Exponential Decay and Ionization Thresholds in Non-Relativistic Quantum Electrodynamics

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Abstract

Spatial localization for quantum mechanical particles (electrons) interacting with quantized radiation (photons) is studied at energies below the ionization threshold. We give two definitions of the ionization threshold. One in terms of minimal energies of non-localized states, and a second one in terms of spectral data of cluster Hamiltonians. We show that these definitions agree, and that all states in the spectral subspace of energies below the ionization threshold decay exponentially in the particle coordinates. The latter result is derived from a new, general result on exponential decay tailored to fit our problem, but applicable to many non-relativistic quantum systems outside quantum electrodynamics as well.

1 Introduction

If an atom or molecule is in a state with total energy below the ionization threshold, then all electrons are well localized near the nuclei. In non-relativistic quantum mechanics this finds its mathematical expression in the fact that the spectrum of the Hamilton operator below the ionization threshold is discrete and all eigenfunctions decay exponentially. When the electrons are coupled to the quantized radiation field, then there is no discrete spectrum anymore and the ground state is the only eigenfunction. Nevertheless, all states in the spectral subspace of energies below the ionization threshold are exponentially well localized as functions of the electron coordinates. To prove this is the main purpose of this paper. Localization of the electrons below the ionization threshold is necessary to justify the dipole approximation [2], and it plays an important role in proving existence of a ground state [2, 3, 7] and for Rayleigh scattering [5].

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The ionization threshold is the least energy that an atom or molecule can achieve in a state where one or more electrons have been moved "infinitely far away" from the nuclei. To give a more precise definition we need to introduce a mathematical model for atoms and molecules. A (pure) state of N electrons and an arbitrary number of transversal photons shall be described by a vector in the Hilbert space $\mathcal{H}_N = \mathcal{H}_{\mathrm{el}} \otimes \mathcal{F}$, where $\mathcal{H}_{el}$ is the antisymmetric tensor product of N copies of $L^2(\mathbb{R}^3; \mathbb{C}^2)$, appropriate for N spin-1/2 fermions, and $\mathcal{F}$ is the bosonic Fock space over $L^2(\mathbb{R}^3, \mathbb{C}^2; dk)$. The nuclei are static, point-like particles without spin. Let H_N denote the Hamilton operator generating the time evolution in $\mathcal{H}_N$, and let H_N^0 be the same Hamiltonian without external potentials (nuclei). We assume that the dynamics of the electrons is non-relativistic and that the forces between material particles (electrons and nuclei) drop off to zero with increasing distance. In view of the latter assumption a natural definition for the ionization threshold $\tau(H_N)$ is

$$\tau(H_N) := \min_{N' \geq 1} \{E_{N-N'} + E^0_{N'}\},$$

where $E_{N-N'} = \inf \sigma(H_{N-N'})$, $E^0_{N'} = \inf \sigma(H^0_{N'})$, and $E_{N=0} = 0$. Let m be the mass of the electron and let $|x| = (\sum_{j=1}^n x_j^2)^{1/2}$ for $x \in \mathbb{R}^n$. We prove that, for all real numbers λ and β with $\lambda + \beta^2/(2m) < \tau(H_N)$,

$$\left\| e^{\beta|x|} E_\lambda(H_N) \right\| < \infty, \tag{1}$$

and that in states with energy above $\tau(H_N)$ the electrons will not be localized in general. Thus $\tau(H_N)$ is in fact a threshold energy separating localized from non-localized states. The question of whether the binding energy $\tau(H_N) - E_N$ is positive or not, is not addressed in this paper, see however [7].

The proof consists of two independent parts. First we give an alternative definition of the ionization threshold which better captures the idea of a localization threshold, and we prove exponential decay below it. Then we show that the two definitions agree.

The alternative definition is as follows. Let $D_R = \{\varphi \in D(H) |\, \varphi(x) = 0, \text{ if } |x| < R\}$, and define a threshold energy $\Sigma(H_N)$ by

$$\Sigma(H_N) = \lim_{R \to \infty} \inf_{\varphi \in D_R,\, \|\varphi\|=1} \langle \varphi, H_N \varphi \rangle \,. \tag{2}$$

Delocalization above $\Sigma(H_N)$ is obvious, and localization below $\Sigma(H_N)$ will be derived from the only assumptions that H_N is self-adjoint, bounded from below, and that

$$[[H_N, f], f] = -2|\nabla f|^2 \tag{3}$$

for all bounded smooth functions $f(x)$ with bounded first derivatives. The latter assumption is satisfied for the positive Laplacian $(-\Delta)$, and hence for all operators $-\Delta + I$ with $[[I, f], f] = 0$. Examples include the commonly traded models of non-relativistic atoms coupled to quantized radiation, as well as many Schrödinger opartors outside quantum electrodynamics.

