BINDING CONDITIONS FOR ATOMIC N-ELECTRON SYSTEMS IN NON-RELATIVISTIC QED

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Abstract. We examine the binding conditions for atoms in non-relativistic QED, and prove that removing one electron from an atom requires a positive energy. As an application, we establish the existence of a ground state for the Helium atom.

Dedicated to Professor G. Zhislin, on the occasion of his seventieth birthday.

1. Introduction

One of the most fundamental results in the spectral theory of multiparticle Schrödinger operators is the proof of the existence of a ground state for atoms and positive ions. It was accomplished for the Helium atom by T. Kato in 1951 [9], and for an arbitrary atom by G. Zhislin in 1960 [12] (cf. the Zhislin theorem in [11]).

The standard approach to the proof of these results consists of two main parts. The first key ingredient is the HVZ - (Hunziker – van-Winter – Zhislin) theorem, which establishes the location of the essential spectrum, and gives a variational criterion for the existence of a bound state. The latter can be referred to as "binding conditions". The statement is that the bottom of the essential spectrum of the whole system is defined by its decomposition into two clusters. If the infimum of the spectrum of the entire system is, for all nontrivial cluster decompositions, less than the sum of the infima of the spectra of the subsystems, it follows that the whole system possesses a ground state.

For an atom with infinite nuclear mass, this condition can be written as

$$E^V(N) < E^V(N') + E^0(N-N') \quad \text{for all} \quad N' < N, \tag{1}$$

where $E^V(N)$ is the infimum of the spectrum of the atom, $E^V(N')$ is the infimum of the spectrum of the same atom without $(N-N')$ electrons, and $E^0(N-N')$ is the infimum of the spectrum of the system of $(N-N')$ electrons, which do not interact with the nucleus. Obviously, in the case of Schrödinger operators (in Quantum mechanics) $E^0(N-N') = 0$, and according to the HVZ theorem, it suffices to consider only the decompositions with $N' = N-1$ in (1).

The second key ingredient consists of the construction of a trial state for the Hamiltonian of the whole atom with energy less than $E^V(N-1)$. As noted above, this step was accomplished by T. Kato for Helium, and by G. Zhislin for the general case.

The problem of the existence of the ground states of atoms has attracted new attention in the context of non-relativistic quantum electrodynamics in the more recent literature. Bach, Fröhlich and Sigal [2] first established the existence of the ground state for the ultraviolet regularized Pauli-Fierz Hamiltonian of an atom, for sufficiently small values of some constants in the theory.

It was subsequently established in [8] that the criterion for the existence of the ground state of multiparticle Schrödinger operators can be extended to hold for Pauli-Fierz Hamiltonians in non-relativistic QED, for arbitrary values of the parameters of the theory. [1]

The problem, however, of devising a mathematically rigorous proof of the fact that the binding conditions are fulfilled for atoms apart from the one electron case, which was covered by [8], has turned out to be very complicated. To clarify the main obstacles, let us recall the basic idea underlying the proofs of the Kato and Zhislin theorems.

If the system is separated into a pair of clusters, one of which contains $N-1$ electrons close to the nucleus, and the other comprises a single electron far away, there is an attractive Coulomb potential that acts on the separated particle. If the latter is localized in a ball of radius R centered at some point with distance bR from the origin, and the subsystem with $N-1$ electrons is localized in a ball of radius R centered at the origin, the intercluster Coulomb interaction can be estimated as CR^{-1} with $C<0$ for $b>N$. At the same time, localizing the subsystems in these balls requires an energy CR^{-2} in the case of Schrödinger operators. For large R, the Coulomb term is obviously dominant, and the binding condition is fulfilled.

This is contrasted by the situation in non-relativistic QED, where the particles have to be localized together with the quantized radiation field. One can expect, on the basis of dimensional analysis [8], that such a localization requires an energy CR^{-1}, which makes it impossible to establish the dominance of the Coulomb interaction by scaling arguments.

In the work at hand, it is demonstrated how this obstacle can be overcome. We prove that if the self-energy operator T_0, restricted to states with total momentum 0, possesses a ground state, it is possible to construct a state consisting of an electron coupled to a photon field, localized in a ball of radius R with energy $\Sigma_0 + o(R^{-1})$, where Σ_0 is the self-energy of an electron. Hence, similarly as for Schrödinger operators, the localization term $o(R^{-1})$ can again be compensated by the attractive Coulomb potential. This implies that the binding condition is fulfilled for decompositions into clusters with $N-1$ and 1 particles.

Existence of the ground state of T_0 has been recently established for sufficiently small values of the fine structure constant [3]. It was proved earlier in [8] that for the decomposition into clusters with zero electrons and N electrons, the binding condition is also fulfilled. Thus, if an atom or a positive ion has only two electrons, the ground state exists.

If an atom has more than two electrons, one must also verify the binding conditions for $1 < N - N' < N$. We note that in contrast to the quantum mechanical case, a system of K electrons coupled to a photon field may have an energy smaller than the self-energy of an electron multiplied by a factor K.

To control this case, it would be sufficient to combine a straightforward modification of the method developed in this paper with a generalization of the results of [8], and to apply it to the case of a system without external potential, after separating the center of mass motion. This generalization is, however, beyond the scope of the present work.

The first proof of the existence of the ground states for all atoms in non-relativistic QED has, besides numerous other important results, been accomplished by Bach, Fröhlich and Sigal in [2], by a completely different approach. To compare the results in [2] for Helium to the results of the work at hand, we remark that the units used in our paper correspond to those in [8], which differ from the ones in [2]. Furthermore, we emphasize that while

[1]A detailed review of numerous further results connected to the existence of ground states, mostly in Nelson-type models, can be found in [8]. Furthermore, also cf. [7]

the ultraviolet cutoff in the quantized vector potential employed in [2] is, in our units, incorporated at a value $\Lambda \sim \alpha$, where α denotes the fine structure constant, we are studying the corresponding case for an ultraviolet cutoff at $\Lambda \sim 1$. The parameter that accounts for the strength of the perturbation produced by the photon field is in [2] assumed to be much smaller than a constant that depends on the ionization energy of the atom, the latter being computed for the Schrödinger operator of the electron subsystem. One of the key issues in the work at hand is to devise a proof that also encompasses the strongly nonperturbative regime, where this parameter is allowed to be much larger than the ionization energy. This is achieved mainly based on the parameter independence of the results of [8], as well as of the methods developed in the present paper, in addition to exploiting the existence of the ground state of T_0 for small α.

2. Definitions and main results

We consider the Pauli-Fierz Hamiltonian H_N for a system of N electrons in an external electrostatic potential, coupled to the quantized electromagnetic radiation field,

$$\begin{aligned} H_N = & \sum_{\ell=1}^{N} \Big\{ \big(-i\nabla_{x_\ell} \otimes I_f + \sqrt{\alpha} A_f(x_\ell) \big)^2 + \sqrt{\alpha}\sigma \cdot B_f(x_\ell) + V(x_\ell) \otimes I_f \Big\} \\ & + \frac{1}{2} \sum_{1 \le k,\ell \le N} W(|x_k - x_\ell|) \otimes I_f + I_{el} \otimes H_f. \end{aligned} \tag{2}$$

The operator H_N acts on the Hilbert space $\mathcal{H} := \mathcal{H}_N^{el} \otimes \mathcal{F}$, where $\mathcal{H}_N^{el}$, for $N < \infty$, is the Hilbert space of N non-relativistic electrons, given by the totally antisymmetric wave functions in $(L^2(\mathbb{R}^3) \otimes \mathbb{C}^2)^N$, where $\mathbb{R}^3$ is the configuration space of a single electron, and $\mathbb{C}^2$ accomodates its spin.

We will describe the quantized electromagnetic field by use of the Coulomb gauge condition. Accordingly, the one-photon Hilbert space is given by $L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$, where $\mathbb{R}^3$ denotes either the photon momentum or configuration space, and $\mathbb{C}^2$ accounts for the two independent transversal polarizations of the photon. The photon Fock space is then defined by

$$\mathcal{F} = \bigoplus_{n \in \mathbb{N}} \mathcal{F}_s^{(n)},$$

where the n-photons space $\mathcal{F}_s^{(n)} = \bigotimes_s^n \left(L^2(\mathbb{R}^3) \otimes \mathbb{C}^2 \right)$ is the symmetric tensor product of n copies of $L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$.

We use units such that $\hbar = c = 1$, and where the mass of the electron equals $m = 1/2$. The electron charge is then given by $e = \sqrt{\alpha}$, with $\alpha \approx 1/137$ denoting the fine structure constant. As usual, we will consider α as a parameter.

The operator that couples an electron to the quantized vector potential is given by

$$A_f(x) = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \frac{\zeta(|k|)}{2\pi |k|^{1/2}} \varepsilon_\lambda(k) \Big[e^{ikx} \otimes a_\lambda(k) + e^{-ikx} \otimes a_\lambda^*(k) \Big] \mathrm{d}k =: D(x) + D^*(x),$$

where by the Coulomb gauge condition, $\mathrm{div} A_f = 0$. The operators a_λ, a_λ^* satisfy the usual commutation relations

$$[a_\nu(k), a_\lambda^*(k')] = \delta(k-k')\delta_{\lambda,\nu}, \quad [a_\nu(k), a_\lambda(k')] = 0,$$

and there exists a unique unit ray $\Omega_f \in \mathcal{F}$, the Fock vacuum, which satisfies $a_\lambda(k)\Omega_f = 0$ for all $k \in \mathbb{R}^3$ and $\lambda \in \{1,2\}$. The vectors $\varepsilon_\lambda(k) \in \mathbb{R}^3$ are the two orthonormal polarization vectors perpendicular to k,

$$\varepsilon_1(k) = \frac{(k_2, -k_1, 0)}{\sqrt{k_1^2 + k_2^2}} \qquad \text{and} \qquad \varepsilon_2(k) = \frac{k}{|k|} \wedge \varepsilon_1(k).$$

The function $\zeta(|k|)$ describes the *ultraviolet cutoff* on the wavenumbers k. We assume ζ to be of class C^1, with compact support.

The operator that couples an electron to the magnetic field $B_f = \mathrm{curl} A_f$ is given by

$$\begin{aligned} B_f(x) &= \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \frac{\zeta_\Lambda(|k|)}{2\pi |k|^{1/2}} k \times i\varepsilon_\lambda(k) \Big[e^{ikx} \otimes a_\lambda(k) + e^{-ikx} \otimes a_\lambda^*(k) \Big] \mathrm{d}k \\ &=: K(x) + K^*(x). \end{aligned}$$

In Equation (2), $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ is the 3-component vector of Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The photon field energy operator H_f is given by

$$H_f = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} |k| a_\lambda^*(k) a_\lambda(k) \mathrm{d}k.$$

The potentials V and W are relatively $-\Delta$ bounded with relative bound zero and satisfy for positive γ, γ_0 and r_0 the following conditions:

$$V(x) \le -\frac{\gamma_0}{|x|}, \qquad |x| > r_0, \tag{3}$$

$$W(x) \le \frac{\gamma_1}{|x|}, \qquad |x| > r_0. \tag{4}$$

One of the main assumptions of the work at hand is the existence of a ground state of the one electron self-energy operator with total momentum $P = 0$. For its precise formulation, let us consider the case of a free electron coupled to the quantized electromagnetic field. The self-energy operator T is given by

$$T = \big(-i\nabla_x \otimes I_f + \sqrt{\alpha} A_f(x) \big)^2 + \sqrt{\alpha}\sigma \cdot B_f(x) + I_{el} \otimes H_f.$$

We note that this system is translationally invariant, that is, T commutes with the operator of total momentum

$$P_{tot} = p_{el} \otimes I_f + I_{el} \otimes P_f,$$

where p_{el} and $P_f = \sum_{\lambda=1,2} \int k a_\lambda^*(k) a_\lambda(k) \mathrm{d}k$ denote the electron and the photon momentum operators.

Let $\mathcal{H}_P \cong \mathbb{C}^2 \otimes \mathcal{F}$ denotes the fibre Hilbert space corresponding to conserved total momentum P. For any fixed value P of the total momentum, the restriction of T to the fibre space $\mathcal{H}_P$ is given by (see e.g. [3])

$$T(P) = (P - P_f + \sqrt{\alpha} A_f(0))^2 + \sqrt{\alpha}\sigma \cdot B_f(0) + H_f. \tag{5}$$

We denote $\Sigma = \inf \sigma(T)$ and $\Sigma_0 = \inf \sigma(T(0))$. The following assumptions will be used to formulate the main result

Condition $\mathfrak{C}_1$.

i) $\Sigma = \Sigma_0$

ii) Σ_0 is an eigenvalue of $T(0)$, with associated eigenspace $\mathcal{E}_{\Sigma_0}$.

iii) There exists $\Omega_0 \in \mathcal{E}_{\Sigma_0}$ with a finite expectation number of photons, i.e.

$$\langle N_f \Omega_0, \Omega_0 \rangle < c,$$

where $N_f = \sum_{\lambda=1,2} \int a^*_\lambda(k) a_\lambda(k) \mathrm{d}k$.

iv) The above eigenfunction Ω_0 fulfills, for $\lambda = 1, 2$ and some $p_0 \in (6/5, 2]$

$$\|\nabla_k a_\lambda(k)\Omega_0\| \in L^{p_0}(\mathbb{R}^3) + L^2(\mathbb{R}^3)$$

Condition i) was studied by Fröhlich for a spinless Pauli-Fierz model, [6], who proved that in this case, it is fulfilled for all $\alpha > 0$.

For the case including the $\sigma \cdot B$ term, it was proved in [4] that for small α, the condition is also fulfilled.

The existence of the eigenspace $\mathcal{E}_{\Sigma_0}$ in ii) was recently proved for sufficiently small α [3], [4].

Finally, it will be proved in the present paper that for small α, the function Ω_0 possesses the properties iii) and iv). Thus, we conclude that there exists a number α_0, such that at least for all $\alpha \le \alpha_0$, condition $\mathfrak{C}_1$ is fulfilled.

The second main set of assumptions required for our analysis is given as follows. For $M \in \mathbb{N}$, let H_M denote the Pauli-Fierz Hamiltonian for M electrons defined in (2).

