]. For any self-adjoint operator $A$ and any $n \in \mathbb{N}$, this functional calculus yields the identity

$$g_\varepsilon(A) = \sum_{k=0}^{n-1} \int_{-\infty}^{\infty} g_\varepsilon^{(k)}(\lambda) \frac{d\lambda}{\pi k!} \text{Im}\{i^k(A - \lambda - i)^{-1}\} + \int_{0}^{1} \mu^{n-1} d\mu \int_{-\infty}^{\infty} g_\varepsilon^{(n)}(\lambda) \frac{d\lambda}{\pi (n-1)!} \text{Im}\{i^n(A - \lambda - i\mu)^{-1}\}.\hspace{1cm} (VI.15)$$

We choose $n = 3$ and $A := \Lambda^{-2}k^2 = \Lambda^{-2}\mathcal{F} \circ (-\Delta) \circ \mathcal{F}^* =: \Lambda^{-2}(-\Delta_x)$ and obtain

$$g_\varepsilon(A) = \int_{-\infty}^{\infty} \left[g_\varepsilon(\lambda) - \frac{1}{2}g_\varepsilon''(\lambda)\right] \frac{d\lambda}{\pi} \text{Im}\{(A - \lambda - i)^{-1}\} \hspace{1cm} (VI.16)$$

$$+ \int_{-\infty}^{\infty} g_\varepsilon'(\lambda) \frac{d\lambda}{\pi} \text{Re}\{(A - \lambda - i)^{-1}\}$$

$$- \int_{0}^{1} \mu^2 d\mu \int_{-\infty}^{\infty} g_\varepsilon''(\lambda) \frac{d\lambda}{2\pi} \text{Re}\{(A - \lambda - i\mu)^{-1}\}.$$

We observe that due to the support properties of $g_\varepsilon$ and its derivatives and the definition of $A = \Lambda^{-2}k^2$, we have

$$\chi_{\sigma, \Lambda} = g_\varepsilon(A) \chi_{\sigma, \Lambda} = \chi_{\sigma, \Lambda} g_\varepsilon(A), \quad g_\varepsilon(A) \overline{\chi_{(1+\varepsilon)\Lambda}} = \overline{\chi_{(1+\varepsilon)\Lambda}} g_\varepsilon(A) = 0,$$ \hspace{1cm} (VI.17)
which implies that

\[ X_3 = \| \chi_{(1+\varepsilon)\Lambda} \phi(x) \chi_{\Lambda} \|_{L^1([h_0])} = \| \chi_{(1+\varepsilon)\Lambda} \phi(x) g \chi_{\Lambda} \|_{L^1([h_0])} \]

\[ \leq \int_{-\infty}^{\infty} \frac{d\lambda}{\pi} (|g_{\lambda}(\lambda)| + |g'_{\lambda}(\lambda)|) \left\| [R(\lambda + i\mu), \phi(x)] \chi_{\Lambda} \right\|_{L^1([h_0])} \]

\[ + \int_0^1 \frac{d\lambda}{\pi} d\mu \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} |g'''_{\lambda}(\lambda)| \left\| [R(\lambda + i\mu), \phi(x)] \chi_{\Lambda} \right\|_{L^1([h_0])}. \]

where \( R(z) := ( - \Lambda^{-2} \Delta_x - z )^{-1} \), with \( z \in \mathbb{C} \setminus \mathbb{R} \). Now, note that

\[ [R(z), \phi(x)] = \Lambda^{-2} R(z) [\Delta_x, \phi(x)] R(z) \]

\[ = \Lambda^{-2} R(z) (\nabla_x \cdot \nabla \phi(x) + \nabla \phi(x) \cdot \nabla_x) R(z), \]

and hence

\[ \left\| [R(\lambda + i\mu), \phi(x)] \chi_{\Lambda} \right\|_{L^1([h_0])} \]

\[ \leq \frac{2}{\Lambda^2} \left\| \nabla_x R(\lambda + i\mu) \right\|_{B[\mathbb{H}_0]} \left\| R(\lambda + i\mu) \right\|_{B[\mathbb{H}_0]} \left\| \nabla \phi(x) \chi_{\Lambda} \right\|_{L^1([h_0])} \]