The second part of the proof, that $\tau(H_N) = \Sigma(H_N)$, is the hard part. The inequality $\tau(H_N) \leq \Sigma(H_N)$ requires localizing both the electrons and the photons, and in particular their field energy. This was done in [7, 6]. To show that $\tau(H_N) \geq \Sigma(H_N)$ we construct suitable (compactly supported) minimizers φ_0 and φ_∞^R of $H_{N-N'}$ and $H^0_{N'}$, respectively, where φ_∞^R is localized at a distance R from the origin. We than merge these states into a single state $\psi_R \in \mathcal{H}_N$. The problem is to do this in such a way that $\langle \psi_R, H_N \psi_R \rangle = \langle \varphi_0, H_{N-N'}\varphi_0 \rangle + \langle \varphi_\infty^R, H^0_{N'} \varphi_\infty^R \rangle + o(1)$ as $R \to \infty$.

In the context of QED the first result of the form (1) is due to Bach, Fröhlich and Sigal [2], who proved exponential binding for small coupling and away from the ionization threshold of H_N with *zero* coupling. The threshold energy $\tau(H_N)$ was introduced in [7] where it was shown that E_N is an eigenvalue of H_N if $\tau(H_N) > E_N$. The paper [7] also contains an easy argument showing that *eigenvectors* of H_N with eigenvalues below $\tau(H_N)$ exhibit the exponential decay implied by (1). For N-particle Schrödinger operators the exponential decay (1) with τ being the least point of the essential spectrum was proved by O'Conner in 1973 [9], and the equivalence of the two definitions for the ionization threshold is shown as part of modern proofs of the HVZ Theorem [8]. See Agmon's book [1] for more results on the exponential decay of solutions of second order elliptic equations.

Section 2 contains the general theorem on exponential decay in an abstract Hilbert space setting. In Section 3 this result is applied to quantum electrodynamics and the main result on equality of the thresholds is formulated. Its proof is given in Section 4. The Appendix collects technical results and notations used in the proofs.

2 The Abstract Argument

In this section $q : D \times D \to \mathbb{C}$ denotes a densely defined, closable, semi-bounded quadratic form with domain $D \subset \mathcal{H}$ in a Hilbert space $\mathcal{H}$. We assume that $\mathcal{H}$ is a closed subspace of $L^2(\mathbb{R}^n) \otimes \mathcal{F}$, that is invariant with respect to multiplication with bounded (measurable) functions that only depend on $|x|$, $x \in \mathbb{R}^n$. Here $\mathcal{F}$ is an arbitrary, additional Hilbert space. In our applications $\mathcal{F}$ will be the tensor product of spin and Fock space and $\mathcal{H}$ the subspace with the symmetry required by the nature of the particles.

On the quadratic form q we make the further assumption, that for all $f \in C^\infty(\mathbb{R}^n;\mathbb{R})$ with $f, \nabla f \in L^\infty(\mathbb{R}^n)$ and with $f(x) = f(|x|)$, there exist constants a and b such that

$$\begin{aligned} &(i) && fD \subset D \\ &(ii) && |q(f\varphi, f\varphi)| \leq a q(\varphi,\varphi) + b\langle \varphi, \varphi\rangle \\ &(iii) && q(f^2\varphi,\varphi) + q(\varphi, f^2\varphi) - 2q(f\varphi, f\varphi) = -2\langle \varphi, |\nabla f|^2 \varphi \rangle \end{aligned}$$

for all $\varphi \in D$. Requirements (i) and (ii) are mild technical assumptions which ensure that property (iii) extends to all φ in the domain of the closure of q. Equation (iii) is the basis of the so called IMS (localization) formula for Schrödinger operators. To verify it in the case where q is defined in terms of a symmetric operator $\tilde{H} : D \subset \mathcal{H} \to \mathcal{H}$ it is useful to note that $f^2\tilde{H} + \tilde{H}f^2 - 2f\tilde{H}f = [[\tilde{H}, f], f]$. Assumption (iii) then becomes

$$[[\tilde{H}, f], f] = -2|\nabla f|^2$$

which holds for the positive Laplacian $(-\Delta)$ and hence for all operators $-\Delta + I$ in $\mathcal{H}$ with $[[I, f], f] = 0$. Some examples, other than those in the next section, are $\tilde{H} = (-i\nabla + A(x))^2 + V(x)$ with a classical vector potential $A(x)$ and scalar potential $V(x)$ (choose $\mathcal{F} = \mathbb{C}$), and Schrödinger operators with restricted domains $\Omega \subset \mathbb{R}^n$ $(\mathcal{H} = L^2(\Omega) \subset L^2(\mathbb{R}^n) \otimes \mathbb{C})$, or with a translational symmetry $(\mathcal{F} = L^2(\mathbb{R}))$ such as in wave guides defined by potential wells.