Condition $\mathfrak{C}_2$.

i) The operator H_M has a ground state

$$\Upsilon \in \mathcal{H} = \mathcal{H}^{el}_M \otimes \mathcal{F}, \tag{6}$$

with a finite expectation number of photons.

ii) For $\lambda = 1, 2$ and some $p_0 \in (6/5, 2]$,

$$\|(I_{el} \otimes \nabla_k a_\lambda(k))\Upsilon\| \in L^{p_0}(\mathbb{R}^3) + L^2(\mathbb{R}^3).$$

iii) Let x_i $i = 1, \ldots M$ be the position vectors of the electrons. Then,

$$\left(\sum_{i=1}^{M} |x_i| \otimes I_f \right) \Upsilon \in \mathcal{H}.$$

For $M \in \mathbb{N}$, let

$$E_M = \inf \sigma(H_M).$$

The main result of this article is the following

Theorem 2.1. *For $N \in \mathbb{N}$, let the Conditions $\mathfrak{C}_1$ and $\mathfrak{C}_2$ with $M = N - 1$ be fulfilled, and assume that the potentials V and W satisfy* (3) *and* (4)*, with $\gamma_0/\gamma_1 > (N-1)$. Then,*

$$E_N < E_{N-1} + \Sigma. \tag{7}$$

Remark 2.1. *If one assumes that the system with M electrons satisfies the binding condition of* [8]*, it was shown in* [8] *that this system possesses a ground state which satisfies all the conditions of $\mathfrak{C}_2$. In particular, the ground state of the Hydrogen atom fulfills $\mathfrak{C}_2$.*

This Theorem shows that under the above stated conditions, removing one electron from the system costs energy. In this sense, the system is stable with respect to the given type of ionization.

The conditions on the potential $V(x)$ and $W(x)$ cover a large number of models in atomic and molecular physics. In particular, for $V(x) = -\beta Z/|x|$ and $W = \beta/|x|$, the operator H_N describes an atom or ion with N electrons.

In the physical case, β is equal to the Sommerfeld fine structure constant α. However, we would like to emphasize that the proof of the Theorem is valid for all values of $\beta > 0$, even in the strongly nonperturbative regime $0 < \beta \ll \alpha$.

Theorem 2.1 states that as long as the number of electrons N is less than $Z + 1$ (neutral atoms and positive ions), ionization by separation of one electron is energetically disadvantageous.

If was earlier proved in [8] that removal of all electrons from the atom also leads to an increase of the energy.

Combining these two results for the case $N = 2$, and the binding condition in [8, Theorem 3.1], yields

Theorem 2.2. *The Pauli-Fierz Hamiltonian for Helium*

$$H_2 = \sum_{\ell=1}^{2} \left\{ \left(-i\nabla_{x_\ell} \otimes I_f + \sqrt{\alpha} A_f(x_\ell)\right)^2 + \sqrt{\alpha}\sigma \cdot B_f(x_\ell) - \tfrac{2\alpha}{|x_\ell|} \otimes I_f \right\} + \tfrac{\alpha}{|x_1 - x_2|} \otimes I_f + I_{el} \otimes H_f$$

has a ground state for all $\alpha \leq \alpha_0$.

Notice that the conditions on the potential $V(x)$ require only some type of behaviour at infinity. Therefore, instead of one nucleus with Coulomb potential of charge Z, one can consider a system of nuclei

$$V(x) = \sum_{i=1}^{k} \frac{\alpha Z_i}{|x - R_i|}$$

with the same total charge, in the infinite mass approximation. In particular, for Hydrogen molecules as well as for all molecular ions with two electrons, Theorem 2.1 implies the existence of a ground state for all $\alpha \leq \alpha_0$.

3. Properties of the ground state of $T(0)$.

This section addresses the main properties of the self-energy operator $T(0)$ that are required for the present analysis. In particular, existence of a ground state $\Omega_0 \in \mathbb{C}^2 \otimes \mathcal{F}$, finiteness of the expected photon number with respect to Ω_0, and regularity of $a_\lambda(k)\Omega_0$ are discussed.

3.1. **Existence Theorem.**

In the following theorem, existence of a ground state of $T(0)$, and bounds on the associated expected photon kinetic energy are established.

Theorem 3.1. *For* α *sufficiently small,* $\Sigma_0 = \inf\sigma(T(0))$ *is a degenerate eigenvalue, bordering to absolutely continuous spectrum, which satisfies*

$$|\Sigma_0| \leq c\alpha\ .$$

Let $\mathcal{E}_{\Sigma_0} = \ker(T(0) - \Sigma_0) \subset \mathbb{C}^2 \otimes \mathcal{F}$ denote its eigenspace. Then, $\dim_{\mathbb{C}} \mathcal{E}_{\Sigma_0} = 2$, and for any $\Omega_0 \in \mathcal{E}_{\Sigma_0}$, normalized by $\langle \Omega_0, \Omega_f \rangle = 1$, the estimate

$$\|\Omega_0\| \leq 1 + c\sqrt{\alpha}$$

is satisfied. Furthermore,

$$\|A_f(0)\Omega_0\| \ , \ \|H_f^{1/2}\Omega_0\| \leq c\sqrt{\alpha} \tag{8}$$

hold. All constants are uniform in α.

For the spinless case, both results are proved in [3] by use of the operator-theoretic renormalization group based on the smooth Feshbach map, cf. [1]. For the case including spin, an outline of the proof is given in the Appendix of [4], while a publication containing the detailed proof is in preparation. The bound on $\|A_f(0)\Omega_0\|$ follows straightforwardly from the one on $\|H_f\Omega_0\|$.

3.1.1. *Expected photon number.* Using Theorem 3.1, we may next bound the expected photon number with respect to Ω_0.

Theorem 3.2. *For α sufficiently small, and $\Omega_0 \in \mathcal{E}_{\Sigma_0}$ defined as in Theorem 3.1, $\Omega_0 \in \mathrm{Dom}(N_f^{1/2})$, where $N_f = \sum_{\lambda=1,2} \int a_\lambda^*(k) a_\lambda(k) \mathrm{d}k$ is the photon number operator, and*

$$\|N_f^{1/2}\Omega_0\|^2 < c\sqrt{\alpha} \ .$$

In particular,

$$\|\chi(|k| < 1) a_\lambda(k)\Omega_0\| \leq c\sqrt{\alpha}|k|^{-1} \ .$$

All constants are uniform in α.

Proof. We first remark that the integral $\int dk \|a_\lambda(k)\Omega_0\|^2$ is ultraviolet finite, since

$$\begin{aligned} \int \chi(|k| \geq 1) \|a_\lambda(k)\Omega_0\|^2 \mathrm{d}k \ &< \ \int \chi(|k| \geq 1)|k| \|a_\lambda(k)\Omega_0\|^2 \mathrm{d}k \\ &\leq \ \langle \Omega_0, H_f \Omega_0 \rangle \\ &\leq \ c\alpha \ , \end{aligned} \tag{9}$$

using (8). We may thus assume that the domain of the integral is the unit ball $B_1(0)$. For $|k| < 1$, we employ a similar argument as in [6, 2, 8]. Using

$$\big(: T(0) : - \Sigma_0' \big) a_\lambda(k) \Omega_0 = \big[: T(0) : , \, a_\lambda(k) \big] \Omega_0 \ ,$$

where $: (\,\cdot\,) :$ denotes Wick ordering, and

$$\Sigma_0' := \Sigma_0 - \langle A_f(0)^2 \rangle_{\Omega_f} = \inf \sigma(: T(0) :) \ ,$$

we obtain

$$\begin{aligned} a_\lambda(k)\Omega_0 \ &= \ \sqrt{\alpha} R(k) \Big(k \cdot A_f(0) + \frac{\zeta(|k|)}{|k|^{1/2}} \epsilon_\lambda(k) \cdot P_f \\ &\quad + \frac{\zeta(|k|)}{|k|^{1/2}} ik \wedge \epsilon_\lambda(k) \cdot \sigma + \sqrt{\alpha} \frac{\zeta(|k|)}{|k|^{1/2}} \epsilon_\lambda(k) \cdot A_f(0) \Big) \Omega_0 \ , \end{aligned} \tag{10}$$

where

$$R(k) := \Big(H_f + |k| + \frac{1}{2}(P_f + k)^2 - \Sigma_0' \Big)^{-1} \ . \tag{11}$$

Clearly, $\langle \Omega_f, : T(0) : \Omega_f \rangle = 0$, and a standard variational argument shows that $\Sigma_0' < 0$ for $\alpha > 0$. Hence, $0 < R(k) < (H_f + |k|)^{-1}$, and

$$\|R(k)P_f\| \le \|R(k)H_f\| \le 1 \,.$$

Thus, using $\|R(k)|k|\| \le 1$ and theorem 3.1,

$$\begin{aligned} \|\chi(|k|<1)a_\lambda(k)\Omega_0\| &\le c\sqrt{\alpha}\chi(|k|<1)\Big(\|A_f(0)\Omega_0\| + 2|k|^{-1/2}\|\Omega_0\| \\ &\qquad + \sqrt{\alpha}|k|^{-1}\|A_f(0)\Omega_0\|\Big) \\ &\le c\sqrt{\alpha}|k|^{-1} \,. \end{aligned} \tag{12}$$

The right hand side is in $L^2(B_1(0))$, and the assertion is established. □

For the case of a confined electron, it was proved in [8] that the corresponding estimate exhibits a $|k|^{-1/2}$ singularity instead of $|k|^{-1}$ as present here, owing to the exponential decay of the particle wave function.

Furthermore, if the conserved momentum P is non-zero, there exists a ground state $\Omega_P(\kappa)$ for a regularized version of the model, which includes an infrared cutoff below $0 < \kappa \ll 1$ in $A_f(0)$ (some requirements on the cutoff function are necessary, cf. [3]). Then, with all modifications implemented, the additional term

$$\sqrt{\alpha}R(k)\frac{\zeta(|k|)}{|k|^{1/2}}P \cdot \epsilon_\lambda(k)\;\Omega_P(\kappa)$$

enters the right hand side of (10). Therefore, $\langle \Omega_P(\kappa), N_f \Omega_P(\kappa)\rangle$ is logarithmically infrared divergent in the limit $\kappa \to 0$, for all $|P| > 0$, and in fact, $\Omega_P(\kappa)$ does not converge to an element in Fock space.

3.1.2. *Regularity properties of the ground state.* Next, we derive a result about the regularity of $a_\lambda(k)\Omega_0$ in momentum space, which is, in our further discussion, used for photon localization estimates in position space.

Theorem 3.3. *For α sufficiently small, let $\Omega_0 \in \mathcal{E}_{\Sigma_0}$. Then,*

$$\|\nabla_k a_\lambda(k)\Omega_0\| \in L^p(\mathbb{R}^3) + L^2(\mathbb{R}^3) \,,$$

for $1 \le p < \frac{3}{2}$.

Proof. We proceed similarly as in [8]. To begin with, we differentiate the right hand side of (10) with respect to k, and observe that

$$|\nabla_k R(k)| \le (1 + H_f + |k|)R^2(k) \,, \tag{13}$$

since $|P_f| \le H_f$.

Let us first bound the ultraviolet part of $\|\nabla_k a_\lambda(k)\Omega_0\|$. For $|k| \ge 1$,

$$\begin{aligned} \|\chi(|k|\ge 1)\nabla_k a_\lambda(k)\Omega_0\| &= \sqrt{\alpha}\|\chi(|k|\ge 1)\nabla_k R(k) k\cdot A_f(0)\Omega_0\| \\ &\le \Big(\|\chi(|k|\ge 1)(1+H_f+|k|)R(k)\| + |k|^{-1}\Big) \\ &\qquad \|\sqrt{\alpha}\chi(|k|\ge 1)R(k)k\cdot A_f(0)\Omega_0\| \\ &\le 2\sqrt{\alpha}\|\chi(|k|\ge 1)a_\lambda(k)\Omega_0\| \,, \end{aligned} \tag{14}$$

and consequently, by Theorem 3.2,

$$\int_{|k|\geq 1} \|\nabla_k a_\lambda(k)\Omega_0\|^2 \mathrm{d}k \leq c\alpha \ . \tag{15}$$

We may thus restrict our discussion to the case $|k| < 1$.

Differentiating with respect to k, the photon polarization vectors satisfy

$$|\nabla_k \epsilon_\lambda(k)| \leq \frac{c}{\sqrt{k_1^2 + k_2^2}}. \tag{16}$$

Recalling that the cutoff function ζ is of class C^1, and using Theorem 3.2, one straightforwardly deduces that there exists a constant c which is uniform in α, such that

$$\begin{aligned} \|\chi(|k|<1)\nabla_k a_\lambda(k)\Omega_0\| &\leq c\sqrt{\alpha}\Big(\frac{1}{|k|^2} + \frac{1}{|k|\sqrt{k_1^2+k_2^2}}\Big) \\ &\leq \frac{c\sqrt{\alpha}}{|k|\sqrt{k_1^2+k_2^2}} \ . \end{aligned} \tag{17}$$

Here, one again uses $\|R(k)P_f\| \leq \|R(k)H_f\| \leq 1$, and $\|R(k)|k|\| \leq 1$, in addition to (13). Thus, by the Hölder inequality,

$$\begin{aligned} &\Big(\int_{|k|<1} \|\nabla_k a_\lambda(k)\Omega_0\|^p \mathrm{d}k\Big)^{1/p} \\ &\leq \ C\sqrt{\alpha}\Big(\int_{|k|<1} \frac{1}{|k|^{r/2}(k_1^2+k_2^2)^{r/2}}\,\mathrm{d}k\Big)^{1/r}\Big(\int_{|k|<1}\frac{1}{|k|^{r^*/2}}\,\mathrm{d}k\Big)^{1/r^*} \ , \end{aligned} \tag{18}$$

with $\frac{1}{p} = \frac{1}{r} + \frac{1}{r^*}$. The integrals on the right hand side of (18) are bounded for the choices $1 \leq r^* < 6$, and $1 \leq r < 2$, which implies that $1 \leq p < \frac{3}{2}$, corresponding to the exponent expected from scaling. □

In the case of a confined electron, [8], the bound analogous to (17) is $\frac{c\sqrt{\alpha}}{|k|^{1/2}\sqrt{k_1^2+k_2^2}}$. The reason for the fact that it is by a factor $|k|^{1/2}$ less singular is stated in a previous remark. Consequently, in [8], the inequality corresponding to (18) likewise requires the choice $r < 2$, but in contrast, r^* can be chosen arbitrarily large. Therefore, the result proved in [8] holds for $\frac{1}{p} > \frac{1}{2} + \frac{1}{\infty} = \frac{1}{2}$, that is, $1 \leq p < 2$.

4. Self-energy of localized states with total momentum $P = 0$

The goal of this chapter is to arrive at a sharp upper bound on the infimum of the quadratic form of the operator $T(0)$, when restricted to states where all photons are localized in a ball of radius R centered at the origin.

To this end, we recall that for the Schrödinger operator $-\Delta$ corresponding to a free electron, the infimum of the spectrum on the whole space is zero, whereas the infimum on functions supported in a ball of radius R, with Dirichlet boundary conditions, is C/R^2.

The main result of this section is the following.

