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Existence of Atoms and Molecules in Non-Relativistic Quantum Electrodynamics

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Abstract

We show that the Hamiltonian describing N nonrelativistic electrons with spin, interacting with the quantized radiation field and several fixed nuclei with total charge Z, has a ground state when $N < Z+1$. The result holds for any value of the fine structure constant α and for any value of the ultraviolet cutoff Λ on the radiation field. There is no infrared cutoff. The basic mathematical ingredient in our proof is a novel localization of the electromagnetic field in such a way that the errors in the energy are of smaller order than $1/L$, where L is the localization radius.

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1 Introduction

The existence of atoms and molecules in the framework of the Schrödinger equation was proved by Zhislin [14] for fixed nuclei when $N < Z + 1$. That is to say, the bottom of the spectrum of the N-electron Hamiltonian is a genuine N-particle bound state that satisfies Schrödinger's equation with some energy E, for each choice of the locations of the nuclei. (Here N is the number of electrons, each of charge $-e$, and Ze is the total charge of one or more fixed, positively charged nuclei.) The main physical result of the present paper is the proof of the same thing when account is taken of the ever-present quantized electromagnetic field. The interaction of this field with the electrons (but not the field itself) necessarily has an ultraviolet cutoff $|k| \leq \Lambda$ (in order to have finite quantities), but we emphasize that no infrared cutoff is used here.

If the fine structure constant $\alpha = e^2/\hbar c$ and Λ are small enough, the result follows from [1], but our result holds for *all values* of these parameters. In a recent paper Barbaroux, Chen and Vugalter [3] developed a new method that shows the existence of ground states for two-electron molecules with $2 < Z + 1$ (e.g., the Helium atom). Although they do not have to require that the perturbation is small when compared to the ionization energy as in [1], they have to impose restrictions on the various parameters since their works relies on the existence of the zero momentum ground state of the Hamiltonian of an electron interacting only with the radiation field. This has been established in [4] but only for sufficiently small coupling constants. The method of [3] is different from ours.

Our work (and [3]) relies on earlier work with Griesemer [7] where it was shown that a ground state exists provided a "binding condition" is satisfied, and it is this condition that is proved in [3] for the restricted $N = 2$ case and for the general case here for $N < Z + 1$. If $E^V(N)$ denotes the bottom of the spectrum of the Hamiltonian $H^V(N)$, which includes the Coulomb attraction of the electrons to the fixed nuclei of various positive charges $Z_1 e, \ \ldots, \ Z_K e$ with $Z = \sum Z_j$, and if $E^0(N)$ denotes the bottom of the spectrum of $H^0(N)$ — the "free-electron" Hamiltonian in which there are no nuclei, but the electron-electron Coulomb repulsion is included — then the *binding condition* is

$$\boxed{E^V(N) < \min\left\{E^V(N') + E^0(N - N') : 0 \leq N' < N\right\} \ .} \tag{1.1}$$

This binding condition, incidentally, is the same condition that Zhislin derived for the Schrödinger equation without the quantized electromagnetic field, and which he verified for $N < Z + 1$.

The inclusion of the quantized electromagnetic field presents two main difficulties. One is that if the bottom of the spectrum contains an eigenvalue it is *not* an isolated eigenvalue, as it was in [14]. Rather, the bottom of the spectrum is always the bottom of the essential spectrum because one can create arbitrarily many, arbitrarily soft photons. It is not easy to find an eigenvalue when it lies in the continuum. This problem was solved in [7] under condition (1.1).

The second main problem, which complicates the proof of (1.1), comes from the fact that each electron carries a virtual cloud of photons. This cloud may have substantial energy and when two electrons are near each other (whether bound or not) the interference of the photon clouds must be taken into account. In general, this is a highly non-perturbative effect. Our way around this difficulty is to prove that the photon clouds can be localized (i.e., effectively eliminated outside a ball of radius L surrounding the electron or the atom) in such a way that the error induced in the energy of the cloud is smaller than $L^{-(1+\varepsilon)}$, and thus the direct Coulomb interaction, which goes as L^{-1}, is dominant — as it was in the original paper [14]. A closely related effect is that even in the absence of an external potential electrons interact with each other. In such a case their dynamics is governed by H^0, which contains the electron-electron Coulomb repulsion. Nevertheless, it is not inconceivable that the quantized field, which interacts simultaneously with all the electrons, might cause binding among the "free" electrons. While this is unlikely it has never been disproved and we must not assume in our proof that $E^0(N) = NE^0(1)$.

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2 Basic Definitions and Concepts

The Hamiltonian under consideration, in appropriate units, is the Pauli-Fierz Hamiltonian and is given by

$$H^V(N) = \sum_{j=1}^{N} \Big[(p_j + \sqrt{\alpha} A(x_j))^2 + \frac{g}{2}\sqrt{\alpha}\, \sigma_j \cdot B(x_j) + V(x_j) \Big] + \alpha \sum_{i<j} \frac{1}{|x_i - x_j|} + H_f \ . \tag{2.1}$$

Here, g is some constant (close to 2, physically) and the vector σ_j is the set of three Pauli spin matrices for electron j. (Owing to the ultraviolet cutoff there is no restriction to $|g| \leq 2$, as there would be without a cutoff [12].) The operator p_j denotes $-i\nabla$ acting on the coordinate of the j-th electron.

The potential V is the potential of $K \geq 1$ nuclei with positive charges $Z_1, \ldots, Z_K$ and locations $R_1, \ldots, R_K \in \mathbb{R}^3$.

$$V(x) = -\sum_{j=1}^{K} Z_j |x - R_j|^{-1} \ . \tag{2.2}$$

Remark: The truth of our main theorem (3.1) — and its proof — does not require that $V(x)$ be given by (2.2). In addition to the general condition [7, eq. (5)], we need only the condition that there is some radius ρ such that $\langle V(x) \rangle \leq -Z/|x|$ for $|x| > \rho$, where $\langle \ \cdot \ \rangle$ denotes spherical average. Similarly, the repulsion $|x_i - x_j|^{-1}$ can be replaced by $W(x_i - x_j)$ provided $\langle W(x) \rangle \leq 1/|x|$ for all $|x| > \rho$.

The free Hamiltonian $H^0(N)$ is similar to $H^V(N)$, but without the attraction to the nuclei, i.e.,

$$H^0(N) = \sum_{i=1}^{N} \left[(p_i + \sqrt{\alpha} A(x_i))^2 + \frac{g}{2} \sqrt{\alpha}\, \sigma_i \cdot B(x_i) \right] + \alpha \sum_{i<j} \frac{1}{|x_i - x_j|} + H_f \ . \tag{2.3}$$

Note that the Coulomb repulsion among the electrons is included. The reason for including the Coulomb repulsion is (as stated above) that we do not know whether the electrons bind to each other through the interaction with the electromagnetic field, i.e., the electrons may not separate in the lowest energy state (if there is one).

The (ultraviolet cutoff) magnetic vector potential is defined by

$$A(x) = \frac{1}{2\pi} \sum_{\lambda=1}^{2} \int \frac{\varepsilon_\lambda(k)}{\sqrt{|k|}} \widehat{\chi}_\Lambda(k) \left(\widehat{a}_\lambda(k) e^{ik \cdot x} + \widehat{a}^*_\lambda(k) e^{-ik \cdot x} \right) dk \ , \tag{2.4}$$

where the function $\widehat{\chi}_\Lambda$ is a smooth, radial function in k space, that vanishes outside the ball whose radius is the ultraviolet cutoff Λ. We denoted the creation and destruction operators of photons of momentum k and polarization λ by $\widehat{a}_\lambda(k)$ and $\widehat{a}^*_\lambda(k)$. This unusual notation is used since we shall later introduce the creation and destruction operators in configuration space, $a_\lambda(y)$ and $a^*_\lambda(y)$, which act on the Fourier transformed functions in Fock space.

The magnetic field is $B(x) = \mathrm{curl}A(x)$. The operators $\widehat{a}_\lambda, \widehat{a}^*_\lambda$ satisfy the usual commutation relations

$$[\widehat{a}_\lambda(k), \widehat{a}^*_\nu(q)] = \delta(k-q)\delta_{\lambda,\nu} \ , \quad [\widehat{a}_\lambda(k), \widehat{a}_\nu(q)] = 0, \quad \text{etc} \tag{2.5}$$

and the vectors $\varepsilon_\lambda(k)$ are the two possible orthonormal polarization vectors perpendicular to k and to each other.

The vectors $\varepsilon_\lambda(k)$ have to be discontinuous functions of k on every sphere of fixed $|k|$-value because it is not possible to "comb the hair on a sphere". However, the only physical quantity,

$$\sum_{\lambda=1}^{2} \varepsilon^i_\lambda(k)\varepsilon^j_\lambda(k) = \delta_{i,j} - \frac{k_i k_j}{|k|^2} \ , \tag{2.6}$$

is discontinuous only at the point $k = 0$. For the rest of this paper we choose the polarizations vectors to be

$$\begin{aligned} \varepsilon_1(k) &= \frac{(k_2, -k_1, 0)}{\sqrt{k_1^2 + k_2^2}} \ , \\ \varepsilon_2(k) &= \frac{k}{|k|} \wedge \varepsilon_1(k) \ . \end{aligned} \tag{2.7}$$

Let us emphasize here that some smoothness of the function $\widehat{\chi}_\Lambda$ is essential for our arguments since this guarantees that the coupling functions

$$h^i_\lambda(y) = \frac{1}{2\pi} \int \frac{\widehat{\chi}_\Lambda(k)}{\sqrt{|k|}} \varepsilon^i_\lambda(k) e^{-ik\cdot y} dk \tag{2.8}$$

has a suitable decay as $|y| \to \infty$. If we did not have the discontinuous function $\varepsilon^i_\lambda(k)$ in (2.8) then $h(y)$ would decay as $|y|^{-5/2}$ as $|y| \to \infty$. (Proof: $|k|^{-1/2}$ is the Fourier transform of $|y|^{-5/2}$ in the sense of distributions [10, Theorem 5.9]. The Fourier transform of $\widehat{\chi}_\Lambda$ is real analytic and decays faster than any inverse power of $|y|$. Hence, the convolution of χ with $|y|^{-5/2}$ decays like $|y|^{-5/2}$. With a sharp cutoff it would decay only like $|y|^{-2}$ which turns out to be insufficient for a good localization of the photon states.

This analysis of h shows that we have to be circumspect about the choice of the polarization vectors. Their discontinuity will spoil the $|y|^{-5/2}$ decay, but it is important to get better decay than $|y|^{-2}$. In Lemma B.1 of Appendix B it is shown that with our choice (2.7) of the polarization vectors the coupling functions have sufficient decay in the sense that $\int |y|^{2\gamma} |h^i_\lambda(y)|^2 dy$ is finite for all $\gamma < 1$. Thus, in an average sense, the coupling functions decay

almost as fast as $|y|^{-5/2}$. We made no attempt to optimize the choice of the polarization vectors.

While polarization is physically measurable, the polarization vectors are not. They are merely a basis. It is odd, therefore, that their mathematical definition plays a role in the spatial localization of the photon field that we shall construct, and which is central to our proof of the binding condition. It would be better to start with a formalism that contains only "divergence-free" vector fields as the dynamical variables instead of trying to define them with the aid of unphysical polarization vectors. In particular, the Fock space would be built over the L^2-space of divergence-free vector fields instead of $L^2 \otimes \mathbb{C}^2$. We shall not explore this here, but we mention that the localization of a divergence-free vector field, which preserves the divergence-free property is also a subtle matter.

The field energy, H_f, sometimes called $d\Gamma(\omega)$, is given by

$$H_f = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} |k| \widehat{a}^*_\lambda(k) \widehat{a}_\lambda(k) dk \tag{2.9}$$

There is no cutoff in H_f. The energy of a photon is $|k|$.

Another unbounded operator of interest is the number operator

$$\mathcal{N} = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \widehat{a}^*_\lambda(k) \widehat{a}_\lambda(k) dk \ . \tag{2.10}$$

The physical Hilbert space for this system is given by

$$\mathcal{H}(N) = \wedge^N L^2(\mathbb{R}^3; \mathbb{C}^2) \otimes \mathcal{F} \tag{2.11}$$

where the wedge indicates that the electron wave functions are antisymmetric under the exchange of the particle labels. Thus, the functions in the space $\mathcal{H}(N)$ obey the Pauli exclusion principle. The photon Fock space is $\mathcal{F}$. We denote the inner product of two states Ψ and Φ in the space $\mathcal{H}(N)$ or in Fock space alone by

$$(\Psi, \Phi) \qquad \text{and} \qquad \langle \Psi, \Phi \rangle \ , \tag{2.12}$$

respectively. If Ψ and Φ are in $\mathcal{H}(N)$ then $\langle \Psi, \Phi \rangle$ makes sense and defines a summable function of $x_1, s_1, \ \ldots \ , x_N, s_N$, where x_j, s_j are the space-spin variables of the j-th electron.

It is desirable that the above Hamiltonians be selfadjoint on certain domains and this has been worked out, e.g., in [9]. In this paper we will always

be talking about the Friedrichs extension of the symmetric operators $H^{\#}(N)$ (where $\#$ is 0 or V). The form domain will consist of all states for which each term in the operators has a finite expectation value. Accordingly, we define the ground state energy $E^{\#}(N)$ for the Hamiltonian $H^{\#}(N)$ by

$$E^{\#}(N) = \inf \left\{ \left(\Psi, H^{\#}(N)\Psi \right) : \Psi \in \mathcal{H}(N) \ , \|\Psi\| = 1 \right\} \ . \tag{2.13}$$

The numbers $E^{\#}(N)$ are finite. This follows from Lemma A.4 in [7] together with the fact that the Coulomb potential is form bounded with respect to $p^2 = -\Delta$.