Given $R > 0$ let $D_R = \{\varphi \in D : \varphi(x) = 0 \text{ for } |x| < R\}$ and define

$$\Sigma_R = \inf_{\varphi \in D_R,\, \|\varphi\|=1} q(\varphi, \varphi) \quad \text{and} \quad \Sigma = \lim_{R\to\infty} \Sigma_R. \tag{4}$$

The numbers Σ_R are finite, because, by (i), D_R is not empty. But Σ may take on the value $+\infty$.

Theorem 1. *Let q be a semi-bounded, closable, quadratic form on $\mathcal{H}$ satisfying assumptions (i), (ii), and (iii) above, and let H denote the unique self-adjoint operator associated with the closure of the form q. If λ and β are real numbers with $\lambda + \beta^2 < \Sigma$, then*

$$\left\| e^{\beta|x|} E_\lambda(H) \right\| < \infty,$$

where $E_\lambda(H)$ is the resolution of the identity for H.

Remarks. (1) For Schrödinger operators $-\Delta + V$ on open domains $\Omega \subset \mathbb{R}^n$ with Dirichlet boundary conditions and with $V_- \ll -\Delta$ the above theorem implies that the spectrum below Σ is discrete. In fact $(-\Delta+1)^{-1/2}e^{-\beta|x|}$ is compact and hence so is $E_\lambda(H) = [(H+i)^{-1/2}(-\Delta + 1)^{1/2}][(-\Delta+1)^{-1/2}e^{-\beta|x|}][e^{\beta|x|}E_\lambda(H)][E_\lambda(H)(H+i)^{1/2}]$ for $\lambda + \beta^2 < \Sigma$.

(2) Everything in this section equally holds for any norm $|x|$ on $\mathbb{R}^n$ that is induced by an inner product $x \cdot y$, if Δ is used to denote the Laplace-Beltrami operator with respect to the metric $g(x, y) = x \cdot y$.

The following proof is inspired by the proof of binding in Bach et al.[2].

Proof. Let $Q(H) \subset \mathcal{H}$ denote the form domain of H, i.e., the domain of the closure of q. We use q to denote the closure of q as well. $Q(H)$ is the closure of D with respect to the form norm $\|\cdot\|_q$ associated with q. By assumptions (i) and (ii), multiplication with a bounded function

$f \in C^\infty(\mathbb{R}^n)$ with bounded derivatives is a bounded linear operator on $(D, \|\cdot\|_q)$ and hence extends to a bounded linear operator on $(Q(H), \|\cdot\|_q)$. In particular

$$fQ(H) \subset Q(H) \tag{5}$$

and (iii) extends from D to $Q(H)$.

Let $E = \inf\sigma(H)$ and suppose $\lambda \geq E$. Otherwise the assertion of the theorem is trivial. First we show that

$$H_R := H + \max\{\Sigma_R - E, 0\}\chi_{2R} \geq \Sigma_R - \frac{C}{R^2} \tag{6}$$

where χ_{2R} denotes the characteristic function of the set $\{x : |x| \leq 2R\}$ and C is a constant. Pick $j_1, j_2 \in C^\infty(\mathbb{R}_+)$ with $j_1^2 + j_2^2 \equiv 1$, $\text{supp}(j_1) \subset \{t \leq 2\}$ and $\text{supp}(j_2) \subset \{t \geq 1\}$. Let $j_{i,R}(x) = j_i(|x|/R)$. Then by (5) and since (iii) holds on $Q(H)$,

$$\begin{aligned} H_R &= \frac{1}{2}\sum_{i=1}^{2}\left(j_{i,R}^2 H_R + H_R j_{i,R}^2\right) \\ &= \sum_{i=1}^{2} j_{i,R} H_R j_{i,R} - \sum_{i=1}^{2}|\nabla j_{i,R}|^2 \end{aligned}$$

in the sense of forms on $Q(H)$. By definition of Σ_R and the construction of $j_{i,R}$,

$$\begin{aligned} &j_{1,R}\, H_R\, j_{1,R} \geq j_{1,R}(H + \Sigma_R - E)j_{1,R} \geq \Sigma_R j_{1,R}^2 \\ &j_{2,R}\, H_R\, j_{2,R} \geq j_{2,R} H j_{2,R} \geq \Sigma_R j_{2,R}^2. \end{aligned}$$

Hence (6) follows.