\[ \leq \frac{4}{\mu^2 \Lambda} \left\| \nabla \phi(x) \chi_{\Lambda} \right\|_{L^1([h_0])}, \]

using that, for all \( \lambda \in [-2, 2] \) and \( \mu \in (0, 1) \),

\[ \left\| R(\lambda + i\mu) \right\|_{B[\mathbb{H}_0]} = \sup_{r > 0} \left\{ \left| (r/\Lambda)^2 - \lambda - i\mu \right|^{-1} \right\} = \frac{1}{\mu}, \]

\[ \left\| \nabla_x R(\lambda + i\mu) \right\|_{B[\mathbb{H}_0]} = \Lambda \sup_{r > 0} \left\{ \left| (r/\Lambda)^2 - \lambda - i\mu \right|^{-1} \right\} \leq \frac{2\Lambda^3}{\mu}. \]

Inserting (VI.20) into (VI.18) and additionally taking (VI.13)-(VI.14), as well as \( \varepsilon \in (0, 1) \) into account, we arrive at

\[ X_3 \leq \frac{C}{\varepsilon^2 \Lambda} \left\| \nabla \phi(x) \chi_{\Lambda} \right\|_{L^1([h_0])}, \]

for some universal constant \( C < \infty \). To estimate the trace norm on the right side of (VI.23) we first conjugate the operators by a suitable unitary dilatation, which
implements the change of length scale \((x, k) \mapsto (Lx, k/L)\) and does not change the norm, and then apply Inequality \(\text{(VI.1)}\) with \(p = 1\). These steps lead us to

\[
\|\nabla \phi(x) \chi_{\sigma, L}(k)\|_{L^1[\mathbb{R}]} = \|\nabla \phi(Lx) \chi_{\sigma, L}(k/L)\|_{L^1[\mathbb{R}]} = \|\nabla \phi(Lx) \chi_{L \sigma, L}(k/L)\|_{L^1[\mathbb{R}]},
\]

where we use that \(\nabla \phi\) is supported in \(B(0, L)\), hence \(x \mapsto \nabla \phi(Lx)\) is supported in \(B(0, 1) \subseteq Q\), and in the sum \(\sum_{\beta \in \mathbb{Z}^3} \|\nabla \phi(Lx) 1_{Q+\beta}\|_2\) only the term corresponding to \(\beta = 0\) contributes. Now, \(\text{Vol}[B(0, L) \cap (Q + \gamma)] \leq \text{Vol}[(Q + \gamma)] = 1\) and \(\text{Vol}[B(0, L) \cap (Q + \gamma)] \leq \text{Vol}[(Q + \gamma)] = 0\) unless \(|\gamma| \leq L \Lambda + \sqrt{3}\) which implies that

\[
\sum_{\gamma \in \mathbb{Z}^3} \sqrt{\text{Vol}[B(0, L \Lambda) \cap (Q + \gamma)]} \leq \sum_{\gamma \in \mathbb{Z}^3} 1_{B(0, L \Lambda + \sqrt{3})}(\gamma) \leq \frac{4\pi}{3} (L \Lambda + 3)^3,
\]

using that \(\frac{3}{2} \sqrt{3} \leq 3\). Furthermore, \(\|\nabla \phi(Lx)\|_2 = L^{-3/2} \|\nabla \phi(x)\|_2\), and thus

\[
\|\nabla \phi(x) \chi_{\sigma, L}(k)\|_{L^1[\mathbb{R}]} \leq \frac{4\pi C_{BS}}{3 L^{3/2}} (L \Lambda + 3)^3 \|\nabla \phi\|_2. \tag{VI.26}
\]

Inserting this into \(\text{(VI.23)}\) we finally obtain

\[
X_3 \leq \frac{C (L \Lambda + 1)^3}{\varepsilon^2 L^{3/2} \Lambda} \|\nabla \phi\|_2, \tag{VI.27}
\]

for a suitable constant \(C < \infty\). Estimate \(\text{(VI.3)}\) now follows from inserting \(\text{(VI.6)}, \text{(VI.10)}, \text{(VI.11)}\), and \(\text{(VI.27)}\) into \(\text{(VI.6)}\).
VII  Lower Bound on $X(\Theta_{\phi,\alpha})$