A few remarks concerning the Fock space $\mathcal{F}$ are in order. It is built over the space $L^2(\mathbb{R}^3)\otimes\mathbb{C}^2$; the second factor takes into account the polarizations. Let $\{f_i\}$, $i = 1, 2, \ldots$, be an orthonormal basis for $L^2(\mathbb{R}^3)\otimes\mathbb{C}^2$. Then, vectors of the form

$$|i_1, m_1; \ \ldots \ ; i_n, m_n\rangle = \frac{1}{\sqrt{m_1! \cdots m_n!}} \ a^*(f_{i_1})^{m_1} \cdots a^*(f_{i_n})^{m_n} |0\rangle \ , \tag{2.14}$$

constitute an orthonormal basis for $\mathcal{F}$, the occupation number basis. In (2.14) n is an arbitrary nonnegative integer (with $n = 0$ denoting the vacuum vector $|0\rangle$) , the indices $i_1, \cdots, i_n$ are all different, the m_i are all positive integers, $a^*(f)$ is an abbreviation for $\sum_\lambda a^*_\lambda(f_\lambda)$ and $f_\lambda = f(k, \lambda)$ is a function in L^2. Thus, any state $\Phi \in \mathcal{F}$ can be uniquely written as

$$\Phi = \sum_{n\geq 0} \sum_{i_1<i_2< \ \cdots \ <i_n} \sum_{m_1, \ \ldots \ ,m_n} \phi_{i_1,m_1; \ \ldots \ ;i_n,m_n} \ |i_1, m_1; \ \ldots \ ; i_n, m_n\rangle \ , \tag{2.15}$$

where the $n = 0$ term in (2.15) is just $\phi_0|0\rangle$ with $\phi_0 \in \mathbb{C}$. The inner product is given by

$$\langle \Phi, \Phi \rangle = \sum_{n\geq 0} \sum_{i_1<i_2< \ \cdots \ <i_n} \sum_{m_{i_1}, \ \ldots \ ,m_{i_n}} |\phi_{i_1,m_1; \ \ldots \ ;i_n,m_n}|^2 \ . \tag{2.16}$$

This representation has the advantage that the symmetry in the photon variables is automatically taken care of. It is particularly useful when dealing with product states. Consider a state Φ whose photons are all **localized** in a closed region $\mathcal{Y} \subset \mathbb{R}^3$. This means that all the $f_i(y, \lambda)$ appearing in (2.14) and in (2.15) vanish if $y \notin \mathcal{Y}$. Likewise, consider a state Ψ whose photons are all localized in a closed region $\mathcal{Z} \subset \mathbb{R}^3$ which is disjoint from $\mathcal{Y}$. Pick an orthonormal basis $\{f_k\}$ in $L^2(\mathcal{Y}) \otimes \mathbb{C}^2$ and an orthonormal basis $\{g_\ell\}$ in $L^2(\mathcal{Z}) \otimes \mathbb{C}^2$. Clearly, the two algebras of creation and annihilation operators generated by $a^{\#}(f_k)$ and $a^{\#}(g_\ell)$ commute. If

$$\Phi = \sum_{n\geq 0} \sum_{i_1<i_2< \ \cdots \ <i_n} \sum_{p_1, \ \ldots \ ,p_n} \phi_{i_1,p_1; \ \ldots \ ;i_n,p_n} \ |i_1, p_1; \ \ldots \ ; i_n, p_n\rangle_{\mathcal{Y}} \tag{2.17}$$

and

$$\Psi = \sum_{n\geq 0} \sum_{j_1<j_2<\cdots<j_n} \sum_{q_1,\ \cdots\ ,q_n} \psi_{j_1,q_1;\ \cdots\ ;j_k,q_k}\ \ |j_1,q_1;\ \ldots\ ;j_k,q_k\rangle_{\mathcal{Z}} \quad (2.18)$$

then we define the product state Ξ by

$$\Xi = \sum \phi_{i_1,p_1;\ \cdots\ ;i_m,p_m}\psi_{j_1,q_1;\ \cdots\ ;j_k,q_k}\ \ |i_1,p_1;\ \ldots;i_m,p_m\rangle_{\mathcal{Y}} \otimes\ |j_1,q_1;\ \ldots;j_k,q_k\rangle_{\mathcal{Z}} \quad (2.19)$$

where

$$|i_1,p_1;\ \cdots\ ;i_m,p_m\rangle_{\mathcal{Y}} \otimes |j_1,q_1;\ \cdots\ ;j_k,q_k\rangle_{\mathcal{Z}} = \frac{1}{\sqrt{p_1!\cdots p_m!}\sqrt{q_1!\cdots q_k!}}\, a^*(f_{i_1})^{p_1}\cdots a^*(f_{i_m})^{p_m} a^*(g_{j_1})^{q_1}\cdots a^*(g_{j_k})^{q_k}|0\rangle \quad (2.20)$$

By a simple calculation we find that

$$\langle \Xi, \Xi\rangle = \langle \Phi, \Phi\rangle \langle \Psi, \Psi\rangle\ . \quad (2.21)$$

Further, if f is a function supported in $\mathcal{Y}$, then

$$\langle \Xi, a^*(f)a(f)\Xi\rangle = \langle \Phi, a^*(f)a(f)\Phi\rangle \langle \Psi, \Psi\rangle\ . \quad (2.22)$$

Likewise, if f is supported in $\mathcal{Y}$ and g in $\mathcal{Z}$, then

$$\langle \Xi, a^*(f)a(g)\Xi\rangle = \langle \Phi, a^*(f)\Phi\rangle \langle \Psi, a(g)\Psi\rangle\ . \quad (2.23)$$

Quite generally, we have, for normal-ordered, bilinear expressions, the following formulas (in which β, γ denote linear forms in the annihilation operators a, and hence β^*, γ^* are linear forms in the creation operators):

$$\begin{aligned}
\langle \Xi, \beta\,\gamma\,\Xi\rangle &= \langle \Psi, \beta\,\gamma\,\Psi\rangle \langle \Phi, \Phi\rangle + \langle \Psi, \Psi\rangle \langle \Phi, \beta\,\gamma\,\Phi\rangle \\
&\quad + \langle \Psi, \beta\,\Psi\rangle \langle \Phi, \gamma\,\Phi\rangle + \langle \Psi, \gamma\,\Psi\rangle \langle \Phi, \beta\,\Phi\rangle \\
\langle \Xi, \beta^*\,\gamma^*\,\Xi\rangle &= \langle \Psi, \beta^*\,\gamma^*\,\Psi\rangle \langle \Phi, \Phi\rangle + \langle \Psi, \Psi\rangle \langle \Phi, \beta^*\,\gamma^*\,\Phi\rangle \\
&\quad + \langle \Psi, \beta^*\,\Psi\rangle \langle \Phi, \gamma^*\,\Phi\rangle + \langle \Psi, \gamma^*\,\Psi\rangle \langle \Phi, \beta^*\,\Phi\rangle \\
\langle \Xi, \beta^*\,\gamma\,\Xi\rangle &= \langle \Psi, \beta^*\,\gamma\,\Psi\rangle \langle \Phi, \Phi\rangle + \langle \Psi, \Psi\rangle \langle \Phi, \beta^*\,\gamma\,\Phi\rangle \\
&\quad + \langle \Psi, \beta^*\,\Psi\rangle \langle \Phi, \gamma\,\Phi\rangle + \langle \Psi, \gamma\,\Psi\rangle \langle \Phi, \beta^*\,\Phi\rangle
\end{aligned} \quad (2.24)$$

A formula of the type (2.24) does *not exist* for anti-normal-ordered products $\beta\gamma^*$. We shall have no need of such terms, however, because the only source of such terms is $A(x_i)^2$ in the electron kinetic energy. If we denote the part of (2.4) coming from $\widehat{a}_\lambda(k)$ by $\beta(x)$ and the remainder by $\beta^*(x)$ (see (2.29)) then

$$A(x)^2 = \beta(x)^2 + \beta^*(x)^2 + 2\beta^*(x)\beta(x) + C \tag{2.25}$$

where

$$C = \frac{1}{2\pi^2}\int \frac{|\widehat{\chi}_\Lambda(k)|^2}{|k|}dk \ . \tag{2.26}$$

Thus, apart from a fixed, finite number αNC, which is strictly proportional to N, (and which is, therefore, independent of any decomposition of the system into clusters) we can (and henceforth shall) replace $A(x_i)^2$ by the normal-ordered

$$:A(x_i)^2: = \beta(x_i)^2 + \beta^*(x_i)^2 + 2\beta^*(x_i)\beta(x_i) \ . \tag{2.27}$$

Formulas (2.24) continue to hold for vectors Φ in the physical Hilbert space $\mathcal{H}(N)$, with the replacement of $\langle\ ,\ \rangle$ by $(\ ,\ )$. In this case, the coefficients, $\phi_{i_1,m_1;\ \ldots\ ;i_n,m_n}$, are (antisymmetric) functions of the electron space-spin coordinates, $x_i,\ s_i$.

It is convenient to introduce the operators given by

$$a_\lambda(y) = \frac{1}{(2\pi)^3}\int \widehat{a}_\lambda(k)e^{ik\cdot y}dk \ . \tag{2.28}$$

Then the vector potential can be written as

$$A^i(x) = \sum_{\lambda=1}^{2} a_\lambda(h^i_\lambda(x-\cdot)) + a^*_\lambda(h^i_\lambda(x-\cdot)) \ . \tag{2.29}$$

The action of the operators $a_\lambda(h^i_\lambda(x-\cdot))$ is given by

$$\begin{aligned}[a_\lambda(h^i_\lambda(x-\cdot))\Psi]_n(y_1,\lambda_1;\cdots;y_n,\lambda_n)\\ = \sqrt{n+1}\int \overline{h^i_\lambda(x-y)}[\Psi]_{n+1}(y,\lambda;y_1,\lambda_1;\cdots;y_n,\lambda_n)dy \ .\end{aligned} \tag{2.30}$$

A convenient expression for $a_\lambda(h^i_\lambda(x-\cdot))$ is the formula

$$a_\lambda(h^i_\lambda(x-\cdot)) = \int a_\lambda(y)\overline{h^i_\lambda(x-y)}dy \ . \tag{2.31}$$

The number operator and the field energy can be expressed in terms of the operators $a_\lambda(x)$ by

$$(\Phi, \mathcal{N}\Phi) = (2\pi)^3 \sum_{\lambda=1}^{2} \int \|a_\lambda(x)\Phi\|^2 dx \ , \tag{2.32}$$

and

$$(\Phi, H_f\Phi) = (2\pi)^3 \sum_{\lambda=1}^{2} \left(a_\lambda(\cdot)\Phi, \sqrt{-\Delta}\ a_\lambda(\cdot)\Phi \right) \tag{2.33}$$

which by eq. 7.12(4) in [10] can be rewritten as

$$4\pi \sum_{\lambda=1}^{2} \int \frac{\|a_\lambda(x)\Phi - a_\lambda(y)\Phi\|^2}{|x-y|^4} dxdy \ . \tag{2.34}$$

By the previous considerations we have for the product state Ξ that

$$\begin{aligned} \sum_\lambda (a_\lambda(x)\Xi, a_\lambda(y)\Xi) = \\ \sum_\lambda (a_\lambda(x)\Phi, a_\lambda(y)\Phi)\,(\Psi,\Psi) + (\Phi,\Phi) \sum_i (a_\lambda(x)\Psi, a_\lambda(y)\Psi) \\ + \sum_\lambda (a_\lambda(x)\Phi, \Phi)\,(\Psi, a_\lambda(y)\Psi) + \sum_\lambda (\Phi, a_\lambda(y)\Phi)\,(a_\lambda(x)\Psi, \Psi) \ , \end{aligned} \tag{2.35}$$

and hence we obtain for the field energy of Ξ the expression

$$\begin{aligned} (\Xi, H_f\Xi) = (\Phi, H_f\Phi)\,(\Psi,\Psi) + (\Phi,\Phi)\,(\Psi, H_f\Psi) \\ - 8\pi \sum_\lambda \Re \left[\int \frac{(a_\lambda(x)\Phi, \Phi)\,(\Psi, a_\lambda(y)\Psi) + (\Phi, a_\lambda(y)\Phi)\,(a_\lambda(x)\Psi, \Psi)}{|x-y|^4} \right] dxdy \ . \end{aligned} \tag{2.36}$$

The x integration in the first term of the last integral runs over the set $\mathcal{Y}$ while the y integration runs over the set $\mathcal{Z}$ and similarly in the second term the x integration runs over the set $\mathcal{Z}$ while the y integration runs over the set $\mathcal{Y}$. Hence the last expression is well defined as long as the distance between the sets $\mathcal{Y}$ and $\mathcal{Z}$ is positive. This term expresses the fact that the field energy is a nonlocal operator and this nonlocality is one of the main obstacles to be overcome.

In general, the states Φ and Ψ will depend on the position and spin variables of the various electrons and hence the product state (2.19) has to be antisymmetrized over the electron labels. It is straightforward to check

that the expression (2.36) continues to hold also for such states. (When different groups of electrons are involved an antisymmetrization is required, however, as discussed in (3.8).)

We need one more concept before stating our main theorem. It will be necessary to localize both the electrons and the photon field. As far as the electrons are concerned it is useful to define what we mean by a **symmetrized product of n domains** in $\mathbb{R}^3$. If $B_1, \dots B_n$ are n domains (open sets) in $\mathbb{R}^3$ then the symmetrized product, Ω, is a domain in $(\mathbb{R}^3)^n$ given by

$$\Omega(B_1, \dots, B_n) = \bigcup_{\pi \in S_n} B_{\pi 1} \times B_{\pi 2} \times \cdots \times B_{\pi n} \ , \tag{2.37}$$

where S_n is the group of permutations of n labels. It might be useful to illustrate this when $n = 2$. Then we have $B_1 \subset \mathbb{R}^3$, $B_2 \subset \mathbb{R}^3$ and $\Omega(B_1, B_2) = (B_1 \times B_2) \cup (B_2 \times B_1)$. This is different from $(B_1 \cup B_2) \times (B_2 \cup B_1)$. Physically it means there is one particle in each domain B_i, but the label of the particle is indeterminate. If the domains overlap there may be several particles in one domain, of course.

3 The Main Theorem

The following is our main theorem. The proof given in this section uses several inequalities derived later on in this paper, but we present the proof now in order to make the main ideas clear without too many technicalities.

THEOREM 3.1 (Binding in Atoms). *The strict inequality (1.1) holds for all $N < Z + 1$, all g, all α and all Λ. In particular this implies that there exists a normalized ground state $\Phi(N)$ in $\mathcal{H}(N)$ for the Hamiltonian $H^V(N)$, i.e., $(\Phi(N), H(N)\Phi(N)) = E^V(N)$, and it satisfies $H^V(N)\Phi(N) = E^V(N)\Phi(N)$.*

See the remark after eq. (2.2).

PROOF: Our proof has three main parts. The first is the construction of a good trial function for $N - N'$ (with $0 \leq N' < N$) localized, 'free' electrons and localized photons accompanying these localized electrons. The second part is the construction of a good trial function for N' localized electrons 'bound' to the given, fixed nuclei, together with localized photons. The third part consists in the construction of a trial function which is a product of these two functions and then showing that the energy is lowered (by a greater amount than the localization errors) because of a negative

Coulomb energy between the 'bound' system (consisting of electrons and nuclei) and the localized 'free' electrons. One difficulty in part 3 is that although the photons in the two regions are localized in separate regions, there is still a residual interaction between the two fields, given by the last term in (2.36), which has to be considered. This interaction comes from the fact that multiplication by $|k|$ in Fourier space is a nonlocal operation in position space.

The general argument proceeds by induction. We know from [7] that one electron binds. Assuming that the binding condition holds for M electrons, all $1 \leq M \leq N-1$, we have to show that it holds for N electrons, i.e., $E^V(N) < \min\{E^V(N') + E^0(N-N') : 0 \leq N' < N\}$. Using [7, Theorem 2.1] we may assume that the Hamiltonian $H^V(M)$ has a ground state for all $1 \leq M \leq N-1$. By the second part of [7, Theorem 3.1] we know that $E^V(N) < E^0(N)$ for all N, since $Z > 0$ and the attractive Coulomb potential is strictly negative.

*Part*1. From now on we set

$$n = N - N' \, .$$

Given $0 \leq N' < N$ we shall construct a normalized state $\Phi(n)$ for the free electron Hamiltonian $H^0(n)$ with the property that the n electrons are localized in a symmetrized product Ω of some balls of radius R_0 while the field is localized in balls with the same center but with radius $L > 2R_0$. The construction of $\Phi(n)$ is done in Theorem 4.3. It lies in the physical Hilbert space $\mathcal{H}(n)$ and has an energy given by

$$\frac{\big(\Phi(n), H^0(n)\Phi(n)\big)}{(\Phi(n), \Phi(n))} \leq E^0(n) + \frac{Cn}{(L-2R_0)^\gamma}\left(\frac{R_0}{L^\gamma}\right)(1+|\log(\Lambda R_0)|) + \frac{2\pi^2 n^2}{R_0^2} \, , \tag{3.1}$$

for any $\gamma < 1$, where C is some constant independent of L and R_0. (It does depend on γ and on n, but n is bounded by N).

In (3.1) the term $(Cn/(L-2R_0)^\gamma)\,(R_0/L^\gamma)\,(1+|\log(\Lambda R_0)|)$ comes from the energy needed to localize the field in n balls of radius L. The last term comes from the kinetic energy needed to localize n electrons in the n balls of radius R_0 (Lemma 4.1).