Now let $\Delta := [\inf\sigma(H), \lambda]$ with λ as in the statement of the theorem and pick $R \in \mathbb{R}$ so large that $\lambda + \beta^2 < \Sigma_R - C/R^2$. Keep this R fixed in the following. Let $\delta := \Sigma_R - C/R^2 - \beta^2 - \lambda > 0$, and choose a function $g_\Delta \in C_0^\infty(\mathbb{R})$ such that $g_\Delta \equiv 1$ on Δ and $\text{supp}(g_\Delta) \subset (-\infty, \lambda + \delta/2]$. Then, by (6), $g_\Delta(H_R) = 0$ and therefore

$$g_\Delta(H) = g_\Delta(H) - g_\Delta(H_R) \tag{7}$$

We now show that $e^{\beta|x|}(g_\Delta(H) - g_\Delta(H_R))$ is bounded. To this end, we define

$$f(x) := \frac{\beta\langle x\rangle}{1 + \varepsilon\langle x\rangle}, \qquad \langle x\rangle = (1 + |x|^2)^{1/2}$$

and show that, $e^f(g_\Delta(H) - g_\Delta(H_R))$ is bounded uniformly in $\varepsilon > 0$. Note that $f \in C^\infty(\mathbb{R}^n)$, is bounded and that $|\nabla f| \leq \beta$. Let $\tilde{g}_\Delta$ be the almost analytic extension $\tilde{g}_\Delta(x + iy) = (g_\Delta(x) + iyg'_\Delta(x))\gamma(y)$ where $\gamma \in C_0^\infty(\mathbb{R})$ equals one in a neighborhood of $y = 0$. By the almost analytic functional calculus (see [4])

$$g_\Delta(H) = -\frac{1}{\pi}\int \frac{\partial\tilde{g}}{\partial\bar{z}}(z - H)^{-1}\, dx\, dy$$

and hence, using (7) and a resolvent identity we can write

$$e^f g_\Delta(H) = \frac{1}{\pi}\int \frac{\partial \tilde{g}}{\partial \bar{z}} e^f (z-H_R)^{-1} e^{-f} e^f (\Sigma_R - E)\chi_{2R}(z-H)^{-1}\,dx\,dy$$

whose norm we estimate from above as

$$\begin{aligned} \|e^f g_\Delta(H)\| \;&\leq\; \sup_{z\in \mathrm{supp}(\tilde{g})} \|e^f(z-H_R)^{-1}e^{-f}\|\,\|e^f\chi_{2R}\|_\infty(\Sigma_R - E) \\ &\quad \times \frac{1}{\pi}\int \left|\frac{\partial \tilde{g}}{\partial \bar{z}}\right| \|(z-H)^{-1}\|\,dx\,dy. \end{aligned}$$

The norm $\|e^f\chi_{2R}\|_\infty$ is bounded uniformly in $\varepsilon > 0$ and the integral is finite. To estimate $\|e^f(z-H_R)^{-1}e^{-f}\|$ let $H_{R,f} := e^f H_R e^{-f}$ with domain $D(H_{R,f}) = e^f D(H)$ and note that

$$(z-H_{R,f})^{-1} = e^f(z-H_R)^{-1}e^{-f}$$

as can easily be seen by direct computation. In particular, the resolvent sets $\rho(H_{R,f})$ and $\rho(H_R)$ coincide. Let $\varphi \in D(H_{R,f}) \subset Q(H)$ and $\|\varphi\| = 1$. Then

$$\begin{aligned} 2\,\mathrm{Re}\,\langle \varphi, H_{R,f}\varphi\rangle &= \langle \varphi, (e^f H_R e^{-f} + e^{-f} H_R e^f)\varphi\rangle \\ &= \langle \varphi, e^{-f}(e^{2f} H_R + H_R e^{2f})e^{-f}\varphi\rangle \\ &= 2\,\langle \varphi, (H_R - |\nabla f|^2)\varphi\rangle \end{aligned}$$

where (iii) was used in the last equation. In conjunction with (6) this shows that, for $z \in \mathrm{supp}(\tilde{g})$,

$$\mathrm{Re}\,\langle \varphi, (H_{R,f} - z)\varphi\rangle \geq \Sigma_R - C/R^2 - \beta^2 - \mathrm{Re}(z) \geq \delta/2 \tag{8}$$

and hence that $\|(H_{R,f} - z)\varphi\| \geq \delta/2\|\varphi\|$. Since $\rho(H_{R,f}) = \rho(H_R) \supset \mathrm{supp}(\tilde{g})$, it follows that

$$\|(z - H_{R,f})^{-1}\| \leq 2/\delta$$

for $z \in \mathrm{supp}(\tilde{g})$, which completes the proof. □

3 Atoms Coupled to Quantized Radiation

In this section we apply the abstract result of the previous section to systems of N charged, non-relativistic quantum particles, interacting with the quantized radiation field. Since we are mainly interested in the case of electrons in the field of static nuclei, the bulk of the exposition deals with this case. At the end we comment on the more general case of particles from different species.