Theorem 4.1. *For all $R > 0$, there exists a function $\Phi^R \in \mathfrak{D}(T(0))$, such that*
i) The n photonic components $\Phi_n^R(y_1, \dots, y_n; \lambda_1, \dots, \lambda_n)$ fulfill

$$\mathrm{supp}\Phi_n^R \subset \{(y_1, \dots, y_n; \lambda_1, \dots, \lambda_n) \mid \sup_i |y_i| < R\}$$

ii)

$$\langle T(0)\Phi^R, \Phi^R\rangle \leq \left(\Sigma_0 + \frac{c(R)}{R}\right) \|\Phi^R\|^2 \ , \tag{19}$$

where $c(R)$ tends to zero as R tends to infinity.
iii)The function Φ^R has the following additional properties. For all $\varepsilon > 0$ and all $|x| > 2R$,

$$|\langle D(x)\Phi^R, \Phi^R\rangle| \leq \frac{c(|x|)}{|x|}\|\Phi\|^2 \ , \tag{20}$$

$$|\langle D(x)^2\Phi^R, \Phi^R\rangle| \leq \frac{c(|x|)}{|x|^2}\|\Phi\|^2 \ , \tag{21}$$

$$|\langle D^*(x)D(x)\Phi^R, \Phi^R\rangle| \leq \frac{c(|x|)}{|x|^2}\|\Phi\|^2 \ , \tag{22}$$

and

$$|\langle K(x)\Phi^R, \Phi^R\rangle| \leq \frac{c(|x|)}{|x|}\|\Phi\|^2 \tag{23}$$

where $c(|x|)$ tends to zero, uniformly in R, as $|x|$ tends to infinity.

Before addressing the proof of Theorem 4.1, we shall first demonstrate how it can be employed to construct a state in $\mathcal{H}_1 \otimes \mathcal{F}$ that accounts for a system consisting of an electron coupled to a photonic field, localized in a ball of radius R centered at a fixed point b, with energy close to the self-energy Σ_0. For that purpose, let us, for given $x \in \mathbb{R}^3$, define the shift operator $\tau_x : \mathcal{F} \to \mathcal{F}$, which, for $\phi = (\phi_0, \phi_1, \dots, \phi_n, \dots) \in \mathcal{F}$, is given by

$$\tau_x\phi_n(y_1, \dots, y_n; \lambda_1, \dots, \lambda_n) = \phi_n(y_1 - x, \dots, y_n - x; \lambda_1, \dots, \lambda_n).$$

Theorem 4.2. *Let f be a real valued function in $C_0^2(\mathbb{R}^3) \otimes \mathbb{C}^2$, supported in the unit ball centered at the origin. For $R > 0$ and $b \in \mathbb{R}^3$, we define $\Theta^{R,b} \in \mathcal{H}_1 \otimes \mathcal{F}$ by*

$$\Theta^{R,b} = \frac{f(\frac{x}{R} - b) \otimes \tau_x\Phi^R}{\|f(\frac{x}{R}) \otimes \Phi^R\|}. \tag{24}$$

Then, for all $\varepsilon > 0$ and R large enough independent of b, we have

$$\left\langle \left((i\nabla_x \otimes I_f + \sqrt{\alpha}A_f(x))^2 + \sqrt{\alpha}\sigma.B_f(x) + I_{el} \otimes H_f\right) \Theta^{R,b}, \Theta^{R,b}\right\rangle \leq \Sigma_0 + \frac{\varepsilon}{R}. \tag{25}$$

Proof of Theorem 4.2. For a real valued function f, let $f^{R,b}(x) := f(x/R - b)$. Obviously,

$$\begin{aligned} &\left\langle \left((i\nabla_x \otimes I_f + \sqrt{\alpha}A_f(x))^2 + \sqrt{\alpha}\sigma.B_f(x) + I_{el} \otimes H_f\right) \Theta^{R,b}, \Theta^{R,b}\right\rangle = \\ &\frac{1}{\|f(\frac{x}{R}) \otimes \Phi^R\|^2} \left(\langle -\Delta_x f^{R,b}, f^{R,b}\rangle \|\Phi^R\|^2 + \|f\|^2 \langle T(0)\Phi^R, \Phi^R\rangle\right). \end{aligned} \tag{26}$$

According to Theorem 4.1, the second term on the right hand side can be estimated by

$$\frac{\|f\|^2\langle T(0)\Phi^R, \Phi^R\rangle}{\|f^{R,b}(x) \otimes \Phi^R\|^2} \leq \Sigma_0 + \frac{c(R)}{R} \ .$$

For the first term on the right hand side of (26), we have

$$\frac{\langle -\Delta_x f^{R,b}, f^{R,b}\rangle}{\|f^{R,b}(x)\|^2} \leq \frac{c}{R^2} \ ,$$

which completes the proof of the Theorem.

4.1. **Localization estimates.** In order to prove Theorem 4.1, we consider the ground state Ω_0 of the self-energy operator $T(0)$ at zero momentum, and act on it with two spatial localization functions $\mathcal{U}^{\mathcal{R}}$ and $\mathcal{V}^{\mathcal{R}}$, which constitute a partition of unity $(\mathcal{U}^{\mathcal{R}})^2 + (\mathcal{V}^{\mathcal{R}})^2 = 1$ on $\mathcal{F}$. This yields a state for which all photons are inside the ball of radius R, and another state for which all photons are outside the ball of radius $R/2$.

Clearly, the expectation of $T(0)$ with respect to Ω_0 is not equal to the sum of the expectations with respect to the two localized states. The difference, which is usually called the localization error, must be estimated to obtain an upper bound on the self-energy of the localized state. In the present subsection, we estimate the localization errors for different terms in the operator $T(0)$.

Let us to begin with define spatial cutoff functions u and v as follows. We pick $u \in C_0^\infty(\mathbb{R}_+)$ such that

$$u(x) = \begin{cases} 1 & \text{if } x \in [0, 1/2] \\ 0 & \text{if } x \geq 1 \end{cases} , \tag{27}$$

$0 \leq u \leq 1$ and $v := \sqrt{1 - u^2} \in C^2(\mathbb{R}_+)$.

For $Y = (y_1, y_2, \ldots, y_n) \in \mathbb{R}^n$, we denote $\|Y\|_\infty = \max_{1 \leq i \leq n} |y_i|$. For $n \in \mathbb{N}$ and all $Y \in \mathbb{R}^n$, we also define $u_n^R(Y) = u(\frac{\|Y\|_\infty}{R})$ and $v_n^R(Y) = \sqrt{1 - u_n^R(Y)^2}$.

Next, we introduce a pair of operators $\mathcal{U}^{\mathcal{R}}$ and $\mathcal{V}^{\mathcal{R}}$ on $\mathcal{F}$ by

$$\mathcal{U}^R \psi = \big(\psi_0, u_1^R(y_1)\psi_1(y_1), \ldots, u_n^R((y_1, \ldots y_n))\psi(y_1, \ldots y_n), \ldots\big) \tag{28}$$

and

$$\mathcal{V}^R \psi = \big(\psi_0, v_1^R(y_1)\psi_1(y_1), \ldots, v_n^R((y_1, \ldots y_n))\psi(y_1, \ldots y_n), \ldots\big) , \tag{29}$$

where we have omitted the polarization indices from the notation.

4.1.1. *Localization error for the field energy H_f.*

Lemma 4.1. *There exists $c < \infty$ such that for all $\varepsilon > 0$, and all R large enough,*

$$\langle H_f \mathcal{U}^R \psi, \mathcal{U}^R \psi \rangle + \langle H_f \mathcal{V}^R \psi, \mathcal{V}^R \psi \rangle - \langle H_f \psi, \psi \rangle \leq \langle N_f \psi, \psi \rangle \left(\frac{\varepsilon}{R} + \frac{c}{\varepsilon R} \frac{\|\mathcal{V}^{R/2}\psi\|^2}{\|\psi\|^2} \right) \tag{30}$$

holds for $\psi \in \mathfrak{Q}(H_f) \cap \mathfrak{Q}(N_f)$.

Proof. Since H_f maps each n-photon sector of the Fock space $\mathcal{F}$ into itself, it suffices to estimate the localization error for the n-photon component of ψ. Furthermore, since H_f acts on a function in $\mathcal{F}_s^{(n)}$ as $n|\nabla_{y_1}|$, the statement of the Lemma follows straightforwardly from Lemma 4.2. □

Lemma 4.2. *There exists $c < \infty$ such that for all $\varepsilon > 0$, all R large enough,*

$$\begin{aligned} \langle |\nabla| u(\frac{|y|}{R})\phi, u(\frac{|y|}{R})\phi \rangle + \langle |\nabla| v(\frac{|y|}{R})\phi, v(\frac{|y|}{R})\phi \rangle - \langle |\nabla| \phi, \phi \rangle \\ \leq \left(\frac{\varepsilon}{R} + \frac{c}{\varepsilon R} \frac{\|\phi \chi(|y| > R)\|^2}{\|\phi\|^2} \right) . \end{aligned} \tag{31}$$

holds for all $\phi \in C_0^\infty(\mathbb{R}^3)$.

Proof. By [10, Theorem 9], we have

$$\begin{aligned}
&\langle|\nabla|\phi,\phi\rangle-\langle|\nabla|u(\frac{|y|}{R})\phi,u(\frac{|y|}{R})\phi\rangle-\langle|\nabla|v(\frac{|y|}{R})\phi,v(\frac{|y|}{R})\phi\rangle \\
&\qquad=\frac{1}{2\pi^2}\int\frac{|\phi(y)||\phi(z)|}{|y-z|^4}\left(\left|u(\frac{|y|}{R})-u(\frac{|z|}{R})\right|^2+\left|v(\frac{|y|}{R})-v(\frac{|z|}{R})\right|^2\right)\mathrm{d}y\mathrm{d}z.
\end{aligned}\tag{32}$$

Let us consider

$$I=\int\frac{|\phi(y)||\phi(z)|}{|y-z|^4}\left|u(\frac{|y|}{R})-u(\frac{|z|}{R})\right|^2\mathrm{d}y\mathrm{d}z.\tag{33}$$

The term with the function v can be estimated similarly. By symmetry, it suffices to estimate this integral in the region where $|y|\le|z|$. We split the integral I into three parts I_1, I_2, and I_3, respectively, corresponding to the regions $\mathcal{R}_1=\{|z|<R/2\}$, $\mathcal{R}_2=\{|z|>R/2,|y-z|>R/4\}$ and $\mathcal{R}_3=\{|z|>R/2,|y-z|<R/4\}$.

Since $|y|\le|z|$, we have, in the region $\mathcal{R}_1$, $|y|\le|z|<R/2$. Thus, in $\mathcal{R}_1$, we have $u(\frac{|y|}{R})-u(\frac{|z|}{R})=0$. Therefore,

$$I_1=0\ .$$

Now, for all $\varepsilon>0$

$$\begin{aligned}
I_2&\le\varepsilon\int_{\mathcal{R}_2}\frac{|\phi(y)|^2}{|y-z|^4}\mathrm{d}y\mathrm{d}z+\frac{1}{\varepsilon}\int_{\mathcal{R}_2}\frac{|\phi(z)|^2}{|y-z|^4}\mathrm{d}y\mathrm{d}z \\
&\le c\left(\varepsilon\frac{1}{R}\|\phi\|^2+\frac{1}{\varepsilon R}\|\phi\chi(|z|>R/2)\|^2\right)
\end{aligned}\tag{34}$$

where c is a constant independent of ε.

Finally, since the derivative of u is bounded, we have the inequality $|u(|y|/R)-u(|z|/R)|^2\le c|y-z|^2/R^2$. This implies

$$\begin{aligned}
I_3&\le c\int_{\mathcal{R}_3}\frac{|\phi(y)||\phi(z)|}{|y-z|^4}\frac{|y-z|^2}{R^2}\mathrm{d}y\mathrm{d}z \\
&\le\frac{c}{R^2}\int_{\mathcal{R}_3}\frac{\varepsilon|\phi(y)|^2+(1/\varepsilon)|\phi(z)|^2}{|y-z|^2}\mathrm{d}y\mathrm{d}z \\
&\le\frac{c\varepsilon}{R}\|\phi\|^2+\frac{1}{\varepsilon R}\|\phi\chi(|z|>R/2)\|^2.
\end{aligned}\tag{35}$$

□

4.1.2. *Localization error for the operator P_f^2.*

Lemma 4.3. *There exists $c<\infty$ such that for all $\varepsilon>0$ and all R large enough,*

$$\langle P_f^2\mathcal{U}^R\psi,\mathcal{U}^R\psi\rangle+\langle P_f^2\mathcal{V}^R\psi,\mathcal{V}^R\psi\rangle-\langle P_f^2\psi,\psi\rangle\le\frac{c}{R^2}\langle N_f\psi,\psi\rangle\tag{36}$$

holds for $\psi\in\mathfrak{Q}(H_f)\cap\mathfrak{Q}(N_f)$.

Proof. The operator P_f^2 maps each n-photon sector into itself. Therefore, it is sufficient to restrict the proof to $\mathcal{F}_s^{(n)}$. We have

$$
\begin{aligned}
&\langle P_f^2 u_n^R \psi_n, u_n^R \psi_n\rangle + \langle P_f^2 v_n^R \psi_n, v_n^R \psi_n\rangle - \langle P_f^2 \psi, \psi\rangle \\
&= \sum_{i,j} \langle \nabla_i \nabla_j u_n^R \psi_n, u_n^R \psi_n\rangle + \langle \nabla_i \nabla_j v_n^R \psi_n, v_n^R \psi_n\rangle - \langle \nabla_i \nabla_j \psi_n, \psi_n\rangle \\
&= \sum_{i,j} \langle u_n^R \nabla_i \nabla_j \psi_n, u_n^R \psi_n\rangle + \langle v_n^R \nabla_i \nabla_j \psi_n, v_n^R \psi_n\rangle - \langle \nabla_i \nabla_j \psi_n, \psi_n\rangle \\
&+ 2\sum_{i,j} \langle (\nabla_i u_n^R)(\nabla_j \psi_n), u_n^R \psi_n\rangle + \langle (\nabla_i v_n^R)(\nabla_j \psi_n), v_n^R \psi_n\rangle \\
&+ \sum_{i,j} \langle \psi_n \nabla_i \nabla_j u_n^R, u_n^R \psi\rangle + \langle \psi_n \nabla_i \nabla_j v_n^R, v_n^R \psi\rangle
\end{aligned}
\tag{37}
$$

Since $(u_n^R)^2 + (v_n^R)^2 = 1$, the first term on the right hand side of (37) is zero. Similarly, by rewriting the second term as

$$
\sum_{i,j} \langle (\nabla_i (u_n^R)^2)(\nabla_j \psi_n), \psi_n\rangle + \langle (\nabla_i (v_n^R)^2)(\nabla_j \psi_n), \psi_n\rangle
$$

we find that it is also zero. Next, we note that $\nabla_i \nabla_j u_n^R = 0$ and $\nabla_i \nabla_j v_n^R = 0$ if $i \neq j$, because the functions u and v depend only on the $\|.\|_\infty$ norm.