In order to complement the upper bound on $X(\Theta_{\phi,\alpha})$ from Section VI by a corresponding lower bound we first derive a general inequality on $X(A)$ of the form $X(A) \geq \text{Tr}[A^{1/2}] - 2\Lambda^{1-p} \text{Tr}[A^{p/2}]$, where $p$ is any exponent between $\frac{1}{2}$ and 1. By another application of the Birman-Solomyak inequality (VI.1) we then estimate the emerging error term by a multiple of $\|\phi\|_p^p$.

We begin by deriving a general lower bound on $X(A)$ only using that $|k| \leq \Lambda - 1$ on $\mathfrak{h}$.

Lemma VII.1. Let $A \geq 0$ be a nonnegative self-adjoint operator on $\mathfrak{h}$ such that $A^{1/2} \in \mathcal{L}[\mathfrak{h}]$ is trace-class and assume that $0 < p < 1$. Then

$$X(A) \geq \text{Tr}[A^{1/2}] - 2\Lambda^{1-p} \text{Tr}[A^{p/2}].$$

(VII.1)

Proof. We recall from Lemma VI.2 that

$$X(A) = \text{Tr}[A^{1/2} \left\{ (k^2 + A)^{1/2} + |k| \right\}^{-1} A^{1/2}]$$

$$= \text{Tr}[A^{1/2} \left\{ K_A + K_0 \right\}^{-1} A^{1/2}],$$

(VII.2)

with $K_A := \sqrt{k^2 + A}$. From the second resolvent identity we derive

$$\frac{1}{K_A + K_0} = \frac{1}{K_A} - \frac{1}{K_A} \frac{K_0}{K_A + K_0}$$

$$= \frac{1}{K_A} - \frac{1}{K_A} \frac{K_0}{K_A} + \frac{1}{K_A} \frac{K_0}{K_A + K_0} \frac{1}{K_A} \frac{1}{K_A}$$

$$\geq \frac{1}{K_A} - \frac{1}{K_A} \frac{1}{K_A},$$

(VII.3)

which implies

$$X(A) \geq \text{Tr}[A^{1/2} K_A^{-1} A^{1/2}] - \text{Tr}[A^{1/2} K_A^{-1} K_0 K_A^{-1} A^{1/2}].$$

(VII.4)

Since

$$K_0 = |k| \leq \Lambda^{1-p}|k|^p \leq \Lambda^{1-p} K_A^{p/2},$$

(VII.5)

and $K_A \geq A^{1/2}$, we have that

$$\text{Tr}[A^{1/2} K_A^{-1} K_0 K_A^{-1} A^{1/2}] \leq \Lambda^{1-p} \text{Tr}[A^{1/2} K_A^{-2(p/2)} A^{1/2}]$$

$$\leq \Lambda^{1-p} \text{Tr}[A^{p/2}].$$

(VII.6)
By operator monotonicity we further have
\[
\frac{A^{1/2} - A^{1/2} K_{A^{-1}} A^{1/2}}{\sqrt{\Lambda^2 + A}} \leq \frac{A}{\sqrt{\Lambda^2 + A}}
\]
\[
= \frac{A^{1/2}}{\sqrt{\Lambda^2 + A}} \left( \sqrt{\Lambda^2 + A} - A^{1/2} \right) = \frac{A^{1/2} \Lambda^2}{\sqrt{\Lambda^2 + A} (\sqrt{\Lambda^2 + A} + A^{1/2})}
\]
\[
\leq \frac{\Lambda^2 A^{1/2}}{\Lambda^2 + A} \leq \frac{\Lambda^2 A^{1/2}}{1 + \frac{A}{\Lambda} p} = \Lambda^{1-p} A^{p/2}. \quad (VII.7)
\]
Inserting (VII.6) and (VII.7) into (VII.4), we arrive at the claim. \(\square\)

As described above, we now use Lemma VII.1 to derive a lower bound on \(X(2\Theta_{\phi,\alpha})\).