In the "standard model" of non-relativistic QED the Hilbert space of a system of N electrons and an arbitrary number of transversal photons is the tensor product

$$\mathcal{H}_N = \wedge_{i=1}^N L^2(\mathbb{R}^3; \mathbb{C}^2) \otimes \mathcal{F}_f$$

of the antisymmetric product of N copies of $L^2(\mathbb{R}^3;\mathbb{C}^2)$ appropriate for N spin-1/2 fermions and $\mathcal{F}_f = \oplus_{n\geq 0} \otimes_s^n L^2(\mathbb{R}^3, dk; \mathbb{C}^2)$ is the bosonic Fock space over $L^2(\mathbb{R}^3, dk; \mathbb{C}^2)$, where the factor $\mathbb{C}^2$ accounts for the two possible polarizations of the transversal photons. Let $\mathcal{D}_N \subset \mathcal{H}_N$ be the subspace of sequences $\varphi = (\varphi_0, \varphi_1, \ldots)$ where

$$\varphi_n \in C_{0,a}^\infty((\mathbb{R}^3 \times \{1,2\})^N; \mathbb{C}) \otimes \otimes_s^n L_0^2(\mathbb{R}^3, \mathbb{C}^2)$$

and $\varphi_n = 0$ for all but finitely many n. The index a indicates that the functions are anti-symmetric with respect to permutations of the N arguments, and $L_0^2(\mathbb{R}^3;\mathbb{C}^2)$ is the space of compactly supported L^2-functions. Clearly $\mathcal{D}_N$ is a dense subspace of $\mathcal{H}_N$.

The Hamilton operator $\tilde{H}_N : \mathcal{D}_N \subset \mathcal{H}_N \to \mathcal{H}_N$ of our system is given by

$$\tilde{H}_N = \sum_{j=1}^N (p_j + \sqrt{\alpha} A(x_j))^2 + \frac{g}{2}\sqrt{\alpha}\sigma_j \cdot B(x_j) + V + H_f. \tag{9}$$

where $p_j = -i\nabla_{x_j}$, $A(x_j)$ is the quantized vector potential in Coulomb gauge evaluated at the point x_j, $B(x_j) = \mathrm{curl} A(x_j)$ is the magnetic field, σ_j the triple of Pauli matrices $(\sigma_j^{(1)}, \sigma_j^{(2)}, \sigma_j^{(3)})$ acting on the spin degrees of freedom of the jth particle, V is a real-valued potential, and H_f is the Hamilton operator of the field energy. The parameter α is the fine structure constant and the coupling constant $g \in \mathbb{R}$ is arbitrary, to allow for a simultaneous treatment of the interesting cases $g = 2$ and $g = 0$.

Formally $A(x)$ is given by

$$A(x) = \sum_{\lambda=1,2} \int_{|k|\leq\Lambda} \frac{1}{\sqrt{|k|}} \varepsilon_\lambda(k) \left[e^{ik\cdot x} a_\lambda(k) + e^{-ik\cdot x} a_\lambda^*(k) \right] d^3k$$

where $\Lambda < \infty$ is an arbitrary but fixed ultraviolett cutoff. For every $k \neq 0$ the two polarization vectors $\varepsilon_\lambda(k) \in \mathbb{R}^3$, $\lambda = 1, 2$ are normalized, orthogonal to k and to each other.

The operators $a_\lambda(k)$ and $a_\lambda^*(k)$ are the usual annihilation and creation operators, satisfying the canonical commutation relations

$$[a_\lambda(k), a_\mu^*(k')] = \delta_{\lambda\mu}\delta(k - k'), \qquad [a_\lambda^\sharp(k), a_\mu^\sharp(k')] = 0.$$

In terms of $a_\lambda(k)$ and $a_\lambda^*(k)$ the field Hamiltonian is given by

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

See Appendix B for mathematically more proper definitions of $A(x)$ and H_f.

The potential V is the sum of the external and the Coulomb two-body potentials for each pair of electrons. However, for the purpose of the results to be proved in this section, it is enough to assume that

$$(H1) \qquad V \in L_{\mathrm{loc}}^2(\mathbb{R}^{3N}; \mathbb{R}), \text{ and } V_- \leq \varepsilon(-\Delta) + C_\varepsilon \text{ for all } \varepsilon > 0,$$

and of course that V is symmetric with respect to permutation of the particle coordinates. The Hamiltonian $\tilde{H}_N$ is a symmetric, densely defined operator and by Lemma 8, it is bounded from below. The quadratic form $q(\varphi,\psi) = \left\langle \varphi, \tilde{H}_N \psi \right\rangle$ with domain $D = \mathcal{D}_N$ is therefore semi-bounded and closable and hence the theory of the previous section applies, once we have verified assumptions (i), (ii), and (iii). The unique self-adjoint operator H_N associated with the closure of the quadratic form q is the Friedrichs' extension of $\tilde{H}_N$. The thresholds Σ_R and Σ associated with the form q are now given by

$$\begin{aligned} \Sigma_R(H_N) &= \inf_{\varphi\in\mathcal{D}_{N,R},\ \|\varphi\|=1} \left\langle \varphi, \tilde{H}_N \varphi \right\rangle \\ \Sigma(H_N) &= \lim_{R\to\infty} \Sigma_R(H_N) \end{aligned}$$

where $\mathcal{D}_{N,R} := \{\varphi \in \mathcal{D}_N : \varphi(X) = 0 \text{ if } |X| < R\}$. The following theorem is a corollary of Theorem 1.