*Part*2. According to the induction assumption at the beginning of this proof we may assume that $1 \leq N' \leq N-1$ and that the Hamiltonian $H^V(N')$ of the bound electrons has a normalized ground state $\Gamma(N')$. By [7, Lemma 6.2] we know that this ground state is exponentially localized in the electron variables, i.e., if we denote by $|X|$ the quantity $\sum_{i=1}^{N'} |x_i|$ then

$$\|e^{\beta|X|}\Gamma(N')\|^2 \leq C_\beta \tag{3.2}$$

for any $\beta^2 < \min\{E^V(N'-m) + E^0(m) : 0 < m \leq N'\} - E^V(N')$.

(Note: An error in the proof of this exponential localization in [7, Lemma 6.2] was discovered by J-M. Barbaroux and the necessary correction was published in [6]. We are grateful to Prof. Barbaroux for pointing out this mistake to us.)

Although it is not necessary to do so, we (strictly) localize $\Gamma(N')$ so that all the electrons are in a common ball of radius R_0. Following that, we localize the photon field in a larger ball of radius $L > R_0$. The field localization is essential. The electron localization is not since it would be possible to use only the exponential decay of $\Gamma(N')$. The localization is done as follows.

Let $\chi \leq 1$ be a smooth cutoff function with support in the unit ball centered at the origin and $\chi(x) = 1$ for $|x| < 1/2$. Let $\Theta = \prod_{i=1}^{N'} \chi(x_i/R_0)$ and $\widetilde{\Gamma}(N') = \Theta\Gamma(N')$. Since $\Gamma(N')$ is a ground state, and hence satisfies the Schrödinger equation, we can deduce that the increase in energy due to the cutoff is bounded as follows.

$$\left(\widetilde{\Gamma}(N'), H^V(N')\widetilde{\Gamma}(N')\right) \leq E^V(N')\left(\widetilde{\Gamma}(N'), \widetilde{\Gamma}(N')\right) + N'\frac{C_\beta \exp(-\beta R_0)}{R_0^2} \ . \tag{3.3}$$

Inequality (3.3) follows from (3.2) and integration by parts as follows. With $\langle\ ,\ \rangle$ denoting inner product in Fock space and dX denoting integration over the space-spin variables, we have

$$\begin{aligned}\int \langle \Theta\Gamma(N'), \sum_j (\nabla_j + iA(x_j))^2 \Theta\Gamma(N')\rangle \ dX = \\ \int \left(\sum_j \Theta\Delta_{x_j}\Theta\right) \langle \Gamma(N'), \Gamma(N')\rangle \ dX \\ + 2\int \sum_j \left(\Theta\nabla_{x_j}\Theta\right) \cdot \langle \Gamma(N'), (\nabla_j + iA(x_j))\Gamma(N')\rangle \ dX \\ + \int \Theta^2 \langle \Gamma(N'), \sum_j (\nabla_j + iA(x_j))^2 \Gamma(N')\rangle dX \ . \end{aligned} \tag{3.4}$$

Since $(\nabla + iA(x))^2$ is a symmetric operator, the left side of (3.4) is real and, therefore, the right side must be real, too. The first term on the right side is real. The third term is also real because $\Gamma(N')$ satisfies the Schrödinger equation, and hence $\langle \Gamma(N'), \sum_j (\nabla_j + iA(x_j))^2 \Gamma(N')\rangle = \langle \Gamma(N'), (-E^V(N') + \text{real potentials})\Gamma(N')\rangle$, which is real. The middle term must, therefore, be

real too (when summed over all particles), and we can replace the integrand by its real part. This means that we can replace $2\langle\Gamma(N'),(\nabla_{x_j}+iA(x_j))\Gamma(N')\rangle$ by $2\Re\langle\Gamma(N'),\nabla_{x_j}\Gamma(N')\rangle=\nabla_{x_j}\langle\Gamma(N'),\Gamma(N')\rangle$ since $\langle\Gamma(N'),iA(x_j)\Gamma(N')\rangle$ is imaginary (because $A(x_j)$ is symmetric).

Now, integrating by parts we can combine the second term with the first to yield $-\int(\nabla_{x_j}\Theta)^2\langle\Gamma(N'),\Gamma(N')\rangle dx_j$. This is the error term (the last term leads to the principal term $E^V(N')\left(\widetilde{\Gamma}(N'),\widetilde{\Gamma}(N')\right)$). This error term can be bounded by replacing $\nabla\chi(x_j/R_0)$ by C/R_0 times the characteristic function of the annulus between $R_0/2$ and R_0, for some constant C. But this characteristic function is bounded by $\exp(-\beta R_0/2)\exp(+\beta|x|)$. Inequality (3.3) then follows from the exponential decay (3.2).

Next one has to show that the error term in (3.3) is small when compared with $\|\widetilde{\Gamma}(N')\|^2$. It follows from the exponential decay that

$$\|\widetilde{\Gamma}(N')\|^2\geq 1-N'C_\beta e^{-\beta R_0}\ . \tag{3.5}$$

To see this note that $\chi(x_i/R_0)^2\geq 1-g_i$, where $g_i=1$ if $|x_i|>R_0/2$ and $g_i=0$ otherwise. Then $\Theta\geq\prod_i(1-g_i)\geq 1-\sum_i g_i$. But $g_i\leq\exp\{-\beta R_0\}\exp\{2\beta|x_i|\}\leq\exp\{-\beta R_0\}\exp\{2\beta|X|\}$. Therefore,

$$\begin{aligned}\|\widetilde{\Gamma}(N')\|^2&\geq\left(\Gamma(N'),\ (1-\sum_i g_i)\Gamma(N')\right)\\&\geq 1-N'\exp\{-\beta R_0\}\left(\Gamma(N'),\ \exp\{-2\beta|X|\}\Gamma(N')\right)\ .\end{aligned}$$

Together, (3.3) and (3.5) imply (for $\exp\{\beta R_0\}>N'\ C_\beta$)

$$\begin{aligned}\frac{\left(\widetilde{\Gamma}(N'),H^V(N')\ \widetilde{\Gamma}(N')\right)}{\left(\widetilde{\Gamma}(N'),\ \widetilde{\Gamma}(N')\right)}&\leq E^V(N')+\frac{N'}{R_0^2}\ \frac{C_\beta}{\exp\{\beta R_0\}-N'\ C_\beta}\\&\leq E^V(N')+\frac{2N'}{R_0^2}\ C_\beta e^{-\beta R_0}\ ,\end{aligned}\tag{3.6}$$

where the last inequality holds provided that R_0 is chosen such that $\beta R_0\geq\log(2N'C_\beta)$.

The next step is to localize the photons in the state $\widetilde{\Gamma}(N')$ in a ball centered at the origin of radius $L>R_0$. This leads to a new state $\Psi(N')$ with

$$\frac{\big(\Psi(N'), H^V(N')\Psi(N')\big)}{(\Psi(N'), \Psi(N'))} \leq E^V(N') + \frac{N'}{R_0^2}\,\frac{C_\beta}{\exp\{\beta R_0\} - N'\,C_\beta} + \frac{CN'}{(L-2R_0)^\gamma}\frac{R_0}{L^\gamma}\ , \quad (3.7)$$

for all $\gamma < 1$ and for R_0 and $L - 2R_0$ large enough.

The construction of this function Ψ is precisely the same as the photon field localization that led to the state $\Phi(n)$. It is carried out in Theorem 4.3.

Thus, $\Psi(N')$ is a state in which all the electrons are localized in a ball of radius R_0 and the photons are all localized in a ball of radius L. Moreover the localization errors are small and given in (3.7).

Part3. Now we put the pieces from Part 1 and Part 2 together and construct a trial function Ξ whose energy will be strictly below $E^V(N') + E^0(n)$.

As mentioned above, since $H^0(n)$ is translation invariant we can, by shifting, make sure that the photons in the state $\Psi(N')$ and the photons in the shifted state $\Phi(n)$, live in disjoint sets. This will be the case when the smallest distance of the centers of the balls $B_1, \dots B_n$ with the center of the ball in which $\Psi(N')$ lives is greater than $2L$.

Now we can form the product state Ξ as indicated in (2.19). The state is symmetric in the photon variables by construction. It has to be antisymmetrized in the electron labels though, i.e., replace the products $\phi_{i_1,p_1;\cdots;i_m,p_m}\psi_{j_1,q_1;\cdots;j_k,q_k}$ in (2.19) by

$$c(N,N')\sum_{\pi\in S_N}(-1)^\pi \phi_{i_1,p_1;\cdots;i_m,p_m}(z_{\pi(1)},\cdots z_{\pi(N-N')}) \times \psi_{j_1,q_1;\cdots;j_k,q_k}(z_{\pi(N-N'+1)},\cdots,z_{\pi(N)})\ . \quad (3.8)$$

where π runs through all the permutations of N elements,

$$c(N,N') = \frac{1}{\sqrt{N!(N-N')!N'!}} \quad (3.9)$$

is the normalization and $z_j = (x_j, s_j)$, the position and spin of the j-th electron. The expression in (3.9) is calculated by noting first that ϕ and ψ are each antisymmetric in their electron coordinates and, second, that there is no overlap between ϕ and ψ because the x variables in the two functions have disjoint support. Informally speaking, the antisymmetrization in (3.8)

has no effect and could be dispensed with for all practical purposes since the operators ∇ and the potentials that we consider here are local operators. If we the Hamiltonian contained nonlocal operators, such as the 'relativistic' $\sqrt{-\Delta}$ then the antisymmetrization (3.8) would have a more profound effect — although (3.9) is still correct.

Next, we calculate (with : : denoting normal ordering)

$$\begin{aligned}(\Xi, H(N)\ \Xi) \\ &= \left(\Xi, \sum_{i=1}^{N}\left[:(p_i+\sqrt{\alpha}A(x_i))^2: + \frac{g}{2}\sqrt{\alpha}\,\sigma_i\cdot B(x_i) + V(x_i)\right]\Xi\right) \\ &\qquad + \left(\Xi, \sum_{i<j}\frac{1}{|x_i-x_j|}\Xi\right) + (\Xi, H_f\Xi) \quad (3.10)\end{aligned}$$

in terms of the normalized $\Phi(n)$ and $\Psi(N')$. The field energy term has been explained previously in equation (2.36) and yields

$$\begin{aligned}(\Xi, H_f\Xi) &= (\Phi(n), H_f\Phi(n)) + \big(\Psi(N'), H_f\,\Psi(N')\big) \\ &\quad + 8\pi\sum_i \Re\int \frac{(a_\lambda(x)\Phi(n), \Phi(n))\,(\Psi(N'), a_\lambda(y)\Psi(N'))}{|x-y|^4}dxdy \\ &\quad + 8\pi\sum_i \Re\int \frac{(\Phi(n), a_\lambda(y)\Phi(n))\,(a_\lambda(x)\Psi(N'), \Psi(N'))}{|x-y|^4}dxdy\ . \quad (3.11)\end{aligned}$$

The Coulomb repulsion term is easily calculated to consist of three terms:

$$\left(\Phi(n), \sum_{N'<i<j\le N}\frac{1}{|x_i-x_j|}\Phi(n)\right)(\Psi(N'), \Psi(N')) + \quad (3.12)$$

$$\left(\Psi(N'), \sum_{1\le i<j\le N'}\frac{1}{|x_i-x_j|}\Psi(N')\right)(\Phi(n), \Phi(n)) + \quad (3.13)$$

$$\sum_{i=1, j=N'+1}^{N', N}\int \frac{\|\Psi(N')\|^2(x_1,..,x_{N'})\|\Phi(n)\|^2(x_{N'+1},..,x_N)}{|x_i-x_j|}d^Nx \quad (3.14)$$

Here the norm signs indicate that the norm has been taken in Fock space and in the spin space.

The electron kinetic energy involves the calculation of terms of the form

$$\begin{aligned}
&\big(\Xi, a(f)^2\Xi\big) \\
&= \big(\Psi(N'), a(f)^2\Psi(N')\big)\,(\Phi(n),\Phi(n)) + \big(\Phi(n), a(f)^2\Phi(n)\big)\,\big(\Psi(N'),\Psi(N')\big) \\
&\qquad + 2\Re\,\big(\Psi(N'), a(f)\Psi(N')\big)\,(\Phi(n), a(f)\Phi(n)) \quad . \qquad (3.15)
\end{aligned}$$

Thus, we have that

$$\begin{aligned}
&\left(\Xi, \sum_{i=1}^{N}\Big[:(p_i+\sqrt{\alpha}A(x_i))^2: + \frac{g}{2}\sqrt{\alpha}\,\sigma_i\cdot B(x_i)\Big]\,\Xi\right) = \\
&\sum_{i=1}^{N'}\Big(\Psi(N'), \Big[:(p_i+\sqrt{\alpha}A(x_i))^2: + \frac{g}{2}\sqrt{\alpha}\,\sigma_i\cdot B(x_i)\Big]\,\Psi(N')\Big)\,(\Phi(n),\Phi(n)) \\
&+ \sum_{i=N'+1}^{N}\Big(\Phi(n), \Big[:(p_i+\sqrt{\alpha}A(x_i))^2: + \frac{g}{2}\sqrt{\alpha}\,\sigma_i\cdot B(x_i)\Big]\,\Phi(n)\Big)\,\big(\Psi(N'),\Psi(N')\big) \\
&+ \alpha\sum_{i=1}^{N'}\int\big(\Phi(n), :A(x_i)^2:\Phi(n)\big)\,\|\Psi(N')\|^2(x_1,\dots,x_{N'})dx_1\cdots dx_{N'} \qquad (3.16) \\
&+ \alpha\sum_{i=N'+1}^{N}\int\big(\Psi(N'), :A(x_i)^2:\Psi(N')\big)\,\|\Phi(n)\|^2(x_{N'+1},..,x_N)dx_{N'+1}\cdot\cdot dx_N \qquad (3.17) \\
&+ 2\alpha\sum_{i=1}^{N'}\int(\Phi(n), A(x_i)\Phi(n))\cdot\big(\Psi(N'), p_i\Psi(N')\big)\,(x_1,\dots,x_{N'})dx_1\cdots dx_{N'} \qquad (3.18) \\
&+ 2\alpha\sum_{i=N'+1}^{N}\int\big(\Psi(N'), A(x_i)\Psi(N')\big)\cdot \\
&\qquad\qquad (\Phi(n), p_i\Phi(n))\,(x_{N'+1},\dots,x_N)dx_{N'+1}\cdots dx_N \qquad (3.19) \\
&+ 2\alpha\sum_{i=1}^{N}\int\big\langle\Psi(N'), A(x_i)\Psi(N')\big\rangle\,\langle\Phi(n), A(x_i)\Phi(n)\rangle\,dx_1\cdots dx_N \qquad (3.20) \\
&+ \frac{g}{2}\sqrt{\alpha}\sum_{i=N'+1}^{N}\int\big(\Psi(N'), B(x_i)\Psi(N')\big)\cdot \\
&\qquad\qquad (\Phi(n), \sigma_i\Phi(n))\,(x_{N'+1},\dots,x_N)dx_{N'+1}\cdots dx_N \qquad (3.21) \\
&+ \frac{g}{2}\sqrt{\alpha}\sum_{i=1}^{N'}\int(\Phi(n), B(x_i)\Phi(n))\cdot \\
&\qquad\qquad \big(\Psi(N'), \sigma_i\Psi(N')\big)\,(x_1,\dots,x_{N'})dx_1\cdots dx_{N'} \quad . \qquad (3.22)
\end{aligned}$$

Finally, the last and most important term

$$\left(\Xi, \sum_{i=1}^{N} V(x_i)\Xi\right) = \left(\Psi(N'), \sum_{i=1}^{N'} V(x_i)\Psi(N')\right)(\Phi(n), \Phi(n)) + \left(\Phi(n), \sum_{i=N'+1}^{N} V(x_i)\Phi(n)\right)\big(\Psi(N'), \Psi(N')\big) \quad . \quad (3.23)$$

Lemma 5.6 allows us to show that the terms (3.16, 3.17) are of order $L^{-2\gamma}$ for any $\gamma < 1$. This follows from the fact that in our trial function the electrons are localized in balls of radius R_0, and so the distance D in Lemma 5.6 between any electron and the localized photon field of the subsystem to which the electron does *not* belong is at least $L - R_0$. Since we can easily choose L large and R_0 to be an arbitrarily chosen small constant times L we conclude, from Lemma 5.6, that these terms are of order $L^{-2\gamma}$ for any $\gamma < 1$.