Thus, we obtain

$$
\begin{aligned}
&\sum_{i,j} \langle \psi_n \nabla_i \nabla_j u_n^R, u_n^R \psi\rangle + \langle \psi_n \nabla_i \nabla_j v_n^R, v_n^R \psi\rangle \\
&\quad = \sum_{i} \langle \psi_n \Delta_i u_n^R, u_n^R \psi\rangle + \langle \psi_n \Delta_i v_n^R, v_n^R \psi\rangle \\
&\quad = n\langle \psi_n \Delta_1 u_n^R, u_n^R \psi\rangle + \langle \psi_n \Delta_1 v_n^R, v_n^R \psi\rangle \\
&\quad \leq n \frac{c}{R^2} \|\psi_n\|^2 ,
\end{aligned}
\tag{38}
$$

where in the last inequality, we used that for some constant c, we have $|\Delta u_n^R| \leq cR^{-2}$ and $|\Delta v_n^R| \leq cR^{-2}$. ∎

4.1.3. *Localization error for $P_f A_f(0)$.*

Lemma 4.4. *Let $\psi \in \mathfrak{Q}(P_f A_f(0)) \cap \mathfrak{D}(P_f) \cap \mathfrak{D}(N_f)$, and assume that for some $p_0 \in (6/5, 2]$,*

$$
\|\nabla_k a_\lambda(k)\psi\|_{\mathcal{F}} \in L^{p_0}(\mathbb{R}^3) + L^2(\mathbb{R}^2).
$$

Then, the inequality

$$
\left| \langle P_f A_f(0) \mathcal{U}^R \psi, \mathcal{U}^R \psi\rangle + \langle P_f A_f(0) \mathcal{V}^R \psi, \mathcal{V}^R \psi\rangle - \langle P_f A_f(0) \psi, \psi\rangle \right| \leq \frac{c}{R^{1+\delta}}
\tag{39}
$$

holds with $\delta = (p_0 - 6/5)/2$.

Proof. Throughout this proof, we will write $\int \mathrm{d}y$ for integration over the y variable, and summation over the polarization λ. Here and in the rest of the paper, we define $G_\lambda(x)$ as the Fourier transform of the vector function

$$
\frac{\varepsilon_\lambda(k)}{|k|^{\frac{1}{2}}} \zeta(k).
$$

In addition, everywhere where it does not lead to any misunderstanding, we will omit the photon polarization index λ.

We have

$$
\begin{aligned}
&\langle P_f D(0)\mathcal{U}^R\psi, \mathcal{U}^R\psi\rangle + \langle P_f D(0)\mathcal{V}^R\psi, \mathcal{V}^R\psi\rangle - \langle P_f D(0)\psi,\psi\rangle \\
&= i\sum_n \sqrt{n+1}\Bigg\{\int G(-y_{n+1})\psi_{n+1}\sum_{i=1}^n \overline{(\nabla_i\psi_n)}\left(u^R_{n+1}u^R_n + v^R_{n+1}v^R_n - 1\right) \mathrm{d}y_1\ldots\mathrm{d}y_{n+1} \\
&\qquad + \int G(-y_{n+1})\psi_{n+1}\overline{\psi_n}\left(\sum_{i=1}^n u^R_{n+1}\nabla_i u^R_n + v^R_{n+1}\nabla_i v^R_n\right)\mathrm{d}y_1\ldots\mathrm{d}y_{n+1}\Bigg\} \\
&=: \sum_n (a_n + b_n) \ .
\end{aligned} \tag{40}
$$

We first estimate the term a_n. We denote $F = u^R_{n+1}u^R_n + v^R_{n+1}v^R_n - 1$. For $|y_{n+1}| \le R/2$, either $\|Y\|_\infty = |y_{n+1}|$ and then $u^R_{n+1}(Y) = u^R_n(y_1,\ldots,y_n) = 1$ and $v^R_{n+1}(Y) = v^R_n(y_1,\ldots,y_n) = 1$, or $\|Y\|_\infty = |y_k|$, for some $k \neq n+1$, and then $u^R_{n+1}(Y) = u^R_n(y_1,\ldots,y_n)$ and $v^R_{n+1}(Y) = v^R_n(y_1,\ldots,y_n)$. In both cases, we get $F = 0$. Thus for $\delta > 0$ sufficiently small, we have

$$
\begin{aligned}
|a_n| &= \left|\sqrt{n+1}\int_{|y_{n+1}|\ge R/2} G(-y_{n+1})\psi_{n+1}\sum_{i=1}^n \overline{(\nabla_i\psi_n)}F\mathrm{d}y_1\ldots\mathrm{d}y_{n+1}\right| \\
&\le \sqrt{n+1}\int_{|y_{n+1}|\ge R/2}(1+|y_{n+1}|)^{1-\delta}|G(-y_{n+1})||\psi_{n+1}|(1+|y_{n+1}|)^{2\delta} \\
&\quad \times \frac{1}{(1+|y_{n+1}|)^{1+\delta}}(P_f\psi)_n\mathrm{d}y_1\ldots\mathrm{d}y_{n+1} \\
&\le \frac{1}{R^{1+\delta}}\int\sqrt{n+1}|\psi_{n+1}|(1+|y_{n+1}|)^{2\delta}(1+|y_{n+1}|)^{1-\delta} \\
&\quad |G(-y_{n+1})||(P_f\psi)_n|\mathrm{d}y_1\ldots\mathrm{d}y_{n+1}
\end{aligned} \tag{41}
$$

Applying the Schwarz inequality, we arrive at

$$
\begin{aligned}
|a_n| \le& \frac{2^{1+\delta}}{R^{1+\delta}}\|\sqrt{n+1}\psi_{n+1}(1+|y_{n+1}|)^{2\delta}\|_{L^2_{n+1}}\ \|(1+|y_{n+1}|)^{1-\delta}G\|_{L^2(\mathrm{d}y_{n+1})} \\
&\|(P_f\psi)_n\|_{L^2_n},
\end{aligned} \tag{42}
$$

where for brevity, $L^2_k := L^2(\mathrm{d}y_1,\ldots,\mathrm{d}y_k)$. According to Lemma 7.1 in the Appendix, one finds that $\|(1+|y_{n+1}|)^{1-\delta}G\|_{L^2(\mathrm{d}y_{n+1})}$ is finite. Therefore,

$$
\sum_n |a_n| \le \frac{c}{R^{1+\delta}}\sum_n\left(\|\sqrt{n+1}\psi_{n+1}(1+|y_{n+1}|)^{2\delta}\|^2_{L^2_{n+1}} + \|(P_f\psi)_n\|^2_{L^2_n}\right) \ . \tag{43}
$$

We note that

$$
\|\nabla_k a_\lambda(k)\psi\|_{\mathcal{F}} \in L^{p_0}(\mathbb{R}^3,\mathrm{d}k) + L^2(\mathbb{R}^3,\mathrm{d}k)
$$

implies

$$
\sum_n (n+1)\|\psi_{n+1}(y,.)\|^2_{L^2_n}(1+|y|)^2 \in L^{q_0/2}(\mathbb{R}^3,\mathrm{d}y) + L^1(\mathbb{R}^3,\mathrm{d}y) \ ,
$$

with $\frac{1}{p_0}+\frac{1}{q_0}=1$, by the Hausdorff-Young inequality. Consequently, one can straightforwardly verify that for $\delta=(p_0-6/5)/2$,

$$\sum_n \|\sqrt{n+1}\psi_{n+1}(1+|y_{n+1}|)^{2\delta}\|^2_{L^2_{n+1}} < c \; . \tag{44}$$

Moreover,

$$\sum_n \|(P_f\psi)_n\|^2_{L^2_n} < c \; , \tag{45}$$

since $\psi \in \mathfrak{D}(P_f)$. Inequalities (43)-(45) imply that

$$\sum_n |a_n| \leq \frac{c}{R^{1+\delta}} \; . \tag{46}$$

Let us turn to the estimate of b_n. If $\max_{i=1,\dots,n}|y_i| \neq |y_{n+1}|$, then

$$\sum_{i=1}^n \Big(u^R_{n+1}(y_1,\dots y_{n+1})\nabla_i u^R_n(y_1,\dots y_n) + v^R_{n+1}(y_1,\dots y_{n+1})\nabla_i v^R_n(y_1,\dots y_n)\Big) = 0 \; .$$

If $\max\{y_1,\dots,y_{n+1}\} = |y_{n+1}|$, then $\nabla_i u^R_n = \nabla_i v^R_n = 0$ for all $(y_1,\dots y_n)$, such that one finds $\max_{k=1,\dots,n}|y_k| > |y_i|$. This means that except on a set of measure zero in $\mathbb{R}^n$, the functions $u^R_{n+1}\nabla_i u^R_n + v^R_{n+1}\nabla_i v^R_n$ have disjoint supports. Therefore,

$$\sum_{i=1}^n u^R_{n+1}\nabla_i u^R_n + v^R_{n+1}\nabla_i v^R_n \leq \frac{c}{R} \; .$$

Moreover, $\nabla_i u^R_N$ and $\nabla_i v^R_N$ have support in the set $\{|y_i| \in [R/2, R]\}$, thus, since from the above, we only have to consider the region where $|y_{n+1}| > \max_{i=1,\dots,n}|y_i|$, we get $|y_{n+1}| > R/2$, hence

$$\begin{aligned} |b_n| &\leq \frac{c}{R}\sqrt{n}\int_{|y_{n+1}|>R/2} |G(-y_{n+1})|\; |\psi_{n+1}|\; |\psi_n| \mathrm{d}y_1\dots\mathrm{d}y_{n+1} \\ &\leq \frac{c}{R}\int_{|y_{n+1}|>R/2} (1+|y_{n+1}|)^{-1/2}|G(-y_{n+1})|(1+|y_{n+1}|)^{1/2} \\ &\times |\psi_n|\sqrt{n}|\psi_{n+1}|\mathrm{d}y_1\dots\mathrm{d}y_{n+1} \; . \end{aligned} \tag{47}$$

Applying the Schwarz inequality and Lemma 7.1, we obtain from (47)

$$\sum_n |b_n| \leq \frac{c}{R^{3/2}}\left(\|\psi\|^2 + \|N_f\psi\|^2\right) . \tag{48}$$

Inequalities (46) and (48) complete the proof of Lemma 4.4. □

4.1.4. *Localization error for $A_f(0)^2$.*

Lemma 4.5. *Let $\psi \in \mathfrak{Q}(A_f(0)^2) \cap \mathfrak{D}(N_f)$, and let for some $p_0 \in (6/5, 2]$*

$$\|\nabla_k a_\lambda(k)\psi\| \in L^{p_0}(\mathbb{R}^3) + L^2(\mathbb{R}^3).$$

Then, the inequality

$$\langle A_f(0)^2\mathcal{U}^R\psi, \mathcal{U}^R\psi\rangle + \langle A_f(0)^2\mathcal{V}^R\psi, \mathcal{V}^R\psi\rangle - \langle A_f(0)^2\psi,\psi\rangle \leq \frac{c}{R^{1+\delta}} \tag{49}$$

holds with $\delta = (p_0-6/5)/2$.

Proof. Using the canonical commutation relations, we have

$$A_f(0)^2 = D(0)^2 + D^*(0)^2 + 2\mathcal{R}eD^*(0)D(0) + cI,$$

where the constant c depends on the ultraviolet cutoff. Therefore, it is sufficient to compute the localization error for $D(0)^2$ and $D^*(0)D(0)$. We have

$$\begin{aligned}
&\langle D(0)^2\mathcal{U}^R\psi, \mathcal{U}^R\psi\rangle + \langle D(0)^2\mathcal{V}^R\psi, \mathcal{V}^R\psi\rangle - \langle D(0)^2\psi, \psi\rangle \\
&= \sum_n \sqrt{n+1}\sqrt{n+2}\int G(y_{n+2})G(y_{n+1})\psi_{n+2}\overline{\psi_n} \\
&\qquad \times \left(u^R_{n+2}u^R_n + v^R_{n+2}v^R_n - 1\right) \mathrm{d}y_1 \ldots \mathrm{d}y_{n+2}
\end{aligned} \tag{50}$$

In the region where $\max_{i=1,\ldots,n+2}|y_i| \neq \max\{|y_{n+1}|, |y_{n+2}|\}$, we find

$$\left(u^R_{n+2}u^R_n + v^R_{n+2}v^R_n - 1\right)(y_1, \ldots, y_{n+2}) = \left((u^R_n)^2 + (v^R_n)^2 - 1\right)(y_1, \ldots, y_n) = 0\ . \tag{51}$$

In the region where $\max_{i=1,\ldots,n+2}|y_i| = |y_{n+2}| \leq R/2$, we have

$$u^R_{n+2}(y_1, \ldots, y_{n+2}) = u^R_n(y_1, \ldots, y_n) = 1$$

and

$$v^R_{n+2}(y_1, \ldots, y_{n+2}) = v^R_n(y_1, \ldots, y_n) = 0.$$

This yields (51) in that case. Similarly, in the region where $\max_{i=1,\ldots,n+2}|y_i| = |y_{n+1}| \leq R/2$, equation (51) holds. Therefore, in (50), it suffices to carry out the integration in the region $\{(y_1, \ldots y_{n+2}) \mid |y_{n+1}| \geq R/2\} \cup \{(y_1, \ldots y_{n+2}) \mid |y_{n+2}| \geq R/2\}$. Let us consider the integral in the first region. The other will be treated the same way. We have

$$\begin{aligned}
&\left|\sqrt{n+2}\sqrt{n+1}\int G(y_{n+2})G(y_{n+1})\psi_{n+2}\overline{\psi_n}\left(u^R_{n+2}u^R_n + v^R_{n+2}v^R_n - 1\right)\mathrm{d}y_1 \ldots \mathrm{d}y_{n+2}\right| \\
&\qquad \leq \frac{2^{1+\delta}}{R^{1+\delta}}\int |G(y_{n+1})|(1+|y_{n+1}|)^{1-\delta}|G(y_{n+2})|\sqrt{n+1}|\psi_n| \\
&\qquad\qquad \times\sqrt{n+2}|\psi_{n+2}|(1+|y_{n+1}|)^{2\delta}\mathrm{d}y_1 \ldots \mathrm{d}y_{n+2}\ .
\end{aligned} \tag{52}$$

Applying the Schwarz inequality and using (44) as in Lemma 4.4, we obtain the estimate

$$\begin{aligned}
&\Big|\sum_n\sqrt{n+1}\sqrt{n+2}\int G(y_{n+2})G(y_{n+1})\psi_{n+2}\overline{\psi_n} \\
&\qquad \left(u^R_{n+2}u^R_n + v^R_{n+2}v^R_n - 1\right)\mathrm{d}y_1 \ldots \mathrm{d}y_{n+2}\Big| \leq c\frac{1}{R^{1+\delta}}.
\end{aligned}$$