Theorem 2. *Assume Hypothesis (H1) is satisfied and let H_N be the Friedrichs' extension of the symmetric operator $\tilde{H}_N : \mathcal{D}_N \subset \mathcal{H}_N \to \mathcal{H}_N$ given by Eq.* (9)*. If λ and β are real numbers with $\lambda + \beta^2 < \Sigma(H_N)$, then*

$$\left\| e^{\beta|X|} E_\lambda(H_N) \right\| < \infty.$$

Proof. It suffices to verify the assumptions (i), (ii) and (iii) in the previous section. Suppose $f \in C^\infty(\mathbb{R}^{3N})$ with $f, \nabla f \in L^\infty(\mathbb{R}^{3N})$, and $f(X) = f(|X|)$. Then $f\mathcal{D}_N \subset \mathcal{D}_N$ is obvious from the definition of $\mathcal{D}_N$. Property (ii) follows from

$$\begin{aligned} f(p_i + \sqrt{\alpha}A(x_i))^2 f &\le 2\|f\|_\infty^2 (p_i + \sqrt{\alpha}A(x_i))^2 + 2\|\nabla_{x_i} f\|_\infty^2 \\ f H_f f &\le \|f\|_\infty^2 H_f \\ f V f &\le \|f\|_\infty^2 V_+, \end{aligned}$$

from Lemma 7 and Lemma 8. The proof of (iii) is a straightforward computation using that $f^2\tilde{H}_N + \tilde{H}_N f^2 - 2f\tilde{H}_N f = [[\tilde{H}_N, f], f]$. $\square$

Remark. The above theorem and its proof can easily be generalized to systems of N particles from $n \le N$ species, with different masses m_i, charges, and spins. Theorem 2 then holds again with the new norm $|X| = \left(\sum_{i=1}^N 2m_i x_i^2\right)^{1/2}$ in the exponential factor.

Our next goal is to establish a relation between $\Sigma(H_N)$ and spectral data of cluster Hamiltonians. To this end, we impose the following additional assumption on V:

$$(H2) \left\{ \begin{array}{l} V(X) = \sum_{i=1}^N v(x_i) + \sum_{i<j} w(x_i - x_j) \quad \text{where } v, w \in L^2_{\text{loc}}(\mathbb{R}^3) \\ \text{and } \lim_{|x|\to\infty} v(x) = 0,\ \lim_{|x|\to\infty} w(x) = 0. \end{array} \right.$$

If the external potential v is associated with a particle sitting at the origin $x = 0$, then these assumptions can be understood as saying that the interaction between spatially separated clusters of particles drops off to zero as the inter-cluster distance increases to infinity. The limitation to two-body forces in (H2) is not necessary.

Theorem 3. *Assume (H1) and (H2), and let* $E_{N-N'} = \inf\sigma(H_{N-N'})$, *and* $E_N^0 = \inf\sigma(H_N^0)$ *where all external potentials are dropped in* H_N^0. *Then*

$$\Sigma(H_N) = \inf_{N'\geq 1}\{E_{N-N'} + E_{N'}^0\}.$$

The proof requires in particular localizing the field energy in neighborhoods of the electrons. In the order to control the localization errors which thereby arise we need an infrared cutoff in the interaction. That is, we first prove the above theorem in the case where all interactions of electrons with photons of energy less than an arbitrary small, but positive constant μ have been dropped from H_N. The theorem then follows in the limit $\mu \to 0$.

4 IR-Cutoff Hamiltonians

In this section we prove Theorem 6, which is Theorem 3 with an infrared cutoff μ in the interaction, and we show how Theorem 3 then follows in the limit $\mu \to 0$.