The terms (3.14, 3.23) taken together are the terms that will give us binding. We shall show that, after averaging over rotations, the two terms add to $-(Z - N')/3L$, which is less than $-$pos. const.$/L$ according to our hypothesis.

'Averaging over rotations' means the following. We fix the state $\Psi(N')$ of the electrons bound to the nuclei and their field, which extends out a distance L from the origin. On the other hand, the state of the n unbound electrons was called $\Phi(n)$, but actually there are infinitely many states we could use. That is, we start with one $\Phi(n)$ and consider all rotations of it about the origin. The average Coulomb interaction (i.e., the average of (3.14) and (3.23)) is the same as if the bound electron state $\Psi(N')$, including the nuclei, was rotated about the origin. However, the average potential generated by the latter average over rotations at a point x would be exactly $(Z - N')/|x|$ *provided* $|x| > L$. This is Newton's theorem [10, Theorem 9.7]. Therefore, there exists a rotation so that the Coulomb interactions (3.14) and (3.23) are as if the inner state were a point charge located at the origin and of strength $Z - N'$.

We now choose $\Phi(n)$ so that one of the balls of radius L in which the n electrons and the field reside is tangent to the ball of radius L in which the bound electrons and field reside. By averaging over rotations we may assume that the Coulomb potential seen by the n electrons is that of a point charge at the origin; since there is at least one of the outer balls that is a distance $2L$ from the origin, and since that ball contains at least one electron, we can safely say that the Coulomb interaction of the outer electrons with the

nuclei, i.e., the sum of the term (3.14) and the last term in (3.23), is less than $-(Z-N')/3L$. (The reason we wrote $Z-N'$ instead of $n(Z-N')$ is that we do not know the positions of the other $n-1$ electrons; they could be very far away.)

To summarize the situation thus far, we have a negative Coulomb attraction of order CL^{-1}, where C is a fixed constant. We have various localization errors of order $L^{-2\gamma}$, R_0^{-2} and also $(R_0/L^\gamma)(L-2R_0)^{-\gamma}(1+|\log(\Lambda R_0)|)$. These latter terms can be made arbitrarily small compared to CL^{-1} if we choose $1>\gamma>3/4$ and

$$L^{2\gamma-1} >> R_0 >> L^{1/2} \ . \tag{3.24}$$

Finally, there are the terms (3.11) and (3.18 – 3.22) which involve expectation values of linear operators $a^\#$ in $\Phi(n)$ and in $\Psi(N')$. These are dangerous looking terms; on the face of it they appear to possibly be of order L^{-1}, but we can make them all effectively vanish!

To eliminate these terms we can make an anti-unitary transformation on $\Psi(N')$ (or else on $\Phi(n)$, but not on both) that will not alter the energy of each subunit or alter the Coulomb interaction. This anti-unitary is simply to replace $a^\#$ by $-a^\#$ and, simultaneously use complex conjugation to change $\Psi(N')$ to its complex conjugate $\overline{\Psi(N')}$. In addition we apply the unitary operator $\mathcal{W}=\prod_{i=1}^{N'}\sigma_i^{(2)}$, where σ^2 is the second Pauli matrix in the usual basis in which σ^2 has purely imaginary elements and σ^1 and σ^3 are real.

The effect of applying this anti-unitary is to replace (3.11) and (3.18 – 3.22) by their negatives, whereas all other energy terms remain unchanged. Note that the anti-unitary when applied to $\Psi(N')$ changes the sign of one of the factors in (3.18 – 3.22) only. It changes the sign of $(\Psi(N'),p_i\Psi(N'))$ because of the complex conjugation and it changes the sign of $(\Psi(N'),\sigma_i\Psi(N'))$ because of complex conjugation and $\mathcal{W}$. The terms $(\Psi(N'),A(x_i)\Psi(N'))$ and $(\Psi(N'),B(x_i)\Psi(N'))$ change their sign because of the change of sign of the $a^\#$'s. Thus, each of this terms can be negated, and one choice or the other will make *the sum* (but perhaps not each individual term) of (3.11) and (3.18 – 3.22) non-positive. □

4 Localization Estimates for 'Free' Electrons and Photons

The main result of this section is Theorem 4.3 which shows how to construct a state in which the 'free' electrons and the field are localized. This was used

in Part 1 of the proof of Theorem 3.1. Part 2 of the proof of Theorem 3.1 also uses the part of Theorem 4.3 relating to the field localization.

The proofs in this section rely, in part, on the commutator estimates of Sects. 5 and 6. The Hamiltonian for the n free electrons is given in (2.3).

4.1 Localization of the Electrons, but not the Photons

LEMMA 4.1 (localization of electrons). *Fix a radius $R_0 > 0$. Then there exist (not necessarily disjoint) balls $B_1, \ldots B_n$ in $\mathbb{R}^3$, each of radius R_0, and a normalized vector Ψ in the physical Hilbert space $\mathcal{H}(n)$ such that the electronic part of Ψ is supported in $\Omega(B_1, \ldots, B_n)$ and with an energy*

$$\big(\Psi, H^0(n)\Psi\big) < E^0(n) + b\, n^2 R_0^{-2}, \tag{4.1}$$

where $b = 2\pi^2$ is twice the lowest eigenvalue of the Dirichlet Laplacian in a ball of radius 1.

Conjecture: The proof does not tell us the location of the n balls. If they happen to be distinct then we can replace n^2 by n in (4.1). We conjecture that the theorem can be generally improved in this way, i.e., $n^2 \to n$, with, perhaps, a different value for b.

PROOF: Let $\varepsilon = b n^2 R_0^{-2}/2$ and let Φ be a normalized approximate ground state with error at most $\varepsilon/2$, i.e., $\Phi \in \mathcal{H}$ and $\big(\Phi, H^0\Phi\big) < E^0(n) + \varepsilon/2$. Let B denote the ball of radius R_0 centered at the origin in $\mathbb{R}^3$ and let χ be a normalized, nonnegative, infinitely differentiable function with support in B. Define the function G of $X = (x_1, ..., x_n)$ and $Y = (y_1, ..., y_n)$ by

$$G(X,Y) = \sum_{\pi \in S_n} \prod_{i=1}^{n} \chi(x_i - y_{\pi i}) \ , \tag{4.2}$$

where S_n is the symmetric group. Clearly G is a symmetric function of the X variables and of the Y variables and, therefore, $G(X,Y)\Phi$ is a valid vector in the physical Hilbert space for each choice of Y.

It is obvious that

$$P(X) := \int_{\mathbb{R}^{3n}} G(X,Y)^2 dY \tag{4.3}$$

is simply $n!$ times the permanent of the $n \times n$ hermitian, positive semidefinite matrix $M_{i,j} := \int_{\mathbb{R}^3} \chi(x_i - y)\chi(x_j - y)dy$. It is a general fact that such a

permanent is not less than the product of its diagonal elements; in fact it is not less than the product of the permanent of any principal $(n-m)\times(n-m)$ submatrix and the permanent of its $m\times m$ complement [11], so $P(X)\geq n!$. In particular, a fact that we shall use later is that for each i, $P(X)\geq n!M_{i,i}\widetilde{M}_{i,i}=n!\widetilde{M}_{i,i}$, where $\widetilde{M}_{i,i}$ is the permanent cofactor of $M_{i,i}$, i.e., it is the permanent of the matrix in which the i^{th} row and column is deleted from M. (In our case, the assertion is obvious since every matrix element $M_{i,j}>0$.)

We define $W(X,Y)=G(X,Y)P(X)^{-1/2}$, and using this we define

$$\Psi_Y := W(X,Y)\Phi\ . \tag{4.4}$$

Our Ψ will be be Ψ_Y (up to normalization) for a choice of Y to be determined shortly. Since $P(X)\geq n!$ the multiplier $W(X,Y)$ is C_c^∞.

We proceed analogously to Theorem 3.1 of [7]. Consider

$$\mathcal{E}(Y) := (\Psi_Y, H^0(n)\Psi_Y) - \left[E^0(n)+\varepsilon+b\,n^2R_0^{-2}\right](\Psi_Y,\,\Psi_Y)\ . \tag{4.5}$$

Our goal is to show that $\int\mathcal{E}(Y)dY<0$ for a suitable choice of χ. This will prove that there is a set of Y's of positive measure such that $\Psi_Y\neq 0$ and also $(\Psi_Y,H^0(n)\Psi_Y)/(\Psi_Y,\,\Psi_Y)\leq[E^0(n)+\varepsilon+b\,n^2R_0^{-2}]$, which is what we wish to prove.

It is obvious, from (4.3) that $\int W(X,Y)^2dY=1$ and so

$$\int(\Psi_Y,\,\Psi_Y)\,dY=(\Phi,\,\Phi)=1. \tag{4.6}$$

In a similar fashion one sees that

$$\int(\Psi_Y,[\alpha\sum_{i<j}|x_i-x_j|^{-1}+H_f]\Psi_Y)dY=(\Phi,[\alpha\sum_{i<j}|x_i-x_j|^{-1}+H_f]\Phi)\ . \tag{4.7}$$

Next, we compute

$$\begin{aligned}\|(\nabla_{x_i}+iA(x_i))\Psi_Y\|^2=\|(\nabla_{x_i}W)\Phi\|^2+\Re\left(\Phi,(\nabla_{x_i}W^2)\cdot(\nabla_{x_i}+iA(x_i))\Phi\right)\\ +\|W(\nabla_{x_i}+iA(x_i))\Phi\|^2\ .\end{aligned} \tag{4.8}$$

The middle term vanishes when we integrate over Y since $\int W(X,Y)^2dY=1$ and hence $\int\nabla_{x_i}W(X,Y)^2dY=0$. The last term gives us the required contribution of the kinetic energy to $\int(\Psi_Y,H^0(n)\Psi_Y)dY$ in (4.5), again using the fact that $\int W(X,Y)^2dY=1$. The first term is $(\Phi,F_i(X)\Phi)$, where

$$F_i(X)=\int\left|\nabla_{x_i}\left\{G(X,Y)P(X)^{-1/2}\right\}\right|^2dY\ . \tag{4.9}$$

Our proof is complete if we can show that $F_i(X) \leq 3\varepsilon/2n$, which we shall do next. We start with

$$\nabla_{x_i}\left\{G(X,Y)P(X)^{-1/2}\right\} = P(X)^{-1/2}\nabla_{x_i}G(X,Y) - (1/2)G(X,Y)P(X)^{-3/2}\nabla_{x_i}P(X)\ . \quad (4.10)$$

If we square this and integrate over Y we obtain (recalling that $\nabla_{x_i}P(X) = 2\int G(X,Y)\nabla_{x_i}G(X,Y)dY$ and $\int G(X,Y)^2dY = P(X)$)

$$F_i(X) = \frac{1}{P(X)}\int |\nabla_{x_i}G(X,Y)|^2dY - \frac{1}{4P(X)^2}|\nabla_{x_i}P(X)|^2\ . \quad (4.11)$$

We shall ignore the last term since it is negative.

In order to compute $\nabla_{x_i}G(X,Y)$ let us write

$$G(X,Y) = \sum_{j=1}^{n}\chi(x_i - y_j)\mu_j(X',Y') := \sum_{j=1}^{n}a_j(X,Y), \quad (4.12)$$

where

$$\mu_j(X',Y') = \sum_{\pi\in S_{n-1}}\prod_{\ell\neq i}\chi\left(x_\ell - y_{\pi\ell}\right)\ , \quad (4.13)$$

and where S_{n-1} denotes the set of bijections of $1,\ldots,\hat{i},\ldots,n$ into $1,\ldots,\hat{j},\ldots,n$. Then,

$$\int |\nabla_{x_i}G|^2\,dY = \sum_{j=1}^{n}\sum_{k=1}^{n}\int \nabla_{x_i}a_j\cdot\nabla_{x_i}a_k dY \leq n\sum_{j=1}^{n}\int |\nabla_{x_i}a_j|^2\,dY$$
$$= n\sum_{j=1}^{n}\int |(\nabla\chi)(x_i - y_j)|^2\,dy_j\int \mu_j(X',Y')^2dY' = nC_{i,i}\int |\nabla\chi(x)|^2dx\ , \quad (4.14)$$

where $Y' = (y_1,\ldots,\hat{y_j},\ldots,y_n)$ and where $C_{i,i} = \int \mu(X',Y')^2dY'$ equals $(n-1)!$ times $\widetilde{M}_{i,i}$, the cofactor of $M_{i,i}$ in the permanent of M. However, $P(X) \geq n!M_{i,i}\widetilde{M}_{i,i} = n!M_{i,i}[C_{i,i}/(n-1)!]$, as explained before. Therefore, $P^{-1}\int |\nabla_{x_i}G|^2\,dY \leq n\int |\nabla\chi|^2$. The same inequality holds for any $i = 1,\ldots,n$ which gives us a factor of n^2 altogether.

At this point we wish to choose χ to be the lowest Dirichlet eigenfunction of $-\Delta$ in the ball B. That function is not in $C_c^\infty(B)$, but it can be approximated by such a function so that the error in $n^2\int |\nabla\chi|^2$ is less than $\varepsilon/2$. □

4.2 Localization of Photons

Our next task is to produce a state in which the photons are localized. A definition is needed first. We say that the electromagnetic field in a state Φ is **supported** in a closed subset $\Sigma \subset \mathbb{R}^3$ if each component a_λ of the field satisfies $\|a_\lambda(x)\Phi\| = 0$ for all $x \notin \Sigma$. To construct a localized state from any given state Φ we use the representation (2.15) of Fock space. We suppress the space and spin variables of the electrons for the moment. For a smooth cutoff function $0 \leq j(y) \leq 1$ define the localization operator $\mathcal{J}$ on Fock space in the following manner. $\mathcal{J}\Phi$ is still given by (2.15) but the vector $|i_1, m_1; \cdots ; i_n, m_n\rangle$ is changed to

$$\mathcal{J}|i_1, m_1; \cdots ; i_n, m_n\rangle = \frac{1}{\sqrt{m_1! \cdots m_n!}}\, a^*(jf_{i_1})^{m_1} \cdots a^*(jf_{i_n})^{m_n}|0\rangle \ , \quad (4.15)$$

Clearly, $\mathcal{J}$ is a linear, self-adjoint operator and

$$\|a_\lambda(y)\mathcal{J}\Phi\| = 0 \quad (4.16)$$

for all y that are outside the support of the function $j(y)$. Note that $\mathcal{J}$ is a contraction, i.e., $\|\mathcal{J}\Phi\| \leq \|\Phi\|$ for all Φ.

To work effectively with the operator $\mathcal{J}$ the following commutation relations will be useful later. Since the electron variables are not relevant for the calculation, we suppress them here.