**Theorem VII.2.** There exists a universal constant \(C < \infty\) such that, for all \(\alpha, L > 0\), all \(0 \leq \sigma \leq 1 \leq \Lambda < \infty\), all \(0 < \varepsilon \leq 1\) and all \(\phi = |\phi| \in Y_L\), the estimate
\[
\frac{1}{2} X(2\Theta_{\phi,\alpha}) \geq \sqrt{\frac{4\alpha}{9\pi}} (\Lambda^3 - \sigma^3) \|\phi\|_1 - \frac{C \alpha^{1/4} \Lambda^{1/2} (L \Lambda + 1)^3}{L^{3/2}} \sqrt{\|\phi\|_1}
\]  
holds true.

**Proof.** We first use that \(A \mapsto X(A)\) is monotonically increasing. Since
\[
\Theta_{\phi,\alpha} = \Phi_{\phi,\alpha}^* \Phi_{\phi,\alpha} = \frac{\alpha}{(2\pi)^3} P_C \chi_{\sigma,\Lambda} \phi(x)^2 \chi_{\sigma,\Lambda} P_C \quad (VII.9)
\]
\[
\geq \frac{\alpha}{(2\pi)^3} P_C \chi_{\sigma,\Lambda} \phi(x) \chi_{\sigma,\Lambda} P_C \chi_{\sigma,\Lambda} \phi(x) \chi_{\sigma,\Lambda} P_C
\]
\[
= \left[ (2\pi)^{-3/2} P_C \chi_{\sigma,\Lambda} \phi(x) \chi_{\sigma,\Lambda} P_C \right]^2,
\]
we obtain from Lemma VII.1 with \(p = \frac{1}{2}\) that
\[
\frac{1}{2} X(2\Theta_{\phi,\alpha}) \geq \frac{1}{2} X \left( \left[ (2\alpha)^{1/2} (2\pi)^{-3/2} P_C \chi_{\sigma,\Lambda} \phi(x) \chi_{\sigma,\Lambda} P_C \right]^2 \right)
\]
\[
\geq \frac{(2\alpha)^{1/2}}{2(2\pi)^{3/2}} \text{Tr} \left( P_C \chi_{\sigma,\Lambda} \phi(x) \chi_{\sigma,\Lambda} P_C \right)
\]
\[
- \frac{(2\alpha)^{1/4} \Lambda^{1/2}}{(2\pi)^{3/4}} \text{Tr} \left( [P_C \chi_{\sigma,\Lambda} \phi(x) \chi_{\sigma,\Lambda} P_C]^{1/2} \right). \quad (VII.10)
\]
\[
\geq \sqrt{\frac{4\alpha}{9\pi}} (\Lambda^3 - \sigma^3) \|\phi\|_1 - \frac{(2\alpha)^{1/4} \Lambda^{1/2}}{(2\pi)^{3/4}} \sqrt{\|\phi(x)\chi_{\sigma,\Lambda}(k)\|_{L^1([0])}.}
\]
To estimate the second term on the right side of (VII.10) we proceed as in (VI.23)-(VI.26). After unitary rescaling \((x, k) \mapsto (Lx, k/L)\), we apply (VI.1) again and get
\[
\| \sqrt{\varphi(x)} \chi_{\sigma, \Lambda}(k) \|_{L^1(b_0)} = \| \sqrt{\varphi(Lx)} \chi_{\sigma, \Lambda}(k) \|_{L^1(b_0)} \\
\leq C_{\text{BS}}(1) \| \sqrt{\varphi(Lx)} \|_{2;1} \| \chi_{\sigma, \Lambda}(k) \|_{2;1} \\
\leq \frac{4\pi C_{\text{BS}}(1)}{3} (LA + 3)^3 \| \sqrt{\varphi(Lx)} \|_{2;1},
\]
where the last estimate results from (VI.24)-(VI.25). Since \(x \mapsto \varphi(Lx)\) is supported in \(B(0, 1) \subseteq Q = [-\frac{1}{2}, \frac{1}{2}]^3\), we further have
\[
\| \sqrt{\varphi(Lx)} \|_{2;1} = \sum_{\beta \in \mathbb{Z}^3} \| \sqrt{\varphi(Lx)} \cdot 1_{Q+\beta} \|_2 = \| \sqrt{\varphi(Lx)} \|_2 \\
= \| \varphi(Lx) \|_1^{1/2} = L^{-3/2} \| \varphi \|_1^{1/2}.
\]
Finally, inserting (VII.12) into (VII.11), we arrive at (VII.8). \(\Box\)
VIII  Asymptotics of the Lieb-Loss Energy

