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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 (Self-energy of electrons in non-perturbative QED. Preprint arXiv:math-ph/9908020 and mp-arc #99–305, 1999) approximated 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 ϕ_{el} and ψ_{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 $\Lambda \to \infty$.

1. 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 [11,15], and about seventy years ago quantum electrodynamics (QED) was formulated by Feynman, Schwinger, Tomonaga, and Dyson [16,18,34,38], 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. The original (relativistic) QED was shown to be perturbatively renormalizable [17], but its nonperturbative renormalizability is wide open. One alternative route to approach the ultraviolet problem is to resort to simpler models, especially those that replace the relativistic by a nonrelativistic particle, known as *nonrelativistic QED* or *Pauli–Fierz Hamiltonians*. In fact, 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 [5–7, 9, 21] for these models. The construction of the ultraviolet limit has been successfully carried out for some of these models, notably the Nelson model by a Gross transformation [23, 33], the spin-boson Hamiltonian [14], and Fröhlich Hamiltonians [22, 22, 30]. Another alternative is to replace the fully interacting model by an effective mean-field theory [19, 20, 25].

One approach among these is a simplifying variational model proposed by Lieb and Loss in 1999 [31]. Their starting point is the Pauli–Fierz Hamiltonian

$$H_{\alpha,\Lambda} \;=\; \frac{1}{2}\Big(\tfrac{1}{i}\vec{\nabla}_x - \alpha^{1/2}\vec{A}_\Lambda(x)\Big)^2 + H_{\rm ph} \tag{1.1}$$

of a nonrelativistic spinless particle (modeling the electron), minimally coupled to the quantized radiation field. Here, $\frac{1}{i}\vec{\nabla}_x$ is the (particle) momentum operator, and $\vec{A}_\Lambda(x) = \int_{|k|\leq\Lambda} \big(e^{-ik\cdot x}a^*(k) + e^{ik\cdot x}a(k)\big)\frac{\varepsilon(k)\,dk}{(2\pi)^{3/2}\,|k|^{1/2}}$ is the magnetic vector potential in Coulomb gauge and cut off for momenta larger than Λ in magnitude. Moreover, $H_{\rm ph} = \int |k|\, a^*(k)\, a(k)\, dk$ 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 $\mathrm{dom}[H_{0,0}] \subseteq \mathcal{H}_{\rm el}\otimes\mathcal{F}_{\rm ph}$ of the noninteracting Hamiltonian $H_{0,0} = \frac{1}{2}(-\Delta)\otimes\mathbf{1}_{\rm ph} + \mathbf{1}_{\rm el}\otimes H_{\rm ph}$, see [26, 28], where $\mathcal{H}_{\rm el} = L^2(\mathbb{R}^3)$ is the space of square-integrable functions on $\mathbb{R}^3$, and $\mathcal{F}_{\rm ph}$ 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 Sect. 2 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,

$$E_{\rm gs}(\alpha,\Lambda) \;:=\; \inf\Big\{\langle\Psi\,|H_{\alpha,\Lambda}\Psi\rangle \;\Big|\; \Psi\in\mathcal{H}_{\rm el}\otimes\mathcal{F}_{\rm ph},\;\; \|\Psi\|=1\Big\}. \tag{1.2}$$

Lieb and Loss restricted [31] the variation in (1.2) to wave functions of product form $\Psi = \phi\otimes\psi$, with normalized $\phi\in\mathcal{H}_{\rm el}$ and $\psi\in\mathcal{F}_{\rm ph}$, to obtain a new approximation and upper bound $E_{\rm LL}(\alpha,\Lambda) \geq E_{\rm gs}(\alpha,\Lambda)$ to the ground state energy, i.e.,

$$E_{\rm LL}(\alpha,\Lambda) := \inf\Big\{\mathcal{E}_{\alpha,\Lambda}(\phi,\psi) \;\Big|\; \phi\in\mathcal{H}_{\rm el},\; \psi\in\mathcal{F}_{\rm ph},\; \|\phi\|=\|\psi\|=1\Big\}, \tag{1.3}$$

$$\mathcal{E}_{\alpha,\Lambda}(\phi,\psi) := \big\langle\phi\otimes\psi\big|H_{\alpha,\Lambda}(\phi\otimes\psi)\big\rangle. \tag{1.4}$$

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 $E_{\mathrm{gs}}(\alpha, \Lambda) \to \infty$, as $\Lambda \to \infty$. We henceforth refer to Eqs. (1.3)–(1.4) as the **Lieb–Loss Model**.

In Theorem 1.1 in [31], Lieb and Loss proved the existence of two universal constants $C_1, C_2 \in \mathbb{R}^+$ such that

$$C_1\, \alpha^{1/2}\, \Lambda^{3/2} \ \le\ E_{\mathrm{LL}}(\alpha, \Lambda) \ \le\ C_2\, \alpha^{2/7}\, \Lambda^{12/7}. \tag{1.5}$$

This is the first of a series of results of Lieb and Loss in [31], 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. Lieb and Loss also demonstrate in [31] that the bounds in (1.5) hold true for the actual ground state-energy $E_{\mathrm{gs}}(\alpha, \Lambda)$, too, and they sketch an argument that up to a multiplicative constant, the right side of (1.5) is also a lower bound to $E_{\mathrm{LL}}(\alpha, \Lambda)$. Note that the Lieb–Loss model does not take the renormalization of the electron mass into account, and the actual value of $E_{\mathrm{LL}}(\alpha, \Lambda)$ is of limited quantitative use in physics. The significance of Eq. (1.5), however, lies in the fact that the formal perturbation expansion of the ground state about the photon vacuum yields $E_{\mathrm{gs}}(\alpha, \Lambda) \sim C\alpha\Lambda^2$. In contrast, Eq. (1.5) 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 the derivation of the asymptotics of $E_{\mathrm{LL}}(\alpha, \Lambda)$, as $\Lambda \to \infty$ or $\alpha \to 0$. That is, for any given $0 < \alpha \leq 1$ and $\Lambda \geq 1$, we first reduce the minimization of $\mathcal{E}_{\alpha,\Lambda}$ over pairs (ϕ, ψ) of normalized vectors in $\mathcal{H}_{\mathrm{el}} \times \mathcal{F}_{\mathrm{ph}}$ to a minimization over normalized positive vectors $\phi \equiv |\phi| \in \mathcal{H}_{\mathrm{el}}$, by showing that $E_{\mathrm{LL}}(\alpha, \Lambda) = \inf_{\phi \in \mathcal{H}_{\mathrm{el}},\, \|\phi\|=1} \mathcal{E}_{\alpha,\Lambda}\big(|\phi|, U_{|\phi|}\Omega\big)$, where $\Omega \in \mathcal{F}_{\mathrm{ph}}$ is the normalized vacuum vector and $U_{|\phi|}$ is a Bogoliubov transformation that parametrically depends on $|\phi|$. We then compare the *effective* energy functional $\widehat{\mathcal{E}}_{\alpha,\Lambda}\big(|\phi|\big) := \mathcal{E}_{\alpha,\Lambda}\big(|\phi|, U_{|\phi|}\Omega\big)$ to the auxiliary classical functional

$$\mathcal{F}_\beta(\phi) \ := \frac{1}{2}\big\|\vec{\nabla}\phi\big\|_2^2 + \beta\, \|\phi\|_1, \tag{1.6}$$

for $\beta := (\frac{4\alpha}{9\pi})^{1/2}\Lambda^3$ and 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

$$F_\beta \ := \inf\big\{\mathcal{F}_\beta(\phi) \ \big|\ \phi \in Y, \quad \|\phi\|_2 = 1\big\} \tag{1.7}$$

satisfies the scaling relation

$$F_\beta \ = \ \beta^{4/7}\, F_1, \tag{1.8}$$

and in [24], the second author shows that the infimum in (1.7) is actually attained and strictly positive, in particular,

$$F_1 \ > \ 0. \tag{1.9}$$

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

Theorem 1.1. *There exists a universal constant $C < \infty$ such that for all $\alpha > 0$ and $\Lambda \geq 1$, the estimate*

$$-C\,\alpha^{\frac{4}{49}}\Lambda^{-\frac{4}{49}} \;\leq\; \frac{E_{\mathrm{LL}}(\alpha,\Lambda)}{(\frac{4}{9\pi})^{2/7}\,F_1\,\alpha^{2/7}\,\Lambda^{12/7}} - 1 \;\leq\; C\,\alpha^{\frac{4}{105}}\Lambda^{-\frac{4}{105}} \tag{1.10}$$

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 Sect. 3.3.

(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 $\vec{A}_\sigma$. We do not give details of the argument but refer the reader to [6].

(2) We first analyze the functional $\mathcal{E}_{\alpha,\Lambda}$. A direct computation yields

$$\mathcal{E}_{\alpha,\Lambda}(\phi,\psi) \;=\; \frac{1}{2}\big\|\vec{\nabla}\phi\big\|_2^2 + \Big\langle\psi\Big|\;\mathbb{H}\big(|\phi|^2,\,\mathrm{Im}\{\overline{\phi}\,\vec{\nabla}\phi\}\big)\psi\Big\rangle_{\mathcal{F}}, \tag{1.11}$$

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

$$\begin{aligned}\mathbb{H}[\rho,\vec{v}] \;:=\; & H_{\mathrm{ph}} + \frac{\alpha}{2}\int \rho(x)\,\vec{A}^2_{\sigma,\Lambda}(x)\,d^3x \\ & +\sqrt{\alpha}\int \vec{v}(x)\cdot\vec{A}_{\sigma,\Lambda}(x)\,d^3x.\end{aligned} \tag{1.12}$$

In Theorem 4.4, in Sect. 4.1, we demonstrate that by a suitably chosen Weyl transformation W_ϕ, the term linear in the fields, i.e., proportional to $\vec{v} = \mathrm{Im}\{\overline{\phi}\,\vec{\nabla}\phi\}$, 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 ϕ. More precisely,

$$\mathcal{E}_{\alpha,\Lambda}\big(\phi,\psi\big) \;\geq\; \mathcal{E}_{\alpha,\Lambda}\big(|\phi|, W_\phi\psi\big). \tag{1.13}$$

Defining

$$\widehat{\mathcal{E}}_{\alpha,\Lambda}\big(\phi\big) \;:=\; \inf\Big\{\mathcal{E}_{\alpha,\Lambda}(\phi,\psi)\;\Big|\;\psi\in\mathcal{F}_{\mathrm{ph}},\;\|\psi\| = 1\Big\}, \tag{1.14}$$

we therefore have that

$$\widehat{\mathcal{E}}_{\alpha,\Lambda}\big(\phi\big) \;\geq\; \widehat{\mathcal{E}}_{\alpha,\Lambda}\big(|\phi|\big). \tag{1.15}$$

We pause to remark that due to (1.15), the ground state energies of the Hamiltonian operators in Eqs. (1.7) and (1.9) in [31] coincide. Hence, Theorems 1.1 and 1.2 in [31] are actually bounds on the same number. Our present result in Theorem 1.1 sharpens this as the constants C_1 and C_2 in [31, Theorem 1.2] are shown to agree and the difference to be of lower order in Λ and higher order in α.

We further remark that there is an alternative derivation of (1.15) by using that the semigroup generated by $H_{\alpha,\Lambda}$ is positivity improving, if the Hilbert space is represented as a space of square-integrable functions of the particle position and the magnetic vector potential, as was shown by Hiroshima in [27,29]. This leads to a variant of the diamagnetic inequality which can be used to establish (1.15) (see also Eq. (14.4) in [37]).

(3) Equation (1.15) guarantees that we can assume without loss of generality that $\phi = |\phi| \geq 0$, and in this case,

$$\mathcal{E}_{\alpha,\Lambda}(\phi, \psi) \;=\; \frac{1}{2}\|\vec{\nabla}\phi\|_2^2 + \Big\langle \psi \Big| \, \Big(H_{\rm ph} + \frac{\alpha}{2} \int |\phi(x)|^2 \, \vec{A}_\Lambda^2(x) \, d^3x \Big) \, \psi \Big\rangle_{\mathcal{F}}. \tag{1.16}$$

In Theorem 4.5, in Sect. 4.2, we give an alternative proof for the observation of Lieb and Loss that

$$\inf \Big\{ \Big\langle \psi \Big| \, \Big(H_{\rm ph} + \frac{\alpha}{2} \int |\phi(x)|^2 \, \vec{A}_\Lambda^2(x) \, d^3x \Big) \, \psi \Big\rangle_{\mathcal{F}} \, \Big| \, \psi \in \mathcal{F}_{\rm ph}, \; \|\psi\| = 1 \Big\}$$
$$= \frac{1}{2} {\rm Tr}\big\{ \sqrt{-\Delta_x + 2\Theta_{|\phi|,\alpha}} \; - \; \sqrt{-\Delta_x} \big\}, \tag{1.17}$$

where $\Theta_{\phi,\alpha} := \alpha(2\pi)^{-3} P_C \chi_{\sigma,\Lambda} (\hat{\phi}*)^* (\hat{\phi}*) \chi_{\sigma,\Lambda} P_C$, with $\chi_{\sigma,\Lambda} := \mathbf{1}[\sigma^2 \leq -\Delta_x \leq \Lambda^2]$ being the characteristic function of momenta with magnitude between σ and Λ, $\hat{\phi}*$ denoting convolution with $\hat{\phi}$, and $P_C := \mathbf{1}\Big[(\vec{\nabla}_x \cdot) = 0 \Big]$ being the projection onto divergence-free vector fields, i.e., vector fields in Coulomb gauge.

The heart of the proof of Theorem 4.5 is the determination of the Bogoliubov transformation $\mathbb{U}_{B_*(\phi)}$ which diagonalizes the quadratic effective Hamiltonian $\mathbb{H}(|\phi|^2, 0)$ on the left side of (1.17). While the general procedure to determine $\mathbb{U}_{B_*(\phi)}$ is well-known, the details of the explicit computation are involved. As a future project, it is planned to conjugate the (fully interacting) Hamiltonian with $\mathbb{U}_{B_*(\phi)}$ and to separate in the obtained operator $\mathbb{U}_{B_*(\phi)} H_{\alpha,\Lambda} \mathbb{U}^*_{B_*(\phi)}$, the diagonalized quadratic part from a remainder which, hopefully, is less singular than the former in the ultraviolet limit.

(4) Inserting (1.17) into (1.14)–(1.15), we arrive at

$$\widehat{\mathcal{E}}_{\alpha,\Lambda}(\phi) \;=\; \frac{1}{2}\big\|\vec{\nabla}\phi\big\|_2^2 + \frac{1}{2} X(2\Theta_{\phi,\alpha}), \tag{1.18}$$

for $\phi = |\phi| \geq 0$, where

$$X(A) \;:= {\rm Tr}\Big(\sqrt{|k|^2 + A} - |k| \Big) \quad \text{and} \tag{1.19}$$

$$\Theta_{\phi,\alpha} \;:= \frac{\alpha}{(2\pi)^3} \, P_C \, \chi_{\sigma,\Lambda} \, \phi(x)^2 \, \chi_{\sigma,\Lambda} \, P_C, \tag{1.20}$$

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

(5) In Sect. 5, we introduce the infima

$$E_{\rm LL}^{(L)}(\alpha, \Lambda) \;:= \inf \Big\{ \widehat{\mathcal{E}}_{\alpha,\Lambda}(\phi_L) \, \Big| \, \phi_L \in Y_L \Big\}, \tag{1.21}$$

$$F_\beta^{(L)} \;:= \inf \Big\{ \mathcal{F}_\beta(\phi_L) \, \Big| \, \phi_L \in Y_L \Big\}, \tag{1.22}$$

of the Lieb–Loss functional $E_{\mathrm{LL}}(\alpha,\Lambda)(\phi_L)$ and the auxiliary functional $\mathcal{F}_\beta(\phi_L)$ under variation only over compactly supported functions $\phi_L \in Y_L := H^1(B(0,L))$ and compare these infima to $E_{\mathrm{LL}}(\alpha,\Lambda)$ and F_β by means of the IMS localization formula. Here, $B(x,r) \subseteq \mathbb{R}^3$ denotes the open ball of radius $r > 0$ centered at $x \in \mathbb{R}^3$, as usual. More specifically, we prove in Theorem 5.1 that

$$E_{\mathrm{LL}}^{(L)}(\alpha,\Lambda) \;-\; C\,L^{-2} \le E_{\mathrm{LL}}(\alpha,\Lambda) \;\le\; E_{\mathrm{LL}}^{(L)}(\alpha,\Lambda), \tag{1.23}$$

$$F_\beta^{(L)} \;-\; C\,L^{-2} \le F_\beta \;\le\; F_\beta^{(L)}, \tag{1.24}$$

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

(6) The sixth step carried out in Sects. 6 and 7 is to find upper and lower bounds for all compactly supported $\phi = |\phi| \in Y_L := H^1\big(B(0,L)\big)$ on $X(\Theta_{\phi_L,\alpha})$. In Theorem 6.1, we prove the existence of a universal constant $C < \infty$ such that, for all $0 < \varepsilon \le 1$, $L \ge 1/\Lambda$, and $\phi \in Y_L$,

$$\frac{1}{2}X(2\Theta_{\phi,\alpha}) \;-\; \sqrt{\frac{4\alpha}{9\pi}}\,\Lambda^3\,\|\phi_L\|_1 \\ \le C\big(\varepsilon\,\alpha^{\frac12}\,\Lambda^3 + \alpha^{\frac12}\,\sigma^{\frac32}\,\Lambda^{\frac32}\big)\,\|\phi_L\|_1 \;+\; C\,\varepsilon^{-2}\,\Lambda^2\,L^{\frac32}\,\|\nabla\phi_L\|_2. \tag{1.25}$$

This is complemented by the lower bound in Theorem 7.2 which asserts that there exists a universal constant $C < \infty$ such that, for all $L \ge 1/\Lambda$ and $\phi \in Y_L$,

$$\frac{1}{2}X(2\Theta_{\phi,\alpha}) \;-\; \sqrt{\frac{4\alpha}{9\pi}}\,\Lambda^3\,\|\phi_L\|_1 \;\ge\; -C\,\alpha^{\frac14}\,\Lambda^{\frac72}\,L^{\frac32}\,\|\phi_L\|_1^{\frac12}. \tag{1.26}$$

(7) Estimates (1.25) and (1.26) suggest to compare the functional $\widehat{\mathcal{E}}_{\alpha,\Lambda}(\phi) = \frac12\|\vec\nabla\phi\|_2^2 + \frac12 X(2\Theta_{\phi,\alpha})$ to $\mathcal{F}_{\beta(\alpha,\Lambda)}(\phi) = \frac12\|\vec\nabla\phi\|_2^2 + \beta(\alpha,\Lambda)\|\phi\|_1$ with $\beta(\alpha,\Lambda) := \sqrt{\frac{4\alpha}{9\pi}}\Lambda^3$ which is done in Sect. 8. Indeed, this leads us to introduce the family of auxiliary functionals $(\mathcal{F}_\beta)_{\beta>0}$, defined on $Y := H^1(\mathbb{R}^3) \cap L^1(\mathbb{R}^3) \subset H^1(\mathbb{R}^3)$ as

$$\mathcal{F}_\beta(\phi) \;:=\; \frac12\big\|\vec\nabla\phi\big\|_2^2 + \beta\,\|\phi\|_1, \tag{1.27}$$

and their infima

$$F_\beta \;:=\; \inf\big\{\mathcal{F}_\beta(\phi)\;\big|\;\phi\in Y,\;\;\|\phi\|_2 = 1\big\}. \tag{1.28}$$

This family of functionals is analyzed by direct methods of the calculus of variations in detail by the second author in a separate paper [24], and here we describe its properties only briefly.