LEMMA 4.2 (Commutation relations for $\mathcal{J}$). *For any f in the single photon Hilbert space $L^2(\mathbb{R}^3; \mathbb{C}^2)$ we have (with $a_\lambda(f) = \int a_\lambda(y)\overline{f(y)}dy$, as before) that*

$$a_\lambda(f)\mathcal{J} = \mathcal{J}a_\lambda(jf), \qquad \mathcal{J}a^*_\lambda(f) = a^*_\lambda(jf)\mathcal{J} \quad (4.17)$$

$$[a_\lambda(f), \mathcal{J}] = \mathcal{J}a_\lambda((j-1)f), \qquad [a^*_\lambda(f), \mathcal{J}] = -a^*_\lambda((j-1)f)\mathcal{J} \ . \quad (4.18)$$

PROOF: For any state Ψ in the Fock space we have that

$$\begin{aligned}
&[a_\lambda(f)\mathcal{J}\Psi]_n\,(y_1, \lambda_1; \ldots ; , y_n\lambda_n) \\
&\quad = \sqrt{n+1}\prod_{k=1}^{n} j(y_k) \int \overline{f(y)}j(y)\,[\Psi]_{n+1}\,(y, \lambda; y_1, \lambda_1; \ldots ; y_n, \lambda_n)dy \\
&\qquad\qquad = [\mathcal{J}a_\lambda(jf)\Psi]_n\,(y_1, \lambda_1; \ldots ; y_n, \lambda_n) \ . \quad (4.19)
\end{aligned}$$

All the relations follow immediately from this. □

4.3 Localization of the Photons and the Electrons Together

One would like to think that most of the photons ought to be localized near the electrons. This will be the case provided one replaces the state Ψ of Lemma 4.1 by the ground state for the Hamiltonian $H^0(n)$ restricted to the states that vanish outside the set Ω. Moreover, this state will have an energy close to the energy $E^0(n)$. The following theorem makes this precise.

THEOREM 4.3 (Localized photons and free electrons). *Fix radii $R_0 > 0$ and $L > 2R_0$. Then there exist (not necessarily disjoint) balls $B_1, \dots B_n$ in $\mathbb{R}^3$, each of radius R_0 and a normalized vector $\Phi(n)$ in the physical Hilbert space $\mathcal{H}(n)$ such that the electronic part of $\Phi(n)$ is supported in $\Omega(B_1, \dots, B_n)$ and the electromagnetic field is supported in $\Sigma = \cup_{i=1}^n P_i$ where P_i is a ball concentric with B_i but with radius L.*

The energy of $\Phi(n)$ satisfies

$$\big(\Phi(n), H^0(n)\Phi(n)\big) < E^0(n) + b\,\frac{n^2}{R_0^2} + c\frac{n}{(L-2R_0)^\gamma}\left(\frac{R_0}{L^\gamma}\right)(1 + |\log(\Lambda R_0)|), \tag{4.20}$$

for any $\gamma < 1$ and where $b = 2\pi^2$ is twice the lowest eigenvalue of the Dirichlet Laplacian in a ball of radius 1. The constant c depends only on γ and is independent of R_0 and L.

PROOF: We start with the wave function Ψ given by Lemma 4.1. This fixes the balls $B_1, \dots B_n$, and hence the symmetrized product $\Omega(B_1, \dots B_n)$. The next step is to redefine the Hamiltonian $H^0(n)$ by restricting the Hilbert space to the balls, i.e., we replace the space $\wedge L^2(\mathbb{R}^3; \mathbb{C}^2)$ by the subspace of $L^2(\Omega; \otimes_1^n \mathbb{C}^2)$ consisting of functions that are antisymmetric under the exchange of particle labels. (This makes sense because Ω is symmetric under exchange of particle coordinates.) The Laplacian is replaced by the Dirichlet Laplacian.

A physical way to say this is that we add an infinite potential outside Ω. This is not a sum of single particle potentials, but that is immaterial. The point is that by the methods of [7] there is a bound state, i.e., there is a state $\Phi_D(n)$ with lowest energy $E_D^0(n)$ (the letter D stands for 'Dirichlet') that satisfies Schrödinger's equation. (In fact, the methods of [7] are not needed to establish the existence of a ground state in this case since all finite energy states are evidently localized; this was noted earlier in [5], [1] and [8]. However, [7] is needed for the photon localization in the next step.)

This ground state will obviously have a lower energy than the Ψ given by

Lemma 4.1 since that Ψ automatically satisfies the Dirichlet boundary conditions, that is $\big(\Phi_D(n), H^0(n)\Phi_D(n)\big) \leq (E^0(n) + b\,n^2 R_0^{-2})\,(\Phi_D(n), \Phi_D(n))$.

Next, we localize the photons in the set Σ. A standard IMS localization yields two smooth functions $j_1(y), j_2(y)$ with

$$j_1(y)^2 + j_2(y)^2 = 1 \tag{4.21}$$

with support of $j_1(y)$ in Σ, We also require that $j_1(y)$ is identically equal to 1 on the set $\cup_{i=1}^n Q_i$ where, for each i, Q_i is a ball of radius $L/2$, concentric with P_i. Moreover we can assume that $|\nabla j_i(y)| \leq C/L$ for some constant C and $i = 1, 2$. We define $\mathcal{J}\Phi_D(n)$ by using j_1 in (4.15) and, with the help of (4.16), we use the localized state $\mathcal{J}\Phi_D(n)$, appropriately normalized, as a trial function. This function will be the required function $\Phi(n)$ of our theorem.

The energy of the state $\mathcal{J}\Phi_D(n)$ can be compared with the energy of $\Phi_D(n)$ by using the commutator formula

$$\big(\mathcal{J}\Phi_D(n), (H^0(n) - E_D^0(n))\mathcal{J}\Phi_D(n)\big) = \big(\mathcal{J}\Phi_D(n), [H^0(n), \mathcal{J}]\Phi_D(n)\big)\ . \tag{4.22}$$

An important point about having a *ground state* $\Phi_D(n)$ is that one can derive infrared bounds for this state (see Sects. 5 and 6). All that is needed is that Φ_D is a ground state, i.e., it satisfies the Schrödinger equation in order to apply the 'pull through formula'.

Lemma 5.2 shows that the norm $\|\mathcal{J}\Phi_D\|$ is close to one and Lemma 5.5 shows that the right side of (4.22) is bounded as

$$\begin{aligned}&\big(\mathcal{J}\Phi_D(n), [H^0(n), \mathcal{J}]\Phi_D(n)\big)\\ &\qquad \leq \frac{C}{(L - 2R_0)^\gamma}\left(\frac{R_0}{L^\gamma}\right)(1 + |\log(\Lambda R_0)|)\,(\mathcal{J}\Phi_D(n), \mathcal{J}\Phi_D(n))\ ,\end{aligned} \tag{4.23}$$

for any $\gamma < 1$, where the constant C depends on γ but not on R_0 and L. This shows that $\Phi(n) = \mathcal{J}\Phi_D(n)/\|\mathcal{J}\Phi_D(n)\|$ satisfies (4.20). □

5 Commutator and Related Estimates

In this section we prove various results stated in the previous sections, particularly Lemma 5.5 which is used in the proof of Theorem 4.3. We also prove Lemma 5.6, which is not a commutator estimate; it is simpler. It is

needed to bound the terms (3.16) and (3.17), as we stated just after eq. (3.23).

We will deal mainly with the Dirichlet ground state associated with electrons localized in the set $\Omega(B_1, \dots B_n)$. The bounds for the ground state describing electrons exponentially localized near the nuclei is easier and follows in the same fashion.

In this section and the next we denote the Dirichlet ground state $\Phi_D(n)$ simply by Φ in order to simplify the notation.

Recall the definitions of j_1, j_2 in (4.21) and of the operator $\mathcal{J}$ in (4.15) which is defined by substituting j_1 for j. An important operator in our analysis is the outer photon number, given by

$$\mathcal{N}_{\text{out}} = \sum_{\lambda=1}^{2} \int_{j_2(y)>0} a^*_\lambda(y) a_\lambda(y) dy \tag{5.1}$$

or, in terms of matrix elements,

$$(\Phi, \mathcal{N}_{\text{out}} \Phi) := \sum_{\lambda=1}^{2} \int_{j_2(y)>0} \|a_\lambda(y)\Phi\|^2 dy \tag{5.2}$$

We start with the following bound, which is a consequence of the infrared bounds proved in Sect. 6. It is used in the proofs of Lemmas 5.2, 5.3 and 5.4.

LEMMA 5.1 (Photon number is small far away from the electrons). *For the Dirichlet ground state Φ of the free electrons localized in $\Omega(B_1, \dots B_n)$ we have the bound (with C independent of R_0 and L)*

$$(\Phi, \mathcal{N}\Phi) \leq C(1 + |\log(\Lambda R_0)|) \ , \tag{5.3}$$

and for all $\gamma < 1$, the bound

$$(\Phi, \mathcal{N}_{\text{out}}\Phi) \leq C \left(\frac{R_0}{L^\gamma}\right)^2 \|\Phi\|^2 \tag{5.4}$$

where the constant C depends on n, Λ, γ but not on R_0 and L. Likewise, for the ground state Ψ of the bound system given by the Hamiltonian $H^V(N')$ we have that (with C independent of R_0 and L)

$$(\Psi, \mathcal{N}\Psi) \leq C \ , \tag{5.5}$$

and for all $\gamma < 1$ and $L > 2R_0$ that

$$(\Psi, \mathcal{N}_{\text{out}}\Psi) \leq C \left(\frac{1}{L^{2\gamma}}\right) \|\Psi\|^2 \ , \tag{5.6}$$

where the constant C depends only on γ.

Our goal is to prove inequality (4.23), which is Lemma 5.5 of this section. To do so, we shall need the following three lemmas, in which $\mathcal{J}$ is defined with j_1. Recall that $0 \leq j_1(y) \leq 1$ and $j_1(y) = 1$ for $y \in \bigcup_{i=1}^n Q_i$ (see the proof of Theorem 4.3).

LEMMA 5.2. *For the normalized ground state Φ, we have for all $0 < \gamma < 1$ that*

$$1 - \|\mathcal{J}\Phi\|^2 \leq C \left(\frac{R_0}{L^\gamma}\right)^2 \tag{5.7}$$

where C is a constant that depends on γ, n, Λ but not on R_0 and L. Moreover, for an arbitrary state Ψ,

$$(\mathcal{J}\Psi, \mathcal{N}_{\text{out}}\ \mathcal{J}\Psi) \leq (\Psi, \mathcal{N}_{\text{out}}\ \Psi)\ . \tag{5.8}$$

PROOF: Formula (5.8) is immediate from

$$(\mathcal{J}\Psi, \mathcal{N}_{\text{out}}\mathcal{J}\Psi) = \sum_{n=1}^{\infty} n \| \prod_{l=1}^{n} j(y_l) \prod_{l=1}^{n} \chi_{j_2(y_l)>0} [\Psi]_n \|^2\ . \tag{5.9}$$

Next, note that

$$1 - \prod_{k=1}^{n} j_1^2(y_k) = \sum_{l=1}^{n} \prod_{k=1}^{l-1} j_1^2(y_k) j_2^2(y_l) \tag{5.10}$$

(by definition the empty product equals 1). This is proved by inserting $j_2^2(y_n) = 1 - j_1^2(y_n)$ on the left side of (5.10) and then repeating the process inductively. In particular, we have that

$$1 - \prod_{k=1}^{n} j_1^2(y_k) \leq \sum_{l=1}^{n} j_2^2(y_l)\ , \tag{5.11}$$

from which we obtain

$$1 - \|\mathcal{J}\Phi\|^2 \leq (\Phi, \mathcal{N}_{\text{out}}\Phi) \leq C \left(\frac{R_0}{L^\gamma}\right)^2 \tag{5.12}$$

by Lemma 5.1. □

LEMMA 5.3. *For the ground state Φ and for every $L > 2R_0$ we have that*

$$\left| \left(\mathcal{J}\Phi, \sum_{i=1}^{n} \left[(p_i + A(x_i))^2, \mathcal{J} \right] \Phi \right) \right| \leq\ C \frac{1}{(L - 2R_0)^\gamma} \left(\frac{R_0}{L^\gamma}\right) (1 + |\log(\Lambda R_0)|) \|\mathcal{J}\Phi\|^2\ , \tag{5.13}$$

for all $\gamma < 1$. C is a constant that depends on γ, n, Λ but not on R_0 and L. (Note that it makes no difference whether we use $(p_i + A(x_i))^2$ or use its normal ordering since the commutator of a_i and a_i^* is proportional to the identity operator, which commutes with $\mathcal{J}$.)

PROOF: We first calculate the commutator of $(p + A(x))^2$ with $\mathcal{J}$.

$$\sum_{i=1}^{n} \left[(p_i + A(x_i))^2, \mathcal{J}\right] =$$
$$\sum_{i=1}^{n} \left(2p_i \cdot ([a_i, \mathcal{J}] + [a_i^*, \mathcal{J}]) + [a_i a_i, \mathcal{J}] + [a_i^* a_i^*, \mathcal{J}] + 2[a_i^* a_i, \mathcal{J}]\right) \ , \quad (5.14)$$

where we abbreviated $a_\lambda(h_\lambda^j(x_i - \cdot))$ by a_i and likewise for a_i^*.(Note that the index $j \in \{1, 2, 3\}$ of the coupling function is unimportant and will be suppressed from now on.)

Step 1. The term $\sum_{i=1}^{n} (\mathcal{J}\Phi, 2p_i \cdot [a_i, \mathcal{J}]\Phi)$ is bounded, by Schwarz's inequality, by

$$2 \left(\sum_{i=1}^{n} \|p_i \mathcal{J}\Phi\|^2\right)^{1/2} \left(\sum_{i=1}^{n} \|[a_i, \mathcal{J}]\Phi\|^2\right)^{1/2} . \quad (5.15)$$

The first factor can be estimated simply in terms of the energy while the second factor will deliver the necessary decay in L. Using Lemma 4.2 the problem is reduced to estimating, for each fixed $X = (x_1, \ldots, x_n) \in \Omega$ and each i (with $\|\cdot\|$ denoting the norm in Fock space only)

$$\begin{aligned} &\|\mathcal{J} a(h(x_i - \cdot)(j_1(\cdot) - 1))\Phi\| \\ &\quad \leq \|a(h(x_i - \cdot)(j_1(\cdot) - 1))\Phi\| \leq \int (1 - j_1(y)) \ \|h(x_i - y)a(y)\Phi\| dy \\ &\quad \leq \int (1 - j_1(y)) \ |h(x_i - y)| \|a(y)\Phi\| dy \\ &\quad \leq \left(\int (1 - j_1(y)) \ |h(x_i - y)|^2 dy\right)^{1/2} \left(\int (1 - j_1(y)) \|a(y)\Phi\|^2 dy\right)^{1/2} . \end{aligned} \quad (5.16)$$

The first factor in (5.16) can be bounded, using Lemma B.1, by

$$\left(\int (1 - j_1(y)) \ \frac{1}{(L - 2R_0)^{2\gamma}} |x_i - y|^{2\gamma} |h(x_i - y)|^2 dy\right)^{1/2} \leq \frac{C}{(L - 2R_0)^\gamma} \quad (5.17)$$

since, whenever $1 - j_1(y) \neq 0$, the distance between x_i and y is at least $d = (L/2) - R_0$, by construction. If we now square (5.16) and integrate over X we get the desired decay estimate for (5.15).

For the second factor in (5.16) we note that $1 - j_1(y) \leq j_2(y)^2$. This, together with Lemma 5.1, yields

$$\left(\sum_{i=1}^{n} \| \mathcal{J} a(h(x_i - \cdot)(j_1(\cdot) - 1))\Phi \|^2 \right)^{1/2} \leq \frac{C}{(L - 2R_0)^\gamma} \left(\frac{R_0}{L^\gamma} \right) \tag{5.18}$$

for all $\gamma < 1$.