We turn to the proof of the main result of this paper, Theorem VIII.1, stated below again for the reader’s convenience. In our proof a key role is played by the scaling relation the effective energy $F[\beta]$ obeys. $F[\beta]$ is defined in (V.5) as the infimum of the functional $F_\beta > 0$ over $L^2$-normalized functions in $H^1(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$. In [19] one of us showed that this infimum is attained for some $\phi_\beta$ and hence is actually a minimum. A major issue in this regard is non-reflexivity of the $L^1$-space precluding a naive application of the direct method of the calculus of variations. This was remedied by using the theory of uniform convex spaces and the Milman-Pettis theorem. Subsequently an explicit characterization of the minimizer (up to spherical rearrangement) can be given in terms of a Bessel function. In particular,

$$F[1] > 0 \quad \text{(VIII.1)}$$

is a positive constant, and it is then not difficult to see that $F[\beta]$ scales as

$$F[\beta] = \beta^{4/7} F[1], \quad \text{(VIII.2)}$$

for all $\beta > 0$.

**Theorem VIII.1.** There exists a universal constant $C < \infty$ such that, for all $\alpha > 0$ and $\Lambda \geq 1$, the estimate

$$-C \alpha^{\frac{4}{10}} \Lambda^{-\frac{4}{10}} \leq \frac{E_{LL}(\alpha, \Lambda)}{F_1 \alpha^{2/7} \Lambda^{12/7}} - 1 \leq C \alpha^{\frac{4}{105}} \Lambda^{-\frac{4}{105}} \quad \text{(VIII.3)}$$

holds true.

**Proof.** We first take the infrared limit $\sigma \to 0$. Note that $E_{LL}$, $E_{LL}^{(L)}$, $F$, $F^{(L)}$, $X(2\Theta_{\phi,\alpha})$, and all error terms are continuous at $\sigma = 0$, and we can simply set $\sigma := 0$ everywhere. Then Theorems VI.1 and VII.2 with $p = 1/2$ yield

$$\frac{1}{2} X(2\Theta_{\phi,\alpha}) - \sqrt{\frac{4\alpha}{9\pi}} \Lambda^3 \|\phi\|_1 \leq C \varepsilon \Lambda^3 \|\phi\|_1 + C \alpha^{1/2} \varepsilon^{-2} L^{3/2} \Lambda^2 \|\nabla \phi\|_2, \quad \text{(VIII.4)}$$

$$\frac{1}{2} X(2\Theta_{\phi,\alpha}) - \sqrt{\frac{4\alpha}{9\pi}} \Lambda^3 \|\phi\|_1 \geq - C \alpha^{1/4} L^{3/2} \Lambda^{7/2} \|\phi\|_1^{1/2}, \quad \text{(VIII.5)}$$

some constant $C_1 < \infty$ and any $\phi = |\phi| \in Y_L$ with $\|\phi\|_2 = 1$, provided that $L \geq \Lambda^{-1}$. 