– For fixed $\beta > 0$, the functional $\mathcal{F}_\beta$ possesses a minimizer, which is unique up to translations, nonnegative, spherically symmetric and decreasing. In particular, its infimum F_β is attained and hence a strictly positive minimum.

- For all $\beta > 0$, both energy and minimizer are uniquely determined by their scaling behavior in β 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.
- The scaling relation $F_\beta = \beta^{4/7} F_1$ and the numerical value of $F_1 > 0$ can also be obtained in the following way: Introduce $\phi_\lambda(x) := \lambda^{3/2}\phi(\lambda x)$, for any $\phi \in Y$ with $\|\phi\|_2 = 1$ and $\lambda > 0$, so that $\|\phi_\lambda\|_2 = 1$, too. Then, $\mathcal{F}_\beta(\phi_\lambda) = \frac{\lambda^2}{2}\|\vec{\nabla}\phi\|_2^2 + \beta\lambda^{-3/2}\|\phi\|_1$, and a minimization over $\lambda > 0$ yields
$$\begin{aligned} \mathcal{F}_\beta(\phi) \;&\geq\; \frac{7}{4}\Big(\frac{2}{3}\Big)^{3/7} \beta^{4/7} \Big(\|\nabla\phi\|_2^2 \, \|\phi\|_1^{4/3}\Big)^{3/7} \\ &\geq\; \frac{7}{4}\Big(\frac{2}{3}\Big)^{3/7} \beta^{4/7}\, C_3^{-3/7}, \end{aligned} \tag{1.29}$$
where the last step uses Nash's inequality in three spatial dimensions, and C_3 is the optimal constant computed in [12]. Moreover, in [12] it is shown that the lower bound (1.29) is attained, and therefore $F_1 = \frac{7}{4}(\frac{2}{3})^{3/7} C_3^{-3/7} > 0$. We are grateful to one of the anonymous referees for pointing this short derivation out to us.

In Sect. 8, we use the information on the auxiliary functional and especially the scaling relation $F_\beta = \beta^{4/7} F_1$ to finally derive (1.10), formulated again as (8.3) in Theorem 8.1. In order to simultaneously control the errors on the right side of (1.25) and the localization error of order $\mathcal{O}(L^{-2})$, we choose $\varepsilon := \alpha^{4/105}\Lambda^{-4/105}$ and $L := \alpha^{17/105}\Lambda^{-88/105}$ and arrive at the upper bound in (1.10). Similarly, we choose $L := \alpha^{9/49}\Lambda^{-40/49}$ to obtain the lower bound in (1.10) from (1.26) and the localization estimate.

Note that the lower bound suggests that the length scale $\ell(\alpha, \Lambda)$ of the particle in the ground state of the Lieb–Loss model is of order $\ell(\alpha, \Lambda) \approx \alpha^{\tau - 1}\Lambda^{-\tau}$, with $\tau = \frac{40}{49} \approx 0.82$.

2. 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
$$H_{\alpha,\sigma,\Lambda} \;:=\; \frac{1}{2}\Big(i\vec{\nabla} + \sqrt{\alpha}\vec{A}_{\sigma,\Lambda}(x)\Big)^2 + H_{\mathrm{ph}}, \tag{2.1}$$
which we define here as a quadratic form on $\mathrm{H}^1(\mathbb{R}^3) \otimes \mathcal{D}(N_{\mathrm{ph}}^{1/2})$, where $\mathrm{H}^1(\mathbb{R}^3) \subseteq L^2(\mathbb{R}^3)$ is the Sobolev space of square-integrable functions whose gradient is square-integrable, as well, and $\mathcal{D}(N_{\mathrm{ph}}^{1/2}) \subseteq \mathfrak{F}_{\mathrm{ph}}$ denotes the subspace of finite

photon number expectation value of the photon Fock space $\mathfrak{F}_{\rm ph}$. The latter is the boson Fock space over the one-photon Hilbert space $\mathfrak{h}$, i.e., it is the orthogonal sum $\mathfrak{F}_{\rm ph} = \bigoplus_{n=0}^{\infty} \mathfrak{F}_{\rm ph}^{(n)}$ of n-photon sectors, where $\mathfrak{F}_{\rm ph}^{(0)} := \mathbb{C} \cdot \Omega$ is the one-dimensional vacuum sector spanned by the normalized vacuum vector Ω, and for $n \geq 1$, the n-photon sector $\mathfrak{F}_{\rm ph}^{(n)} := \mathcal{S}_n[\mathfrak{h}_{\rm pol}^{\otimes n}] \subseteq \mathfrak{h}_{\rm pol}^{\otimes n}$, is the subspace of the n-fold tensor product of $\mathfrak{h}_{\rm pol}$ of totally symmetric vectors.

The one-photon Hilbert space $\mathfrak{h}_{\rm pol} := L^2(S_{\sigma,\Lambda} \times \mathbb{Z}_2)$ is the space of square-integrable, divergence-free vector fields $\vec{k} \mapsto \vec{\epsilon}(\vec{k},+)f(k,+) + \vec{\epsilon}(\vec{k},-)f(k,-)$ 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 parameterized by the polarization vectors $\vec{\epsilon}(k,\pm) \perp k$ that are chosen so as to form an orthonormal frame $\big(\vec{k}/|\vec{k}|, \vec{\epsilon}(\vec{k},+), \vec{\epsilon}(\vec{k},-)\big)$ in $\mathbb{C} \otimes \mathbb{R}^3$, for all $\vec{k} \in S_{\sigma,\Lambda} \backslash \{\vec{0}\}$. Of course, the map $k \to \vec{\epsilon}(k)$ 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 (2.1), the field Hamiltonian

$$H_{\rm ph} \ = \ \mathrm{d}\Gamma(|k|) \ = \ \int |k| \, a^*(k) \, a(k) \, dk \tag{2.2}$$

represents the energy of the radiation field, and

$$\vec{A}_{\sigma,\Lambda}(x) \ = \ (2\pi)^{-\frac{3}{2}} \int \frac{\vec{\epsilon}(k)}{|k|^{\frac{1}{2}}} \big(a^*(k) \, e^{-ik\cdot x} \ + \ a(k) \, e^{ik\cdot x} \big) \, dk \tag{2.3}$$

is the quantized vector potential (in Coulomb gauge). In (2.2), (2.3), we denote elements of $S_{\sigma,\Lambda} \times \mathbb{Z}_2 \ni (\vec{k},\tau)$ by $k := (\vec{k},\tau)$ and then further $-k := (-\vec{k},\tau)$, $|k| := |\vec{k}|$, $k \cdot x := k_1 x_1 + k_2 x_2 + k_3 x_3$, $\int F(k) \, dk := \sum_{\tau=\pm} \int_{\sigma \leq |\vec{k}| < \Lambda} F(\vec{k},\tau) \, d^3k$. Furthermore, we use creation and annihilation operators $a^*(k)$ and $a(k)$, for $k \in S_{\sigma,\Lambda} \times \mathbb{Z}_2$, in (2.2) and (2.3). These are operator-valued distributions constituting a Fock representation of the canonical commutation relations (CCR) on $\mathfrak{F}_{\rm ph}$, i.e.,

$$\big[a(k_1), \, a(k_2)\big] = \big[a^*(k_1), \, a^*(k_2)\big] \ = \ 0 \, , \tag{2.4}$$

$$\big[a(k_1), \, a^*(k_2)\big] = \delta(k_1 - k_2) \, , \quad a(k_1)\Omega \ = \ 0, \tag{2.5}$$

for all $k_1 = (\vec{k}_1, \tau_1), k_2 = (\vec{k}_2, \tau_2) \in S_{\sigma,\Lambda} \times \mathbb{Z}_2$ (integrated over k_1 and k_2 against test functions), where $\delta(k_1 - k_2) = \delta^3(\vec{k}_1 - \vec{k}_2) \, \delta_{\tau_1,\tau_2}$. Finally, the photon number operator entering the definition of the domain $\mathcal{D}(N_{\rm ph}^{1/2})$ is given by $N_{\rm ph} := \int a^*(k) a(k) \, dk$.

The Lieb–Loss model is defined by the Lieb–Loss (energy) functional $\mathcal{E}_{\alpha,\sigma,\Lambda} : \mathrm{H}^1(\mathbb{R}^3) \times \mathcal{D}(N_{\rm ph}^{1/2}) \to \mathbb{R}$ 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 $\psi \in \mathfrak{F}_{\rm ph}$ in the Rayleigh–Ritz principle, i.e.,

$$\mathcal{E}_{\alpha,\sigma,\Lambda}(\phi,\psi) \ := \ \big\langle \phi \otimes \psi \, \big| \, H_{\alpha,\sigma,\Lambda}(\phi \otimes \psi) \big\rangle. \tag{2.6}$$

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

$$\mathcal{E}_{\alpha,\sigma,\Lambda}(\phi, \psi) \;=\frac{1}{2}\|\vec{\nabla}\phi\|_2^2 + \Big\langle \psi \Big| \, \mathbb{H}\big(|\phi|^2, \; \mathrm{Im}\{\overline{\phi}\,\vec{\nabla}\phi\}\big)\, \psi \Big\rangle_{\mathfrak{F}}, \tag{2.7}$$

where $\langle \cdot | \cdot \rangle_{\mathfrak{F}}$ denotes the scalar product on the photon Fock space $\mathfrak{F}_{\mathrm{ph}}$ and, for fixed $\rho : \mathbb{R}^3 \to \mathbb{R}^+$ and $\vec{v} : \mathbb{R}^3 \to \mathbb{R}^3$, the quadratic Hamiltonian $\mathbb{H}[\rho, \vec{v}]$ is given as

$$\mathbb{H}[\rho, \vec{v}] \;:=\; H_{\mathrm{ph}} + \frac{\alpha}{2}\int \rho(x)\, \vec{A}_{\sigma,\Lambda}^{\,2}(x)\, d^3x + \sqrt{\alpha}\int \vec{v}(x)\cdot \vec{A}_{\sigma,\Lambda}(x)\, d^3x. \tag{2.8}$$

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 $r := |\phi| \in \mathrm{H}^1(\mathbb{R}^3; \mathbb{R}_0^+)$ and choose $\gamma \in \mathrm{H}^1(\mathbb{R}^3; \mathbb{R})$, for a given $\phi \in \mathrm{H}^1(\mathbb{R}^3; \mathbb{C})$, so that

$$\phi \;=\; r\, e^{i\gamma}, \qquad |\phi|^2 \;= r^2, \qquad \mathrm{Im}\{\overline{\phi}\,\vec{\nabla}\phi\} \;=\; r^2\,\vec{\nabla}\gamma, \tag{2.9}$$

$$\|\vec{\nabla}\phi\|_2^2 \;=\; \|\vec{\nabla}r\|_2^2 + \|r\vec{\nabla}\gamma\|_2^2, \tag{2.10}$$

and thus

$$\mathcal{E}_{\alpha,\sigma,\Lambda}(r\, e^{i\gamma}\;,\; \psi) \;=\frac{1}{2}\|\vec{\nabla}r\|_2^2 + \frac{1}{2}\|r\vec{\nabla}\gamma\|_2^2 + \Big\langle \psi \Big| \, \mathbb{H}\big(r^2, \; r^2\,\vec{\nabla}\gamma\big)\, \psi \Big\rangle_{\mathfrak{F}}. \tag{2.11}$$

Although convenient, the explicit parametrization of Couloumb 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

$$\begin{aligned}\mathfrak{h} &:= P_C\big[L^2(S_{\sigma,\Lambda}; \mathbb{C}\otimes\mathbb{R}^3)\big] \\ &= \Big\{ f \in L^2(S_{\sigma,\Lambda}; \mathbb{C}\otimes\mathbb{R}^3) \;\Big|\; \forall \vec{k} \in S_{\sigma,\Lambda}: \quad \vec{k} \perp f(\vec{k}) \Big\}\end{aligned} \tag{2.12}$$

of divergence-free, square-integrable vector fields, where $P_C \in \mathcal{B}\big[L^2(S_{\sigma,\Lambda}; \mathbb{C}\otimes\mathbb{R}^3)\big]$ is the orthogonal projection acting as $\big[P_C f\big](\vec{k}) := P_{\vec{k}}^{\perp} f(\vec{k}) := f(\vec{k}) - P_{\vec{k}} f(\vec{k})$, 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

$$\Xi : \; \mathfrak{h}_{\mathrm{pol}} \;\to\; \mathfrak{h}, \quad \big[\Xi f\big](\vec{k}) \;:=\; \vec{\epsilon}(\vec{k}, +)\, f(\vec{k}, +) + \vec{\epsilon}(\vec{k}, -)\, f(\vec{k}, -) \tag{2.13}$$

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 $\mathfrak{F}_{\mathrm{ph}} := \mathfrak{F}_b[\mathfrak{h}]$, the bosonic Fock space over divergence-free vector fields. On $\mathfrak{F}_{\mathrm{ph}}$, we have a Fock representation of the CCR of the form

$$\big[a(\vec{k}_1,\nu_1),\, a(\vec{k}_2,\nu_2)\big] \; = \big[a^*(\vec{k}_1,\nu_1),\, a^*(\vec{k}_2,\nu_2)\big] \;=\; 0\,, \tag{2.14}$$

$$\big[a(\vec{k}_1,\nu_1),\, a^*(\vec{k}_2,\nu_2)\big] \; = \delta(\vec{k}_1-\vec{k}_2)\,\big(P^{\perp}_{\vec{k}_1}\big)_{\nu_1,\nu_2}\,, \quad a(k_1)\Omega \;=\; 0, \tag{2.15}$$

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

$$\big[a(f),\, a(g)\big] \; = \big[a^*(f),\, a^*(g)\big] \;=\; 0\,, \tag{2.16}$$

$$\big[a(f),\, a^*(g)\big] \; = \big\langle f \,\big|\, P_C\, g\big\rangle\,, \quad a(f)\Omega \;=\; 0, \tag{2.17}$$

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

$$a^*(f) \;:=\; \sum_{\nu=1}^{3} \int f_\nu(\vec{k})\, a^*(\vec{k},\nu)\, d^3k\,, \quad a(f) \;:=\; \sum_{\nu=1}^{3} \int \overline{f_\nu(\vec{k})}\, a(\vec{k},\nu)\, d^3k. \tag{2.18}$$

for all $f = (f_1, f_2, f_3)^t \in \mathfrak{h}$. In this representation, the operator $\vec{A}_{\sigma,\Lambda}(x)$ of the magnetic vector potential becomes $\vec{\mathbb{A}}(x) = \big(\mathbb{A}_1(x),\, \mathbb{A}_2(x),\, \mathbb{A}_3(x)\big)$, with

$$\begin{aligned}\mathbb{A}_\mu(x) &= a^*\big(m_\mu(x)\big) + a\big(m_\mu(x)\big)\\ &= \sum_{\nu=1}^{3} \int \Big\{ m_{\mu,\nu}(x,\vec{k})\, a^*(\vec{k},\nu) + \overline{m_{\mu,\nu}(x,\vec{k})}\, a(\vec{k},\nu)\Big\} d^3k,\end{aligned} \tag{2.19}$$

$$m_{\mu,\nu}(x,\vec{k}) \;:= \frac{\mathbf{1}\big[\sigma \le |\vec{k}| < \Lambda\big]}{(2\pi)^{3/2}\, |\vec{k}|^{1/2}}\, \big(P^{\perp}_{\vec{k}}\big)_{\mu,\nu}\, e^{-ik\cdot x}, \tag{2.20}$$

and the Hamiltonian $\mathbb{H}\big(r^2,\, r^2\,\vec{\nabla}\gamma\big)$ in (2.11) turns into

$$\begin{aligned}&\mathbb{H}\big(r^2,\, r^2\,\vec{\nabla}\gamma\big)\\ &\quad= H_{\mathrm{ph}} + \frac{\alpha}{2} \int \big(r(x)\,\vec{\mathbb{A}}(x)\big)^2\, d^3x + \sqrt{\alpha} \int \big(r(x)\,\vec{\nabla}\gamma(x)\big)\cdot\big(r(x)\,\vec{\mathbb{A}}(x)\big)\, d^3x.\end{aligned} \tag{2.21}$$

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

3. Bogoliubov Transformations

Next, we analyze the infimum of $\psi \mapsto \big\langle \psi \,\big|\, \mathbb{H}\big[r^2, r^2\vec{\nabla}\gamma\big]\psi\big\rangle$, as $\psi \in \mathcal{D}(N_{\mathrm{ph}}^{1/2})$ varies over normalized states, by means of Bogoliubov 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

$$[Jf](\vec{k}) \;:=\; \overline{f(-\vec{k})} \tag{3.1}$$

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

3.1. Antiunitary Maps and Generalized Field Operators

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

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

$$\mathsf{J}^2 \;=\; \mathbf{1}_{\mathsf{h}} \quad \textit{and} \quad \forall\, f,g \in \mathsf{h}: \;\; \langle \mathsf{J}(f)|\mathsf{J}(g)\rangle_{\mathsf{h}} \;=\; \langle g|f\rangle_{\mathsf{h}}. \tag{3.2}$$

Given an *antiunitary involution* $\mathsf{J} : \mathsf{h} \to \mathsf{h}$, we can define the maximal J-invariant subspace

$$\mathsf{h}_{\mathbb{R}} \;=\; \big\{ f \in \mathsf{h} \,\big|\, \mathsf{J}f = f \,\big\} \;\subseteq\; \mathsf{h}, \tag{3.3}$$

which is a $\mathbb{R}$-linear subspace of h. Writing $f \in \mathsf{h}$ as $f = f_1 + if_2$, with $f_1 := \frac{1}{2}(f + \mathsf{J}f) \in \mathsf{h}$ and $f_2 := \frac{1}{2i}(f - \mathsf{J}f) \in \mathsf{h}$, we obtain a direct sum decomposition $\mathsf{h} = \mathsf{h}_{\mathbb{R}} \oplus i\mathsf{h}_{\mathbb{R}}$. Similar to antiunitary operators $\mathsf{h} \to \mathsf{h}^*$, antiunitary involutions $\mathsf{h} \to \mathsf{h}$ are not unique. This gives us freedom to make a suitable choice for the problem to solve, namely (3.1) in the present case.