The infrared cutoff Hamiltonians $H_{N,\mu}$, $\mu > 0$ are defined in the same way as H_N with the only difference that the vector potential $A(x)$ and the magnetic field $B(x)$ in H_N are replaced by

$$A_\mu(x) = \sum_{\lambda=1,2}\int_{\mu\leq|k|\leq\Lambda}\frac{1}{\sqrt{|k|}}\varepsilon_\lambda(k)\left[e^{ik\cdot x}a_\lambda(k) + e^{-ik\cdot x}a_\lambda^*(k)\right]d^3k$$

and $B_\mu(x) = \mathrm{curl}A_\mu(x)$. To separate the soft, non-interacting photons from the interacting ones we use that $\mathcal{F}_f$ is isomorphic to $\mathcal{F}_i \otimes \mathcal{F}_s$ where $\mathcal{F}_i$ and $\mathcal{F}_s$ denote the bosonic Fock spaces over $L^2(|k| \geq \mu)$ and $L^2(|k| < \mu)$ respectively. Let $\mathcal{H}_i = \wedge^N L^2(\mathbb{R}^3;\mathbb{C}^2)\otimes\mathcal{F}_i$. Then the Hamilton operator can be written as

$$H_{N,\mu} = H_\mu^i \otimes 1 + 1 \otimes H_f^s \qquad \text{on} \quad \mathcal{H} = \mathcal{H}_i \otimes \mathcal{F}_s \tag{10}$$

if we identify $\mathcal{F}$ with $\mathcal{F}_i \otimes \mathcal{F}_s$. Let $\mathcal{F}_{s,n}$ denote the subspace of $\mathcal{F}_s$ with precisely n soft bosons and let Ω_s be the vacuum of $\mathcal{F}_s$. Then (10) and the positivity of $H_f^s = H_f\restriction\mathcal{F}_s$ show that

$$\begin{aligned}\inf\sigma(H_{N,\mu}) &= \inf_{n\geq 0}\left(\inf\sigma(H_{N,\mu}\restriction\mathcal{H}_i\otimes\mathcal{F}_{s,n})\right)\\ &= \inf\sigma(H_{N,\mu}\restriction\mathcal{H}_i\otimes[\Omega_s]),\end{aligned} \tag{11}$$

where $[\Omega_s]$ is the space spanned by Ω_s. This will allow us to drop the soft bosons in all approximate energy minimizers.

Lemma 4. *There exists a constant* $C_{N,\Lambda}$, *depending on* Λ, N, g *and* α, *such that*

$$\pm(H_N - H_{N,\mu}) \leq \mu^{1/2}C_{N,\Lambda}\left\{\sum_{i=1}^N p_i^2 + H_f + 1\right\} \qquad \textit{for} \quad 0\leq\mu\leq 1.$$

Proof. By definition of H_N and $H_{N,\mu}$,

$$\begin{aligned} H_N - H_{N,\mu} &= \sum_{i=1}^{N} 2\sqrt{\alpha} p_i \cdot \big(A(x_i) - A_\mu(x_i)\big) + \alpha\big(A(x_i) - A_\mu(x_i)\big)\big(A(x_i) + A_\mu(x_i)\big) \\ &\quad + \frac{g}{2}\sqrt{\alpha}\sigma \cdot \big(B(x_i) - B_\mu(x_i)\big) \end{aligned}$$

where we used that $A(x)$ and $A_\mu(x)$ commute. The differences $A(x) - A_\mu(x)$ and $B(x) - B_\mu(x)$ can be seen as a vector potential and a magnetic field with an *ultraviolett* cutoff μ. Hence the lemma follows from Lemma 7 with $\Lambda = \mu$ and $\varepsilon = \mu^{1/2}$. □

Lemma 5. *(i) $\Sigma(H) < \infty$ if and only if $\Sigma(H_\mu) < \infty$ and in this case there exists a constant C_Λ depending on the parameters Λ, N, α, and g, such that*

$$|\Sigma(H_{N,\mu}) - \Sigma(H_N)| \leq C_\Lambda \mu^{1/2}, \qquad \textit{if } \mu \leq 1.$$

(ii) There exists a constant C_Λ depending on the parameters Λ, N, α, and g, such that

$$|\tau(H_{N,\mu}) - \tau(H_N)| \leq C_\Lambda \mu^{1/2}, \qquad \textit{if } \mu \leq 1.$$

Proof. By Lemma 4 and Lemma 8, there exist constants C and D, independent of μ, such that

$$H_{N,\mu} \leq H_N + \mu^{1/2}(CH_N + D) \qquad \text{for} \quad \mu \leq 1.$$

It follows that

$$\Sigma(H_{N,\mu}) \leq \Sigma(H_N) + \mu^{1/2}(C\Sigma(H_N) + D) \qquad \text{for} \quad \mu \leq 1$$

and, in particular, that $\Sigma(H_{N,\mu}) < \infty$ if $\Sigma(H_N) < \infty$. Since the roles of $H_{N,\mu}$ and H_N are interchangeable, (i) follows. The proof of (ii) is similar. □