We have

$$\begin{aligned}
&\langle D^*(0)D(0)\mathcal{U}^R\psi, \mathcal{U}^R\psi\rangle + \langle D^*(0)D(0)\mathcal{V}^R\psi, \mathcal{V}^R\psi\rangle - \langle D^*(0)D(0)\psi, \psi\rangle \\
&= \sum_n (n+1)\int G(y_{n+1})\overline{G(z_{n+1})}\psi_{n+1}(y_1, \ldots, y_n, y_{n+1})\overline{\psi_{n+1}}(y_1, \ldots, y_n, z_{n+1}) \\
&\qquad \times\Big(u^R_{n+1}(y_1, \ldots, y_n, y_{n+1})u^R_{n+1}(y_1, \ldots, y_n, z_{n+1}) \\
&\qquad + v^R_{n+1}(y_1, \ldots, y_n, y_{n+1})v^R_n(y_1, \ldots, y_n, z_{n+1}) - 1\Big)\mathrm{d}y_1 \ldots \mathrm{d}y_{n+1}\mathrm{d}z_{n+1}
\end{aligned}$$

As before, in the region where both y_{n+1} and z_{n+1} are less than $R/2$, the expression inside the integral is zero. Without any loss of generality, we may assume that $y_n + 1 > R/2$. In that case, the expression above is bounded by

$$\begin{aligned}(n+1)R^{1+\delta}\|\psi_{n+1}(y_1,\dots,y_n,y_n+1)\chi(|y_n+1|\geq R/2)G(-y_n+1)\|^2\\ +(n+1)R^{-(1+\delta)}\|\psi_{n+1}(y_1,\dots,y_n,z_n+1)G(-z_n+1)\|^2\end{aligned}$$

Similarly to (52), we obtain

$$\|\psi_{n+1}(y_1,\dots,y_n,y_n+1)\chi(|y_n+1|\geq R/2)G(-y_n+1)\|^2 \leq R^{-2(1+\delta)}\|\psi_{n+1}\|^2.$$

Therefore,

$$\langle D^*(0)D(0)\mathcal{U}^R\psi,\mathcal{U}^R\psi\rangle + \langle D^*(0)D(0)\mathcal{V}^R\psi,\mathcal{V}^R\psi\rangle - \langle D^*(0)D(0)\psi,\psi\rangle \leq \frac{c}{R^{1+\delta}}.$$

This concludes the proof. □

4.1.5. *Localization error for the operator $\sigma.B_f(0)$.*

Lemma 4.6. *Let $\psi \in \mathfrak{Q}(\sigma.B_f(0)) \cap \mathfrak{D}(N_f)$, and assume that there exists $p_0 \in (6/5, 2]$, such that*

$$\|\nabla_k a_\lambda(k)\psi\| \in L^{p_0}(\mathbb{R}^3) + L^2(\mathbb{R}^3).$$

Then, the inequality

$$\langle \sigma.B_f(0)\mathcal{U}^R\psi,\mathcal{U}^R\psi\rangle + \langle \sigma.B_f(0)\mathcal{V}^R\psi,\mathcal{V}^R\psi\rangle - \langle \sigma.B_f(0)\psi,\psi\rangle \leq \frac{c}{R^{1+\delta}} \tag{53}$$

holds with $\delta = (p_0 - 6/5)/2$.

The proof of Lemma 4.6 is similar to the one of Lemma 4.5, with a large number of simplifications.

4.2. **Proof of Theorem 4.1.** We let

$$\Phi^R := \mathcal{U}^R\Omega_0, \tag{54}$$

where Ω_0 is a normalized ground state eigenfunction of the operator $T(0)$, and where $\mathcal{U}^R$ is defined in (28). We recall that we have $\langle T(0)\Omega_0,\Omega_0\rangle = \Sigma_0\|\Omega_0\|^2$. We would like to show that the value of the quadratic form associated to $T(0)$ at Φ^R is, for large R, close to the value of the quadratic form associated to $T(0)$ at Ω_0.

First, we notice that Ω_0 fulfills all the conditions of Lemmata 4.1-4.6 which implies that

$$\langle T(0)\Omega_0,\Omega_0\rangle = \langle T(0)\mathcal{U}^R\Omega_0,\mathcal{U}^R\Omega_0\rangle + \langle T(0)\mathcal{V}^R\Omega_0,\mathcal{V}^R\Omega_0\rangle + \frac{C(R)}{R},$$

where $C(R)$ tends to zero as R tends to infinity. Thus, since $\langle T(0)\mathcal{V}^R\Omega_0,\mathcal{V}^R\Omega_0\rangle \geq \Sigma_0\|\mathcal{V}^R\Omega_0\|^2$, we obtain

$$\begin{aligned}\langle T(0)\Phi^R,\Phi^R\rangle &\leq \Sigma_0 + \frac{|C(R)|}{R} - \Sigma_0\langle T(0)\mathcal{V}^R\Omega_0,\mathcal{V}^R\Omega_0\rangle\\ &\leq \Sigma_0(1-\|\mathcal{V}^R\Omega_0\|^2) + \frac{|C(R)|}{R} = \Sigma_0\|\Phi^R\|^2 + \frac{|C(R)|}{R}\ ,\end{aligned}$$

which proves ii) of Theorem 4.1.

To complete the proof of Theorem 4.1, it suffices to prove the two Inequalities (20) and (23). Let us start with (20).

$$
\begin{aligned}
|\langle D(x)\Phi^R,\Phi^R\rangle| &\le \sum_n \sqrt{n+1}\int |G(x-y_{n+1})|\ |\Phi^R_{n+1}|\ |\Phi^R_n| \mathrm{d}y_1\mathrm{d}y_{n+1}\\
&= \sum_n \sqrt{n+1}\frac{2}{|x|}\int_{|y_{n+1}|\le R} |G(x-y_{n+1})|(1+|x-y_{n+1}|)|\Phi^R_{n+1}|\\
&\qquad\qquad \times \frac{(1+|y_{n+1}|)^{2\delta}}{(1+|y_{n+1}|)^{2\delta}}|\Phi^R_n|\mathrm{d}y_1\mathrm{d}y_{n+1}
\end{aligned}
$$

By applying the Schwarz inequality, we get

$$
\begin{aligned}
|\langle D(x)\Phi^R,\Phi^R\rangle| &\le \sum_n \sqrt{n+1}\int |G(x-y_{n+1})|\ |\Phi^R_{n+1}|\ |\Phi^R_n| \mathrm{d}y_1\mathrm{d}y_{n+1}\\
&= \sum_n \frac{2}{|x|}\|G(x-y_{n+1})(1+|x-y_{n+1}|)(1+|y_{n+1}|)^{-2\delta}\Phi^R_n\|\\
&\qquad\qquad \times\|\sqrt{n+1}(1+|y_{n+1}|)^{2\delta}\Phi^R_{n+1}\|
\end{aligned}
\tag{55}
$$

We recall that from Lemma 7.1 that $|G(x-y_{n+1})(1+|x-y_{n+1}|)|\in L^r(\mathbb{R}^3)$ for all $r>2$. Therefore, for $p>3/(3-2\delta)$, and q given by $1/p+1/q=1$, we have $\|(1+|y_{n+1}|)^{-2\delta}\|_q<\infty$. Thus,

$$
\begin{aligned}
&\|G(x-y_{n+1})(1+|x-y_{n+1}|)(1+|y_{n+1}|)^{-2\delta}\Phi^R_n\|\\
&\le\ \|G(x-y_{n+1})(1+|x-y_{n+1}|)\chi(|y_{n+1}|\le R)\|_p\|(1+|y_{n+1}|)^{-2\delta}\|_q\|\Phi^R_n\|.
\end{aligned}
$$

Moreover, for $|x|>2R$, the norm $\|G(x-y_{n+1})(1+|x-y_{n+1}|)\chi(|y_{n+1}|\le R)\|_p$ tends to zero as $R\to\infty$. This estimate together with (55) yields

$$
|\langle D(x)\Phi^R,\Phi^R\rangle| \ \le\ \frac{2}{|x|}\varepsilon(x)\sum_n\left(\|\Phi^R_n\|^2+\|\sqrt{n+1}(1+|y_{n+1}|)^{2\delta}\Phi^R_{n+1}\|^2\right)
$$

Conditions $\mathfrak{C}_1iii)$ and $\mathfrak{C}_1iv)$ together with the above inequality conclude the proof of (20) if we pick $\delta=(p_0-6/5)/2$. The proofs of (21), (22), and (23) are similar.

5. Approximate ground state for a system with an external potential

In the present section, we consider the Pauli-Fierz Hamiltonian for M electrons with an external potential

$$
\begin{aligned}
H_M = &\sum_{\ell=1}^{M}\left\{\left(-i\nabla_{x_\ell}\otimes I_f+\sqrt{\alpha}A_f(x_\ell)\right)^2+\sqrt{\alpha}\sigma\cdot B_f(x_\ell)+V(x_\ell)\otimes I_f\right\}\\
&+\frac{1}{2}\sum_{1\le k,\ell\le M} W(x_k-x_\ell)\otimes I_f+I_{el}\otimes H_f\ ,
\end{aligned}
$$

acting on $\mathcal{H}=\mathcal{H}^{el}_M\otimes\mathcal{F}$. The brackets $\langle\,\cdot\,,\,\cdot\,\rangle$ will from here on denote the scalar product on $\mathcal{H}$. Furthermore, for the rest of this section, we will write operators of the form $I_{el}\otimes A_f$ or $B_{el}\otimes I_f$ on $\mathcal{H}$ simply as A_f or B_{el}, respectively, in order not to overburden the notation. The precise meaning will be clear from the context.

We assume that the Condition $\mathfrak{C}_2$ is fulfilled for this system, which implies, in particular, that the operator H_M has a ground state. We will construct an approximation to the ground state which is spatially localized with respect to the electron and photon variables, and whose energy is close to the ground state energy.

5.1. **Localization of the electrons.** We start with localization in the electron configuration space. To this end, we recall from (6) that Υ denotes the ground state of H_M. For u given by (27), we define $\Upsilon^R = (\Upsilon_0^R, \Upsilon_1^R, \ldots, \Upsilon_n^R, \ldots) \in \mathcal{H} = \mathcal{H}_M^{el} \otimes \mathcal{F}$ by

$$\Upsilon_n^R = u\left(\frac{2\sqrt{\sum_{i=1}^M |x_i|^2}}{R}\right)\Upsilon_n \,,$$

where Υ_n is the n-photon component of Υ. Notice that on the support of Υ^R, we have $|x_i| \leq R/2$ for $i = 1, \ldots, M$.

Lemma 5.1. *For all $R > 1$,*

$$\langle H_M \Upsilon^R, \Upsilon^R\rangle \leq E_M + \frac{c}{R^2} \tag{56}$$

$$1 - \frac{c}{R^2} \leq \|\Upsilon^R\| \leq 1 \tag{57}$$

The proof of this Lemma follows immediately from standard localization error estimates for Schrödinger operators [5], and the Condition $\mathfrak{C}_2$ iii).

5.2. **Localization of photons.** Our next goal is to localize all photons in a ball of radius $2R$ centered at the origin. For this purpose, we define the function $\Psi^R = (\Psi_1^R, \Psi_2^R, \ldots \Psi_n^R, \ldots) \in \mathcal{H}_M^{el} \otimes \mathcal{F}$ as

$$\Psi^R = \mathcal{U}^{2R}\Upsilon^R. \tag{58}$$

where $\mathcal{U}^R$ straightforwardly extends the operator defined on $\mathcal{F}$ in (28) to $\mathcal{H}_M^{el} \otimes \mathcal{F}$.

We note here that the localization radius for photons is chosen to be four times larger than that for the electrons. The consequence is that the contribution of the "external" photons to the magnetic vector-potential will be negligible within the region where the electrons are localized.

Similarly to Lemma 4.1, we find that there exists $c < \infty$, such that for all $\varepsilon > 0$, and all R large enough,

$$\begin{aligned} &\langle H_f \mathcal{U}^{2R}\Upsilon^R, \mathcal{U}^{2R}\Upsilon^R\rangle + \langle H_f \mathcal{V}^{2R}\Upsilon^R, \mathcal{V}^{2R}\Upsilon^R\rangle - \langle H_f \Upsilon^R, \Upsilon^R\rangle \\ &\qquad \leq \langle N_f \Upsilon^R, \Upsilon^R\rangle \left(\frac{\varepsilon}{R} + \frac{c}{\varepsilon R}\frac{\|\mathcal{V}^R\Upsilon^R\|^2}{\|\Upsilon^R\|^2}\right). \end{aligned} \tag{59}$$

Obviously, it suffices to compute the localization error only for the operator

$$(-i\nabla_{x_1} + \sqrt{\alpha}A_f(x_1))^2 + \sqrt{\alpha}\sigma \cdot B_f(x_1) + H_f.$$

In the rest of this section, we will denote $x = x_1$.

Lemma 5.2. *The following estimate holds*

$$\begin{aligned} &\left|\langle \mathcal{U}^{2R}\Upsilon^R, i\nabla_x A_f(x)\mathcal{U}^{2R}\Upsilon^R\rangle + \langle \mathcal{V}^{2R}\Upsilon^R, i\nabla_x A_f(x)\mathcal{V}^{2R}\Upsilon^R\rangle - \langle \Upsilon^R, i\nabla_x A_f(x)\Upsilon^R\rangle\right| \\ &\qquad \leq \frac{c}{R^{1+\delta}}\left(\|N_f\Upsilon^R\|^2 + \|\nabla_x \Upsilon^R\|^2\right), \end{aligned} \tag{60}$$

where $\delta = (p_0 - 6/5)/2$ and p_0 is given by $\mathfrak{C}_2$ ii).