40
We first derive the upper bound in (VIII.3). From (VIII.4) we obtain
\[
\hat{E}_{\alpha,\Lambda}(\phi) = \frac{1}{2} \|\nabla \phi\|_2^2 + \frac{1}{2} X(2\Theta,\alpha) \\
\leq \frac{1}{2} (1 + \delta) \|\nabla \phi\|_2^2 + \sqrt{\frac{4\alpha}{9\pi}} \Lambda^3 (1 + C_2 \varepsilon) \|\phi\|_1 + C_2 \alpha \delta^{-1} \varepsilon^{-4} L^3 \Lambda^4 \\
\leq (1 + \delta) F_{\beta_2}(\phi) + C_2 \alpha \delta^{-1} \varepsilon^{-4} L^3 \Lambda^4, \tag{VIII.6}
\]
where \( F_{\beta} \) is defined in (V.4) and
\[
\beta_2 := \frac{\beta_0}{1 + \delta}, \quad \beta_0 \equiv \beta(\alpha, \Lambda) = \sqrt{\frac{4\alpha}{9\pi}} \Lambda^3, \tag{VIII.7}
\]
for some \( C_2 < \infty \) and all \( 0 < \delta \leq 1 \). Taking the infimum over all \( \phi = |\phi| \in Y_L \) with \( \|\phi\|_2 = 1 \) in (VIII.6), we further have
\[
E_{LL}(\alpha, \Lambda) \leq (1 + \delta) F_{\beta}(\phi) + C_2 \alpha \delta^{-1} \varepsilon^{-4} L^3 \Lambda^4. \tag{VIII.8}
\]
The localization estimates (V.II)-(V.III) now imply
\[
E_{LL}(\alpha, \Lambda) \leq (1 + \delta) F[\beta_2] + C_2 \alpha \delta^{-1} \varepsilon^{-4} L^3 \Lambda^4 + C_3 L^{-2}, \tag{VIII.9}
\]
for some constant \( C_3 < \infty \). From the scaling relation (VIII.2), we get
\[
(1 + \delta) F[\beta_2] = (1 + \delta) \beta_2^{4/7} F[1] = (1 + C_2 \varepsilon)^{4/7} (1 + \delta)^{3/7} \beta_0^{4/7} F[1] \\
\leq (1 + C_4 \varepsilon + C_4 \delta) F[\beta_0], \tag{VIII.10}
\]
for some \( C_4 < \infty \), and inserting this into (VIII.9), we arrive at the intermediate estimate, stating that there exists a universal constant \( C_5 < \infty \), such that
\[
\frac{E_{LL}(\alpha, \Lambda)}{F[\beta(\alpha, \Lambda)]} - 1 \leq C_5 \left( \varepsilon + \delta + \alpha^{-2/7} L^{-2} \Lambda^{-12/7} + \alpha^{5/7} \delta^{-1} \varepsilon^{-4} L^3 \Lambda^{16/7} \right) \tag{VIII.11}
\]
holds for all \( \varepsilon, \delta \in (0, 1] \), \( \alpha > 0 \), \( \Lambda \geq 1 \), and \( L > \Lambda^{-1} \). As \( \alpha \) enters the right side of (VIII.11) only in negative powers, we may assume \( \alpha \in (0, 1] \) w.l.o.g. To meet these requirements, we set
\[
\varepsilon := \delta := \alpha^r \Lambda^{-s} \quad \text{and} \quad L := \alpha^{-t} \Lambda^{-u}, \tag{VIII.12}
\]
for some positive constants \( r, s, t, u \).
for \( r, s, t, u \geq 0 \) to be chosen later. Then
\[
\varepsilon + \delta + \alpha^{-\frac{5}{7}} L^{-2} \Lambda^{-\frac{15}{7}} + \alpha^{\frac{1}{7}} \delta^{-1} \varepsilon^{-4} L^{3} \Lambda^{\frac{16}{7}} \]
\[
= 2 \alpha^r \Lambda^{-s} + \alpha^{2t-\frac{2}{7}} \Lambda^{2-2u} + \alpha^{\frac{5}{7} - 5r - 3t} \Lambda^{5s + 3u - \frac{2}{7}} \leq 4 \alpha^{a/7} \Lambda^{-b/7},
\]
with
\[
a := \min \{ 7r, 14t - 2, 5 - 35r - 21t \}, \quad (VIII.14)
\]
\[
b := \min \{ 7s, 14u - 2, 5 - 35s - 21u \}. \quad (VIII.15)
\]
We choose \( r, s, t, u \) so that all three terms in both (VIII.14) and (VIII.15) are equal, i.e., \( r := s := 4/105 \) and \( t := u := 17/105 \). This yields \( a = b = 4/15 \) and hence the upper bound
\[
\frac{E_{LL}(\alpha, \Lambda)}{F[\beta(\alpha, \Lambda)]} - 1 \leq 4C_5 \alpha^{\frac{4}{105}} \Lambda^{-\frac{4}{105}}, \quad (VIII.16)
\]
in (VIII.3).