Next, $(\mathcal{J}\Phi, 2\sum_{i=1}^{n} p_i \cdot [a_i^*, \mathcal{J}]\Phi) = -2\sum_{i=1}^{n} ([a_i, \mathcal{J}]\mathcal{J}\Phi, p_i\Phi)$ and this can be estimated in the same fashion as before except that the estimate is in terms of

$$(\mathcal{J}\Phi, \mathcal{N}_{\text{out}}\mathcal{J}\Phi)$$

instead of $(\Phi, \mathcal{N}_{\text{out}}\Phi)$. On account of Lemma 5.2, this is bounded by

$$(\Phi, \mathcal{N}_{\text{out}}\Phi) \ .$$

Hence, we obtain the same kind of bound as in (5.18), i.e., for all $\gamma < 1$,

$$| \sum_{i=1}^{n} (\mathcal{J}\Phi, 2p_i \cdot [a_i^*, \mathcal{J}]\Phi) | \leq \frac{C}{(L - 2R_0)^\gamma} \left(\frac{R_0}{L^\gamma} \right) \ .$$

Step 2. Returning to (5.14) we concentrate on the term $[a_i a_i, \mathcal{J}]$ which can be written as $a_i[a_i, \mathcal{J}] + [a_i, \mathcal{J}]a_i$. Using Schwarz's inequality

$$(\mathcal{J}\Phi, a_i[a_i, \mathcal{J}]\Phi) = (a_i^*\mathcal{J}\Phi, [a_i, \mathcal{J}]\Phi) \leq \|a_i^*\mathcal{J}\Phi\| \ \|[a_i, \mathcal{J}]\Phi\| \ . \tag{5.19}$$

The second factor is treated in precisely the same fashion as in Step 1. The first factor cannot be estimated directly in terms of the energy, since the function $\mathcal{J}\Phi$ is not an eigenfunction. This will be dealt with below where we estimate the term $\|a^*\mathcal{J}^2\Phi\|$.

The term

$$(\mathcal{J}\Phi, [a_i, \mathcal{J}]a_i\Phi) \ , \tag{5.20}$$

can be written, using Lemma 4.2, as

$$\begin{aligned} &(\mathcal{J}\Phi, \mathcal{J}a(h(x_i - \cdot)(j_1(\cdot) - 1))a(h(x_i - \cdot))\Phi) \\ &\qquad = \left(\mathcal{J}^2\Phi, a(h(x_i - \cdot))a(h(x_i - \cdot)(j_1(\cdot) - 1))\Phi\right) \end{aligned} \tag{5.21}$$

which, again using Schwarz's inequality, can be bounded by

$$\|a^*(h(x_i - \cdot))\mathcal{J}^2\Phi\| \, \|a(h(x_i - \cdot)(j_1(\cdot) - 1))\Phi\| \, . \tag{5.22}$$

As before, the first factor cannot be estimated in terms of the energy, since $\mathcal{J}^2\Phi$ is not an eigenstate. Note, however, that

$$\|a^*\mathcal{J}^2\Phi\|^2 = \|a\mathcal{J}^2\Phi\|^2 + \|h\|^2\|\mathcal{J}^2\Phi\|^2 \, . \tag{5.23}$$

and the first term on the right side can be estimated by

$$\|h\|^2 \left(\mathcal{J}^2\Phi, \mathcal{N}\mathcal{J}^2\Phi\right) \leq \|h\|^2 \left(\Phi, \mathcal{N}\Phi\right) \, . \tag{5.24}$$

This follows from the formula

$$\mathcal{N} = \sum_{j=1}^{\infty} a^*(f_j)a(f_j) \, , \tag{5.25}$$

which is valid for any orthonormal basis $\{f_j\}$, in which we pick $f_1(y) = h(x-y)/\|h(x-\cdot)\|$, and from (5.9). (Here h is an abbreviation for the coupling functions.) Thus, using Lemma 5.1,

$$|\sum_{i=1}^{n} (\mathcal{J}\Phi, [a_i a_i, \mathcal{J}]\Phi)| \leq C\frac{1}{(L-2R_0)^\gamma}\left(\frac{R_0}{L^\gamma}\right)(1 + |\log(\Lambda R_0)|) \, . \tag{5.26}$$

Step 3. By taking adjoints the third term in (2), $\sum_{i=1}^n [a_i^* a_i^*, \mathcal{J}]$ leads to the expression

$$-\sum_{i=1}^{n} ([a_i a_i, \mathcal{J}]\mathcal{J}\Phi, \Phi) \tag{5.27}$$

and can be dealt with in the same fashion as in Step 2. It remains to analyze $\sum_{i=1}^n [a_i^* a_i, \mathcal{J}] = \sum_{i=1}^n a_i^*[a_i, \mathcal{J}] + [a_i^*, \mathcal{J}]a_i$. The first term is estimated using

$$(a_i\mathcal{J}\Phi, [a_i, \mathcal{J}]\Phi) \leq \|a_i\mathcal{J}\Phi\| \, \|[a_i, \mathcal{J}]\Phi\| \, , \tag{5.28}$$

while the second one can be written as

$$-([a_i, \mathcal{J}]\mathcal{J}\Phi, a_i\Phi) \tag{5.29}$$

which, once more by Schwarz's inequality, can be bounded by

$$\|[a_i, \mathcal{J}]\mathcal{J}\Phi\| \, \|a_i\Phi\| \, . \tag{5.30}$$

Both these terms have been estimated previously. □

We come now to the third lemma needed for the proof of Lemma 5.5. This lemma concerns only the real part of a commutator expectation value (5.31), but this is all we need for Lemma 5.5. The reason is that the total commutator in Lemma 5.5 is manifestly real, since $\Phi(n)$ is an eigenstate of $H^0(n)$ and $\mathcal{J}$ is selfadjoint. On the other hand, the piece of the commutator considered in Lemma 5.3 is also manifestly real and the only other part of $H^0(n)$ to be considered is the potential energy terms, which commute with $\mathcal{J}$. Therefore, the commutator expectation value in (5.31) is, in fact, real. The proof of Lemma 5.4 is greatly simplified, however, by being able to ignore the (non-existent) imaginary part.

LEMMA 5.4 (Commutator of $\mathcal{J}$ with the field energy). *The ground state Φ satisfies the bound*

$$\Re\left(\mathcal{J}\Phi, [H_f, \mathcal{J}]\,\Phi\right) \leq \frac{C}{L}\left(\frac{R_0}{L^\gamma}\right)\left(1 + |\log(\Lambda R_0)|\right)^{1/2} \tag{5.31}$$

for any $\gamma < 1$. C is a constant that depends on γ, n, Λ but not on R_0 and L.

PROOF: It is convenient to write the field energy of a state Φ in the form

$$(\Phi, H_f\Phi) = (2\pi)^3 \sum_\lambda \left(a_\lambda(\cdot)\Phi, \sqrt{-\Delta}\; a\lambda(\cdot)\Phi\right) = 4\pi \sum_\lambda \int \frac{\|a_\lambda(x)\Phi - a_\lambda(y)\Phi\|^2}{|x-y|^4} dxdy \ , \tag{5.32}$$

(see [10, Eq. 7.12(4)]). Next, we note that the commutator expression (5.31) is given by

$$(\mathcal{J}\Phi, H_f\mathcal{J}\Phi) - \Re\left(\mathcal{J}\Phi, \mathcal{J}H_f\Phi\right) = 4\pi \sum_\lambda \int \frac{\|a_\lambda(x)\mathcal{J}\Phi - a_\lambda(y)\mathcal{J}\Phi\|^2}{|x-y|^4} dxdy$$
$$- 4\pi \sum_\lambda \Re \int \frac{\left(a_\lambda(x)\mathcal{J}^2\Phi - a_\lambda(y)\mathcal{J}^2\Phi, a_\lambda(x)\Phi - a_\lambda(y)\Phi\right)}{|x-y|^4} dxdy \ . \tag{5.33}$$

First, we investigate the numerator of the sum of the two integrands, which is

$$(a_\lambda(x)\mathcal{J}\Phi, a_\lambda(x)\mathcal{J}\Phi) - \Re\left(a_\lambda(x)\mathcal{J}^2\Phi, a_\lambda(x)\Phi\right)$$
$$- \Re\left(a_\lambda(x)\mathcal{J}\Phi, a_\lambda(y)\mathcal{J}\Phi\right) + \Re\left(a_\lambda(x)\mathcal{J}^2\Phi, a_\lambda(y)\Phi\right) \tag{5.34}$$

plus the same thing with y and x exchanged. For brevity's sake we have omitted the sums over λ here and in the following. We note that the x-x terms (and likewise the y-y terms) cancel. This follows from

$$\begin{aligned}(a_\lambda(x)\mathcal{J}\Phi, a_\lambda(x)\mathcal{J}\Phi) - \Re\left(a_\lambda(x)\mathcal{J}^2\Phi, a_\lambda(x)\Phi\right) = \\ (a_\lambda(x)\mathcal{J}\Phi, a_\lambda(x)\mathcal{J}\Phi) - \Re\left(\mathcal{J}a_\lambda(x)\mathcal{J}\Phi, a_\lambda(x)\Phi\right) - \Re\left([a_\lambda(x),\mathcal{J}]\,\mathcal{J}\Phi, a_\lambda(x)\Phi\right) \\ = \Re\left(a_\lambda(x)\mathcal{J}\Phi, [a_\lambda(x),\mathcal{J}]\,\Phi\right) - \Re\left([a_\lambda(x),\mathcal{J}]\,\mathcal{J}\Phi, a_\lambda(x)\Phi\right)\ , \quad (5.35)\end{aligned}$$

which, together with Lemma 4.2, yields

$$\begin{aligned}(j_1(x)-1)\Re\left(a_\lambda(x)\mathcal{J}\Phi, \mathcal{J}a_\lambda(x)\Phi\right) - (j_1(x)-1)\Re\left(\mathcal{J}a_\lambda(x)\mathcal{J}\Phi, a_\lambda(x)\Phi\right) \\ = (j_1(x)-1)\left[\Re\left(a_\lambda(x)\mathcal{J}\Phi, \mathcal{J}a_\lambda(x)\Phi\right) - \Re\left(a_\lambda(x)\mathcal{J}\Phi, \mathcal{J}a_\lambda(x)\Phi\right)\right] = 0\ . \quad (5.36)\end{aligned}$$

Now we deal with last two terms in (5.34).

$$\begin{aligned}\Re\left(a_\lambda(x)\mathcal{J}^2\Phi, a_\lambda(y)\Phi\right) - \Re\left(a_\lambda(x)\mathcal{J}\Phi, a_\lambda(y)\mathcal{J}\Phi\right) \\ = \Re\left([a_\lambda(x),\mathcal{J}]\,\mathcal{J}\Phi, a_\lambda(y)\Phi\right) + \Re\left(a_\lambda(x)\mathcal{J}\Phi, \mathcal{J}a_\lambda(y)\Phi\right) \\ - \Re\left(a_\lambda(x)\mathcal{J}\Phi, a_\lambda(y)\mathcal{J}\Phi\right) \\ = \Re\left([a_\lambda(x),\mathcal{J}]\,\mathcal{J}\Phi, a_\lambda(y)\Phi\right) + \Re\left(a_\lambda(x)\mathcal{J}\Phi, [\mathcal{J}, a_\lambda(y)]\,\Phi\right)\ . \quad (5.37)\end{aligned}$$

Again, by Lemma 4.2, this equals

$$(j_1(x)-1)\Re\left(a_\lambda(x)\mathcal{J}\Phi, \mathcal{J}a_\lambda(y)\Phi\right) - (j_1(y)-1)\Re\left(a_\lambda(x)\mathcal{J}\Phi, \mathcal{J}a_\lambda(y)\Phi\right)\ . \quad (5.38)$$

Commuting the $\mathcal{J}$ once more with the a's leads to

$$\begin{aligned}(j_1(x)-1)\Re\left([a_\lambda(x),\mathcal{J}]\,\Phi, \mathcal{J}a_\lambda(y)\Phi\right) - (j_1(y)-1)\Re\left([a_\lambda(x),\mathcal{J}]\,\Phi, \mathcal{J}a_\lambda(y)\Phi\right) \\ + \{j_1(x)-j_1(y)\}\,\Re\left(\mathcal{J}a_\lambda(x)\Phi, \mathcal{J}a_\lambda(y)\Phi\right)\ . \quad (5.39)\end{aligned}$$

We do not have to worry about the last term, since it is the product of a symmetric and an antisymmetric term in the variables x and y, and thus its x-y integral with $|x-y|^{-4}$ in (7) vanishes. The other term, using Lemma 4.2, is of the form

$$\left\{(j_1(x)-1)^2 - (j_1(y)-1)(j_1(x)-1)\right\}\Re\left(\mathcal{J}a_\lambda(x)\Phi, \mathcal{J}a_\lambda(y)\Phi\right)\ . \quad (5.40)$$

Taking into account the terms with x and y exchanged we find that (5.33) equals

$$4\pi\sum_\lambda \int \frac{(j_1(x)-j_1(y))^2\,\Re\left(\mathcal{J}a_\lambda(x)\Phi, \mathcal{J}a_\lambda(y)\Phi\right)}{|x-y|^4}dxdy\ . \quad (5.41)$$

Now we use Lemma 5.1 to get an estimate on the size of (5.41). Recall that the function $j_1(x)$, which defines $\mathcal{J}$ and which is defined in (4.21), is identically equal to 1 on $\cup_{1=1}^n Q_i$, where Q_i is the ball of radius $L/2$ equicentered with the ball B_i. Moreover $j_1(x) = 0$ whenever the distance of x to the center of every B_i exceeds L. Write $1 = \chi_1 + \chi_2 + \chi_3$ where χ_1 is the characteristic function of $\cup_{1=1}^n Q_i$ and χ_2 is the characteristic function of the shell between $\cup_{1=1}^n Q_i$ and $\Sigma = \cup_{1=1}^n P_i$. Finally, χ_3 is the characteristic function of the outside region (on which $j_2(x) = 1$ and $j_1(x) = 0$). We note, for later use, that $\int \chi_1 \leq CnL^3$ and $\int \chi_2 \leq CnL^3$, where C is a universal constant.

Next, we analyze each of the terms

$$T_{i,j} = 4\pi \int \frac{(j_1(x) - j_1(y))^2 \chi_i(x)\chi_j(y) \Re \left(\mathcal{J}a_\lambda(x)\Phi, \mathcal{J}a_\lambda(y)\Phi\right)}{|x-y|^4} dxdy \ . \tag{5.42}$$

Clearly, $T_{1,1} = T_{3,3} = 0$. To bound the other $T_{i,j}$'s we recall that

$$(j_1(x) - j_1(y))^2 \leq \frac{C}{L^2}|x-y|^2 \ . \tag{5.43}$$

With this and Schwarz's inequality, $T_{i,j}$ is bounded by

$$\begin{aligned} T_{i,j} &\leq \frac{C}{L^2} \int \frac{\chi_i(x)\|\mathcal{J}a_\lambda(x)\Phi\| \ \chi_j(y)\|\mathcal{J}a_\lambda(y)\Phi\|}{|x-y|^2} dxdy \\ &\leq \frac{C}{L^2} \int \frac{\chi_i(x)\|a_\lambda(x)\Phi\| \ \chi_j(y)\|a_\lambda(y)\Phi\|}{|x-y|^2} dxdy. \end{aligned} \tag{5.44}$$

Denote $\|a_\lambda(x)\Phi\|$ by $f(x)$. Consider the terms $i = 3$ and $j = 1, 2$. Using the Hardy-Littlewood-Sobolev inequality (see [10, Theorem 4.3] with $1/2 + 5/6 + 2/3 = 2$), we get the bound

$$T_{3,j} \leq \frac{C}{L^2}\|\chi_3 f\|_2 \|\chi_j f\|_{6/5} \ , \quad j = 1, 2 \ . \tag{5.45}$$

By Hölder's inequality

$$\|\chi_j f\|_{6/5} \leq \|\chi_j\|_3 \|f\|_2 \leq Cn^{1/3}L\|f\|_2 \ , \tag{5.46}$$

and hence, for $j = 1, 2$,

$$T_{3,j} \leq \frac{Cn^{1/3}}{L}(\Phi, \mathcal{N}\Phi)^{1/2}(\Phi, \mathcal{N}_{\text{out}}\Phi)^{1/2} \ . \tag{5.47}$$

Note that $\|\chi_3 f\|_2$ is proportional to $(\Phi, \mathcal{N}_{\text{out}}\Phi)^{1/2}$ while $\|f\|_2$ is proportional to $(\Phi, \mathcal{N}\Phi)^{1/2}$.