Proof. The proof of this Lemma is very similar to the one of Lemma 4.4.

$$
\begin{aligned}
&\big|\langle \mathcal{U}^{2R}\Upsilon^R, i\nabla_x D(x)\mathcal{U}^{2R}\Upsilon^R\rangle + \langle \mathcal{V}^{2R}\Upsilon^R, i\nabla_x D(x)\mathcal{V}^{2R}\Upsilon^R\rangle - \langle \Upsilon^R, i\nabla_x D(x)\Upsilon^R\rangle\big| \\
&\quad \le \int_{|x|\le\frac{R}{2}} \mathrm{d}x \sum_n \sqrt{n+1}\int |G_\lambda(x-y_{n+1})|\, |\Upsilon^R_{n+1}|\, |\nabla_x \Upsilon^R_n| \\
&\quad \times (u_n^{2R}u_{n+1}^{2R} + v_n^{2R}v_{n+1}^{2R} - 1)\mathrm{d}y_1\ldots\mathrm{d}y_{n+1}.
\end{aligned}
\tag{61}
$$

Similarly to Lemma 4.4, we show that $(u_n^{2R}u_{n+1}^{2R} + v_n^{2R}v_{n+1}^{2R} - 1)$ is nonzero only if $|y_{n+1}| \ge R$. This implies $|x-y_{n+1}| \ge |y_{n+1}|/2 \ge R/2$. Therefore, the integral in (61) can be estimated by

$$
\begin{aligned}
&\frac{1}{R^{1+\delta}}\int_{|x|\le\frac{R}{2}} \mathrm{d}x \sum_n \sqrt{n+1}\|\Upsilon^R_{n+1}(1+|y_{n+1}|)^{2\delta}\| \\
&\quad \times \|\sum_\lambda G_\lambda(x-y_{n+1})(1+|x-y_{n+1}|)^{1-\delta}\|\ \|\nabla_x\Upsilon^R_n\|
\end{aligned}
\tag{62}
$$

Since the term $\|\nabla_x\Upsilon^R\|$ is finite, the rest of the proof is not different from the one of Lemma 4.4. ∎

Similarly to Lemmata 4.5 and 4.6 and the above Lemma 5.2, one can prove that

$$
\big|\langle \mathcal{U}^{2R}\Upsilon^R, A^2(x)\mathcal{U}^{2R}\Upsilon^R\rangle + \langle \mathcal{V}^{2R}\Upsilon^R, A^2(x)\mathcal{V}^{2R}\Upsilon^R\rangle - \langle \Upsilon^R, A^2(x)\Upsilon^R\rangle\big| \le \frac{c}{R^{1+\delta}} \tag{63}
$$

and

$$
\begin{aligned}
&\big|\langle \mathcal{U}^{2R}\Upsilon^R, \sigma\cdot B_f(x)\mathcal{U}^{2R}\Upsilon^R\rangle + \langle \mathcal{V}^{2R}\Upsilon^R, \sigma\cdot B_f(x)\mathcal{V}^{2R}\Upsilon^R\rangle - \langle \Upsilon^R, \sigma\cdot B_f(x)\Upsilon^R\rangle\big| \\
&\qquad \le \frac{c}{R^{1+\delta}}
\end{aligned}
\tag{64}
$$

Theorem 5.1 (Energy of the approximate ground state)**.** *For arbitrarily fixed $\varepsilon > 0$ and R large enough, the following statements hold.*
i)

$$
E_M\|\Psi^R\|^2 \le \langle H_M\Psi^R, \Psi^R\rangle \le E_M\|\Psi^R\|^2 + \frac{\varepsilon}{R}\|\Psi^R\|^2 \tag{65}
$$

ii) Let $z \in \mathbb{R}^3$ be an external variable, i.e., the function Ψ^R does not depend on z. Then, for $|z| > 4R$

$$
|\langle D(z)\Psi^R, \Psi^R\rangle| \le \frac{c(z)}{|z|}\ , \tag{66}
$$

$$
|\langle D(z)^2\Psi^R, \Psi^R\rangle| \le \frac{c(z)}{|z|^2}\ , \tag{67}
$$

$$
|\langle D^*(z)D(z)\Psi^R, \Psi^R\rangle| \le \frac{c(z)}{|z|^2}\ , \tag{68}
$$

and

$$
|\langle K(z)\Psi^R, \Psi^R\rangle| \le \frac{c(z)}{|z|}\ , \tag{69}
$$

where $c(z)$ is a function independent of R that tends to zero as $|z|$ tends to infinity.

Proof. Applying Lemma 5.1, and Inequalities (60), (63), (64), we obtain

$$\langle H_M \mathcal{U}^{2R}\Upsilon^R, \mathcal{U}^{2R}\Upsilon^R\rangle + \langle H_M \mathcal{V}^{2R}\Upsilon^R, \mathcal{V}^{2R}\Upsilon^R\rangle - \frac{\varepsilon}{R} \leq E_M + \frac{c}{R^2} \tag{70}$$

Using $E_M\|\mathcal{V}^{2R}\Upsilon^R\|^2 \leq \langle H_M \mathcal{V}^{2R}\Upsilon^R, \mathcal{V}^{2R}\Upsilon^R\rangle$, we get

$$\langle H_M \mathcal{U}^{2R}\Upsilon^R, \mathcal{U}^{2R}\Upsilon^R\rangle \leq E_M\|\mathcal{U}^{2R}\Upsilon^R\|^2 + \frac{\varepsilon}{R} + \frac{c}{R^2} \tag{71}$$

Since $\|\Upsilon^R\| \to 1$ as $R \to \infty$, we get (65).

The proof of ii) is analogous to the proof of Lemma 5.2 and Theorem 4.1 iii). □

6. Proof of Theorem 2.1

The previous discussion enables us to construct a normalized trial function $\Gamma^{R,b} \in \mathcal{H}_N^{el} \otimes \mathcal{F}$. For given $N \in \mathbb{N}$, we define $\tilde{\Psi}^{R,N-1}$ as

$$\tilde{\Psi}^{R,N-1} = \frac{\Psi^R}{\|\Psi^R\|},$$

where Ψ^R is the function defined in Section 5.2 for a system of $M = N-1$ electrons. As a natural candidate for a trial state for the proof of Theorem 2.1, one could consider the state $\varphi = (\varphi_0, \varphi_1, \dots)$ defined by

$$\begin{aligned}\varphi_n = \sum_{j=0}^{n} &\Theta_j^{R,b}(y_1, \dots, y_j, \lambda_1, \dots, \lambda_j, x_N, s_N)\, \cdot \\ &\times \tilde{\Psi}_{n-j}^{R,N-1}(y_{j+1}, \dots, y_n, \lambda_{j+1}, \dots, \lambda_n, x_1, \dots, x_{N-1}, s_1, \dots, s_{N-1}).\end{aligned} \tag{72}$$

However, since the components φ_n are neither symmetric in the photon, nor antisymmetric in the electron variables, our next goal is to symmetrize the function φ_n in the photon variables, and to antisymmetrize it in the electron variables.

We denote by $S_{n,j}$ the set of $\binom{n}{j}$ possible partitions g of the set of n indices $\{1, \dots, n\}$ into two subsets C_1 and C_2 with j and $n-j$ elements respectively. Let $i_1(g), \dots, i_j(g)$ be the indices in C_1 and $i_{j+1}(g), \dots, i_n(g)$ in C_2. We define the function

$$\begin{aligned}(\Pi_{n,j}^p(g)&\Theta_j^{R,b}\tilde{\psi}_{n-j}^{R,N-1})(y_1, \dots, y_n, \lambda_1, \dots, \lambda_n, x, s) \\ &:= \Theta_j^{R,b}(y_{i_1}, \dots, y_{i_j}, \lambda_{i_1}, \dots, \lambda_{i_j}, x_N, s_N) \\ &\times \tilde{\psi}_{n-j}^{R,N-1}(y_{i_{j+1}}, \dots, y_{i_n}, \lambda_{i_{j+1}}, \dots, \lambda_{i_n}, x_1, \dots, x_{N-1}, s_1, \dots s_{N-1})\,.\end{aligned}$$

Evidently,

$$\tilde{\Gamma}_n^{R,b} := \sum_{j=0}^{n} \binom{n}{j}^{-1/2} \sum_{g \in S_{n,j}} \Pi_{n,j}^p(g)\Theta_j^{R,b}\tilde{\Psi}_{n-j}^{R,N-1} \tag{73}$$

is symmetric with respect to the permutation of photon variables.

To construct a combination of the functions $\tilde{\Gamma}_n^{R,b}$ which is antisymmetric in the electron variables, let us consider the set of all transpositions π_i $i = 1, \dots, N$, which exchange a pair of electron variables (x_i, s_i) with (x_N, s_N), including the trivial transposition $(x_N, s_N) \leftrightarrow (x_N, s_N)$. For an arbitrary function $\varphi(x_1, \dots, x_N, s_1, \dots, s_N)$, let

$$(\Pi_i^{el}\varphi)(x_1, \dots, x_N, s_1, \dots, s_N) := \varphi(\pi_i(x_1, \dots, x_N, s_1, \dots, s_N)).$$

Then, we define

$$\Gamma_n^{R,b}=\sum_{j=0}^{n}N^{-1/2}\binom{n}{j}^{-1/2}\sum_{i=1}^{N}\sum_{g\in S_{n,j}}(-1)^{\kappa(i)}\Pi_i^{el}\Pi_{n,j}^{p}(g)\Theta_j^{R,b}\tilde{\Psi}_{n-j}^{R,N-1},\tag{74}$$

where $\kappa(i)=0$ if $i=N$, and $\kappa(i)=1$ otherwise. Obviously,

$$\Gamma^{R,b}=(\Gamma_0^{R,b},\Gamma_1^{R,b},\dots,\Gamma_n^{R,b},\dots)\in\mathcal{H}_N^{el}\otimes\mathcal{F}.$$

Notice that $\Gamma^{R,b}$ is a normalized function in $\mathcal{H}_N^{el}\otimes\mathcal{F}$, since if $|b|>5R$, the summands in (74) have for different i disjoint supports in electron variables, and thus

$$\|\Gamma^{R,b}\|^2=\|\tilde{\Gamma}^{R,b}\|^2=1\tag{75}$$

and

$$(H_N\Gamma^{R,b},\ \Gamma^{R,b})=(H_N\tilde{\Gamma}^{R,b},\ \tilde{\Gamma}^{R,b}).$$

Although the state $\tilde{\Gamma}^{R,b}$ is not antisymmetric in all electron variables, the quadratic form of H_N at $\tilde{\Gamma}^{R,b}$ is well-defined.

Furthermore, both functions $\Theta^{R,b}$ and $\tilde{\Psi}^{R,N-1}$ have a finite expectation number of photons, say, N_1 and N_2, respectively. Evidently, this implies that $\Gamma^{R,b}$ has a finite expected photon number N_1+N_2.

We remark that for $|b|>5R$, and each of the terms in the sum

$$\Pi_i^{el}\sum_{g\in S_{n,j}}\Pi_{n,j}^{p}(g)\Theta_j^{R,b}\tilde{\psi}_{n-j}^{R,N-1},$$

$\Theta_j^{R,b}$ and $\tilde{\psi}_{n-j}^{R,N-1}$ have disjoint supports, thus one finds

$$(H_N\Gamma^{R,b},\ \Gamma^{R,b})=(H_N\tilde{\Gamma}^{R,b},\ \tilde{\Gamma}^{R,b}),$$

where, as we recall from (73), $\tilde{\Gamma}^{R,b}=(\tilde{\Gamma}_0^{R,b},\tilde{\Gamma}_1^{R,b},\dots)$ is the state prior to antisymmetrization in the electron variables. Hence, instead of estimating the quadratic form of the operator H_N with respect to the state $\Gamma^{R,b}$, we may estimate it with respect to $\tilde{\Gamma}^{R,b}$. Although this state is not antisymmetric in all electron variables, the quadratic form is well-defined.

We recall that in our notation for the state $\tilde{\Gamma}^{R,b}$, the variables (x_N,s_N) are the arguments of $\Theta^{R,b}$, while $(x_1,\dots,x_{N-1},s_1,\dots,s_{N-1})$ are the arguments of $\tilde{\psi}^{R,N-1}$, and furthermore, that $\|\tilde{\Gamma}^{R,b}\|=1$.

Lemma 6.1. *For $|b|>8R$, there exists $c>0$ independent of R such that the following estimate holds*

$$\langle H_f\Gamma^{R,b},\Gamma^{R,b}\rangle\leq\langle H_f\Theta^{R,b},\Theta^{R,b}\rangle+\langle H_f\tilde{\Psi}^{R,N-1},\tilde{\Psi}^{R,N-1}\rangle+c\frac{R^{3/2}}{|b|^{5/2}}\langle N_f\Gamma^{R,b},\Gamma^{R,b}\rangle$$

Proof. We have

$$H_f\tilde{\Gamma}_n^{R,b}=n|\nabla_{y_1}|\sum_{j=0}^{n}\binom{n}{j}^{-1/2}\sum_{g\in S_{n,j}}\Pi_{n,j}^{p}(g)\Theta_j^{R,b}\tilde{\Psi}_{n-j}^{R,N-1}\ .\tag{76}$$

Let us start with one of the functions in the sum (76). We take for example the expression $n|\nabla_{y_1}|\Theta_j^{R,b}(y_1,\dots,y_j)\tilde{\Psi}_{n-j}^{R,N-1}(y_{j+1},\dots,y_n)$. All other terms can be treated similarly.

In the quadratic form $\langle H_f \tilde{\Gamma}^{R,b}, \tilde{\Gamma}^{R,b}\rangle$, this term appears twice, in

$$n\Big\langle |\nabla_{y_1}| \Theta_j^{R,b}(y_1,\dots,y_j)\tilde{\Psi}_{n-j}^{R,N-1}(y_{j+1},\dots,y_n), \\ \Theta_j^{R,b}(y_1,\dots,y_j)\tilde{\Psi}_{n-j}^{R,N-1}(y_{j+1},\dots,y_n)\Big\rangle,$$

and in

$$n\Big\langle |\nabla_{y_1}| \Theta_j^{R,b}(y_1,\dots,y_j)\tilde{\Psi}_{n-j}^{R,N-1}(y_{j+1},\dots,y_n), \\ \Theta_{j-1}^{R,b}(y_2,\dots,y_j)\tilde{\Psi}_{n-j+1}^{R,N-1}(y_1,y_{j+1},\dots,y_n)\Big\rangle. \tag{77}$$

All other cross terms appearing in the quadratic form $\langle H_f \tilde{\Gamma}^{R,b}, \tilde{\Gamma}^{R,b}\rangle$ that contain the function $n|\nabla_{y_1}|\Theta_j^{R,b}(y_1,\dots,y_j)\tilde{\Psi}_{n-j}^{R,N-1}(y_{j+1},\dots,y_n)$ are zero, because at least for one variable, the supports of the functions in the scalar product are disjoint. Let us now estimate (77). The function

$$\Theta_j^{R,b}(y_1,\dots,y_j)\tilde{\Psi}_{n-j}^{R,N-1}(y_{j+1},\dots,y_n)$$

is supported in the region $\{|y_1| \geq |b| - 2R\}$ whereas

$$\Theta_{j-1}^{R,b}(y_2,\dots,y_j)\tilde{\Psi}_{n-j+1}^{R,N-1}(y_1,y_{j+1},\dots,y_n)$$

is supported in the region $\{|y_1| \leq 2R\}$. Applying Lemma 7.2 with $|b| > 8R$, we arrive at

$$\begin{aligned} & n\Big|\Big\langle |\nabla_{y_1}| \Theta_j^{R,b}(y_1,\dots,y_j)\tilde{\Psi}_{n-j}^{R,N-1}(y_{j+1},\dots,y_n), \\ &\qquad \Theta_{j-1}^{R,b}(y_2,\dots,y_j)\tilde{\Psi}_{n-j+1}^{R,N-1}(y_1,y_{j+1},\dots,y_n)\Big\rangle\Big| \\ &\leq c\, n\frac{R^{3/2}}{|b|^{5/2}}\Big(\|\Theta_j^{R,b}(y_1,\dots,y_j)\tilde{\Psi}_{n-j}^{R,N-1}(y_{j+1},\dots,y_n)\|^2 \\ &\qquad + \|\Theta_{j-1}^{R,b}(y_2,\dots,y_j)\tilde{\Psi}_{n-j+1}^{R,N-1}(y_1,y_{j+1},\dots,y_n)\|^2\Big), \end{aligned} \tag{78}$$

which implies

$$\begin{aligned} &\langle H_f \tilde{\Gamma}^{R,b}, \tilde{\Gamma}^{R,b}\rangle \leq c\frac{R^{3/2}}{|b|^{5/2}}\langle N_f \tilde{\Gamma}^{R,b}, \tilde{\Gamma}^{R,b}\rangle \\ &\quad + \sum_n n\sum_{j=0}^n \binom{n}{j}^{-1} \sum_{g\in S_{n,j}} \langle |\nabla_{y_1}| \Pi_{n,j}^p(g)\Theta_j^{R,b}\tilde{\Psi}_{n-j}^{R,N-1}, \Pi_{n,j}^p(g)\Theta_j^{R,b}\tilde{\Psi}_{n-j}^{R,N-1}\rangle. \end{aligned} \tag{79}$$