To define Bogoliubov transformations it is convenient to use *generalized creation and annihilation operators* which were first introduced by Araki and Shiraishi in [2,3] to describe the second quantization of one-body Hamiltonians. Bogoliubov transformations are also discussed in detail in [8,36]. Given an antiunitary involution $\mathsf{J} : \mathsf{h} \to \mathsf{h}$, the generalized creation and annihilation (field) operators $A^*_{\mathsf{J}}, A_{\mathsf{J}} : \mathsf{h} \oplus \mathsf{h} \to \mathcal{B}[\mathcal{D}(\mathsf{N}^{1/2}); \mathfrak{F}_b(\mathsf{h})]$ are defined by

$$A^*_{\mathsf{J}}(f \oplus \mathsf{J}g) \;:=\; a^*(f) + a(g) \quad \text{and} \quad A_{\mathsf{J}}(f \oplus \mathsf{J}g) \;:=\; a(f) + a^*(g), \tag{3.4}$$

for any $f, g \in \mathsf{h}$. Note that

$$A_{\mathsf{J}}(F) \;=\; A^*_{\mathcal{J}}(\mathcal{J}F), \quad \text{with} \quad \mathcal{J} \;:=\; \begin{pmatrix} 0 & \mathsf{J} \\ \mathsf{J} & 0 \end{pmatrix} \tag{3.5}$$

being an antiunitary involution on $\mathsf{h}\oplus\mathsf{h}$. The vectors in $\mathsf{h}\oplus\mathsf{h}$ which are invariant under $\mathcal{J}$ are of the form $y \oplus \mathsf{J}y$, with $y \in \mathsf{h}$. They form a real subspace

$$(\mathsf{h} \oplus \mathsf{h})_{\mathcal{J}} \;:=\; \big\{ G \in \mathsf{h} \oplus \mathsf{h} \,\big|\, G = \mathcal{J}G \,\big\} \;=\; \big\{ y \oplus \mathsf{J}y \,\big|\, y \in \mathsf{h} \,\big\} \;=\; \mathsf{q}[\mathsf{h}], \tag{3.6}$$

where $\mathsf{q} : \mathsf{h} \to (\mathsf{h} \oplus \mathsf{h})_{\mathcal{J}}$ is the real-linear map

$$\mathsf{q} \;:=\; \begin{pmatrix} \mathbf{1} \\ \mathsf{J} \end{pmatrix}, \quad \text{with adjoint} \quad \mathsf{q}^* : (\mathsf{h} \oplus \mathsf{h})_{\mathcal{J}} \to \mathsf{h}, \; \mathsf{q}^* \;=\; \big(\mathbf{1},\, \mathsf{J}\big). \tag{3.7}$$

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

$$\big[A_{\mathsf{J}}(F),\, A^*_{\mathsf{J}}(F')\big] \;=\; \big\langle F \,\big|\, \mathcal{S}F' \big\rangle, \tag{3.8}$$

where $\mathcal{S}$ is a natural symplectic form on $\mathsf{h} \oplus \mathsf{h}$ given by

$$\mathcal{S} := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3.9}$$

3.2. Second Quantization and Bogoliubov Transformations

Next, we introduce the *second quantization* of one-photon operators. Let $\mathsf{J} : \mathsf{h} \to \mathsf{h}$ be an antiunitary involution and $\{F_i\}_{i=1}^{\infty} \subseteq \mathsf{h} \oplus \mathsf{h}$ an orthonormal basis. For $T = T^* \in \mathcal{B}[\mathsf{h} \oplus \mathsf{h}]$ and $y \in \mathsf{h}$, we define their second quantization $\mathrm{d}\Gamma_{\mathsf{J}}[T, y] \in \mathcal{B}[\mathcal{D}(N_{\mathrm{ph}}); \mathfrak{F}_{\mathrm{ph}})]$ by

$$\mathrm{d}\Gamma_{\mathsf{J}}[T, y] := \sum_{i,j=1}^{\infty} \langle F_i | \, T F_j \rangle \, A_{\mathsf{J}}^*(F_i) \, A_{\mathsf{J}}(F_j) + \sum_{i=1}^{\infty} \big\{ \langle F_i | \mathsf{q}(y) \rangle \, A_{\mathsf{J}}^*(F_i) + \overline{\langle F_i | \, \mathsf{q}(y) \rangle} \, A_{\mathsf{J}}(F_i) \big\}. \tag{3.10}$$

Note that the definition (3.10) of $\mathrm{d}\Gamma_{\mathsf{J}}[T, y]$ is independent of the choice of the orthonormal basis $\{F_i\}_{i=1}^{\infty} \subseteq \mathsf{h} \oplus \mathsf{h}$. Moreover, $\mathrm{d}\Gamma_{\mathsf{J}}[T, y]$ is self-adjoint on $\mathcal{D}(N_{\mathrm{ph}})$ and $\mathrm{d}\Gamma_{\mathsf{J}}[T, y]$ is semibounded, provided $T \geq 0$. Finally, $[a(f), a(g)] = 0$ and $[a^*(f), a^*(g)] = 0$ imply that $\mathrm{d}\Gamma_{\mathsf{J}}\big[\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right), y\big] = \mathrm{d}\Gamma_{\mathsf{J}}\big[\left(\begin{smallmatrix} a & \mathsf{J} b^* \mathsf{J} \\ \mathsf{J} c^* \mathsf{J} & d \end{smallmatrix}\right), y\big]$, and we can and will henceforth always assume that

$$b^* = \mathsf{J} \, b \, \mathsf{J}, \quad \text{for} \quad T = T^* = \left(\begin{smallmatrix} a & b \\ b^* & d \end{smallmatrix}\right) = \left(\begin{smallmatrix} a & b \\ \mathsf{J} b \mathsf{J} & d \end{smallmatrix}\right). \tag{3.11}$$

A second advantage of the generalized creation and annihilation operators is that their use eases the definition of Bogoliubov transformations. We recall that *Bogoliubov transformations* are unitary transformations $\widehat{\mathbb{U}}$ on Fock space $\mathfrak{F}_{\mathrm{ph}}$ which preserve (3.7) and are linear in the field operators, i.e., they act as

$$\widehat{\mathbb{U}} \, a^*(f) \, \widehat{\mathbb{U}}^* := a^*(Uf) + a(\mathsf{J} V f) + \langle \eta | f \rangle, \tag{3.12}$$

for all $f \in \mathsf{h}$, where U and V are linear operators on h and $\eta \in \mathsf{h}$. The Bogoliubov transformations form a group which is the semidirect product of the group of *homogenous Bogoliubov transformations* and the group of *Weyl transformations*. That is, every Bogoliubov transformation $\widehat{\mathbb{U}}$ can be written as a composition

$$\widehat{\mathbb{U}} = \mathbb{U}_B \, \mathbb{W}_\eta = \mathbb{W}_\mu \, \mathbb{U}_B \tag{3.13}$$

of a homogeneous Bogoliubov transformation $\mathbb{U}_B$ and a Weyl transformation $\mathbb{W}_\eta$ or a composition of a Weyl transformation $\mathbb{W}_\mu$ and $\mathbb{U}_B$, but with $\mu \neq \eta$, in general.

Homogeneous Bogoliubov transformations $\mathbb{U}_B$ are the special case $\eta = 0$ of (3.12). In terms of the generalized field operators, they assume the form

$$\mathbb{U}_B \, A_J^*(F) \, \mathbb{U}_B^* := A_J^*(BF), \quad B \equiv B(U, V) := \begin{pmatrix} U & \mathsf{J} V \mathsf{J} \\ V & \mathsf{J} U \mathsf{J} \end{pmatrix}, \tag{3.14}$$

where the form of B is determined by (3.5), i.e., $\mathcal{J} B = B \mathcal{J}$, and (3.12). Note that this makes explicit use of the antiunitary involution $\mathsf{J} : \mathsf{h} \to \mathsf{h}$. The homogeneous Bogoliubov transformation $\mathbb{U}_B$ is unitary iff it leaves the CCR invariant and preserves the norm of the vacuum vector $\Omega \in \mathfrak{F}_{\rm ph}$, which is equivalent to

$$B^* \mathcal{S} B = \mathcal{S}, \quad B \mathcal{S} B^* = \mathcal{S}, \quad \text{and} \quad \mathrm{Tr}\big(V^* V\big) < \infty. \tag{3.15}$$

The second identity in (3.15) 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 $\mathrm{d}\Gamma_{\mathsf{J}}[T, y]$ of T and y transforms under a homogeneous Bogoliubov transformation $\mathbb{U}_B$ with $B \equiv B(U, V)$ as

$$\mathbb{U}_B \, \mathrm{d}\Gamma_{\mathsf{J}}[T,\ y] \, \mathbb{U}_B^* \ = \ \mathrm{d}\Gamma_{\mathsf{J}}\big[BTB^*,\ \tfrac{1}{2}\mathsf{q}^* B \mathsf{q}(y)\big]. \tag{3.16}$$

Weyl transformations $\mathbb{W}_\eta$ are the special case $U = \mathbf{1}_{\mathsf{h}}$ and $V = 0$ of (3.12). They act on the generalized field operators as

$$\mathbb{W}_\eta \, A_J^*(F) \, \mathbb{W}_\eta^* \ := \ A_J^*(F) + \langle \mathsf{q}(\eta) \,|\, F \rangle. \tag{3.17}$$

The unitarity of $\mathbb{W}_\eta$ is equivalent to the requirement $\eta \in \mathsf{h}$. Another simple computation shows that the second quantization $\mathrm{d}\Gamma_{\mathsf{J}}[T, y]$ of T and y transforms under a Weyl transformation $\mathbb{W}_\eta$ as

$$\mathbb{W}_\eta \, \mathrm{d}\Gamma_{\mathsf{J}}[T,\ y] \, \mathbb{W}_\eta^* \ = \ \mathrm{d}\Gamma_{\mathsf{J}}\Big[T,\ y + \tfrac{1}{2}\mathsf{q}^* T \mathsf{q}(\eta)\Big] + \langle \eta |\ \mathsf{q}^* T \mathsf{q}(\eta) \rangle + 4\mathrm{Re}\langle \eta | y \rangle. \tag{3.18}$$

3.3. The Lieb–Loss Model in Terms of Second Quantization

We turn to the analysis of the Lieb–Loss model. Note that $\mathrm{d}\Gamma_{\mathsf{J}}[T, y]$ depends on the choice of the antiunitary involution $\mathsf{J} : \mathfrak{h} \to \mathfrak{h}$. For the analysis of the Lieb–Loss model it is of key importance to choose the antiunitary involution $J : \mathfrak{h} \to \mathfrak{h}$ with corresponding real-linear map $q : \mathfrak{h} \to (\mathfrak{h} \oplus \mathfrak{h})_J$ as

$$\forall\, f \in \mathfrak{h},\ \vec{k} \in S_{\sigma,\Lambda} : \quad [Jf](\vec{k}) \ := \ \overline{f(-\vec{k})} \tag{3.19}$$

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 J-invariant vectors, as is discussed below.

We identify $\mathbb{H}(r^2, r^2 \vec{\nabla}\gamma)$ with $\mathrm{d}\Gamma_J[T_{r,\alpha}, y_{r,\gamma,\alpha}]$, for suitably chosen $T_{r,\alpha}$ and $y_{r,\gamma,\alpha}$. We state the result in form of Lemma 3.1.

Lemma 3.1. *Let $J : \mathfrak{h} \to \mathfrak{h}$ be defined by (3.19) and $r, \gamma \in H^1(\mathbb{R}^3)$. Then, the Lieb–Loss functional (2.11) is given by*

$$\mathcal{E}_{\alpha,\sigma,\Lambda}(r\, e^{i\gamma}\ ,\ \psi) \ = \frac{1}{2}\|\vec{\nabla} r\|_2^2 + \frac{1}{2}\|r \vec{\nabla}\gamma\|_2^2 + \frac{1}{2}\Big\langle \psi \Big|\ \mathrm{d}\Gamma_J\big[T_{r,\alpha},\ y_{r,\gamma,\alpha}\big]\ \psi \Big\rangle_{\mathfrak{F}}, \tag{3.20}$$

where

$$T_{r,\alpha} \ := \ |k|^{-1/2} \begin{pmatrix} 2|k|^2 + \Theta_{r,\alpha} & \Theta_{r,\alpha} \\ \Theta_{r,\alpha} & \Theta_{r,\alpha} \end{pmatrix} |k|^{-1/2}, \tag{3.21}$$

with $|k|$ *denoting the multiplication operator* $\big[|k|f\big](\vec{k}) := |k|f(\vec{k})$ *(Fourier multiplier), and* $\Theta_{r,\alpha}$ *being a nonnegative,* J*-invariant, self-adjoint Hilbert–Schmidt operator,* $\Theta_{r,\alpha} = \Theta^*_{r,\alpha} = \Theta^T_{r,\alpha} = J\Theta_{r,\alpha}J \geq 0$ *given by*

$$\Theta_{r,\alpha} = \Phi^*_{r,\alpha}\,\Phi_{r,\alpha}, \quad \Phi_{r,\alpha} \;=\; (\hat{r}*)\,P_C\,\chi_{\sigma,\Lambda}, \tag{3.22}$$

$$\Phi_{r,\alpha}(\vec{p},\mu\,;\,\vec{k},\nu) := \alpha^{1/2}\,(2\pi)^{-3/2}\,\hat{r}(\vec{p}-\vec{k})\,\big(P^{\perp}_{\vec{k}}\big)_{\mu,\nu}\,\chi_{\sigma,\Lambda}(\vec{k}), \tag{3.23}$$

where $\big[\chi_{\sigma,\Lambda}f\big](\vec{k}) := \mathbf{1}[\sigma \leq |\vec{k}| < \Lambda]\,f(\vec{k})$ *is a multiplication operator, and* $\hat{r}*$ *is the convolution operator* $[\hat{r}*f](\vec{k}) = \int \hat{r}(\vec{k}-\vec{k}')\,f(\vec{k}')\,d^3k'$*, where* $\hat{r} \equiv \mathcal{F}[r]$ *denotes the Fourier transform* $\mathcal{F}[r](\vec{k}) := (2\pi)^{-3/2}\int e^{-ik\cdot x}\,r(x)\,d^3x$ *of* r*, normalized as to preserve the* L^2*-scalar product.*

Furthermore, $y_{r,\gamma,\alpha} = J[y_{r,\gamma,\alpha}] \in \mathfrak{h}_{\mathbb{R}}$ *is given by*

$$y_{r,\gamma,\alpha} = |k|^{-1/2}\,\Phi^*_{r,\alpha}\,\mathcal{F}[r\,\vec{\nabla}\gamma] \quad \Leftrightarrow$$

$$y_{r,\gamma,\alpha}(\vec{k},\nu) := \sum_{\mu=1}^{3}\int |\vec{k}|^{-1/2}\,\Phi^*_{r,\alpha}\big(\vec{k},\nu;\vec{p},\mu\big)\,\mathcal{F}\big[r\,\partial_\mu\gamma\big](\vec{p})\,d^3p. \tag{3.24}$$

Proof. We first observe that

$$\begin{aligned}\frac{\alpha}{2}\int \big(r(x)\,\vec{\mathbb{A}}(x)\big)^2\,d^3x &= \sum_{\mu=1}^{3}\int \frac{\alpha}{2}\Big[a^*\big(r(x)\,m_\mu(x)\big) + a\big(r(x)\,m_\mu(x)\big)\Big]^2\,d^3x \\ &= \sum_{\mu=1}^{3}\frac{\alpha}{2}\int A^*_J\Big(q\big[r(x)\,m_\mu(x)\big]\Big)\,A_J\Big(q\big[r(x)\,m_\mu(x)\big]\Big)\,d^3x \\ &= \frac{1}{2}\,\mathrm{d}\Gamma_J\left[|k|^{-1/2}\begin{pmatrix}\Theta_{r,\alpha} & \Theta_{r,\alpha}\\ \Theta_{r,\alpha} & \Theta_{r,\alpha}\end{pmatrix}|k|^{-1/2}\,,\;0\right],\end{aligned} \tag{3.25}$$

where $\Theta_{r,\alpha} : \mathfrak{h} \to \mathfrak{h}$ is the bounded operator given by the integral kernel

$$|\vec{k}|^{-1/2}\,\Theta_{r,\alpha}(\vec{k},\nu\,;\,\vec{k}',\nu')\,|\vec{k}|^{-1/2} \;:=\; \sum_{\mu=1}^{3}\int \alpha\,r^2(x)\,m_{\mu,\nu}(x,\vec{k})\,m_{\mu,\nu'}(x,\vec{k}')\,d^3x, \tag{3.26}$$

recalling the definition $m_{\mu,\nu}(x,\vec{k}) := (2\pi)^{-3/2}|\vec{k}|^{-1/2}\chi_{\sigma,\Lambda}(\vec{k})\big(P^{\perp}_{\vec{k}}\big)_{\mu,\nu}e^{-ik\cdot x}$ from (2.20). As $J(e^{ik\cdot x}e_\nu) = e^{ik\cdot x}e_\nu$, we have that $J[r(x)m_\mu(x)] = r(x)m_\mu(x)$ and hence

$$\Theta_{r,\alpha} \;=\; J\,\Theta_{r,\alpha} \;=\; \Theta_{r,\alpha}\,J \;=\; J\,\Theta_{r,\alpha}\,J. \tag{3.27}$$