The next term to consider is $i = 2$ and $j = 1, 2, 3$. Again, H-L-S leads to the bound

$$T_{2,j} \leq \frac{C}{L^2} \|\chi_j f\|_2 \|\chi_2 f\|_{6/5} \ , \ j = 1, 2, 3 \ . \tag{5.48}$$

Applying Hölder's inequality yields

$$\|\chi_2 f\|_{6/5} \leq \|\chi_2\|_3 \ \|\chi_2 f\|_2 \leq C n^{1/3} L \|\chi_2 f\|_2 \ , \tag{5.49}$$

and hence the term with $i = 2$ and $j = 1, 2, 3$ is also bounded above by

$$\frac{C n^{1/3}}{L} (\Phi, \mathcal{N}\Phi)^{1/2} (\Phi, \mathcal{N}_{\text{out}}\Phi)^{1/2} \ , \tag{5.50}$$

where we used $(\Phi, \mathcal{N}_{\text{out}}\Phi)^{1/2} \geq \|\chi_2 f\|_2$. It is the term $(\Phi, \mathcal{N}\Phi)$ which yields the logarithmic term in formula (5.31).

Finally, the term $i = 1$, $j = 2$ is the same as $i = 2$, $j = 1$, and the term $i = 1$, $j = 3$ is the same as $i = 3$, $j = 1$, both of which have been already treated.

Collecting the estimates we have shown that

$$\Re \left(\mathcal{J}\Phi, [H_f, \mathcal{J}]\, \Phi \right) \leq \frac{C n^{1/3}}{L} (\Phi, \mathcal{N}\Phi)^{1/2} (\Phi, \mathcal{N}_{\text{out}}\Phi)^{1/2}$$

which, by Lemma 5.1, proves the lemma. □

We are now ready to prove the estimate stated at the end of the proof of Theorem 4.3, i.e.,

LEMMA 5.5. *For all $L > 2R_0$ we have the estimate*

$$\frac{\left(\mathcal{J}\Phi(n), \left[H^0(n), \mathcal{J} \right] \Phi(n) \right)}{(\mathcal{J}\Phi(n), \mathcal{J}\Phi(n))} \leq \frac{C}{(L - 2R_0)^\gamma} \left(\frac{R_0}{L^\gamma} \right) (1 + |\log(\Lambda R_0)|) \tag{5.51}$$

for all $\gamma < 1$. The constant C depends on n, Λ, γ but not on R_0 and L.

PROOF: The lemma is a direct consequence of Lemmas 5.2, 5.3 and 5.4. □

LEMMA 5.6 (Bound on the error terms). *For each fixed $x \in \mathbb{R}^3$,*

$$(\mathcal{J}\Phi, a(h(x - \cdot))^2 \mathcal{J}\Phi) \leq C_\gamma \frac{1}{D^{2\gamma}} \max \{ (\Phi, \mathcal{N}\Phi), \ 1 \} , \tag{5.52}$$

for any $\gamma < 1$, where D is the distance of x to the support of j_1. The same estimate holds for $a^*(h(x - \cdot))^2$ and for $a^*(h(x - \cdot))a(h(x - \cdot))$ in place of $a(h(x - \cdot))^2$.

PROOF: Using Lemma 4.2,

$$(\mathcal{J}\Phi, a(h(x-\cdot))^2\mathcal{J}\Phi) = (\mathcal{J}\Phi, \mathcal{J}a(h(x-\cdot)j_1(\cdot))^2\Phi) = (a^*(h(x-\cdot)j_1(\cdot))\mathcal{J}^2\Phi, a(h(x-\cdot)j_1(\cdot))\Phi). \quad (5.53)$$

By Schwarz's inequality this is bounded above by

$$\|(a^*(h(x-\cdot)j_1(\cdot))\mathcal{J}^2\Phi\| \, \|a(h(x-\cdot)j_1(\cdot))\Phi)\| \ . \quad (5.54)$$

Similar to the proof of Lemma 5.3, the second factor in (5.54) can be bounded as follows.

$$\begin{aligned}\|a(h(x-\cdot)j_1(\cdot))\Phi\| &\leq \int j_1(y) \ \|h(x-y)a(y)\Phi\|dy \\ &\leq \int j_1(y) \ |h(x-y)|\|a(y)\Phi\|dy \\ &\leq \left(\int j_1(y)^2 \ |h(x-y)|^2dy\right)^{1/2} \left(\int \|a(y)\Phi\|^2dy\right)^{1/2} .\end{aligned} \quad (5.55)$$

The second factor here is $(\Phi, \mathcal{N}\Phi)^{1/2}$ while the first factor can be estimated, using the fact that the support of j_1 and the point x are a distance D apart, as

$$\frac{1}{D^\gamma}\left(\int j_1(y)^2 \ |x-y|^{2\gamma}|h(x-y)|^2dy\right)^{1/2} \leq \frac{C}{D^\gamma} \quad (5.56)$$

by Lemma B.1.

The first factor in (5.54) can be bounded as follows.

$$\|(a^*(h(x-\cdot)j_1(\cdot))\mathcal{J}^2\Phi\|^2 = (\mathcal{J}^2\Phi, a(h(x-\cdot)j(\cdot))a^*(h(x-\cdot)j_1(\cdot))\mathcal{J}^2\Phi) \quad (5.57)$$

$$= (\mathcal{J}^2\Phi, [a(h(x-\cdot)j_1(\cdot)), a^*(h(x-\cdot)j_1(\cdot))]\mathcal{J}^2\Phi) + \|a(h(x-\cdot)j_1(\cdot))\mathcal{J}^2\Phi\|^2 . \quad (5.58)$$

The first (commutator) term in (5.58) equals $\int |h(x-y)|^2 j_1(y)^2 dy \ \|\mathcal{J}^2\Phi\|^2$, which is bounded by $C/D^{2\gamma}$. The second term was treated in (5.55) and is thus bounded by $C/D^{2\gamma}(\Phi, \mathcal{N}\Phi)$. (Note that $(\Phi, \mathcal{N}\Phi) \geq (\mathcal{J}\Phi, \mathcal{N}\mathcal{J}\Phi)$.)

It is immediate that similar estimates hold when aa is replaced by a^*a^* or by a^*a. □

6 Infrared Bounds

In this section we prove Lemma 5.1. It will follow from infrared bounds similar to the ones proved in [1] and [7], which have been proved to hold for

the electrons bound to the Coulomb potential. Those infrared bounds are not sufficient, however, for the localized wave function of the 'free' electrons. The chief reason for this insufficiency is that we need to know the dependence of the constants in the infrared bounds on the parameter R_0. Ultimately, the trouble stems from the fact that we do not know the positions of the n localized electrons, not even remotely. Thus, a direct application of the estimates in [7] would lead to constants that can grow conceivably as R_0^2 or even faster for large R_0. This problem does not occur for the the bound electrons since, in that case, the electrons are localized by the Coulomb potential and the infrared bounds do not depend on the parameter R_0. The theorem below holds for the localized electrons, as well as for the bound electrons. The proof for bound electrons is easier and is omitted.

As in Sect. 5 the Dirichlet ground state $\Phi_D(n)$ for the 'free' electrons localized in in $\Omega(B_1, \ldots, B_n)$ is denoted simply by Φ. Its energy is $E_D^0(n)$. The ground state for the bound system with Hamiltonian $H^V(N')$ is denoted by Ψ.

LEMMA 6.1 (Infrared bounds). *The following infrared bounds hold for* Φ*:*

$$\|\widehat{a}_\lambda(k)\Phi\| \leq \frac{C}{|k|^{3/2}}\widehat{\chi}_\Lambda(k) \ , \tag{6.1}$$

$$\|\widehat{a}_\lambda(k)\Phi\| \leq \frac{CR_0}{|k|^{1/2}}\widehat{\chi}_\Lambda(k) \ . \tag{6.2}$$

The vector $\widehat{a}_\lambda(k)\Phi$ *is a sum of* n *terms of the form* $e^{-ik\cdot Y_j}\widehat{T}_{j,\lambda}(k)$ *where* $\widehat{T}_{j,\lambda}(k)$ *is given by (6.25) and satisfies the estimates*

$$\|\nabla_k \widehat{T}_{j,\lambda}(k)\| \leq \frac{CR_0}{|k|^{1/2}(k_1^2+k_2^2)^{1/2}}\widehat{\chi}_\Lambda(k) + \frac{CR_0}{|k|^{1/2}}\nabla_k\widehat{\chi}_\Lambda(k) \tag{6.3}$$

The vectors Y_j *are defined below. The constant* C *depends on* n*, on the ultraviolet cutoff* Λ *and it is a monotone decreasing function of* R_0*. Similar bounds but without the factor* R_0 *hold for the bound electron ground state* Ψ*.*

PROOF: We prove first the bound (6.2) in detail. As a first step one performs an operator valued gauge transformation (see [7, Eq. 47]) by applying the unitary operator (in which A is the vector potential (2.4))

$$U(x) = \exp[-i\sqrt{\alpha}\sum_{j=1}^{m}\phi_j(x)(x-Y_j)\cdot A(Y_j)] \tag{6.4}$$

to the wave function in each of its variables, i.e.,

$$\Phi \to \widetilde{\Phi} = \prod_{i=1}^{n} U(x_i)\Phi =: \mathcal{U}\Phi \ . \tag{6.5}$$

Here, ϕ_j is a suitably chosen smooth function of compact support and the Y_j are suitably chosen vectors. Note that the factors in the product commute since $A(x)$ commutes with $A(y)$ for all x and y.

Next, we describe the functions ϕ_j. Consider the balls $B_i(2R_0)$, which are concentric with the B_i but with twice the radius, and group them into clusters according to whether they overlap or not. We denote the number of these clusters by m. Such a cluster of balls C_j has a diameter that is bounded above by $4R_0$ times the number of balls in the cluster and hence bounded by $4nR_0$. Denote by Y_j the center of the cluster C_j which is defined to be the center of the smallest ball that contains all the balls $B_i(2R_0)$ belonging to that cluster. We choose functions ϕ_j that are smooth , supported in the union of the balls $B_i(2R_0)$ that belong to the cluster C_j and that are identically one on the union of the balls B_i. In particular $\sum_{j=1}^m \phi_j(x) = 1$ for $x \in \cup_{i=1}^n B_i$.

The gauge transformation $\mathcal{U}$ transforms the Hamiltonian $H^0(n)$ into the Hamiltonian

$$\widetilde{H}^0(n) = \mathcal{U}H^0(n)\mathcal{U}^* = \sum_{i=1}^n \left[(p_i + \sqrt{\alpha}\widetilde{A}(x_i))^2 + \frac{g}{2}\sqrt{\alpha}\,\sigma_i \cdot B(x_i)\right] + \alpha \sum_{i<j} \frac{1}{|x_i - x_j|} + \widetilde{H}_f \tag{6.6}$$

where the new field $\widetilde{A}(x) = \mathcal{U}A(x)\mathcal{U}^* + \alpha^{-1/2}\mathcal{U}p\mathcal{U}^* = A(x) + \alpha^{-1/2}\mathcal{U}p\mathcal{U}^*$ is given by

$$\widetilde{A}(x) = A(x) - \sum_{j=1}^m \phi_j(x)A(Y_j) - \sum_{j=1}^m \nabla\phi_j(x)(x - Y_j) \cdot A(Y_j)\ , \tag{6.7}$$

in which $A(x)$ is still given by (2.4). The transformed field energy $\widetilde{H}_f$ is given as in (2.9) but with $\widehat{a}_\lambda(k)$ replaced by the transformed creation and destruction operators

$$b_\lambda(k, X) = \mathcal{U}\widehat{a}_\lambda(k)\mathcal{U}^* = \widehat{a}_\lambda(k) - i\sqrt{\alpha}w_\lambda(k, X) \tag{6.8}$$

with

$$w_\lambda(k, X) = \sum_{i=1}^n \sum_{j=1}^m \phi_j(x_i)(x_i - Y_j) \cdot \frac{\varepsilon_\lambda(k)}{|k|^{1/2}} e^{-ik\cdot Y_j} \widehat{\chi}_\lambda\,(k)\ . \tag{6.9}$$

As before, the letter X denotes the vector $(x_1, \ldots, x_n)$. We note that

$$\widehat{a}_\lambda(k)\Phi = \mathcal{U}^* \left[\widehat{a}_\lambda(k)\widetilde{\Phi} - i\sqrt{\alpha}w_\lambda(k, X)\widetilde{\Phi}\right]\ . \tag{6.10}$$

Since Φ satisfies the Schrödinger equation we can apply the standard pull-through formula [1, 7] and compute

$$\begin{aligned}
&\left[\widetilde{H}^0(n) - E_D^0(n)\right] \widehat{a}_\lambda(k)\widetilde{\Phi} = \left[\widetilde{H}^0(n), \widehat{a}_\lambda(k)\right] \widetilde{\Phi} = \\
&2\widehat{\chi}_\Lambda(k)\sqrt{\alpha}\,|k|^{-1/2}\varepsilon_\lambda(k)\cdot\sum_{i=1}^{n}(p_i+\sqrt{\alpha}\,\widetilde{A}(x_i))\left\{\sum_{j=1}^{m}(e^{-ik\cdot Y_j}-e^{-ik\cdot x_i})\phi_j(x_i)\right\}\widetilde{\Phi} \\
&\quad + 2\widehat{\chi}_\Lambda(k)\sqrt{\alpha}\sum_{i=1}^{n}\sum_{j=1}^{m}(p_i+\sqrt{\alpha}\,\widetilde{A}(x_i))\cdot\nabla\phi_j(x_i)(x_i-Y_j)\cdot\frac{\varepsilon_\lambda(k)}{\sqrt{|k|}}e^{-ik\cdot Y_j}\widetilde{\Phi} \\
&\qquad + i\frac{g}{2}\widehat{\chi}_\Lambda(k)\sqrt{\alpha}\,\frac{k\wedge\varepsilon_\lambda(k)}{\sqrt{|k|}}\cdot\sum_{i=1}^{n}\sigma_j e^{-ik\cdot x_i}\widetilde{\Phi} - |k|b_\lambda(k,X)\widetilde{\Phi}\ . \quad (6.11)
\end{aligned}$$

The term $\sum_{j=1}^m e^{-ik\cdot x_i}\phi_j(x_i)$ stems from the commutator of $\widehat{a}_\lambda(k)$ with $A(x_i)$, which yields a term proportional to $e^{-ik\cdot x_i}$ without any summation on j. Using, however, the relation $\sum_{j=1}^m \phi_j(x_i) = 1$, which is valid for any x_i in $\cup_{j=1}^n B_j$, we get that $e^{-ik\cdot x_i} = \sum_{j=1}^m e^{-ik\cdot x_i}\phi_j(x_i)$. Note that x_i has to be in $\cup_{j=1}^n B_j$ for, otherwise, $\widetilde{\Phi}$ vanishes.

Likewise, the second term in the above formula appears to have bad infrared behavior, but in order that Φ does not vanish it is necessary that x_i be in one of the balls. But then $\nabla\phi_j(x_i) = 0$ since ϕ_j is constant, and this term does not contribute.