For fixed n and j, in the sum

$$\sum_{g\in S_{n,j}} \langle |\nabla_{y_1}| \Pi_{n,j}^p(g)\Theta_j^{R,b}\tilde{\Psi}_{n-j}^{R,N-1}, \Pi_{n,j}^p(g)\Theta_j^{R,b}\tilde{\Psi}_{n-j}^{R,N-1}\rangle,$$

the variable y_1 appears $\binom{n-1}{j-1}$ times in $\Theta_j^{R,b}$ and $\binom{n-1}{n-j-1}$ times in $\tilde{\Psi}_{n-j}^{R,N-1}$. Therefore, the second term on the right hand side of (79) can be rewritten as

$$
\begin{aligned}
&\sum_n \sum_{j=1}^n n \binom{n}{j}^{-1} \binom{n-1}{j-1} \langle |\nabla_{y_1}| \Theta_j^{R,b}(y_1, \dots, y_j), \Theta_j^{R,b}(y_1, \dots, y_j) \rangle \| \tilde{\Psi}_{n-j}^{R,N-1} \|^2 \\
&\quad + \sum_n \sum_{j=1}^n n \binom{n}{j}^{-1} \binom{n-1}{n-j-1} \| \Theta_j^{R,b} \|^2 \\
&\qquad \langle |\nabla_{y_1}| \tilde{\Psi}_{n-j}^{R,N-1}(y_1, \dots y_{n-j}), \tilde{\Psi}_{n-j}^{R,N-1}(y_1, \dots y_{n-j}) \rangle \\
&= \sum_n \sum_{j=1}^n j \langle |\nabla_{y_1}| \Theta_j^{R,b}(y_1, \dots, y_j), \Theta_j^{R,b}(y_1, \dots, y_j) \rangle \| \tilde{\Psi}_{n-j}^{R,N-1} \|^2 \\
&\quad + \sum_n \sum_{j=1}^n (n-j) \| \Theta_j^{R,b} \|^2 \langle |\nabla_{y_1}| \tilde{\Psi}_{n-j}^{R,N-1}(y_1, \dots y_{n-j}), \tilde{\Psi}_{n-j}^{R,N-1}(y_1, \dots y_{n-j}) \rangle \\
&= \langle H_f \Theta^{R,b}, \Theta^{R,b} \rangle + \langle H_f \tilde{\Psi}^{R,N-1}, \tilde{\Psi}^{R,N-1} \rangle
\end{aligned}
\tag{80}
$$

The relations (79) and (80) imply the statement of the Lemma. □

Lemma 6.2. *For any $\varepsilon > 0$ and $|b|$ large enough,*

$$
\begin{aligned}
&\langle \sum_{\ell=1}^N i \nabla_{x_\ell} A(x_\ell) \tilde{\Gamma}^{R,b}, \tilde{\Gamma}^{R,b} \rangle \\
&\le \langle i \nabla_{x_N} A(x_N) \Theta^{R,b}, \Theta^{R,b} \rangle + \sum_{\ell=1}^{N-1} \langle i \nabla_{x_\ell} A(x_\ell) \tilde{\Psi}^{R,N-1}, \tilde{\Psi}^{R,N-1} \rangle \\
&\quad + \frac{\varepsilon}{2(|b| - 2R)} \left(\| \nabla_{x_N} \Theta^{R,b} \|^2 + \| \Theta^{R,b} \|^2 \right) \\
&\quad + \sum_{\ell=1}^{N-1} \frac{\varepsilon}{2(|b| - 2R)} \left(\| \nabla_{x_\ell} \tilde{\Psi}^{R,N-1} \|^2 + \| \tilde{\Psi}^{R,N-1} \|^2 \right).
\end{aligned}
\tag{81}
$$

Furthermore,

$$
\begin{aligned}
&\langle \sum_{\ell=1}^N \sigma \cdot B(x_\ell) \tilde{\Gamma}^{R,b}, \tilde{\Gamma}^{R,b} \rangle \\
&\le \langle \sigma \cdot B(x_N) \Theta^{R,b}, \Theta^{R,b} \rangle + \sum_{\ell=1}^{N-1} \langle \sigma \cdot B(x_\ell) \tilde{\Psi}^{R,N-1}, \tilde{\Psi}^{R,N-1} \rangle \\
&\quad + \frac{\varepsilon}{(|b| - 2R)} \| \Theta^{R,b} \|^2 + \sum_{\ell=1}^{N-1} \frac{\varepsilon}{(|b| - 2R)} \| \tilde{\Psi}^{R,N-1} \|^2 ,
\end{aligned}
\tag{82}
$$

and

$$\tag{83}\begin{aligned}\Big|\langle\sum_{\ell=1}^{N}D^2(x_\ell)\tilde\Gamma^{R,b},\tilde\Gamma^{R,b}\rangle-\langle D^2(x_N)\Theta^{R,b},\Theta^{R,b}\rangle-\sum_{\ell=1}^{N-1}\langle D^2(x_\ell)\tilde\Psi^{R,N-1},\tilde\Psi^{R,N-1}\rangle\Big|\\ \le\frac{\varepsilon}{(|b|-2R)}\|\Theta^{R,b}\|^2+\sum_{\ell=1}^{N-1}\frac{\varepsilon}{(|b|-2R)}\|\tilde\Psi^{R,N-1}\|^2\end{aligned}$$

Moreover,

$$\tag{84}\begin{aligned}\Big|\langle\sum_{\ell=1}^{N}D^*(x_\ell)D(x_\ell)\tilde\Gamma^{R,b},\tilde\Gamma^{R,b}\rangle-\langle D^*(x_N)D(x_N)\Theta^{R,b},\Theta^{R,b}\rangle\\ -\sum_{\ell=1}^{N-1}\langle D^*(x_\ell)D(x_\ell)\tilde\Psi^{R,N-1},\tilde\Psi^{R,N-1}\rangle\Big|\\ \le\frac{\varepsilon}{(|b|-2R)}\|\Theta^{R,b}\|^2+\sum_{\ell=1}^{N-1}\frac{\varepsilon}{(|b|-2R)}\|\tilde\Psi^{R,N-1}\|^2\end{aligned}$$

Proof. We recall that in $\Theta_j^{R,b}\tilde\Psi_{n-j}^{R,N-1}$, the variable x_1 appears only in the function $\tilde\Psi_{n-j}^{R,N-1}$, and the variable x_N only in $\Theta_j^{R,b}$. Permutations of photon variables do not change this fact. We have, for $k=1,\dots,N$,

$$\tag{85}\begin{aligned}&\Big(D(x_k)\tilde\Gamma^{R,b}\Big)_{n-1}\\ &=\sum_{j=0}^{n}\binom{n}{j}^{-1/2}\sum_{g\in S_{n,j}}\sqrt{n}\langle G(x_k-y_n),\Pi_{n,j}^p(g)\Theta_j^{R,b}\tilde\Psi_{n-j}^{R,N-1}\rangle_{L^2(\mathbb{R}^3\otimes\mathbb{C}^2,\mathrm{d}y_n)}\ ,\end{aligned}$$

where as before, $\mathrm{d}y_n$ means integration with respect to y_n and summation over the associated polarization λ_n.

Let us start with one of the functions $\Pi_{n,j}^p(g)\Theta_j^{R,b}\tilde\Psi_{n-j}^{R,N-1}$ in the sum (73). For fixed g, two variants are possible. Either the index n is in C_1, and the function $\Theta_j^{R,b}$ depends on the photon variable y_n, or the function $\tilde\Psi_{n-j}^{R,N-1}$ depends on y_n. For fixed n and j, the first variant occurs $\binom{n-1}{j-1}$ times, whereas the second one occurs $\binom{n-1}{n-j-1}$ times. Let us consider the function

$$\binom{n}{j}^{-1/2}\Theta_j^{R,b}(x_N,y_1,\dots y_j)\tilde\Psi_{n-j}^{R,N-1}(x_1,\dots x_{N-1},y_{j+1},\dots y_n)$$

In the quadratic form $\langle\sum_{k=1}^N i\nabla_{x_k}D(x_k)\tilde\Gamma^{R,b},\tilde\Gamma^{R,b}\rangle$, it appears only once in the scalar product with

$$\begin{aligned}\sqrt{n}\nabla_{x_k}\overline{G(x_k-y_n)}\binom{n-1}{j-1}^{-1/2}\Theta_j^{R,b}(x_N,y_1,\dots y_j)\\ \times\tilde\Psi_{n-j}^{R,N-1}(x_1,\dots x_{N-1},y_{j+1},\dots y_{n-1})\end{aligned}$$

which, in the case $k \neq N$, is equal to

$$\sqrt{n-j}\begin{pmatrix} n-1 \\ n-j-1 \end{pmatrix}^{-1} \Big\langle \tilde{\Psi}^{R,N-1}_{n-j}(x_1, \dots x_{N-1}, y_{j+1}, \dots y_n), \tag{86}$$
$$\nabla_{x_k}\overline{G(x_k - y_n)}\tilde{\Psi}^{R,N-1}_{n-j-1}(x_1, \dots x_{N-1}, y_{j+1}, \dots y_{n-1})\Big\rangle \|\Theta^{R,b}_j\|^2 \ ,$$

and in the case $k = N$,

$$\sqrt{n-j}\begin{pmatrix} n-1 \\ n-j-1 \end{pmatrix}^{-1}$$
$$\Big\langle \tilde{\Psi}^{R,N-1}_{n-j}(x_1, \dots x_{N-1}, y_{j+1}, \dots y_n)\nabla_{x_N}\Theta^{R,b}_j(x_N, y_1, \dots y_j), \tag{87}$$
$$\overline{G(x_N - y_n)}\tilde{\Psi}^{R,N-1}_{n-j-1}(x_1, \dots x_{N-1}, y_{j+1}, \dots y_{n-1})\Theta^{R,b}_j(x_N, y_1, \dots y_j)\Big\rangle$$

All other terms in (73) with the same j, and with y_n in $\tilde{\Psi}^{R,N-1}_{n-j}$, give the same contribution to $\langle \sum_{k=1}^N i\nabla_{x_k} D(x_k)\tilde{\Gamma}^{R,b}, \tilde{\Gamma}^{R,b}\rangle$. Summing up these $\binom{n-1}{n-j-1}$ contributions in the case $k \neq N$ yields

$$\sqrt{n-j}\Big\langle \tilde{\Psi}^{R,N-1}_{n-j}, \nabla_{x_k}\overline{G(x_k - y_n)}\tilde{\Psi}^{R,N-1}_{n-j-1}\Big\rangle \|\Theta^{R,b}_j\|^2 \ , \tag{88}$$

and in the case $k = N$,

$$\sqrt{n-j}\Big\langle \tilde{\Psi}^{R,N-1}_{n-j}\nabla_{x_N}\Theta^{R,b}_j, \overline{G(x_N - y_n)}\tilde{\Psi}^{R,N-1}_{n-j-1}\Theta^{R,b}_j\Big\rangle \ . \tag{89}$$

If we sum first over $m = n - j$, and then the terms (88) over j, we get

$$\langle \tilde{\Psi}^{R,N-1}, \nabla_{x_k} D(x_k)\tilde{\Psi}^{R,N-1}\rangle \|\Theta^{R,b}\|^2. \tag{90}$$

Let us compute first the sum over $n - j$ of the terms (89), and estimate them according to (66). We obtain for $\varepsilon > 0$, and $|b|$ sufficiently large,

$$\langle |\nabla_{x_N}\Theta^{R,b}_j|, \frac{c(x_N)}{|x_N|}|\Theta^{R,b}_j|\rangle \leq \frac{\varepsilon}{2(|b| - 2R)}\left(\|\nabla_{x_N}\Theta^{R,b}_j\|^2 + \|\Theta^{R,b}_j\|^2\right), \tag{91}$$

where we used that $|x_N| \geq |b| - 2R$, and $c(x_N)$ tends to zero, as $|x_N|$ tends to infinity. Therefore,

$$\left|\sum_n\sum_j \sqrt{n-j}\Big\langle \tilde{\Psi}^{R,N-1}_{n-j}\nabla_{x_N}\Theta^{R,b}_j, \overline{G(x_N - y_n)}\tilde{\Psi}^{R,N-1}_{n-j-1}\Theta^{R,b}_j\Big\rangle\right| \tag{92}$$
$$\leq \frac{\varepsilon}{2(|b| - 2R)}\left(\|\nabla_{x_N}\Theta^{R,b}\|^2 + \|\Theta^{R,b}\|^2\right)$$

In analogy to (90) and (92), the contribution to $\langle \sum_{k=1}^N i\nabla_{x_k} D(x_k)\tilde{\Gamma}^{R,b}, \tilde{\Gamma}^{R,b}\rangle$ of the terms for which the variable y_n is in $\Theta^{R,b}$, is, for $k = N$, equal to

$$\langle i\nabla_{x_N} D(x_N)\Theta^{R,b}, \Theta^{R,b}\rangle \tag{93}$$

and for $k \neq N$, it can be estimated by

$$\frac{\varepsilon}{2(|b| - 2R)}\left(\|\nabla_{x_k}\tilde{\Psi}^{R,N-1}\|^2 + \|\tilde{\Psi}^{R,N-1}\|^2\right) \tag{94}$$

This completes the proof of (81).