Moreover, using the Plancherel theorem, we have that

$$\Theta_{r,\alpha} \;=\; \Phi^*_{r,\alpha}\,\Phi_{r,\alpha}, \tag{3.28}$$

where $\Phi_{r,\alpha} = \alpha^{1/2}(2\pi)^{-3/2}(\hat{r}*)P_C\chi_{\sigma,\Lambda}|\vec{k}|^{-1/2}$ is defined by the integral kernel

$$\Phi_{r,\alpha}(\vec{p},\mu\,;\,\vec{k},\nu) \;:=\; \frac{\alpha^{1/2}}{(2\pi)^{3/2}}\,\hat{r}(\vec{p}-\vec{k})\,\big(P^{\perp}_{\vec{k}}\big)_{\mu,\nu}\,\chi_{\sigma,\Lambda}(\vec{k}), \tag{3.29}$$

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

$$\mathcal{F}[r](\vec{k}) \;\equiv\; \hat{r}(\vec{k}) \;:=\; \int e^{-ik\cdot x}\, r(x)\, \frac{d^3x}{(2\pi)^{-3/2}} \tag{3.30}$$

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

Similarly, we obtain

$$\begin{aligned} &\alpha^{1/2} \int r^2(x)\, \vec{\nabla}\gamma(x) \cdot \vec{\mathbb{A}}(x)\, d^3x \\ &= \sum_{\mu=1}^{3} \int \alpha^{1/2} \Big\{ a^*\big(r^2(x)\, \partial_\mu\gamma(x)\, m_\mu(x)\big) + a\big(r^2(x)\, \partial_\mu\gamma(x)\, m_\mu(x)\big) \Big\}\, d^3x \\ &= \sum_{\mu=1}^{3} \int \frac{\alpha^{1/2}}{2} \Big\{ A_J^*\big(q[r^2(x)\, \partial_\mu\gamma(x)\, m_\mu(x)]\big) + A_J\big(q[r^2(x)\, \vec{\nabla}\gamma(x)\cdot \vec{m}(x)]\big) \Big\}\, d^3x \\ &= \frac{1}{2}\, \mathrm{d}\Gamma_J\big[0\,,\; y_{r,\gamma,\alpha}\big], \end{aligned} \tag{3.31}$$

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

$$y_{r,\gamma,\alpha}(\vec{k},\nu) := \sum_{\mu=1}^{3} \int r^2(x)\, \partial_\mu\gamma(x)\, \alpha^{1/2}\, m_{\mu,\nu}(x,\vec{k})\, d^3x. \tag{3.32}$$

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

$$y_{r,\gamma,\alpha}(\vec{k},\nu) := \sum_{\mu=1}^{3} \int |\vec{k}|^{-1/2}\, \Phi_{r,\alpha}^*\big(\vec{k},\nu;\vec{p},\mu\big)\, \mathcal{F}\big[r\, \partial_\mu\gamma\big](\vec{p})\, d^3p. \tag{3.33}$$

□

4. Minimization over Photon States

4.1. 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 (3.19) 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 $\frac{1}{2}\|r\vec{\nabla}\gamma\|_2^2$ that vanishes for real ϕ. As is already remarked in Step (2) of the sketch of our Proof of Theorem 1.1 in the introduction, there is an alternative way of showing that the optimal electron wave function is positive by using that the semigroup generated by $H_{\alpha,\Lambda}$ is positivity improving.

We start with a preparatory lemma whose simple proof is omitted.

Lemma 4.1. *Let $\kappa \in \mathcal{B}[\mathfrak{h}]$ be a bounded operator and $\delta \in \mathbb{R}^+$. Then,*

$$\kappa \left(\delta^2 + \kappa^* \kappa\right)^{-1} \kappa^* \;\leq\; \mathbf{1}. \tag{4.1}$$

Lemma 4.2. *Let $J : \mathfrak{h} \to \mathfrak{h}$ be defined by (3.19), $r, \gamma \in H^1(\mathbb{R}^3)$, and $T_{r,\alpha}$, $\Theta_{r,\alpha}$, and $y_{r,\gamma,\alpha} \in \mathfrak{h}_\mathbb{R}$ as in (3.21)–(3.24). Then, there is a unique $\eta_{r,\gamma} \in \mathfrak{h}_\mathbb{R}$ such that*

$$y_{r,\gamma,\alpha} \;=\; \frac{1}{2}\, q^*\, T_{r,\alpha}\, q(\eta_{r,\gamma}). \tag{4.2}$$

Moreover, as a quadratic form,

$$\mathrm{d}\Gamma_J\big[T_{r,\alpha},\; y_{r,\gamma,\alpha}\big] \;\geq\; \mathbb{W}_{\eta_{r,\gamma}}\, \mathrm{d}\Gamma_J\big[T_{r,\alpha},\; 0\big]\, \mathbb{W}^*_{\eta_{r,\gamma}} \;-\; \|r\, \vec{\nabla}\gamma\|_2^2. \tag{4.3}$$

Proof. We first compute that

$$\begin{aligned} q^*\, T_{r,\alpha}\, q &= |k|^{-1/2}\, (\mathbf{1}\;\; J) \begin{pmatrix} 2|k|^2 + \Theta_{r,\alpha} & \Theta_{r,\alpha} \\ \Theta_{r,\alpha} & \Theta_{r,\alpha} \end{pmatrix} \begin{pmatrix} \mathbf{1} \\ J \end{pmatrix} |k|^{-1/2} \\ &= |k|^{-1/2} \left(2|k|^2 + \Theta_{r,\alpha} + J\Theta_{r,\alpha} + \Theta_{r,\alpha}J + J\Theta_{r,\alpha}J\right) |k|^{-1/2}, \end{aligned} \tag{4.4}$$

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

$$2y_{r,\gamma,\alpha} \;=\; |k|^{-1/2} \left(2|k|^2 + \Theta_{r,\alpha} + J\Theta_{r,\alpha} + \Theta_{r,\alpha}J + J\Theta_{r,\alpha}J\right) |k|^{-1/2}\, \eta_{r,\gamma}. \tag{4.5}$$

If J was any general antiunitary map, the determination of $\eta_{r,\gamma}$ from (4.5) appeared to be fairly complicated, but thanks to our choice (3.19) of J we have that $\Theta_{r,\alpha} = J\Theta_{r,\alpha} = \Theta_{r,\alpha}J = J\Theta_{r,\alpha}J$ and $y_{r,\gamma,\alpha} = Jy_{r,\gamma,\alpha}$. Therefore, $y_{r,\gamma,\alpha}$ is an element of $\mathfrak{h}_\mathbb{R}$ which is left invariant by $q^*T_{r,\alpha}q = |k|^{-1/2}\big(2|k|^2 + 4\Theta_{r,\alpha}\big)|k|^{-1/2}$. Moreover, $q^*T_{r,\alpha}q \geq 2|k| \geq 2\sigma \cdot \mathbf{1} > 0$ 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

$$\eta_{r,\gamma} \;=\; |k|^{1/2} \left(|k|^2 + 2\Theta_{r,\alpha}\right)^{-1} |k|^{1/2}\, y_{r,\gamma,\alpha} \;\in\; \mathfrak{h}_\mathbb{R} \tag{4.6}$$

and

$$\begin{aligned} &\big\langle \eta_{r,\gamma} \;\big|\; |k|^{-1/2}\big(|k|^2 + 2\Theta_{r,\alpha}\big)\, |k|^{-1/2}\, \eta_{r,\gamma} \big\rangle \\ &\quad= \big\langle |k|^{1/2}\, y_{r,\gamma,\alpha} \;\big|\; \left(|k|^2 + 2\Theta_{r,\alpha}\right)^{-1} |k|^{1/2}\, y_{r,\gamma,\alpha} \big\rangle \\ &\quad= \Big\langle \mathcal{F}[r\,\vec{\nabla}\gamma] \;\Big|\; \Phi_{r,\alpha} \left(|k|^2 + 2\Phi^*_{r,\alpha}\Phi_{r,\alpha}\right)^{-1} \Phi^*_{r,\alpha}\, \mathcal{F}[r\,\vec{\nabla}\gamma] \Big\rangle \\ &\quad\leq \Big\langle \mathcal{F}[r\,\vec{\nabla}\gamma] \;\Big|\; \mathcal{F}[r\,\vec{\nabla}\gamma] \Big\rangle \;=\; \|r\,\vec{\nabla}\gamma\|_2^2, \end{aligned} \tag{4.7}$$

estimating $\big(|k|^2 + 2\Phi^*_{r,\alpha}\Phi_{r,\alpha}\big)^{-1} \leq \big(\sigma^2 + 2\Phi^*_{r,\alpha}\Phi_{r,\alpha}\big)^{-1}$ and then using Lemma 4.1. We obtain the assertion from here by (3.18). □

As a corollary of Lemma 4.2, we now find the following lower bound on the Lieb–Loss functional defined in (1.4).

Corollary 4.3. *Let $\phi \in H^1(\mathbb{R}^3)$ and $\psi \in \mathfrak{F}_{\mathrm{ph}}$ be normalized wave functions. Then, there exists a unitary Weyl transformation $\mathbb{W}_\phi$ such that*

$$\mathcal{E}_{\alpha,\Lambda}\big(\phi, \psi\big) \;\geq\; \mathcal{E}_{\alpha,\Lambda}\big(|\phi|, \mathbb{W}_\phi\psi\big). \tag{4.8}$$

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

$$\widehat{\mathcal{E}}_{\alpha,\Lambda}(\phi) \ := \ \inf \Big\{ \mathcal{E}_{\alpha,\Lambda}(\phi, \psi) \ \Big| \ \psi \in \mathcal{F}_{\mathrm{ph}}, \ \|\psi\| = 1 \Big\}, \tag{4.9}$$

over photon wave functions [see (1.14)] allows us to restrict the minimization over electron wave functions to nonnegative functions.

Theorem 4.4. *Let $J : \mathfrak{h} \to \mathfrak{h}$ be defined by* (3.19) *and suppose that $\phi \in \mathcal{H}_{\mathrm{el}}$ is normalized and $\phi \in H^1(\mathbb{R}^3)$. Then,*

$$\widehat{\mathcal{E}}_{\alpha,\Lambda}(\phi) \ \geq \ \widehat{\mathcal{E}}_{\alpha,\Lambda}(|\phi|) \ = \ \frac{1}{2}\big\|\vec{\nabla}|\phi|\big\|_2^2 + \frac{1}{2}\inf\big\{\sigma\big(\mathrm{d}\Gamma_J[T_{|\phi|,\alpha}, 0]\big)\big\}, \tag{4.10}$$

where $\sigma(A) \subseteq \mathbb{R}$ denotes the spectrum of a self-adjoint operator A and $T_{|\phi|}$ is as defined in (3.21)*–*(3.23)*.*

4.2. The Ground State Energy of $T_{|\phi|,\alpha}$

In this section, we show that the infimum of the spectrum of $\frac{1}{2}\mathrm{d}\Gamma_J[T_{|\phi|}, 0]$ equals $X(\Theta_{|\phi|,\alpha})$, as defined in (1.19) and (3.21)–(3.23). This fact had already been observed in [31], and we give an alternative and detailed proof here. More specifically, we prove the following theorem in this section.

Theorem 4.5. *Let $J : \mathfrak{h} \to \mathfrak{h}$ be defined by* (3.19)*, suppose that $\phi = |\phi| \in H^1(\mathbb{R}^3)$, and let $T_{\phi,\alpha}$ and $\Theta_{\phi,\alpha}$ be given as in* (3.21)*–*(3.24)*. Then,*

$$\inf\big\{\sigma\big(\mathrm{d}\Gamma_J[T_{\phi,\alpha}, 0]\big)\big\} \ = \ \mathrm{Tr}\Big(\sqrt{|k|^2 + 2\Theta_{\phi,\alpha}} \ - \ |k|\Big). \tag{4.11}$$

Inserting (4.11) into (4.10), we immediately obtain the following Corollary.

Corollary 4.6. *Let $J : \mathfrak{h} \to \mathfrak{h}$ be defined by* (3.19) *and suppose that $\phi = |\phi| \in \mathcal{H}_{\mathrm{el}}$ is normalized and $\phi \in H^1(\mathbb{R}^3)$. Then*

$$\widehat{\mathcal{E}}_{\alpha,\Lambda}(\phi) \ = \ \frac{1}{2}\big\|\vec{\nabla}\phi\big\|_2^2 + \frac{1}{2}\mathrm{Tr}\Big(\sqrt{|k|^2 + 2\Theta_{\phi,\alpha}} \ - \ |k|\Big). \tag{4.12}$$

where $\Theta_{\phi,\alpha}$ is defined in (3.22)*–*(3.23)*.*

Proof (Proof of Theorem IV.5). The first step in our proof rests on an observation made in [4] that given a nonnegative Hamiltonian $\mathbb{H}$ representing an interacting quantum system, it holds true that

$$\inf_{\rho\in\mathrm{qfDM}}\big\{\mathrm{Tr}(\rho^{1/2}\mathbb{H}\rho^{1/2})\big\} \ = \ \inf_{\rho\in\mathrm{qfDM}}\big\{\mathrm{Tr}(\rho^{1/2}\mathbb{H}\rho^{1/2}) \ \big| \ \rho \ \text{ is pure}\big\}, \tag{4.13}$$

where qfDM denotes the set of quasifree density matrices. In other words, for the computation of the Bogoliubov–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 [32]. In Lemma 4.7, the observation from [4] is applied to the Hamiltonian $\mathrm{d}\Gamma_J[T_{\phi,\alpha}, 0]$

and yields the statement that its ground state energy is the lowest vacuum expectation value of all homogeneous Bogoliubov transforms of $\mathrm{d}\Gamma_J[T_{\phi,\alpha}, 0]$,

$$\inf \left\{ \sigma\big(\mathrm{d}\Gamma_J[T_{\phi,\alpha}, 0]\big) \right\} \;=\; \inf \left\{ \big\langle \Omega \big| \mathbb{U}_B \, \mathrm{d}\Gamma_J[T_{\phi,\alpha}, 0] \, \mathbb{U}_B^* \Omega \big\rangle \;\Big|\; B \in \mathrm{Bog}_J[\mathfrak{h}] \right\}, \tag{4.14}$$

where $\mathrm{Bog}_J[\mathfrak{h}]$ is defined in (4.22).

Next, an application of Lemma 4.8 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 (4.14) in terms of $|v|$, where $v \in \mathcal{L}^2[\mathfrak{h}]$ is the lower left matrix entry of B of the Bogoliubov transformation $\mathbb{U}_B$,

$$\begin{aligned} &\big\langle \Omega \big| \mathbb{U}_B \, \mathrm{d}\Gamma_J[T_{\phi,\alpha}, 0] \, \mathbb{U}_B^* \Omega \big\rangle \\ &\quad \geq \inf_{v \in \mathcal{L}^2[\mathfrak{h}],\, v \geq 0} \left\{ \mathrm{Tr}\Big[2|k|^{1/2} \, v^2 \, |k|^{1/2} \;+\; \Theta_{\phi,\alpha}^{1/2} |k|^{-1/2} \big(v - \sqrt{1+v^2} \big)^2 |k|^{-1/2} \Theta_{\phi,\alpha}^{1/2} \Big] \right\}. \end{aligned} \tag{4.15}$$

The infimum on the right side of the lower bound (4.15) is explicitly computed in Lemma 4.9, using $\sigma \cdot \mathbf{1} \leq a := 2|k| \leq \Lambda \cdot \mathbf{1}$, $b := |k|^{-1/2}\Theta_{\phi,\alpha}|k|^{-1/2} \geq 0$, and $d := 0$ again. Consequently,

$$\inf \left\{ \big\langle \Omega \big| \mathbb{U}_B \, \mathrm{d}\Gamma_J[T_{\phi,\alpha}, 0] \, \mathbb{U}_B^* \Omega \big\rangle \;\Big|\; B \in \mathrm{Bog}_J[\mathfrak{h}] \right\} \;\geq\; \mathrm{Tr}\Big[\sqrt{k^2 + 2\Theta_{\phi,\alpha}} \;-\; |k| \Big]. \tag{4.16}$$

We finally define

$$B_* \;:= \begin{pmatrix} \sqrt{1+v_*^2} & -v_* \\ -v_* & \sqrt{1+v_*^2} \end{pmatrix} \;=\; \frac{1}{2} \begin{pmatrix} y_*^{1/2} + y_*^{-1/2} & -y_*^{1/2} + y_*^{-1/2} \\ -y_*^{1/2} + y_*^{-1/2} & y_*^{1/2} + y_*^{-1/2} \end{pmatrix}, \tag{4.17}$$

$$v_* \;:= \frac{1}{2}\big(y_*^{1/2} - y_*^{-1/2} \big) \;\geq\; 0, \qquad y_* \;:=\; |k|^{-1/2} \sqrt{k^2 + 2\Theta_{\phi,\alpha}} \, |k|^{-1/2} \;\geq\; \mathbf{1}, \tag{4.18}$$

in accordance with (4.46) and (4.52). Then, by (4.62), $\Theta_{\phi,\alpha} \in \mathcal{L}^2[\mathfrak{h}]$ implies that $y_* - 1 \in \mathcal{L}^2[\mathfrak{h}]$ which is equivalent to $v_* \in \mathcal{L}^2[\mathfrak{h}]$, thanks to (4.59), and thus $1 - y_*^{-1} = y_* - 1 - 4v_*^2 \in \mathcal{L}^2[\mathfrak{h}]$. Moreover, as $|k|$ and $\Theta_{\phi,\alpha}$ are J-invariant, so are y_* and hence also v_* and $\sqrt{1+v_*^2}$. It follows that $B_* \in \mathrm{Bog}_J[\mathfrak{h}]$ is a homogeneous Bogoliubov transformation. Finally,

$$
\begin{aligned}
&B_* \, T_{\phi,\alpha} \, B_*^* \\
&\quad = B_* \begin{pmatrix} 2|k| & 0 \\ 0 & 0 \end{pmatrix} B_*^* \; + \; B_* \begin{pmatrix} |k|^{-1/2}\Theta_{\phi,\alpha}|k|^{-1/2} & |k|^{-1/2}\Theta_{\phi,\alpha}|k|^{-1/2} \\ |k|^{-1/2}\Theta_{\phi,\alpha}|k|^{-1/2} & |k|^{-1/2}\Theta_{\phi,\alpha}|k|^{-1/2} \end{pmatrix} B_*^* \\
&\quad = \frac{1}{2} \begin{pmatrix} (y_*^{1/2} + y_*^{-1/2}) \, |k| \, (y_*^{1/2} + y_*^{-1/2}) & -(y_*^{1/2} + y_*^{-1/2}) \, |k| \, (y_*^{1/2} - y_*^{-1/2}) \\ +2y_*^{-1/2}|k|^{-1/2}\Theta_{\phi,\alpha}|k|^{-1/2}y_*^{-1/2} & +2y_*^{-1/2}|k|^{-1/2}\Theta_{\phi,\alpha}|k|^{-1/2}y_*^{-1/2} \\ -(y_*^{1/2} - y_*^{-1/2}) \, |k| \, (y_*^{1/2} + y_*^{-1/2}) & (y_*^{1/2} - y_*^{-1/2}) \, |k| \, (y_*^{1/2} - y_*^{-1/2}) \\ +2y_*^{-1/2}|k|^{-1/2}\Theta_{\phi,\alpha}|k|^{-1/2}y_*^{-1/2} & +2y_*^{-1/2}|k|^{-1/2}\Theta_{\phi,\alpha}|k|^{-1/2}y_*^{-1/2} \end{pmatrix},
\end{aligned}
\tag{4.19}
$$

so

$$
\begin{aligned}
&\big\langle \Omega \big| \mathbb{U}_{B_*} \, \mathrm{d}\Gamma_J[T_{\phi,\alpha}, 0] \, \mathbb{U}_{B_*}^* \Omega \big\rangle \;=\; \big\langle \Omega \big| \, \mathrm{d}\Gamma_J[B_* T_{\phi,\alpha} B_*^*, 0] \, \Omega \big\rangle \\
&\quad = \frac{1}{2} \, \mathrm{Tr}\Big[(y_*^{1/2} - y_*^{-1/2}) \, |k| \, (y_*^{1/2} - y_*^{-1/2}) + 2y_*^{-1/2}|k|^{-1/2}\Theta_{\phi,\alpha}|k|^{-1/2}y_*^{-1/2} \Big] \\
&\quad = \frac{1}{2} \, \mathrm{Tr}\Big[|k|^{1/2}(y_* + y_*^{-1} - 2)|k|^{1/2} + 2\Theta_{\phi,\alpha}^{1/2}|k|^{-1/2}y_*^{-1}|k|^{-1/2}\Theta_{\phi,\alpha}^{1/2} \Big] \\
&\quad = \frac{1}{2} \, \mathrm{Tr}\Big[\sqrt{k^2 + 2\Theta_{\phi,\alpha}} - |k| + |k|^{1/2}(y_*^{-1} - 1)|k|^{1/2} + 2\Theta_{\phi,\alpha}|k|^{-1/2}y_*^{-1}|k|^{-1/2} \Big] \\
&\quad = \frac{1}{2} \, \mathrm{Tr}\Big[\sqrt{k^2 + 2\Theta_{\phi,\alpha}} - |k| - \big(k^2 + 2\Theta_{\phi,\alpha}\big)|k|^{-1/2}y_*^{-1}|k|^{-1/2} - |k| \Big] \\
&\quad = \mathrm{Tr}\Big[\sqrt{k^2 + 2\Theta_{\phi,\alpha}} - |k| \Big].
\end{aligned}
\tag{4.20}
$$