Since $\widetilde{H}^0(n) - E_D^0(n)$ is nonnegative the operator $\widetilde{H}^0(n) - E_D^0(n) + |k|$ has a bounded inverse $R(k)$. Thus (6.11) leads to the equation

$$\begin{aligned}
\widehat{a}_\lambda(k)\widetilde{\Phi} &= \sqrt{\alpha}\sum_{j=1}^{m} e^{-ik\cdot Y_j} 2\widehat{\chi}_\Lambda(k)\ |k|^{-1/2}\varepsilon_\lambda(k)\cdot R(k) \\
&\qquad \times\sum_{i=1}^{n}(p_i+\sqrt{\alpha}\widetilde{A}(x_i))(1-e^{ik\cdot(Y_j-x_i)})\phi_j(x_i)\widetilde{\Phi} \\
&+ i\sqrt{\alpha}\sum_{i=1}^{n}\frac{g}{2}\widehat{\chi}_\Lambda(k)\frac{k\wedge\varepsilon_\lambda(k)}{\sqrt{|k|}}\cdot R(k)\sigma_i e^{-ik\cdot x_i}\widetilde{\Phi} + i\sqrt{\alpha}|k|R(k)w_\lambda(k,X)\widetilde{\Phi}\ .
\end{aligned} \quad (6.12)$$

As in [7], simple estimates, using Schwarz's inequality, lead to

$$\|\widehat{a}_\lambda(k)\widetilde{\Phi}\| \le 2\widehat{\chi}_\Lambda(k)\sqrt{\alpha}\ |k|^{1/2}\|R(k)\sum_{i=1}^{n}(p_i+\sqrt{\alpha}\widetilde{A}(x_i))^2R(k)\|^{1/2}$$
$$\times\left(\sum_{i=1}^{n}(\sum_{j=1}^{m}\||x_i-Y_j|\phi_j(x_i)\widetilde{\Phi}\|)^2\right)^{1/2}$$
$$+\frac{|g|}{2}\widehat{\chi}_\Lambda(k)\sqrt{\alpha}\ n|k|^{1/2}\|R(k)\widetilde{\Phi}\|+|k|\|R(k)\|\|w_\lambda(k,X)\widetilde{\Phi}\|\ . \quad (6.13)$$

Note that the index j in the first summand is determined by the ball to which the electron i belongs. Therefore, $|x_i - Y_j| \le 2nR_0$.

Lemma A.1 states that

$$\frac{g\sqrt{\alpha}}{2}\sum_{j=1}^{N}\sigma_j\cdot B(x_j)+H_f+C\ge 0 \quad (6.14)$$

where

$$C=\frac{1}{8\pi^2}g^2\alpha N^2\int\widehat{\chi}_\Lambda(k)^2dk\ . \quad (6.15)$$

Thus we also have that

$$\frac{g\sqrt{\alpha}}{2}\sum_{j=1}^{N}\sigma_j\cdot B(x_j)+\widetilde{H}_f+C\ge 0\ , \quad (6.16)$$

(note that the gauge transformation $\mathcal{U}$ commutes with $B(x)$) and hence

$$\beta := \|R(k)\sum_{i=1}^{n}(p_i+\sqrt{\alpha}\widetilde{A}(x_i))^2R(k)\|$$
$$\le\|R(k)\left(\sum_{i=1}^{n}[(p_i+\sqrt{\alpha}\widetilde{A}(x_i))^2+\frac{g}{2}\sigma_iB(x_i)]+\widetilde{H}_f+C\right)R(k)\|$$
$$=\|R(k)\left(\widetilde{H}^0(n)+C\right)R(k)\|\ . \quad (6.17)$$

Thus, by subtracting and adding $E_D^0-|k|$,

$$\beta\le\|R(k)\left(\widetilde{H}^0(n)-E_D^0(n)+|k|\right)R(k)\|+(|E_D^0(n)-|k||+C)\|R(k)^2\|$$
$$=\|R(k)\|+(|E_D^0(n)-|k||+C)\|R(k)^2\| \quad (6.18)$$

where the constant C depends on Λ and n. For the last term in (6.13) we have that

$$\|w_\lambda(k,X)\widetilde{\Phi}\|\le\widehat{\chi}_\Lambda(k)|k|^{-1/2}\sum_{j=1}^{m}\sum_{i=1}^{n}\||x_i-Y_j|\phi_j(x_i)\widetilde{\Phi}\|\ . \quad (6.19)$$

Since $\|R(k)\| = 1/|k|$, we have that $\|R(k)\widetilde{\Phi}\| \leq 1/|k|$.

By combining these estimates with (6.13) and using $|x_i - Y_j|\phi_j(x_i) \leq 2nR_0$, we obtain the bound

$$\|\widehat{a}_\lambda(k)\widetilde{\Phi}\| \leq CR_0|k|^{-1/2}\|\widetilde{\Phi}\|\widehat{\chi}_\lambda(k) \ , \tag{6.20}$$

where the constant C depends on Λ, n and the energy. This estimate carries over to the state Φ by (6.10) since $w_\lambda(k,X)$ applied to Φ satisfies the same estimate, as we see in (6.19). Note that the energy $E_D^0(n)$ does depend on R_0 but it is monotone decreasing as a function of R_0 (by the variational principle for Dirichlet boundary conditions) and it is uniformly bounded below.

Next, we observe in (6.12) that $\widehat{a}_\lambda(k)\widetilde{\Phi}$ is a sum of m terms of the form $e^{-ik\cdot Y_j}\widehat{S}_j(k)$ where

$$\begin{aligned}\widehat{S}_{j,\lambda}(k) = \sqrt{\alpha}2\widehat{\chi}_\Lambda(k)\ |k|^{-1/2}\varepsilon_\lambda(k)\cdot R(k) \\ \times \sum_{i=1}^n (p_i + \sqrt{\alpha}\widetilde{A}(x_i))(1 - e^{ik\cdot(Y_j - x_i)})\phi_j(x_i)\widetilde{\Phi} \\ + i\sqrt{\alpha}\frac{g}{2}\widehat{\chi}_\Lambda(k)\frac{k\wedge\varepsilon_\lambda(k)}{\sqrt{|k|}}\cdot R(k)\sum_{i=1}^n \sigma_i\phi_j(x_i)e^{-ik\cdot(x_i - Y_j)}\widetilde{\Phi} \\ + i\sqrt{\alpha}\widehat{\chi}_\Lambda(k)|k|^{1/2}\varepsilon_\lambda(k)\cdot R(k)\sum_{i=1}^n \phi_j(x_i)(x_i - Y_j)\widetilde{\Phi} \ ,\end{aligned} \tag{6.21}$$

where we have used the identity

$$\sum_{i=1}^n \sigma_i e^{-ik\cdot x_i}\widetilde{\Phi} = \sum_{j=1}^m e^{-ik\cdot Y_j}\sum_{i=1}^n \sigma_i\phi_j(x_i)e^{-ik\cdot(x_i - Y_j)}\widetilde{\Phi} \ . \tag{6.22}$$

Since by (6.8)

$$\widehat{a}_\lambda(k)\Phi = \mathcal{U}^*\left[\widehat{a}_\lambda(k) - i\sqrt{\alpha}w_\lambda(k,X)\right]\widetilde{\Phi} \ , \tag{6.23}$$

we obtain that

$$\widehat{a}_\lambda(k)\Phi = \sum_{j=1}^n e^{-ik\cdot Y_j}\widehat{T}_{j,\lambda}(k) \tag{6.24}$$

where

$$\widehat{T}_{j,\lambda}(k) = \mathcal{U}^*\left[\widehat{S}_{j,\lambda}(k)\widetilde{\Phi} - i\sqrt{\alpha}w_\lambda(k,X)\right]\widetilde{\Phi} \ . \tag{6.25}$$

Differentiating these expressions with respect to k and proceeding in the same fashion as in the proof of (6.2) yields the estimate (6.3).

Differentiating the polarization vectors (2.7) yields the factor $\sqrt{k_1^2+k_2^2}$ in the denominator of (6.3) . The details of the calculation are the same as the ones in [7] and are omitted. The bound (6.1 is considerable easier, since its proof does not require the gauge transformation. Otherwise the proof is word for word as the one above. Finally, the proof of the infrared bounds for Ψ is a word for word translation of the one given in [7]. Note that the localization radius does not show up in this calculation since the electrons are exponentially localized in the vicinity of the origin. □

Finally, we come to the main application of the infrared bounds proved in this section.

PROOF OF LEMMA 5.1: Using (6.1) we can write

$$(\Phi, \mathcal{N}_{\rm out}\Phi) = \int_{j_2(x)>0} \|a(x)\Phi\|^2 dx = \int_{j_2(x)>0} \|\sum_{j=1}^n T_{j,\lambda}(x-Y_j)\|^2 dx \quad (6.26)$$

which, by Schwarz's inequality is bounded above by

$$\sqrt{n}\sum_{j=1}^n \int_{j_2(x)>0} \|T_{j,\lambda}(x-Y_j)\|^2 dx \ . \quad (6.27)$$

For x in the support of j_2 we have that $|x-Y_j|>L$ and hence

$$\int_{j_2(x)>0} \|T_{j,\lambda}(x-Y_j)\|^2 dx \le \frac{1}{L^{2\gamma}} \int |x|^{2\gamma} \|T_{j,\lambda}(x)\|^2 dx \ . \quad (6.28)$$

This last term can be related to the derivative in k space of the function $\widehat{T}_{j,\lambda}(k)$ by the formula

$$\int |x|^{2\gamma} \|T_{j,\lambda}(x)\|^2 dx = C_\gamma \int \frac{\left(\nabla_k \widehat{T}_{j,\lambda}(k), \nabla_k \widehat{T}_{j,\lambda}(k')\right)}{|k-k'|^{2\gamma+1}} dk dk' \quad (6.29)$$

where the constant C_γ is given by

$$C_\gamma = (4\pi)^{-3/2} \frac{\Gamma(\frac{1+2\gamma}{2})}{\Gamma(1-\gamma)} \ . \quad (6.30)$$

Indeed, writing $Q_{j,\lambda}(x) = xT_{j,\lambda}(x)$ this formula follows from

$$\int |x|^{2\gamma-2} \|Q_{j,\lambda}(x)\|^2 dx = C_\gamma \int \frac{\left(\widehat{Q}_{j,\lambda}(k), \widehat{Q}_{j,\lambda}(k')\right)}{|k-k'|^{2\gamma+1}} dk dk' \quad (6.31)$$

[10, Corollary 5.10] and the fact that

$$\left(\widehat{Q}_{j,\lambda}(k), \widehat{Q}_{j,\lambda}(k')\right) = \left(\nabla_k \widehat{T}_{j,\lambda}(k), \nabla_k \widehat{T}_{j,\lambda}(k')\right) \ . \quad (6.32)$$

Using the bound (6.3) a straightforward calculation shows that the function $\|\nabla_k \widehat{T}_{j,\lambda}(k)\|$ is in L^p for all $p < 2$. (The relevant term in (6.3) is the first term on the right side.) Using Schwarz's inequality and the Hardy-Littlewood-Sobolev inequality [10, Theorem 4.3] we can therefore bound (6.29) by

$$C_p \left[\int \|\nabla_k \widehat{T}_{j,\lambda}(k)\|^p dk \right]^{2/p} \leq C R_0^2 \,, \tag{6.33}$$

with $p = 6/(5-2\gamma)$, which is strictly less than 2 for $\gamma < 1$. To prove (5.3) we write for some $0 < H$

$$(\Phi, \mathcal{N}\Phi) = \sum_\lambda \int_{|k|\leq H} \|\widehat{a}_\lambda(k)\Phi\|^2 dk + \sum_\lambda \int_{H\leq|k|} \|\widehat{a}_\lambda(k)\Phi\|^2 dk \,, \tag{6.34}$$

and, using (6.2) and (6.1) we get

$$C R_0 \int_{|k|\leq H} \frac{1}{|k|} \widehat{\chi}_\Lambda dk + C \int_{H\leq|k|} \frac{1}{|k|^3} \widehat{\chi}_\Lambda dk \,, \tag{6.35}$$

which, optimized over H, leads to (5.3).

The proof for the state Ψ is carried out in precisely the same fashion. □

Appendix A

LEMMA A.1. *On $\wedge^N L^2(\mathbb{R}^3;\mathbb{C}^2) \otimes \mathcal{F}$ we have that*

$$\frac{g\sqrt{\alpha}}{2} \sum_{j=1}^N \sigma_j \cdot B(x_j) + H_f + \frac{1}{8\pi^2} g^2 \alpha N^2 \int \widehat{\chi}_\Lambda(k)^2 dk \geq 0 \,. \tag{A.1}$$

PROOF: The magnetic field operator can be written in the form

$$\sum_{\lambda=1}^2 \int [c_\lambda^*(k)\widehat{a}_\lambda(k) + c_\lambda(k)\widehat{a}_\lambda^*(k)] dk \tag{A.2}$$

where

$$c_\lambda^*(k) = \frac{g\sqrt{\alpha}}{4\pi} \widehat{\chi}_\Lambda(k) \sum_j \frac{ik \wedge \varepsilon_\lambda(k)}{\sqrt{|k|}} \cdot \sigma_j e^{ik\cdot x_j} \,. \tag{A.3}$$

With this notation we can write the Hamiltonian (A.1) as

$$\sum_{\lambda=1}^2 \int |k| \left[\widehat{a}_\lambda^*(k) \otimes I + \frac{1}{|k|} c_\lambda^*(k) \right] \left[\widehat{a}_\lambda(k) \otimes I + \frac{1}{|k|} c_\lambda(k) \right] dk$$
$$- \sum_{\lambda=1}^2 \int \frac{1}{|k|} c_\lambda^*(k) c_\lambda(k) dk \tag{A.4}$$

Here, I denotes the identity operator on spin space. The first term is non-negative and crude estimates on the second yield the lemma. □

Appendix B

In this section we prove the estimates on the coupling functions $h^i_\lambda(y)$ which are defined by

$$h^i_\lambda(y) = \frac{1}{2\pi}\int \frac{1}{\sqrt{|k|}}\varepsilon^i_\lambda(k)\chi_\Lambda(k)e^{ik\cdot x}dk \ . \tag{B.1}$$

It is important to choose the polarization vectors carefully in order that their Fourier transforms (from k-space to y-space) have nice decay properties as $|y|$ tends to infinity. We shall express these decay properties in an integrated form. The reason for that is that the decay is not uniform with respect to the direction of the y variable. Recall the definitions (2.7).

LEMMA B.1 (Decay of the coupling functions). *For any $\gamma < 1$ there is a finite constant $C(\gamma)$ such that*

$$\sum_{i=1}^{3}\sum_{\lambda=1}^{2}\int |y|^{2\gamma}|h^i_\lambda(y)|^2dy \le C(\gamma) \ . \tag{B.2}$$

PROOF: First we compute the gradient of h^i_λ in k-space. It is elementary that

$$|\nabla\frac{1}{\sqrt{|k|}}\varepsilon_\lambda(k)| \le \frac{C}{\sqrt{|k|}\sqrt{k_1^2+k_2^2}} \ , \tag{B.3}$$

where C is some constant. Because χ_Λ is smooth,

$$\sum_{i=1}^{3}\sum_{\lambda=1}^{2}\int |\nabla\frac{1}{\sqrt{|k|}}\varepsilon_\lambda(k)\chi_\Lambda(k)|^p dk \le C(p) \tag{B.4}$$

for any $p < 2$. We proceed as in (6.29), (6.30) and write

$$\sum_{i=1}^{3}\sum_{\lambda=1}^{2}\int |y|^{2\gamma}|h^i_\lambda(y)|^2dy = C_\gamma\sum_{i=1}^{3}\sum_{\lambda=1}^{2}\int \frac{\overline{\nabla\widehat{h}^i_\lambda(k)}\cdot\nabla\widehat{h}^i_\lambda(k')}{|k-k'|^{2\gamma+1}}dkdk' \ . \tag{B.5}$$

Again, by the Hardy-Littlewood-Sobolev inequality [10, Theorem 4.3] this is bounded by

$$C_p\left[\sum_{i=1}^{3}\sum_{\lambda=1}^{2}\int |\nabla\frac{1}{\sqrt{|k|}}\varepsilon_\lambda(k)\chi_\Lambda(k)|^p dk\right]^{2/p} \le C_pC(p)^{2/p} \ , \tag{B.6}$$

where $p = 6/(5-2\gamma) < 2$ if $\gamma < 1$. □

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