Let us next prove the inequality (83). The operator $D^2(x_k)$ acts as

$$\left(D^2(x_k)\tilde{\Gamma}^{R,b}\right)_{n-2} = \sum_{j=0}^{n} \binom{n}{j}^{-1/2} \sum_{g\in S_{n,j}} \sqrt{n}\sqrt{n-1} \times \langle G(x_k-y_n)G(x_k-y_{n-1}), \Pi^p_{n,j}(g)\Theta^{R,b}_j\tilde{\Psi}^{R,N-1}_{n-j}\rangle_{L^2(X,\mathrm{d}y_n)\otimes L^2(X,\mathrm{d}y_{n-1})}\ , \tag{95}$$

where $X := \mathbb{R}^3\otimes\mathbb{C}^2$. Assume that in the decomposition g, we have the indices $n\in C_2$ and $(n-1)\in C_2$. Then, both variables y_n and y_{n-1} appear in the function $\tilde{\Psi}^{R,N-1}_{n-j}$. For fixed n and j, we have $\binom{n-2}{n-j-2}$ such cases. Similar to (88) in the case $k\neq N$, and to (89) in the case $k=N$, we obtain, respectively,

$$\sqrt{n-j}\sqrt{n-1-j}\left\langle\tilde{\Psi}^{R,N-1}_{n-j}, \overline{G(x_k-y_n)}\ \overline{G(x_k-y_{n-1})}\tilde{\Psi}^{R,N-1}_{n-j-2}\right\rangle\|\Theta^{R,b}_j\|^2\ , \tag{96}$$

and

$$\sqrt{n-j}\sqrt{n-j-1}\left\langle\tilde{\Psi}^{R,N-1}_{n-j}\Theta^{R,b}_j, \overline{G(x_N-y_n)}\ \overline{G(x_N-y_{n-1})}\tilde{\Psi}^{R,N-1}_{n-j-1}\Theta^{R,b}_j\right\rangle\ . \tag{97}$$

Now, summing each of these expressions over $m=n-j$ and j, and applying (67), we arrive at

$$\langle D^2(x_k)\tilde{\Psi}^{R,N-1}, \tilde{\Psi}^{R,N-1}\rangle\|\Theta^{R,b}\|^2 \tag{98}$$

for $k\neq N$, and

$$\frac{\varepsilon}{(|b|-2R)^2}\|\Theta^{R,b}\|^2 \tag{99}$$

for $k=N$.

Let us now consider g with $n\in C_1$ and $(n-1)\in C_1$, which implies that the variables y_n and y_{n-1} are in $\Theta^{R,b}_j$. We get

$$\langle D^2(x_N)\Theta^{R,b}, \Theta^{R,b}\rangle\|\tilde{\Psi}^{R,N-1}\|^2 \tag{100}$$

for $k=N$, and

$$\frac{\varepsilon}{(|b|-2R)^2}\|\tilde{\Psi}^{R,N-1}\|^2 \tag{101}$$

for $k\neq N$.

Finally, let us address the case where one of the indices n, $n-1$ belongs to C_1 and the other one to C_2. In this case, one of the variables y_n and y_{n-1} appears in $\tilde{\Psi}^{R,N-1}_{n-j}$, and the other one in $\Theta^{R,b}_j$. We have $2\binom{n-2}{j-1}$ such cases. Note that in each such case, either $|G(x_k-y_n)|$ or $|G(x_k-y_{n-1})|$ is small, and the contribution of the sum of these terms can be estimated as

$$\frac{\varepsilon_1}{|b|-2R}\left(\langle N_f\Theta^{R,b}, \Theta^{R,b}\rangle + \langle N_f\tilde{\Psi}^{R,N-1}, \tilde{\Psi}^{R,N-1}\rangle\right) \leq \frac{\varepsilon}{|b|-2R}\left(\|\Theta^{R,b}\|^2 + \|\tilde{\Psi}^{R,N-1}\|^2\right)\ . \tag{102}$$

The estimates (98)-(102) imply (83)

The proof of (82) is very similar to the one of (81). ∎

6.1. **Proof.** To prove Theorem 2.1, we will show that for suitably chosen parameters R and $|b|$, the trial function $\Gamma^{R,b}$ satisfies

$$\langle H_N \Gamma^{R,b}, \Gamma^{R,b} \rangle < E_{N-1} + \Sigma_0. \tag{103}$$

We recall that

$$\begin{aligned} H_N = & \sum_{\ell=1}^{N} \Big\{ \big(-i\nabla_{x_\ell} + \sqrt{\alpha} A_f(x_\ell)\big)^2 + \sqrt{\alpha}\sigma \cdot B_f(x_\ell) + V(x_\ell) \Big\} \\ & + \frac{1}{2} \sum_{1 \le k, \ell \le N} W(|x_k - x_\ell|) + H_f \ , \end{aligned} \tag{104}$$

and that, as was shown in the previous section, the inequality (103) is equivalent to

$$\langle H_N \tilde{\Gamma}^{R,b}, \tilde{\Gamma}^{R,b} \rangle < E_{N-1} + \Sigma_0.$$

For $M \in \mathbb{N}$, we define

$$I_M(x_1, \dots, x_M) = \sum_{\ell=1}^{M} V(x_\ell) + \frac{1}{2} \sum_{1 \le k, \ell \le M} W(x_k - x_\ell).$$

Obviously, we have

$$\begin{aligned} & \sum_{\ell=1}^{N} \langle -\Delta_\ell \tilde{\Gamma}^{R,b}, \tilde{\Gamma}^{R,b} \rangle + \langle I_N(x_1, \dots, x_n) \tilde{\Gamma}^{R,b}, \tilde{\Gamma}^{R,b} \rangle \\ & = \sum_{\ell=1}^{N-1} \langle -\Delta_\ell \tilde{\Psi}^{R,N-1}, \tilde{\Psi}^{R,N-1} \rangle \\ & + \langle I_{N-1}(x_1, \dots, x_{N-1}) \tilde{\Psi}^{R,N-1}, \tilde{\Psi}^{R,N-1} \rangle + \langle -\Delta \Theta^{R,b}, \Theta^{R,b} \rangle \\ & + \left\langle V(x_N) + \langle \sum_{i=1}^{N-1} W(x_i - x_N) \tilde{\Psi}^{R,N-1}, \tilde{\Psi}^{R,N-1} \rangle \Theta^{R,b}, \Theta^{R,b} \right\rangle \end{aligned} \tag{105}$$

where we used that $\Theta^{R,b}$ and $\tilde{\Psi}^{R,N-1}$ are normalized. On the support of the function $\Theta^{R,b}$, we have $|x_N| \le |b| + R$ and on the support of the function $\tilde{\Psi}^{R,N-1}$, $|x_i - x_N| \ge |b| - 2R$. This implies, for $|b|R^{-1}$ sufficiently large, that on the support of $\tilde{\Gamma}^{R,b}$ (defined in (73)),

$$V(x_N) + \sum_{i=1}^{N-1} W(x_i - x_N) < -\frac{\gamma_0}{|b| + R} + \frac{\gamma_1(N-1)}{|b| - 2R} < -\frac{\nu}{2|b|}, \tag{106}$$

for $\nu = \gamma_0 - \gamma_1(N-1) > 0$. Thus, (105) and (106) yield

$$\begin{aligned} & \sum_{\ell=1}^{N} \langle -\Delta_\ell \tilde{\Gamma}^{R,b}, \tilde{\Gamma}^{R,b} \rangle + \langle I_N(x_1, \dots, x_n) \tilde{\Gamma}^{R,b}, \tilde{\Gamma}^{R,b} \rangle \\ & \le \sum_{\ell=1}^{N-1} \langle -\Delta_\ell \tilde{\Psi}^{R,N-1}, \tilde{\Psi}^{R,N-1} \rangle + \langle I_{N-1}(x_1, \dots, x_{N-1}) \tilde{\Psi}^{R,N-1}, \tilde{\Psi}^{R,N-1} \rangle \\ & + \langle -\Delta \Theta^{R,b}, \Theta^{R,b} \rangle - \frac{\nu}{2|b|}. \end{aligned} \tag{107}$$

Taking into account that $\|\nabla_{x_\ell}\tilde{\Psi}^{R,N-1}\| \leq c\|\tilde{\Psi}^{R,N-1}\|$ ($\ell = 1,\dots N-1$), and that $\|\nabla_{x_N}\Theta^{R,b}\| \leq c\|\Theta^{R,b}\|$, with a constant c independent of R, we derive from (81)

$$\begin{aligned}\Big|\sum_{\ell=1}^{N}\langle\nabla_{x_\ell}A(x_\ell)\tilde{\Gamma}^{R,b},\tilde{\Gamma}^{R,b}\rangle - \sum_{\ell=1}^{N-1}\langle\nabla_{x_\ell}A(x_\ell)\tilde{\Psi}^{R,N-1},\tilde{\Psi}^{R,N-1}\rangle \\ -\langle\nabla_{x_N}A(x_N)\Theta^{R,b},\Theta^{R,b}\rangle\Big| \leq \frac{\varepsilon}{|b|-2R}.\end{aligned} \tag{108}$$

Similarly to (108), and using (21), (22), (67), and (68), we have

$$\begin{aligned}&\sum_{\ell=1}^{N}\langle A^2(x_\ell)\tilde{\Gamma}^{R,b},\tilde{\Gamma}^{R,b}\rangle \\ &\leq \sum_{\ell=1}^{N-1}\langle A^2(x_\ell)\tilde{\Psi}^{R,N-1},\tilde{\Psi}^{R,N-1}\rangle + \langle A^2(x_N)\Theta^{R,b},\Theta^{R,b}\rangle + \frac{\varepsilon}{|b|-2R}\end{aligned} \tag{109}$$

Along the same lines, we have for the magnetic term, using (23) and (69),

$$\begin{aligned}&\sum_{\ell=1}^{N}\langle\sigma\cdot B(x_\ell)\tilde{\Gamma}^{R,b},\tilde{\Gamma}^{R,b}\rangle \\ &\leq \sum_{\ell=1}^{N-1}\langle\sigma\cdot B(x_\ell)\tilde{\Psi}^{R,N-1},\tilde{\Psi}^{R,N-1}\rangle + \langle\sigma\cdot B(x_N)\Theta^{R,b},\Theta^{R,b}\rangle + \frac{\varepsilon}{|b|-2R}.\end{aligned} \tag{110}$$

According to Lemma 6.1 we have

$$\begin{aligned}\langle H_f\tilde{\Gamma}^{R,b},\tilde{\Gamma}^{R,b}\rangle \leq \langle H_f\Theta^{R,b},\Theta^{R,b}\rangle + \langle H_f\tilde{\Psi}^{R,N-1},\tilde{\Psi}^{R,N-1}\rangle \\ +c\frac{R^{3/2}}{|b|^{5/2}}\langle N_f\tilde{\Gamma}^{R,b},\tilde{\Gamma}^{R,b}\rangle\ .\end{aligned}$$

Equality (75) implies that $\langle N_f\tilde{\Gamma}^{R,b},\tilde{\Gamma}^{R,b}\rangle\ \leq c\left(\|\tilde{\Psi}^{R,N-1}\|^2 + \|\Theta^{R,b}\|^2\right)$

Collecting the estimates (107)-(111) we obtain for any $\varepsilon > 0$ and sufficiently large R,

$$\langle H_N\tilde{\Gamma}^{R,b},\tilde{\Gamma}^{R,b}\rangle \leq E_{N-1} + \Sigma_0 - \frac{\nu}{2|b|} + \frac{6\varepsilon}{|b|-2R} + \frac{cR^{3/2}}{|b|^{5/2}}\ . \tag{111}$$

To complete the proof of the Theorem, we pick first R large enough to have $\varepsilon < 48^{-1}\nu$, and then pick $|b|$ sufficiently large to satisfy the inequality $(R|b|^{-1})^{3/2} < \delta(4c)^{-1}$, which implies

$$\langle H_N\tilde{\Gamma}^{R,b},\tilde{\Gamma}^{R,b}\rangle < E_{N-1} + \Sigma_0\ .$$

7. Appendix

Lemma 7.1. *We define G_λ as*

$$G_\lambda(y) = \mathcal{F}\left(\frac{\varepsilon_\lambda(k)}{|k|^{\frac{1}{2}}}\zeta(k)\right)$$

where $\mathcal{F}$ denotes the Fourier transform. Then, for $\lambda = 1,2$ and arbitrary $\varepsilon > 0$, $|G_\lambda(y)(1+|y|)| \in L^{2+\varepsilon}(\mathbb{R}^3)$.

Proof. The statement of the Lemma follows from the Hausdorff-Young inequality, and the fact that for arbitrarily $\varepsilon > 0$, $\left|\nabla_k \frac{\varepsilon_{\lambda,i}(k)}{|k|^{\frac{1}{2}}}\zeta(k)\right|$ is in $L^{2-\varepsilon}(\mathbb{R}^3)$, for $i = 1, 2, 3$, which can be checked directly. □

Lemma 7.2. *Let $\varphi_1(x) \in H^{1/2}(\mathbb{R}^3)$ with support in the ball of radius aR centered at the origin, and $\varphi_2(x) \in H^{1/2}(\mathbb{R}^3)$ with support outside the ball of radius bR centered at the origin. Then for $b > 2a$,*

$$|\langle|\nabla|\varphi_1, \varphi_2\rangle| \leq \frac{1}{3^{1/2}\pi}\frac{a^{3/2}}{R(b-a)^{5/2}}\left(\|\varphi_1\|^2 + \|\varphi_2\|^2\right) \tag{112}$$

Proof. Consider the function u defined in (27). Then, for $\chi_1(x) = u(|x|/(bR))$ and $\chi_2(x) = \sqrt{1-\chi_1^2(x)}$, we have, according to [10, Theorem9]

$$\begin{aligned}
&\langle|\nabla|(\varphi_1+\varphi_2), \varphi_1+\varphi_2\rangle - \langle|\nabla|\varphi_1, \varphi_1\rangle - \langle|\nabla|\varphi_2, \varphi_2\rangle \\
\leq\ &\frac{1}{2\pi^2}\int\int \frac{|\varphi_1(x)+\varphi_2(x)|\ |\varphi_1(y)+\varphi_2(y)|}{|x-y|^4}\sum_{i=1,2}|\chi_i^2(x)-\chi_i^2(y)|\mathrm{d}y\mathrm{d}y
\end{aligned}$$

Since $\chi_1 = 1$ on the support of φ_1, $\chi_1 = 0$ on the support of φ_2, we obtain

$$\begin{aligned}
&\langle|\nabla|(\varphi_1+\varphi_2), \varphi_1+\varphi_2\rangle - \langle|\nabla|\varphi_1, \varphi_1\rangle - \langle|\nabla|\varphi_2, \varphi_2\rangle \\
=\ &2\mathcal{R}e\langle|\nabla|\varphi_1, \varphi_2\rangle \\
\leq\ &\frac{1}{\pi^2}\int\int \frac{|\varphi_1(x)|\ |\varphi_2(y)|}{|x-y|^4}\mathrm{d}y\mathrm{d}y \\
\leq\ &\frac{2}{\pi 3^{1/2}}\frac{a^{3/2}}{R(b-a)^{5/2}}\left(\|\varphi_1\|^2 + \|\varphi_2\|^2\right)
\end{aligned}$$

□

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