□

The proof of Theorem 4.5 given rests on Lemmata 4.7–4.10 which we state and prove below. The first step in our derivation is an observation made in [4] which may be viewed as a generalization of Lieb's variational principle [32].

Lemma 4.7. *Let* $\mathsf{J} : \mathsf{h} \to \mathsf{h}$ *be an antiunitary involution and* $T = T^* \in \mathcal{B}[\mathsf{h} \oplus \mathsf{h}]$ *be nonnegative,* $T \geq 0$*, then*

$$
\inf \big\{ \sigma\big(\mathrm{d}\Gamma_{\mathsf{J}}[T, 0]\big) \big\} \;=\; \inf \Big\{ \big\langle \Omega \big| \mathbb{U}_B \, \mathrm{d}\Gamma_{\mathsf{J}}[T, 0] \, \mathbb{U}_B^* \Omega \big\rangle \; \Big| \; B \in \mathrm{Bog}_{\mathsf{J}}[\mathsf{h}] \Big\}, \tag{4.21}
$$

where

$$
\mathrm{Bog}_{\mathsf{J}}[\mathsf{h}] \;:=\; \left\{ B \;=\; \begin{pmatrix} U & \mathsf{J}V\mathsf{J} \\ V & \mathsf{J}U\mathsf{J} \end{pmatrix} \;\middle|\; B^* \mathcal{S} B = \mathcal{S}, \;\; \mathrm{Tr}(V^* V) < \infty \right\} \tag{4.22}
$$

denotes the set of generators of homogeneous Bogoliubov transformations.

Proof. Suppose that $\mathbb{H} \geq 0$ is a nonnegative Hamiltonian on $\mathcal{F}_{\mathrm{ph}}$ and define its *Bogoliubov–Hartree–Fock energy* by

$$
E_{BHF}(\mathbb{H}) \;:=\; \inf \Big\{ \mathrm{Tr}\{\rho^{1/2} \, \mathbb{H} \, \rho^{1/2}\} \; \Big| \; \rho \in \mathfrak{DM}, \;\; \rho \text{ is quasifree} \Big\}, \tag{4.23}
$$

where $\mathfrak{DM} := \{\rho \in \mathcal{B}[\mathfrak{F}_{\rm ph}] \mid 0 \le \rho \le \mathrm{Tr}\{\rho\} = 1\}$ denotes the set of density matrices on $\mathfrak{F}_{\rm ph}$. In [4], it is shown that the Bogoliubov–Hartree–Fock energy is already obtained by taking the infimum over all *pure* quasifree states,

$$E_{BHF}(\mathbb{H}) \;=\; \inf\Big\{\mathrm{Tr}\{\rho^{1/2}\,\mathbb{H}\,\rho^{1/2}\} \;\Big|\; \rho \in \mathfrak{DM},\ \rho \text{ is quasifree and pure}\Big\}. \tag{4.24}$$

Since $\mathrm{d}\Gamma_J[T_{|\phi|}, 0]$ is quadratic in the field operators, its ground state energy agrees with its Bogoliubov–Hartree–Fock energy,

$$\inf\big\{\sigma\big(\mathrm{d}\Gamma_{\mathsf{J}}[T,0]\big)\big\} \;=\; E_{BHF}\big(\mathrm{d}\Gamma_{\mathsf{J}}[T,0]\big). \tag{4.25}$$

On the other hand, the pure quasifree density matrices $\rho_{\rm pure} \in \mathfrak{DM}$ are precisely the rank-one orthogonal projections $\rho_{\rm pure} = |\mathbb{U}_B^*\mathbb{W}_\eta^*\Omega\rangle\langle\mathbb{U}_B^*\mathbb{W}_\eta^*\Omega|$ onto Bogoliubov and Weyl transforms $\mathbb{U}_B^*\mathbb{W}_\eta^*\Omega$ of the vacuum vector Ω, using that, $\mathbb{U}_B^* = \mathbb{U}_{\mathcal{S}B^*\mathcal{S}}$ is a homogeneous Bogoliubov transformation, for $B \in \mathrm{Bog}_{\mathsf{J}}[\mathsf{h}]$, and $\mathbb{W}_\eta^* = \mathbb{W}_{-\eta}$ is a Weyl transformation, for $\eta \in \mathsf{h}$. Thus, we obtain

$$\begin{aligned}
&\inf\big\{\sigma\big(\mathrm{d}\Gamma_{\mathsf{J}}[T,0]\big)\big\}\\
&\quad= \inf\Big\{\big\langle\Omega\big|\mathbb{W}_\eta\,\mathbb{U}_B\,\mathrm{d}\Gamma_{\mathsf{J}}[T,0]\,\mathbb{U}_B^*\,\mathbb{W}_\eta^*\Omega\big\rangle \;\Big|\; B \in \mathrm{Bog}_{\mathsf{J}}[\mathsf{h}],\ \eta \in \mathsf{h}\Big\}\\
&\quad= \inf\Big\{\big\langle\Omega\big|\mathrm{d}\Gamma_{\mathsf{J}}\big[BTB^*,\ -\tfrac{1}{2}q^*BTB^*q\eta\big]\Omega\big\rangle\\
&\qquad + \langle\eta|q^*BTB^*q\eta\rangle \;\Big|\; B \in \mathrm{Bog}_{\mathsf{J}}[\mathsf{h}],\ \eta \in \mathsf{h}\Big\},
\end{aligned} \tag{4.26}$$

using (3.16) and (3.18). Since

$$\big\langle\Omega\big|\mathrm{d}\Gamma_{\mathsf{J}}\big[BTB^*, -\tfrac{1}{2}q^*BTB^*q\eta\big]\Omega\big\rangle \;=\; \big\langle\Omega\big|\mathrm{d}\Gamma_{\mathsf{J}}\big[BTB^*, 0\big]\Omega\big\rangle \tag{4.27}$$

and

$$\langle\eta|q^*BTB^*q\eta\rangle \;\ge\; 0, \tag{4.28}$$

it follows that the infimum on the right side of (4.26) is attained for $\eta = 0$. ☐

Lemma 4.8. *Let* $\mathsf{j} : \mathsf{h} \to \mathsf{h}$ *be an antiunitary involution. Let* $a \in \mathcal{B}[\mathsf{h}]$ *be a bounded,* $b \in \mathcal{L}^2[\mathsf{h}]$ *a Hilbert–Schmidt, and* $d \in \mathcal{L}^1(\mathsf{h})$ *a trace-class operator such that all three are nonnegative and commute with* j*, i.e.,* $a = \mathsf{j}a\mathsf{j} \ge 0$*,* $b = \mathsf{j}b\mathsf{j} \ge 0$*,* $d = \mathsf{j}d\mathsf{j} \ge 0$*. Furthermore, let* $B \in \mathrm{Bog}_{\mathsf{j}}[\mathsf{h}]$*, with* $\mathrm{Bog}_{\mathsf{j}}[\mathsf{h}]$ *as defined in* (4.22)*. Then,*

$$T \;=\; \begin{pmatrix} a+b & b \\ b & d+b \end{pmatrix} \;\ge\; 0, \tag{4.29}$$

and

$$\begin{aligned}
&\big\langle\Omega\big|\mathbb{U}_B\,\mathrm{d}\Gamma_{\mathsf{j}}[T,0]\,\mathbb{U}_B^*\Omega\big\rangle\\
&\qquad\ge\; \inf\Big\{\mathrm{Tr}\Big[a\,v^2 + b\big(v - \sqrt{1+v^2}\big)^2 + d\,(1+v^2)\Big] \;\Big|\; v \ge 0,\ \mathrm{Tr}(v^2) < \infty\Big\}.
\end{aligned} \tag{4.30}$$

Proof. First, we note that

$$\text{if} \quad \widetilde{T} \;=\; \begin{pmatrix} \tilde{a} & \tilde{b}^* \\ \tilde{b} & \tilde{d} \end{pmatrix}, \quad \text{then} \quad \big\langle \Omega \big| \mathrm{d}\Gamma_{\mathsf{j}}[\widetilde{T}, 0] \Omega \big\rangle \;=\; \mathrm{Tr}(\tilde{d}). \tag{4.31}$$

Next, if $B \in Bog_{\mathsf{j}}[\mathsf{h}]$ is of the form

$$B \;=\; \begin{pmatrix} u & \mathsf{j}v\mathsf{j} \\ v & \mathsf{j}u\mathsf{j} \end{pmatrix}, \tag{4.32}$$

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

$$B\,T\,B^* \;=\; \begin{pmatrix} \begin{matrix} u(a+b)u^* + ub\mathsf{j}v^*\mathsf{j} \\ +\mathsf{j}v\mathsf{j}bu + \mathsf{j}v(d+b)v^*\mathsf{j} \end{matrix} & \begin{matrix} u(a+b)v^* + ub\mathsf{j}u^*\mathsf{j} \\ +\mathsf{j}v\mathsf{j}bv^* + \mathsf{j}v(d+b)u^*\mathsf{j} \end{matrix} \\ & \\ \begin{matrix} v(a+b)u^* + \mathsf{j}u\mathsf{j}bu^* \\ +vb\mathsf{j}v^*\mathsf{j} + \mathsf{j}u(d+b)v^*\mathsf{j} \end{matrix} & \begin{matrix} v(a+b)v^* + vb\mathsf{j}u^*\mathsf{j} \\ +\mathsf{j}u\mathsf{j}bv^* + \mathsf{j}u(d+b)u^*\mathsf{j} \end{matrix} \end{pmatrix}. \tag{4.33}$$

Using (4.31), this yields

$$\begin{aligned} \big\langle \Omega \big| \mathrm{d}\Gamma_{\mathsf{j}}[B^*TB, 0]\Omega \big\rangle &= \mathrm{Tr}\big[v(a+b)v^* + v^*b\mathsf{j}u\mathsf{j} + \mathsf{j}u^*\mathsf{j}bv + u(d+b)u^*\big] \\ &= \mathrm{Tr}\big[av^*v + du^*u\big] + 2\mathrm{Re}\mathrm{Tr}\big[bv^*\mathsf{j}u\mathsf{j}\big]. \end{aligned} \tag{4.34}$$

From the Cauchy–Schwarz inequality for traces, we obtain

$$\big|\mathrm{Tr}\big[bv^*\mathsf{j}u\mathsf{j}\big]\big|^2 \le \mathrm{Tr}\big[b\,v^*\,x^{-1}\,v\big]\,\mathrm{Tr}\big[b\,\mathsf{j}u^*\mathsf{j}\,x\,\mathsf{j}u\mathsf{j}\big] = \mathrm{Tr}\big[b\,v^*\,x^{-1}\,v\big]\,\mathrm{Tr}\big[b\,u^*\mathsf{j}\,x\,\mathsf{j}u\big], \tag{4.35}$$

for any bounded and invertible positive operator $x \ge \mu \cdot \mathbf{1} > 0$.

Next, we remark that due to (3.15), we have

$$u^*\,u - v^*\,v \;=\; \mathsf{j}\,u\,u^*\,\mathsf{j} - v\,v^* \;=\; \mathbf{1}, \quad v^*\,\mathsf{j}\,u \;=\; u^*\,\mathsf{j}\,v, \quad \mathsf{j}\,u\,v^* \;=\; v\,u^*\,\mathsf{j}. \tag{4.36}$$

For any $r > 0$, this implies that

$$(r + vv^*)\,\mathsf{j}u \;= r\mathsf{j}u + vu^*\mathsf{j}v \;=\; \mathsf{j}u\,(r + v^*v), \quad (r + vv^*)\,v \;= v\,(r + v^*v), \tag{4.37}$$

which, in turn, gives

$$(r + vv^*)^{-1}\,\mathsf{j}u \;=\; \mathsf{j}u\,(r + v^*v)^{-1}, \quad (r + vv^*)^{-1}\,v \;= v\,(r + v^*v)^{-1}. \tag{4.38}$$

Writing the square root as an integral over resolvents according to $A^{-1/2} = \frac{1}{\pi}\int_0^\infty (s + A)^{-1}\,\frac{ds}{s^{1/2}}$, (4.38) yields

$$(r + vv^*)^{\pm 1/2}\,\mathsf{j}u \;=\; \mathsf{j}u\,(r + v^*v)^{\pm 1/2}, \quad (r + vv^*)^{\pm 1/2}\,v \;= v\,(r + v^*v)^{\pm 1/2}, \tag{4.39}$$

for all $r > 0$. For small $0 < \varepsilon < 1$, we define

$$x_\varepsilon := (1 + vv^*)^{-1/2}\,(\varepsilon + vv^*)^{1/2} \tag{4.40}$$

and observe that due to (4.39) and (4.36), we have

$$\begin{aligned} u^*\mathsf{j}\,x_\varepsilon\,\mathsf{j}u = u^*\mathsf{j}\,(1 + vv^*)^{-1/2}\,(\varepsilon + vv^*)^{1/2}\,\mathsf{j}u \;&=\; u^*u\,(1 + v^*v)^{-1/2}\,(\varepsilon + v^*v)^{1/2} \\ = (1 + v^*v)^{1/2}\,(\varepsilon + v^*v)^{1/2} & \end{aligned} \tag{4.41}$$

and further

$$v^* x_\varepsilon^{-1} v = v^* (\varepsilon + vv^*)^{-1/2} (1 + vv^*)^{1/2} v = v^* v (\varepsilon + v^* v)^{-1/2} (1 + v^* v)^{1/2}$$
$$\leq (v^* v)^{1/2} (1 + v^* v)^{1/2}. \tag{4.42}$$

Inserting (4.41) and (4.42) into (4.35) and taking the limit $\varepsilon \to 0$, we obtain

$$\big|\mathrm{Tr}\big[b\, v^* \, \mathrm{j} u \mathrm{j}\big]\big| \ \leq \ \mathrm{Tr}\big[b_\pm\, (v^* v)^{1/2} (1 + v^* v)^{1/2}\big]. \tag{4.43}$$

Using this estimate and (4.34), we arrive at

$$\big\langle \Omega \big| \mathrm{d}\Gamma_{\mathrm{j}}[B^* T B, 0] \Omega \big\rangle \ \geq \ \mathrm{Tr}\Big[a\, |v|^2 + b\big(|v| - \sqrt{1 + |v|^2}\big)^2 + d(1 + |v|^2)\Big], \tag{4.44}$$

from which the asserted estimate (4.30) is immediate. □

Lemma 4.9. *Let* $\mathrm{j} : \mathsf{h} \to \mathsf{h}$ *be an antiunitary involution. Let* $a \in \mathcal{B}[\mathsf{h}]$ *be a bounded,* $b \in \mathcal{L}^2[\mathsf{h}]$ *a Hilbert–Schmidt, and* $d \in \mathcal{L}^1(\mathsf{h})$ *a trace-class operator such that* $a = \mathrm{j} a \mathrm{j} \geq \sigma \cdot \mathbf{1} > 0$*, for some* $\sigma > 0$*, and* $b = \mathrm{j} b \mathrm{j} \geq 0$*,* $d = \mathrm{j} d \mathrm{j} \geq 0$*, i.e., all three are nonnegative and commute with* j*. Then,*

$$\inf \Big\{ \mathrm{Tr}\Big[a\, v^2 + b\big(v - \sqrt{1 + v^2}\big)^2 + d\,(1 + v^2)\Big] \ \Big| \ v \geq 0,\ \mathrm{Tr}(v^2) < \infty \Big\}.$$
$$= \ \frac{1}{2}\, \mathrm{Tr}\Big[\Big(\sqrt{a + d}\, (a + d + 4b)\, \sqrt{a + d}\Big)^{1/2} - a + d\Big]. \tag{4.45}$$