We similarly proceed for the lower bound in (VIII.3). From (VIII.5) we obtain
\[
\widehat{E}_{\alpha, \Lambda}(\phi) = \frac{1}{2} \| \nabla \phi \|_2^2 + \frac{1}{2} X(2\Theta_{\phi, \alpha})
\geq \frac{1}{2} \| \nabla \phi \|_2^2 + \sqrt{\frac{4\alpha}{9\pi}} \Lambda^{3} (1 - \delta) \| \phi \|_1 - C_6 \delta^{-1} L^3 \Lambda
\]
\[
= F_{\beta_3}(\phi) - C_6 \delta^{-1} L^3 \Lambda, \quad (VIII.17)
\]
for some \( C_2 < \infty \) and all \( 0 < \delta \leq 1 \), where
\[
\beta_3 := \beta_0 (1 - \delta), \quad \beta_0 \equiv \beta(\alpha, \Lambda) = \sqrt{\frac{4\alpha}{9\pi}} \Lambda^{3}. \quad (VIII.18)
\]
Taking the infimum over all \( \phi = |\phi| \in Y_L \) with \( \| \phi \|_2 = 1 \) in (VIII.17), we further have
\[
E^{(L)}(\alpha, \Lambda) \geq F^{(L)}[\beta_3] - C_6 \delta^{-1} L^3 \Lambda. \quad (VIII.19)
\]
The localization estimates (VII.10)-(VII.11) now imply
\[
E_{LL}(\alpha, \Lambda) \geq F[\beta_3] - C_7 L^{-2} - C_6 \delta^{-1} L^3 \Lambda^4, \quad (VIII.20)
\]
for some constant \( C_7 < \infty \). Again invoking the scaling relation (VIII.2), we get
\[
F[\beta_3] = \beta_3^{4/7} F[1] = (1 - \delta)^{4/7} \beta_0^{4/7} F[1] \geq (1 - \delta) F[\beta_0], \quad (VIII.21)
\]
and thus there exists a constant $C_8 < \infty$ such that

$$
\frac{E_{\text{LL}}(\alpha, \Lambda)}{F[\beta(\alpha, \Lambda)]} - 1 \geq -C_8 \left( \delta + \alpha^{-2/7} L^{-2} \Lambda^{-12/7} + \alpha^{-2/7} \delta^{-1} L^3 \Lambda^{16/7} \right)
$$

(VIII.22)

holds for all $\delta, \alpha \in (0, 1]$, $\Lambda \geq 1$, and $L > \Lambda^{-1}$. Again we set

$$
\delta := \alpha^r \Lambda^{-s} \quad \text{and} \quad L := \alpha^{-t} \Lambda^{-u-1},
$$

(VIII.23)

for $r, s, t, u \geq 0$ to be chosen later and obtain

$$
\delta^* + \alpha^{-\frac{2}{7}} L^{-2} \Lambda^{-\frac{12}{7}} + \alpha^{-\frac{2}{7}} \delta^{-1} L^3 \Lambda^{\frac{16}{7}}
$$

(VIII.24)

$$
= \alpha^r \Lambda^{-s} + \alpha^{2t-\frac{2}{7}} \Lambda^{\frac{2}{7}-2u} + \alpha^{5-3t} \Lambda^{s+3u-\frac{5}{7}} \leq 3 \alpha^{a/7} \Lambda^{-b/7},
$$

with

$$
a := \min \left\{ 7r, 14t - 2, 5 - 7r - 21t \right\},
$$

(VIII.25)

$$
b := \min \left\{ 7s, 14u - 2, 5 - 7s - 21u \right\}.
$$

(VIII.26)

We choose $r, s, t, u$ so that all three terms in both (VIII.14) and (VIII.15) are equal, i.e., $r := s := 4/49$ and $t := u := 9/49$. This yields $a = b = 4/7$ and hence the lower bound

$$
\frac{E_{\text{LL}}(\alpha, \Lambda)}{F[\beta(\alpha, \Lambda)]} - 1 \geq -3C_8 \alpha^{\frac{4}{49}} \Lambda^{-\frac{4}{49}}
$$

(VIII.27)

in (VIII.3).

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