Proof. It is convenient to parametrize v as

$$v \ = \ \frac{1}{2}\big(y^{1/2} - y^{-1/2}\big), \tag{4.46}$$

where $y \geq 1$ is a positive operator defined by (4.46) through functional calculus. Note in passing that y is uniquely determined by v up to $\ker(y - 1)$ and that $y - 1 \in \mathcal{L}^2[\mathsf{h}]$, due to Lemma 4.10 (i). Then,

$$v^2 \ = \ \frac{y}{4} + \frac{y^{-1}}{4} - \frac{1}{2} \quad \text{and} \quad 1 + v^2 \ = \ \frac{y}{4} + \frac{y^{-1}}{4} + \frac{1}{2} \ = \ \Big[\frac{1}{2}\big(y^{1/2} + y^{-1/2}\big)\Big]^2. \tag{4.47}$$

Hence, we have that

$$\sqrt{1 + v^2} \ = \ \frac{1}{2}\big(y^{1/2} + y^{-1/2}\big) \quad \text{and} \quad \big(v - \sqrt{1 + v^2}\big)^2 \ = \ y^{-1}. \tag{4.48}$$

Inserting the parameterization (4.46) into the trace in (4.45), we obtain

$$\mathrm{Tr}\Big[a\, v^2 + b\big(v - \sqrt{1 + v^2}\big)^2 + d\,(1 + v^2)\Big] \ = \ \frac{1}{4}\, \mathcal{G}(y), \tag{4.49}$$

with

$$\mathcal{G}(y) \ := \ \mathrm{Tr}\Big[m^2\, y \ + \ (m^2 + 4b)\, y^{-1} \ + \ 2(d - a)\Big], \tag{4.50}$$

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

$$y_* \ := \ m^{-1} \big(m\, (m^2 + 4b)\, m\big)^{1/2} m^{-1} \tag{4.51}$$

and observe that $y_* - 1 \in \mathcal{L}^2[\mathsf{h}]$, by Lemma 4.10 (ii), and that $y_* \, m^2 \, y_* = m^2 + 4b$ which is equivalent to

$$y_*^{-1} \, (m^2 + 4b) \, y_*^{-1} \;=\; m^2. \tag{4.52}$$

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

$$\mathcal{G}(y) - \mathcal{G}(y_*) \;:=\; \mathrm{Tr}\Big[m^2 \, (y - y_*) \;+\; (m^2 + 4b) \, \big(y^{-1} - y_*^{-1} \big) \Big], \tag{4.53}$$

and the second resolvent equation gives

$$y^{-1} - y_*^{-1} \;=\; -y_*^{-1} \, (y - y_*) \, y_*^{-1} \;+\; y_*^{-1} \, (y - y_*) \, y^{-1} \, (y - y_*) \, y_*^{-1}. \tag{4.54}$$

Thus, (4.52) derives

$$\begin{aligned} \mathcal{G}(y) - \mathcal{G}(y_*) &= \mathrm{Tr}\Big[\big(m^2 - y_*^{-1} \, (m^2 + 4b) \, y_*^{-1} \big) \, (y - y_*) \\ &\qquad + y^{-1/2} \, (y - y_*) \, y_*^{-1} \, (m^2 + 4b) \, y_*^{-1} \, (y - y_*) \, y^{-1/2} \Big] \\ &= \; \mathrm{Tr}\Big[y^{-1/2} \, (y - y_*) \, y_*^{-1} \, (m^2 + 4b) \, y_*^{-1} \, (y - y_*) \, y^{-1/2} \Big] \;\geq\; 0. \end{aligned} \tag{4.55}$$

Finally,

$$\begin{aligned} \mathcal{G}(y_*) &= \mathrm{Tr}\Big[m^2 \, y_* + (m^2 + 4b) \, y_*^{-1} + 2(d - a) \Big] \\ &= 2 \, \mathrm{Tr}\big[m \, y_* \, m + d - a \big] = 2 \, \mathrm{Tr}\Big[\big(m \, (m^2 + 4b) \, m \big)^{1/2} + d - a \Big] \\ &= 2 \, \mathrm{Tr}\Big[\big(\sqrt{a + d} \, (a + d + 4b) \, \sqrt{a + d} \big)^{1/2} - a + d \Big], \end{aligned} \tag{4.56}$$

arriving at (4.45). ◻

Lemma 4.10. *Let* h *be a Hilbert space and* $m, b, y \in \mathcal{B}[\mathsf{h}]$ *be positive bounded operators such that* $b \in \mathcal{L}^2[\mathsf{h}]$ *is Hilbert–Schmidt,* $y \geq 1$*, and* $m \geq \sigma^{1/2} \cdot \mathbf{1}$*, for some* $\sigma > 0$*. Then, the following assertions hold true.*

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

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

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

$$\mathbf{1} \;\leq\; y \;\leq\; \big(1 + 2\|v\|_{\mathcal{B}[\mathsf{h}]} \big)^2 \cdot \mathbf{1}. \tag{4.57}$$

Secondly note that

$$v^2 \;=\; \frac{y}{4} + \frac{y^{-1}}{4} - \frac{1}{2} \;=\; \frac{1}{4y} (y - 1)^2, \tag{4.58}$$

and taking (4.57) into account, we arrive at *(i)* because

$$\mathrm{Tr}\big[v^2\big] \;\le\; \mathrm{Tr}\big[(y-1)^2\big] \;\le\; 4\big(1+2\|v\|_{\mathcal{B}[\mathsf{h}]}\big)^2\,\mathrm{Tr}\big[v^2\big]. \tag{4.59}$$

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

$$A^{-1/2} \;=\; \frac{1}{\pi}\int_0^\infty (s+A)^{-1}\,\frac{ds}{s^{1/2}}, \tag{4.60}$$

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

$$\begin{aligned}
y-1 &= m^{-1}\Big[\big(m^4+4mbm\big)^{1/2} - m^2\Big]\,m^{-1} \\
&= \frac{1}{\pi}\int_0^\infty m^{-1}\left\{\frac{m^4+4mbm}{s+m^4+4mbm} - \frac{m^4}{s+m^4}\right\}m^{-1}\,\frac{ds}{s^{1/2}} \\
&= \frac{1}{\pi}\int_0^\infty m^{-1}\left\{\big(s+m^4\big)^{-1} - \big(s+m^4+4mbm\big)^{-1}\right\}m^{-1}\,s^{1/2}\,ds \\
&= \frac{4}{\pi}\int_0^\infty \left\{R_s\,b\,R_s - 4R_s\,bm\,\big(s+m^4+4mbm\big)^{-1}\,mb\,R_s\right\}s^{1/2}\,ds \\
&\le \frac{4}{\pi}\int_0^\infty \left\{R_s\,b\,R_s\right\}s^{1/2}\,ds.
\end{aligned} \tag{4.61}$$

Consequently,

$$\begin{aligned}
&\mathrm{Tr}\big[(y-1)^2\big] \\
&\quad\le \frac{16}{\pi^2}\int_0^\infty\int_0^\infty \mathrm{Tr}\big[\sqrt{R_s}\,\sqrt{R_t}\,b\,\sqrt{R_t}\,R_s\,\sqrt{R_t}\,b\,\sqrt{R_t}\,\sqrt{R_s}\big]\,\sqrt{s}\,\sqrt{t}\,ds\,dt \\
&\quad\le \frac{16}{\pi^2}\int_0^\infty\int_0^\infty \mathrm{Tr}\big[\sqrt{R_s}\,\sqrt{R_t}\,b^2\,\sqrt{R_t}\,\sqrt{R_s}\big]\,\frac{\sqrt{s}\,ds}{s+\sigma^2}\,\frac{\sqrt{t}\,dt}{t+\sigma^2} \\
&\quad\le \frac{16}{\pi^2}\left(\int_0^\infty \frac{\sqrt{s}\,ds}{(s+\sigma^2)^2}\right)^2\mathrm{Tr}\big[b^2\big] \;=\; \frac{16}{\pi^2\,\sigma^2}\left(\int_0^\infty \frac{\sqrt{r}\,ds}{(r+1)^4}\right)^2\mathrm{Tr}\big[b^2\big] \;<\; \infty.
\end{aligned} \tag{4.62}$$

□

5. Localization Estimates

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

$$\widehat{\mathcal{E}}_{\alpha,\Lambda}(\phi) \;=\; \frac{1}{2}\big\|\vec{\nabla}\phi\big\|_2^2 + \frac{1}{2}X(2\Theta_{\phi,\alpha}), \tag{5.1}$$

where $\phi = |\phi| \in \mathcal{H}_{\mathrm{el}}$ is normalized and $\phi \in H^1(\mathbb{R}^3)$, $\Theta_{\phi,\alpha}$ is defined in (3.22)–(3.23), and

$$X(A) \;:=\; \mathrm{Tr}\Big(\sqrt{|k|^2+A} \;-\; |k|\Big), \tag{5.2}$$

for positive operators $A \geq 0$. Recall that, according to Theorem 4.4 and Corollary 4.6, the Lieb–Loss energy defined in Eqs. (1.3)–(1.4) is given by

$$E_{\mathrm{LL}}(\alpha, \Lambda) \;=\; \inf\big\{\widehat{\mathcal{E}}_{\alpha,\Lambda}(\phi) \;\big|\; \phi = |\phi| \in H^1(\mathbb{R}^3),\; \|\phi\|_2 = 1\big\}. \tag{5.3}$$

Ultimately, we compare $\widehat{\mathcal{E}}_{\alpha,\Lambda}$ and its infimum $E_{\mathrm{LL}}(\alpha, \Lambda)$ to $\mathcal{F}_{\beta(\alpha,\Lambda)}$ and its infimum $F_{\beta(\alpha,\Lambda)}$, respectively, where

$$\mathcal{F}_\beta(\phi) := \frac{1}{2}\big\|\vec{\nabla}\phi\big\|_2^2 \;+\; \beta\,\|\phi\|_1, \tag{5.4}$$

$$F_\beta := \inf\big\{\mathcal{F}_\beta(\phi) \;\big|\; \phi = |\phi| \in H^1(\mathbb{R}^3) \cap L^1(\mathbb{R}^3),\; \|\phi\|_2 = 1\big\}, \tag{5.5}$$

$$\beta(\alpha, \Lambda) := \sqrt{\frac{4\alpha}{9\pi}}\;\Lambda^3. \tag{5.6}$$

In the present section, we demonstrate that the minimization in (5.3) 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 5.1 that

$$E_{\mathrm{LL}}^{(L)}(\alpha, \Lambda) \;:=\; \inf\Big\{\widehat{\mathcal{E}}_{\alpha,\Lambda}(\phi) \;\Big|\; \phi = |\phi| \in Y_L,\; \|\phi\|_2 = 1\Big\}, \tag{5.7}$$

approximates $E_{\mathrm{LL}}(\alpha, \Lambda)$, 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,

$$Y_L \;:=\; H^1\big(B(0, L)\big) \;\subseteq\; H^1(\mathbb{R}^3) \cap L^1(\mathbb{R}^3) \;\subseteq\; H^1(\mathbb{R}^3) \;=:\; Y, \tag{5.8}$$

and we correspondingly approximate F_β by

$$F_\beta^{(L)} \;:=\; \inf\big\{\mathcal{F}_\beta(\phi) \;\big|\phi = |\phi| \in Y_L,\; \|\phi\|_2 = 1\big\}. \tag{5.9}$$

Theorem 5.1. *There exists a universal constant $C < \infty$ such that for all $\alpha, \beta, L > 0$, $\sigma \geq 0$, and $\Lambda \geq 1$,*

$$E_{\mathrm{LL}}^{(L)}(\alpha, \Lambda) - \frac{C}{L^2} \leq E_{\mathrm{LL}}(\alpha, \Lambda) \;\leq\; E_{\mathrm{LL}}^{(L)}(\alpha, \Lambda), \tag{5.10}$$

$$F_\beta^{(L)} - \frac{C}{L^2} \leq F_\beta \;\leq\; F_\beta^{(L)}, \tag{5.11}$$

with $E_{\mathrm{LL}}(\alpha, \Lambda)$, $F(\alpha, \Lambda)$, $E_{\mathrm{LL}}^{(L)}(\alpha, \Lambda)$, and $F^{(L)}(\alpha, \Lambda)$ as in (5.3), (5.5), (5.7), and (5.9), respectively.

Proof. The inequalities $E_{\mathrm{LL}}(\alpha, \Lambda) \leq E_{\mathrm{LL}}^{(L)}(\alpha, \Lambda)$ and $F_\beta \leq F_\beta^{(L)}$ 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 (5.10) on $E_{\mathrm{LL}}(\alpha, \Lambda)$, we pick a smooth and compactly supported function $\eta \in C_0^\infty(\mathbb{R}^3; \mathbb{R}_0^+)$, chosen such that $\mathrm{supp}(\eta) \subseteq B(0, 1)$ and $\|\eta\|_2 = 1$. Then, we define

$$\eta_{L,z}(x) \;:=\; L^{-\frac{3}{2}}\,\eta\big[L^{-1}(x - z)\big], \tag{5.12}$$

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

$$\rho_L(z) \;:=\; \|\eta_{L,z}\, \phi\|_2^2, \quad \phi_{L,z}(x) \;:=\; \begin{cases} \frac{\eta_{L,z}(x)\,\phi(x)}{\sqrt{\rho_L(z)}} & \text{if } \rho_L(z) > 0, \\ 0 & \text{if } \rho_L(z) = 0, \end{cases} \tag{5.13}$$

and observe that ρ_L is a probability density on $\mathbb{R}^3$. A variant of the IMS localization formula [13] now yields

$$\begin{aligned} \|\nabla\phi\|_2^2 \;&=\int \big\|\nabla(\eta_{L,z}\phi)\big\|_2^2\, d^3z \;-\; \int |\nabla\eta_{L,z}|^2\, d^3z \\ &=\int \|\nabla\phi_{L,z}\|_2^2\; \rho_L(z)\, d^3z \;-\; \frac{\|\nabla\eta\|_2^2}{L^2}. \end{aligned} \tag{5.14}$$

Note that

$$\Phi_{\phi,\alpha}^*\, \Phi_{\phi,\alpha} \;=\int \big\{\Phi_{\phi_{L,z},\alpha}^*\, \Phi_{\phi_{L,z},\alpha}\big\}\; \rho_L(z)\, d^3z, \tag{5.15}$$

and since $A \mapsto X(A)$ is concave according to Lemma 5.3 (ii), we obtain

$$X\big(\Phi_{\phi,\alpha}^*\, \Phi_{\phi,\alpha}\big) \;\geq\; \int X\big(\Phi_{\phi_{L,z},\alpha}^*\, \Phi_{\phi_{L,z},\alpha}\big)\; \rho_L(z)\, d^3z. \tag{5.16}$$

Consequently,

$$\begin{aligned} \widehat{\mathcal{E}}_{\alpha,\Lambda}(\phi) \;&\geq \int \widehat{\mathcal{E}}_{\alpha,\Lambda}(\phi_{L,z})\; \rho_L(z)\, d^3z \;-\; \frac{\|\nabla\eta\|_2^2}{L^2} \\ &\geq \int E_{\mathrm{LL}}^{(L)}(\alpha,\Lambda)\; \rho_L(z)\, d^3z \;-\; \frac{\|\nabla\eta\|_2^2}{L^2} \;=\; E_{\mathrm{LL}}^{(L)}(\alpha,\Lambda) \;-\; \frac{\|\nabla\eta\|_2^2}{L^2}. \end{aligned} \tag{5.17}$$

Taking the infimum over $\phi \in H^1(\mathbb{R}^3)$ concludes the proof of the first inequality in (5.10). The proof of the first inequality in (5.11) is similar. □

For the proof of Theorem 5.1, we supply various properties of $X(A)$ in the following two lemmata. To formulate these it is convenient to denote

$$K_A \;:=\; \sqrt{k^2 + A}\,, \tag{5.18}$$

so that

$$X(A) \;=\; \mathrm{Tr}\big[K_A - K_0\big]. \tag{5.19}$$

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

$$\sigma\cdot\mathbf{1} \;\leq\; K_0 \;\leq\; K_A \;\leq\; \big(\Lambda + \|A\|_{\mathcal{B}[\mathfrak{h}]}\big)\cdot\mathbf{1}. \tag{5.20}$$

Lemma 5.2. *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,*

$$\mathrm{Tr}\big[(k^2 + A)^{\frac{1}{2}} - |k|\big] \;=\; \mathrm{Tr}\big[A^{\frac{1}{2}}\,\big\{(k^2 + A)^{\frac{1}{2}} + |k|\big\}^{-1} A^{\frac{1}{2}}\big]. \tag{5.21}$$

Proof. Using (5.18)–(5.20), we have that

$$\begin{aligned}\operatorname{Tr}\big[K_A - K_0\big] &= \frac{1}{2}\operatorname{Tr}\Big[\big\{K_A - K_0\big\}\big\{K_A + K_0\big\}\big\{K_A + K_0\big\}^{-1}\Big] \\ &\quad + \frac{1}{2}\operatorname{Tr}\Big[\big\{K_A - K_0\big\}\big\{K_A + K_0\big\}^{-1}\big\{K_A + K_0\big\}\Big] \\ &= \operatorname{Tr}\Big[\big\{K_A^2 - K_0^2\big\}\big\{K_A + K_0\big\}^{-1}\Big] = \operatorname{Tr}\Big[A^{\frac{1}{2}}\big\{K_A + K_0\big\}^{-1}A^{\frac{1}{2}}\Big],\end{aligned} \tag{5.22}$$

where the finiteness of the left side of (5.22) implies finiteness of all following lines. □

Lemma 5.3. *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,*

$$\text{(i)} \qquad X(A) \;\leq\; X(A+B) \;\leq\; X(A) + X(B), \tag{5.23}$$

$$\text{(ii)} \qquad A \;\mapsto\; X(A) \;\; \textit{is concave.} \tag{5.24}$$

Proof. Statement (i) follows from a simple argument using the operator monotonicity of $\mathbb{R}^+ \ni \lambda \mapsto \lambda^{-1/2}$ and Lemma 5.2, and (ii) is a consequence of the concavity of $\mathbb{R}^+ \ni \lambda \mapsto \sqrt{k^2+\lambda} - |k|$, for all $k \in \mathbb{R}^3$. □

6. Upper Bound on $X(2\Theta_{\phi,\alpha})$

We proceed to deriving an upper bound on $E_{\mathrm{LL}}^{(L)}(\alpha, \Lambda)$ defined in (5.7) in terms of $F^{(L)}(\alpha, \Lambda)$ given in (5.9). 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 $\chi_{\sigma,\Lambda} = \mathbf{1}[\sigma \leq |k| < \Lambda]$. 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 [10,35] that, for any $1 \leq p \leq 2$, there exists a universal constant $C_{\mathrm{BS}}(p) < \infty$ such that

$$\|f(x)\, g(i\nabla_x)\|_{\mathcal{L}^p[\mathfrak{h}_0]} \;\leq\; C_{\mathrm{BS}}(p)\, \|f\|_{2;p}\, \|g\|_{2;p}, \tag{6.1}$$

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

$$\|f\|_{2;p} \;:=\; \Big(\sum_{\beta\in\mathbb{Z}^3} \|f \cdot \mathbf{1}_{Q+\beta}\|_2^p\Big)^{1/p} \tag{6.2}$$

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

Theorem 6.1. *There exists a universal constant* $C < \infty$ *such that for all* $\alpha, L > 0$*, all* $0 \le \sigma \le 1 \le \Lambda < \infty$*, all* $0 < \varepsilon \le 1$ *and all* $\phi = |\phi| \in Y_L$*, the estimate*

$$\frac{1}{2} X(2\Theta_{\phi,\alpha}) \le \sqrt{\frac{4\alpha}{9\pi}} \left[\left(\Lambda^3 - \sigma^3\right) + 54\varepsilon\, \Lambda^3 + 5\sigma^{3/2}\, \Lambda^{3/2} \right] \|\phi\|_1 + \frac{C\,\alpha^{1/2} (L\,\Lambda + 1)^3}{\varepsilon^2\, L^{3/2}\, \Lambda} \|\nabla \phi\|_2 \tag{6.3}$$

holds true.

Proof. We first apply Lemma 5.2 and the operator monotonicity of $A \mapsto \sqrt{A}$ and $A \mapsto A^{-1}$ and observe that

$$X(A) \;=\; \mathrm{Tr}\Big[\sqrt{A} \left(\sqrt{k^2 + A} + |k| \right)^{-1} \sqrt{A} \Big] \;\le\; \mathrm{Tr}[\sqrt{A}]. \tag{6.4}$$

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 $\phi(x) := \mathcal{F}\phi\mathcal{F}^* \ge 0$ the corresponding nonnegative multiplication operator, indicating the change from momentum to position space by explicitly keeping the argument "x" for the spatial variable. Using (6.4), the decomposition $\mathbf{1} = \chi_{0,\sigma} + \chi_{\sigma,\Lambda} + \chi_{\Lambda,(1+\varepsilon)\Lambda} + \overline{\chi}_{(1+\varepsilon)\Lambda}$, where $\overline{\chi}_r := \mathbf{1} - \chi_r$, and the triangle inequality for the trace norm, we obtain

$$\begin{aligned} X(2\Theta_{\phi,\alpha}) &= X(2\Phi^*_{\phi,\alpha}\Phi_{\phi,\alpha}) \le \mathrm{Tr}\Big[\sqrt{2\Phi^*_{\phi,\alpha}\Phi_{\phi,\alpha}} \;\Big] = \sqrt{2}\,\|\Phi_{\phi,\alpha}\|_{\mathcal{L}^1[\mathfrak{h}]} \\ &= \frac{(2\alpha)^{1/2}}{(2\pi)^{3/2}} \big\|\phi(x)\, \chi_{\sigma,\Lambda}\, P_C\big\|_{\mathcal{L}^1[\mathfrak{h}]} \\ &\le \frac{(2\alpha)^{1/2}}{(2\pi)^{3/2}} \Big(\big\|\chi_{\sigma,\Lambda}\; \phi(x)\; \chi_{\sigma,\Lambda}\; P_C\big\|_{\mathcal{L}^1[\mathfrak{h}]} + 3X_1 + 3X_2 + 3X_3 \Big), \end{aligned} \tag{6.5}$$

where

$$\begin{aligned} \big\|P_C\; \chi_{\sigma,\Lambda}\; \phi(x)\; \chi_{\sigma,\Lambda}\; P_C\big\|_{\mathcal{L}^1[\mathfrak{h}]} &= \; \big\|\sqrt{\phi(x)}\; \chi_{\sigma,\Lambda}\; P_C\big\|^2_{\mathcal{L}^2[\mathfrak{h}]} \\ &= 2\Big(\mathrm{Vol}[B(0,\Lambda)] - \mathrm{Vol}[B(0,\sigma)]\Big) \left(\int \phi(x)\, d^3x \right) \\ &= \frac{8\pi}{3} \left(\Lambda^3 - \sigma^3\right) \|\phi\|_1 \end{aligned} \tag{6.6}$$

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 $\mathrm{Vol}[M] := \int \mathbf{1}_M(k)\, d^3$ the three-dimensional Lebesgue measure of a measurable set $M \subseteq \mathbb{R}^3$ in (6.6) and henceforth. Furthermore,

$$X_1 := \big\|\chi_{0,\sigma}\; \phi(x)\; \chi_{\sigma,\Lambda}\big\|_{\mathcal{L}^1[\mathfrak{h}_0]}, \tag{6.7}$$

$$X_2 := \big\|\chi_{\Lambda,(1+\varepsilon)\Lambda}\; \phi(x)\; \chi_{\sigma,\Lambda}\big\|_{\mathcal{L}^1[\mathfrak{h}_0]}, \tag{6.8}$$

$$X_3 := \big\|\overline{\chi}_{(1+\varepsilon)\Lambda}\; \phi(x)\; \chi_{\sigma,\Lambda}\big\|_{\mathcal{L}^1[\mathfrak{h}_0]} \tag{6.9}$$

are error terms we proceed to estimate next. Before we remark that the Hilbert space in (6.7)–(6.9) is the space $\mathfrak{h}_0 := L^2(\mathbb{R}^3)$ of complex-valued (scalar) square-integrable functions, as opposed to the one-photon Hilbert space $\mathfrak{h}$ of square-integrable divergence-free vector fields used before. The factors 3 on the right side of (6.5) account for the three components of the latter.

Using the trace inequality $\|AB\|_{\mathcal{L}^1[\mathfrak{h}_0]} \leq \|A\|_{\mathcal{L}^2[\mathfrak{h}_0]} \|B\|_{\mathcal{L}^2[\mathfrak{h}_0]}$ and $(1+\varepsilon)^3 - 1 \leq 3\varepsilon(1+\varepsilon)^2 \leq 12\varepsilon$, we obtain

$$X_1 \leq \big\|\chi_{0,\sigma} \sqrt{\phi(x)}\big\|_{\mathcal{L}^2[\mathfrak{h}_0]} \big\|\sqrt{\phi(x)}\, \chi_{0,\Lambda}\big\|_{\mathcal{L}^2[\mathfrak{h}_0]} \leq \frac{12\pi}{3} \Lambda^{3/2} \sigma^{3/2} \|\phi\|_1, \quad (6.10)$$

$$X_2 \leq \big\|\chi_{\Lambda,(1+\varepsilon)\Lambda} \sqrt{\phi(x)}\big\|_{\mathcal{L}^2[\mathfrak{h}_0]} \big\|\sqrt{\phi(x)}\, \chi_{0,\Lambda}\big\|_{\mathcal{L}^2[\mathfrak{h}_0]} \leq \frac{144\pi}{3} \varepsilon \Lambda^3 \|\phi\|_1, \quad (6.11)$$

similarly to (6.6).

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 $\mathbb{R}_0^-$, $\tilde{g}' \leq 0$, and $\tilde{g} \equiv 0$ on $[1,\infty)$. We then define a smooth function of compact support by

$$g_\varepsilon(\lambda) := \tilde{g}\big(\varepsilon^{-1}(\lambda - 1)\big)\, \tilde{g}\big(\varepsilon^{-1}(-\lambda - 1)\big). \quad (6.12)$$

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

$$\operatorname{supp}(g_\varepsilon) \subseteq: (-2,2), \qquad \|g_\varepsilon\|_\infty = 1 \quad (6.13)$$

$$\operatorname{supp}\big(g_\varepsilon^{(k)}\big) \subseteq (-1-\varepsilon, 1) \cup (1, 1+\varepsilon), \quad \big\|g_\varepsilon^{(k)}\big\|_\infty \leq C_k\, \varepsilon^{-k}, \quad (6.14)$$

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

$$g_\varepsilon(A) = \sum_{k=0}^{n-1} \int_{-\infty}^{\infty} \frac{g_\varepsilon^{(k)}(\lambda)\, d\lambda}{\pi\, k!} \operatorname{Im}\big\{i^k (A - \lambda - i)^{-1}\big\} + \int_0^1 \mu^{n-1}\, d\mu \int_{-\infty}^{\infty} \frac{g_\varepsilon^{(n)}(\lambda)\, d\lambda}{\pi\,(n-1)!} \operatorname{Im}\big\{i^n (A - \lambda - i\mu)^{-1}\big\}. \quad (6.15)$$

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

$$\begin{aligned} g_\varepsilon(A) &= \int_{-\infty}^{\infty} \big[g_\varepsilon(\lambda) - \tfrac{1}{2} g_\varepsilon''(\lambda)\big] \frac{d\lambda}{\pi} \operatorname{Im}\big\{(A - \lambda - i)^{-1}\big\} \\ &\quad + \int_{-\infty}^{\infty} g_\varepsilon'(\lambda) \frac{d\lambda}{\pi} \operatorname{Re}\big\{(A - \lambda - i)^{-1}\big\} \\ &\quad - \int_0^1 \mu^2\, d\mu \int_{-\infty}^{\infty} g_\varepsilon'''(\lambda) \frac{d\lambda}{2\pi} \operatorname{Re}\big\{(A - \lambda - i\mu)^{-1}\big\}. \end{aligned} \quad (6.16)$$

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

$$\chi_{\sigma,\Lambda} = g_\varepsilon(A)\, \chi_{\sigma,\Lambda} = \chi_{\sigma,\Lambda}\, g_\varepsilon(A), \quad g_\varepsilon(A)\, \overline{\chi}_{(1+\varepsilon)\Lambda} = \overline{\chi}_{(1+\varepsilon)\Lambda}\, g_\varepsilon(A) = 0, \quad (6.17)$$

which implies that

$$\begin{aligned} X_3 &= \big\| \overline{\chi}_{(1+\varepsilon)\Lambda}\, \phi(x)\, \chi_{\sigma,\Lambda} \big\|_{\mathcal{L}^1[\mathfrak{h}_0]} = \big\| \overline{\chi}_{(1+\varepsilon)\Lambda}\, \phi(x)\, g_\varepsilon(A)\, \chi_{\sigma,\Lambda} \big\|_{\mathcal{L}^1[\mathfrak{h}_0]} \\ &= \big\| \overline{\chi}_{(1+\varepsilon)\Lambda} \big[g_\varepsilon(A),\, \phi(x) \big]\, \chi_{\sigma,\Lambda} \big\|_{\mathcal{L}^1[\mathfrak{h}_0]} \\ &\leq \int_{-\infty}^{\infty} \frac{d\lambda}{\pi} \big(|g_\varepsilon(\lambda)| + |g_\varepsilon'(\lambda)| + |g_\varepsilon''(\lambda)| \big) \Big\| \big[R(\lambda+i),\, \phi(x) \big]\, \chi_{\sigma,\Lambda} \Big\|_{\mathcal{L}^1[\mathfrak{h}_0]} \\ &\quad + \int_0^1 \mu^2\, d\mu \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi}\, |g_\varepsilon'''(\lambda)|\, \Big\| \big[R(\lambda+i\mu),\, \phi(x) \big]\, \chi_{\sigma,\Lambda} \Big\|_{\mathcal{L}^1[\mathfrak{h}_0]}, \end{aligned} \tag{6.18}$$

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

$$\begin{aligned} \big[R(z),\, \phi(x) \big] &= \Lambda^{-2}\, R(z)\, [\Delta_x, \phi(x)]\, R(z) \\ &= \Lambda^{-2}\, R(z) \big(\nabla_x \cdot \nabla\phi(x) + \nabla\phi(x) \cdot \nabla_x \big)\, R(z), \end{aligned} \tag{6.19}$$

and hence

$$\begin{aligned} &\Big\| \big[R(\lambda+i\mu),\, \phi(x) \big]\, \chi_{\sigma,\Lambda} \Big\|_{\mathcal{L}^1[\mathfrak{h}_0]} \\ &\quad \leq \frac{2}{\Lambda^2}\, \|\nabla_x\, R(\lambda+i\mu)\|_{\mathcal{B}[\mathfrak{h}_0]}\, \|R(\lambda+i\mu)\|_{\mathcal{B}[\mathfrak{h}_0]}\, \|\nabla\phi(x)\, \chi_{\sigma,\Lambda}\|_{\mathcal{L}^1[\mathfrak{h}_0]} \\ &\quad \leq \frac{4}{\mu^2\, \Lambda}\, \|\nabla\phi(x)\, \chi_{\sigma,\Lambda}\|_{\mathcal{L}^1[\mathfrak{h}_0]}, \end{aligned} \tag{6.20}$$

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

$$\|R(\lambda+i\mu)\|_{\mathcal{B}[\mathfrak{h}_0]} = \sup_{r>0} \Big\{ \big| (r/\Lambda)^2 - \lambda - i\mu \big|^{-1} \Big\} \;=\; \frac{1}{\mu}, \tag{6.21}$$

$$\|\nabla_x\, R(\lambda+i\mu)\|_{\mathcal{B}[\mathfrak{h}_0]} = \Lambda \sup_{r>0} \Big\{ (r/\Lambda) \big| (r/\Lambda)^2 - \lambda - i\mu \big|^{-1} \Big\} \;\leq\; \frac{2\Lambda}{\mu}. \tag{6.22}$$

Inserting (6.20) into (6.18) and additionally taking (6.13)–(6.14), as well as $\varepsilon \in (0, 1)$ into account, we arrive at

$$X_3 \;\leq\; \frac{C}{\varepsilon^2\, \Lambda}\, \|\nabla\phi(x)\, \chi_{\sigma,\Lambda}\|_{\mathcal{L}^1[\mathfrak{h}_0]}, \tag{6.23}$$

for some universal constant $C < \infty$. To estimate the trace norm on the right side of (6.23), 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 (6.1) with $p = 1$. These steps lead us to

$$\begin{aligned} \|\nabla\phi(x)\, \chi_{\sigma,\Lambda}(k)\|_{\mathcal{L}^1[\mathfrak{h}_0]} &= \|\nabla\phi(Lx)\, \chi_{\sigma,\Lambda}(k/L)\|_{\mathcal{L}^1[\mathfrak{h}_0]} \\ &= \|\nabla\phi(Lx)\, \chi_{L\sigma,L\Lambda}(k)\|_{\mathcal{L}^1[\mathfrak{h}_0]} \\ &\leq\; C_{\mathrm{BS}}(1)\, \|\nabla\phi\|_{2;1}\, \|\chi_{L\sigma,L\Lambda}\|_{2;1} \\ &= C_{\mathrm{BS}}(1)\, \|\nabla\phi(Lx)\|_2 \sum_{\gamma \in \mathbb{Z}^3} \sqrt{\mathrm{Vol}\big[B(0, L\Lambda) \cap (Q+\gamma) \big]}\,, \end{aligned} \tag{6.24}$$

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 $\sum_{\beta\in\mathbb{Z}^3} \|\nabla\phi(Lx)\, \mathbf{1}_{Q+\beta}\|_2$ only the term corresponding to $\beta = 0$ contributes. Now, $\mathrm{Vol}[B(0,L\Lambda)\cap(Q+\gamma)] \leq \mathrm{Vol}[(Q+\gamma)] = 1$ and $\mathrm{Vol}[B(0,L\Lambda)\cap(Q+\gamma)] \leq \mathrm{Vol}[(Q+\gamma)] = 0$ unless $|\gamma| \leq L\Lambda + \sqrt{3}$ which implies that

$$\begin{aligned}\sum_{\gamma\in\mathbb{Z}^3} \sqrt{\mathrm{Vol}\big[B(0,L\Lambda)\cap(Q+\gamma)\big]} &\leq \sum_{\gamma\in\mathbb{Z}^3} \mathbf{1}_{B(0,L\Lambda+\sqrt{3})}(\gamma) \\ &\leq \mathrm{Vol}\big[B\big(0, L\Lambda + \tfrac{3}{2}\sqrt{3}\big)\big] \\ &\leq \frac{4\pi}{3}\,(L\,\Lambda+3)^3, \end{aligned} \tag{6.25}$$

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

$$\|\nabla\phi(x)\,\chi_{\sigma,\Lambda}(k)\|_{\mathcal{L}^1[\mathfrak{h}_0]} \;\leq\; \frac{4\pi\, C_{\mathrm{BS}}}{3\,L^{3/2}}\,(L\,\Lambda+3)^3\,\|\nabla\phi\|_2. \tag{6.26}$$

Inserting this into (6.23), we finally obtain

$$X_3 \;\leq\; \frac{C\,(L\,\Lambda+1)^3}{\varepsilon^2\,L^{3/2}\,\Lambda}\,\|\nabla\phi\|_2, \tag{6.27}$$

for a suitable constant $C < \infty$. Estimate (6.3) now follows from inserting (6.6), (6.10), (6.11), and (6.27) into (6.6). □

7. Lower Bound on $X(\Theta_{\phi,\alpha})$

In order to complement the upper bound on $X(\Theta_{\phi,\alpha})$ from Sect. 6 by a corresponding lower bound, we first derive a general inequality on $X(A)$ of the form $X(A) \geq \mathrm{Tr}\big[A^{1/2}\big] - 2\Lambda^{1-p}\,\mathrm{Tr}\big[A^{p/2}\big]$, where p is any exponent between $\frac{1}{2}$ and 1. By another application of the Birman–Solomyak inequality (6.1), we then estimate the emerging error term by a multiple of $\|\phi\|_1^p$.

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

Lemma 7.1. *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,*

$$X(A) \;\geq\; \mathrm{Tr}\big[A^{1/2}\big] \;-\; 2\Lambda^{1-p}\,\mathrm{Tr}\big[A^{p/2}\big]. \tag{7.1}$$

Proof. We recall from Lemma 5.2 that

$$\begin{aligned}X(A) &= \mathrm{Tr}\big[A^{1/2}\,\big\{(k^2+A)^{1/2}+|k|\big\}^{-1}\,A^{1/2}\big] \\ &= \mathrm{Tr}\big[A^{1/2}\,\big\{K_A+K_0\big\}^{-1}\,A^{1/2}\big], \end{aligned} \tag{7.2}$$

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

$$\begin{aligned} \frac{1}{K_A + K_0} &= \frac{1}{K_A} - \frac{1}{K_A} K_0 \frac{1}{K_A + K_0} \\ &= \frac{1}{K_A} - \frac{1}{K_A} K_0 \frac{1}{K_A} + \frac{1}{K_A} K_0 \frac{1}{K_A + K_0} K_0 \frac{1}{K_A} \\ &\geq \frac{1}{K_A} - \frac{1}{K_A} K_0 \frac{1}{K_A}, \end{aligned} \tag{7.3}$$

which implies

$$X(A) \geq \mathrm{Tr}\big[A^{1/2} K_A^{-1} A^{1/2}\big] - \mathrm{Tr}\big[A^{1/2} K_A^{-1} K_0 K_A^{-1} A^{1/2}\big]. \tag{7.4}$$

Since

$$K_0 = |k| \leq \Lambda^{1-p} |k|^p \leq \Lambda^{1-p} K_A^{p/2}, \tag{7.5}$$

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

$$\begin{aligned} \mathrm{Tr}\big[A^{1/2} K_A^{-1} K_0 K_A^{-1} A^{1/2}\big] &\leq \Lambda^{1-p} \mathrm{Tr}\big[A^{1/2} K_A^{-2+(p/2)} A^{1/2}\big] \\ &\leq \Lambda^{1-p} \mathrm{Tr}\big[A^{p/2}\big]. \end{aligned} \tag{7.6}$$

By operator monotonicity, we further have

$$\begin{aligned} A^{1/2} - A^{1/2} K_A^{-1} A^{1/2} &\leq A^{1/2} - \frac{A}{\sqrt{\Lambda^2 + A}} \\ &= \frac{A^{1/2}}{\sqrt{\Lambda^2 + A}} \Big(\sqrt{\Lambda^2 + A} - A^{1/2} \Big) = \frac{A^{1/2} \Lambda^2}{\sqrt{\Lambda^2 + A} \left(\sqrt{\Lambda^2 + A} + A^{1/2} \right)} \\ &\leq \frac{\Lambda^2 A^{1/2}}{\Lambda^2 + A} \leq \frac{\Lambda^2 A^{1/2}}{\Lambda^{1+p} A^{(1-p)/2}} = \Lambda^{1-p} A^{p/2}. \end{aligned} \tag{7.7}$$

Inserting (7.6) and (7.7) into (7.4), we arrive at the claim. □

As described above, we now use Lemma 7.1 to derive a lower bound on $X(2\Theta_{\phi,\alpha})$.

Theorem 7.2. *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*

$$\frac{1}{2} X(2\Theta_{\phi,\alpha}) \geq \sqrt{\frac{4\alpha}{9\pi}} \left(\Lambda^3 - \sigma^3\right) \|\phi\|_1 - \frac{C\, \alpha^{1/4} \Lambda^{1/2} (L\Lambda + 1)^3}{L^{3/2}} \sqrt{\|\phi\|_1} \tag{7.8}$$

holds true.

Proof. We first use that $A \mapsto X(A)$ is monotonically increasing. Since

$$\begin{aligned} \Theta_{\phi,\alpha} = \Phi_{\phi,\alpha}^* \Phi_{\phi,\alpha} &= \frac{\alpha}{(2\pi)^3} P_C\, \chi_{\sigma,\Lambda}\, \phi(x)^2\, \chi_{\sigma,\Lambda}\, P_C \\ &\geq \frac{\alpha}{(2\pi)^3} P_C\, \chi_{\sigma,\Lambda}\, \phi(x)\, \chi_{\sigma,\Lambda}\, P_C\, \chi_{\sigma,\Lambda}\, \phi(x)\, \chi_{\sigma,\Lambda}\, P_C \\ &= \big[\alpha^{1/2} (2\pi)^{-3/2} P_C\, \chi_{\sigma,\Lambda}\, \phi(x)\, \chi_{\sigma,\Lambda}\, P_C\big]^2, \end{aligned} \tag{7.9}$$

we obtain from Lemma 7.1 with $p = \frac{1}{2}$ that

$$\begin{aligned} \frac{1}{2} X(2\Theta_{\phi,\alpha}) &\geq \frac{1}{2} X\Big(\big[(2\alpha)^{1/2} \, (2\pi)^{-3/2} \, P_C \, \chi_{\sigma,\Lambda} \, \phi(x) \, \chi_{\sigma,\Lambda} \, P_C \big]^2 \Big) \\ &\geq \frac{(2\alpha)^{1/2}}{2(2\pi)^{3/2}} \operatorname{Tr}\big(P_C \, \chi_{\sigma,\Lambda} \, \phi(x) \, \chi_{\sigma,\Lambda} \, P_C \big) \\ &\quad - \frac{(2\alpha)^{1/4}\Lambda^{1/2}}{(2\pi)^{3/4}} \operatorname{Tr}\big([P_C \, \chi_{\sigma,\Lambda} \, \phi(x) \, \chi_{\sigma,\Lambda} \, P_C]^{1/2} \big). \\ &\geq \sqrt{\frac{4\alpha}{9\pi}} \, \big(\Lambda^3 - \sigma^3 \big) \, \|\phi\|_1 \; - \; \frac{(2\alpha)^{1/4}\Lambda^{1/2}}{(2\pi)^{3/4}} \, \big\| \sqrt{\phi(x)} \, \chi_{\sigma,\Lambda}(k) \big\|_{\mathcal{L}^1[\mathfrak{h}_0]}. \end{aligned} \tag{7.10}$$

To estimate the second term on the right side of (7.10), we proceed as in (6.23)–(6.26). After unitary rescaling $(x, k) \mapsto (Lx, k/L)$, we apply (6.1) again and get

$$\begin{aligned} \big\| \sqrt{\phi(x)} \, \chi_{\sigma,\Lambda}(k) \big\|_{\mathcal{L}^1[\mathfrak{h}_0]} &= \big\| \sqrt{\phi(Lx)} \, \chi_{L\sigma,L\Lambda}(k) \big\|_{\mathcal{L}^1[\mathfrak{h}_0]} \\ &\leq C_{\mathrm{BS}}(1) \, \big\| \sqrt{\phi(Lx)} \big\|_{2;1} \, \big\| \chi_{L\sigma,L\Lambda}(k) \big\|_{2;1} \\ &\leq \frac{4\pi \, C_{\mathrm{BS}}(1)}{3} \, (L\Lambda + 3)^3 \, \big\| \sqrt{\phi(Lx)} \big\|_{2;1}, \end{aligned} \tag{7.11}$$

where the last estimate results from (6.24)–(6.25). Since $x \mapsto \phi(Lx)$ is supported in $B(0, 1) \subseteq Q = [-\frac{1}{2}, \frac{1}{2}]^3$, we further have

$$\begin{aligned} \big\| \sqrt{\phi(Lx)} \big\|_{2;1} &= \sum_{\beta \in \mathbb{Z}^3} \big\| \sqrt{\phi(Lx)} \cdot \mathbf{1}_{Q+\beta} \big\|_2 \; = \; \big\| \sqrt{\phi(Lx)} \big\|_2 \\ &= \|\phi(Lx)\|_1^{1/2} \; = \; L^{-3/2} \, \|\phi\|_1^{1/2}. \end{aligned} \tag{7.12}$$

Finally, inserting (7.12) into (7.11), we arrive at (7.8). □

8. Asymptotics of the Lieb–Loss Energy

We turn to the proof of the main result of this paper, Theorem 1.1, stated below again for the reader's convenience. In our proof, a key role is played by the scaling relation the effective energy F_β obeys. F_β is defined in (5.5) as the infimum of the functional $\mathcal{F}_\beta > 0$ over L^2-normalized functions in $H^1(\mathbb{R}^3) \cap L^1(\mathbb{R}^3)$. In [24], one of us showed that this infimum is attained for some ϕ_β 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,

$$F_1 \; > \; 0 \tag{8.1}$$

is a positive constant, and it is then not difficult to see that F_β scales as

$$F_\beta \;=\; \beta^{4/7}\, F_1, \tag{8.2}$$

for all $\beta > 0$.

Theorem 8.1. *There exists a universal constant $C < \infty$ such that, for all $\alpha > 0$ and $\Lambda \geq 1$, the estimate*

$$-C\,\alpha^{\frac{4}{49}}\Lambda^{-\frac{4}{49}} \;\leq\; \frac{E_{\mathrm{LL}}(\alpha,\Lambda)}{(\frac{4}{9\pi})^{2/7}\,F_1\,\alpha^{2/7}\,\Lambda^{12/7}} \;-\;1\;\leq\; C\,\alpha^{\frac{4}{105}}\Lambda^{-\frac{4}{105}} \tag{8.3}$$

holds true.

Proof. We first take the infrared limit $\sigma \to 0$. Note that E_{LL}, $E_{\mathrm{LL}}^{(L)}$, 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 6.1 and 7.2 with $p = 1/2$ yield

$$\frac{1}{2}X(2\Theta_{\phi,\alpha}) \;-\; \sqrt{\frac{4\alpha}{9\pi}}\;\Lambda^3\,\|\phi\|_1 \;\leq C\,\varepsilon\,\Lambda^3\,\|\phi\|_1 \;+\; C\,\alpha^{1/2}\,\varepsilon^{-2}\,L^{3/2}\,\Lambda^2\,\|\nabla\phi\|_2, \tag{8.4}$$

$$\frac{1}{2}X(2\Theta_{\phi,\alpha}) \;-\; \sqrt{\frac{4\alpha}{9\pi}}\;\Lambda^3\,\|\phi\|_1 \;\geq -\,C\,\alpha^{1/4}\,L^{3/2}\,\Lambda^{7/2}\,\|\phi\|_1^{1/2}, \tag{8.5}$$

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

Next, we derive the upper bound in (8.3). From (8.4), we obtain

$$\begin{aligned}
\widehat{\mathcal{E}}_{\alpha,\Lambda}(\phi) &= \frac{1}{2}\|\nabla\phi\|_2^2 + \frac{1}{2}X(2\Theta_{\phi,\alpha}) \\
&\leq \frac{1}{2}(1+\delta)\,\|\nabla\phi\|_2^2 \;+\; \sqrt{\frac{4\alpha}{9\pi}}\;\Lambda^3\,(1+C_2\varepsilon)\,\|\phi\|_1 \;+\; C_2\,\alpha\,\delta^{-1}\,\varepsilon^{-4}\,L^3\,\Lambda^4 \\
&\leq (1+\delta)\,\mathcal{F}_{\beta_2}(\phi) \;+\; C_2\,\alpha\,\delta^{-1}\,\varepsilon^{-4}\,L^3\,\Lambda^4,
\end{aligned} \tag{8.6}$$

where $\mathcal{F}_\beta$ is defined in (5.4) and

$$\beta_2 \;:=\; \beta_0\,\frac{1+C_2\varepsilon}{1+\delta}\;, \quad \beta_0 \;\equiv\; \beta(\alpha,\Lambda) \;=\; \sqrt{\frac{4\alpha}{9\pi}}\;\Lambda^3, \tag{8.7}$$

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 (8.6), we further have

$$E_{\mathrm{LL}}^{(L)}(\alpha,\Lambda) \;\leq (1+\delta)\,F^{(L)}[\beta_2] \;+\; C_2\,\alpha\,\delta^{-1}\,\varepsilon^{-4}\,L^3\,\Lambda^4. \tag{8.8}$$

The localization estimates (5.10)–(5.11) now imply

$$E_{\mathrm{LL}}(\alpha,\Lambda) \;\leq (1+\delta)\,F_{\beta_2} \;+\; C_2\,\alpha\,\delta^{-1}\,\varepsilon^{-4}\,L^3\,\Lambda^4 \;+\; C_3\,L^{-2}, \tag{8.9}$$

for some constant $C_3 < \infty$. From the scaling relation (8.2), we get

$$\begin{aligned}
(1+\delta)\,F_{\beta_2} = (1+\delta)\,\beta_2^{4/7}\,F_1 \;&=\; (1+C_2\varepsilon)^{4/7}\,(1+\delta)^{3/7}\,\beta_0^{4/7}\,F_1 \\
&\leq (1+C_4\varepsilon+C_4\delta)\,F_{\beta_0},
\end{aligned} \tag{8.10}$$

for some $C_4 < \infty$, and inserting this into (8.9), we arrive at the intermediate estimate, stating that there exists a universal constant $C_5 < \infty$, such that

$$\frac{E_{\mathrm{LL}}(\alpha,\Lambda)}{F_{\beta(\alpha,\Lambda)}} - 1 \leq C_5\Big(\varepsilon + \delta + \alpha^{-2/7} L^{-2} \Lambda^{-12/7} + \alpha^{5/7} \delta^{-1} \varepsilon^{-4} L^3 \Lambda^{16/7}\Big) \tag{8.11}$$

holds for all $\varepsilon, \delta \in (0,1]$, $\alpha > 0$, $\Lambda \geq 1$, and $L > \Lambda^{-1}$. As α enters the right side of (8.11) only in negative powers, we may assume $\alpha \in (0,1]$ w.l.o.g. To meet these requirements, we set

$$\varepsilon := \delta := \alpha^r \Lambda^{-s} \quad \text{and} \quad L := \alpha^{-t} \Lambda^{u-1}, \tag{8.12}$$

for $r, s, t, u \geq 0$ to be chosen later. Then,

$$\begin{aligned} &\varepsilon + \delta + \alpha^{-\frac{2}{7}} L^{-2} \Lambda^{-\frac{12}{7}} + \alpha^{\frac{5}{7}} \delta^{-1} \varepsilon^{-4} L^3 \Lambda^{\frac{16}{7}} \\ &\quad = 2\alpha^r \Lambda^{-s} + \alpha^{2t-\frac{2}{7}} \Lambda^{\frac{2}{7}-2u} + \alpha^{\frac{5}{7}-5r-3t} \Lambda^{5s+3u-\frac{5}{7}} \leq 4\, \alpha^{a/7} \Lambda^{-b/7}, \end{aligned} \tag{8.13}$$

with

$$a := \min\{7r,\ 14t-2,\ 5-35r-21t\}, \tag{8.14}$$

$$b := \min\{7s,\ 14u-2,\ 5-35s-21u\}. \tag{8.15}$$

We choose r, s, t, u so that all three terms in both (8.14) and (8.15) are equal, i.e., $r := s := 4/105$ and $t := u := 17/105$. This yields $a = b = 4/15$ and hence the upper bound

$$\frac{E_{\mathrm{LL}}(\alpha,\Lambda)}{F_{\beta(\alpha,\Lambda)}} - 1 \leq 4C_5\, \alpha^{\frac{4}{105}} \Lambda^{-\frac{4}{105}} \tag{8.16}$$

in (8.3).

We similarly proceed for the derivation of the lower bound in (8.3). From (8.5), we obtain

$$\begin{aligned} \widehat{\mathcal{E}}_{\alpha,\Lambda}(\phi) &= \frac{1}{2}\|\nabla\phi\|_2^2 + \frac{1}{2} X(2\Theta_{\phi,\alpha}) \\ &\geq \frac{1}{2}\|\nabla\phi\|_2^2 + \sqrt{\frac{4\alpha}{9\pi}}\, \Lambda^3 (1-\delta) \|\phi\|_1 - C_6\, \delta^{-1} L^3 \Lambda \\ &= \mathcal{F}_{\beta_3}(\phi) - C_6\, \delta^{-1} L^3 \Lambda, \end{aligned} \tag{8.17}$$

for some $C_2 < \infty$ and all $0 < \delta \leq 1$, where

$$\beta_3 := \beta_0 (1-\delta), \quad \beta_0 \equiv \beta(\alpha,\Lambda) = \sqrt{\frac{4\alpha}{9\pi}}\, \Lambda^3. \tag{8.18}$$

Taking the infimum over all $\phi = |\phi| \in Y_L$ with $\|\phi\|_2 = 1$ in (8.17), we further have

$$E_{\mathrm{LL}}^{(L)}(\alpha,\Lambda) \geq F^{(L)}[\beta_3] - C_6\, \delta^{-1} L^3 \Lambda. \tag{8.19}$$

The localization estimates (5.10)–(5.11) now imply

$$E_{\mathrm{LL}}(\alpha,\Lambda) \geq F_{\beta_3} - C_7 L^{-2} - C_6\, \delta^{-1} L^3 \Lambda^4, \tag{8.20}$$

for some constant $C_7 < \infty$. Again invoking the scaling relation (8.2), we get

$$F_{\beta_3} \;=\; \beta_3^{4/7}\, F_1 \;=\; (1-\delta)^{4/7}\, \beta_0^{4/7}\, F_1 \;\geq\; (1-\delta)\, F_{\beta_0}, \tag{8.21}$$

and thus there exists a constant $C_8 < \infty$ such that

$$\frac{E_{\mathrm{LL}}(\alpha,\Lambda)}{F_{\beta(\alpha,\Lambda)}} - 1 \;\geq\; -C_8\Big(\delta \;+\; \alpha^{-2/7}\, L^{-2}\, \Lambda^{-12/7} \;+\; \alpha^{-2/7}\, \delta^{-1}\, L^3\, \Lambda^{16/7}\Big) \tag{8.22}$$

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

$$\delta \;:=\; \alpha^r \Lambda^{-s} \quad \text{and} \quad L \;:=\; \alpha^{-t}\Lambda^{u-1}\,, \tag{8.23}$$

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

$$\begin{aligned} &\delta + \alpha^{-\frac{2}{7}} L^{-2} \Lambda^{-\frac{12}{7}} + \alpha^{-\frac{2}{7}} \delta^{-1} L^3 \Lambda^{\frac{16}{7}} \\ &= \alpha^r \Lambda^{-s} + \alpha^{2t-\frac{2}{7}} \Lambda^{\frac{2}{7}-2u} + \alpha^{\frac{5}{7}-r-3t} \Lambda^{s+3u-\frac{5}{7}} \;\leq\; 3\,\alpha^{a/7}\,\Lambda^{-b/7}, \end{aligned} \tag{8.24}$$

with

$$a := \min\big\{7r,\; 14t-2,\; 5-7r-21t\big\}, \tag{8.25}$$

$$b := \min\big\{7s,\; 14u-2,\; 5-7s-21u\big\}. \tag{8.26}$$

We choose r, s, t, u so that all three terms in both (8.14) and (8.15) are equal, i.e., $r := s := 4/49$ and $t := u := 9/49$. This yields $a = b = 4/7$ and hence the lower bound

$$\frac{E_{\mathrm{LL}}(\alpha,\Lambda)}{F_{\beta(\alpha,\Lambda)}} - 1 \;\geq\; -3C_8\, \alpha^{\frac{4}{49}}\, \Lambda^{-\frac{4}{49}} \tag{8.27}$$

in (8.3). □

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