Theorem 6. *Under the assumptions (H1), (H2) and (H2) on V one has*

$$\Sigma(H_{N,\mu}) = \tau(H_{N,\mu}) \qquad \textit{for all } \mu > 0.$$

In conjunction with Lemma 5, this theorem proves Theorem 3

Proof of $\Sigma(H_{N,\mu}) \geq \tau(H_{N,\mu})$. This is proved in [7, 6]. For the sake of completeness we repeat the arguments starting from Theorem 9. We may assume that $\Sigma(H_{N,\mu}) < \infty$. By the argument (11) we may restrict $H_{N,\mu}$ to $\mathcal{H}_i \otimes [\Omega_s]$ for the computation of $\Sigma_R(H_{N,\mu})$. By Lemma 8

$$N_f \leq \frac{1}{\mu} H_f \leq \frac{1}{\mu}(2H_{N,\mu} + D) \qquad \textit{on} \quad \mathcal{H}_i \otimes [\Omega_s]$$

and hence by Theorem 9,

$$H_{N,\mu} \geq \tau(H_{N,\mu}) - o(R^0)(H_{N,\mu} + C) \qquad \textit{on} \quad \mathcal{D}_{N,R} \cap (\mathcal{H}_i \otimes [\Omega_s]).$$

It follows that

$$\Sigma_R(H_{N,\mu}) \geq \tau(H_{N,\mu}) - o(R^0)(\Sigma_R(H_{N,\mu}) + C)$$

and the desired result is obtained in the limit $R \to \infty$. □

An important role in the following proof is played by the identification operator $I : \mathcal{F} \otimes \mathcal{F} \to \mathcal{F}$ which collects all photons in the first and second factor of $\mathcal{F} \otimes \mathcal{F}$, and gathers them in a single Fock space. For the precise definition of I and other notations in the following proof not yet introduced, see Appendix B.

Proof of $\Sigma(H_{N,\mu}) \leq \tau(H_{N,\mu})$. In the following the subindex μ is dropped. We need to show that

$$\lim_{R\to\infty} \Sigma_R(H_N) \leq E_{N-N'} + E^0_{N'}$$

for all $N' \geq 1$. The strategy is as follows. First we construct approximate minimizers φ_0 and φ_∞ of $H_{N-N'}$ and $H^0_{N'}$ respectively, with the property that the electrons and the photons described by φ_0 and φ_∞ are compactly supported. Then, by a translation $\varphi_\infty \to T_R\varphi_\infty$ of both the electrons and the photons in φ_∞ we may achieve (ignoring the Pauli principle) that

$$\psi_R = I(\varphi_0 \otimes T_R\varphi_\infty) \in \mathcal{D}_{N,R}, \qquad \text{and } \|\psi_R\| = 1,$$

where $T_R\varphi_\infty$ is still an approximate minimizer of $H^0_{N'}$ by the translation invariance of this Hamiltonian.

Second we show that

$$\langle \psi_R, H_N\psi_R\rangle \leq \langle \varphi_0, H_{N-N'}\varphi_0\rangle + \left\langle \varphi_\infty, H^0_{N'}\varphi_\infty\right\rangle + o(R^0) \qquad R \to \infty$$

which concludes the proof. To incorporate the Pauli principle one needs to anti-symmetrize $I(\varphi_0 \otimes T_R\varphi_\infty)$ with respect to the N electron variables $(x_i, s_i) \in \mathbb{R}^3 \times \{1, 2\}$, $i = 1, \dots, N$. After normalization, this will lead to the same value for the energy $\langle\psi_R, H_N\psi_R\rangle$ as without anti-symmetrization, because the electrons in φ_0 and $T_R\varphi_\infty$ are disjointly supported and the Hamiltonian is local. Thus one does not need to anti-symmetrize.

Let $\varepsilon > 0$ be given and fixed in the following three steps, and let y denote the position operator $y = i\nabla_k$ in the one-photon Hilbert space. For simplicity the irrelevant parameters α and g are dropped henceforth.

Step 1. Given $\varepsilon > 0$ there are normalized states $\varphi_0 \in \mathcal{D}_{N-N'}$ and $\varphi_\infty \in \mathcal{D}_{N'}$ such that

(i) $\langle\varphi_0, H_{N-N'}\varphi_0\rangle < E_{N-N'} + \varepsilon/2$ and $\left\langle\varphi_\infty, H^0_{N'}\varphi_\infty\right\rangle < E^0_{N'} + \varepsilon/2$.

(ii) Both $\left\langle\varphi_0, N_f\varphi_0\right\rangle$ and $\left\langle\varphi_\infty, N_f\varphi_\infty\right\rangle$ are finite and bounded by a constant that is independent of $\varepsilon > 0$.

(iii) φ_0 and φ_∞ have compact support as functions of the electronic configurations $X_{N-N'} \in \mathbb{R}^{3(N-N')}$ and $X_{N'} \in \mathbb{R}^{3N'}$ respectively.

(iv) There exists an R_0 such that

$$\varphi_0 = \Gamma(\chi_{R_0})\varphi_0, \quad \varphi_\infty = \Gamma(\chi_{R_0})\varphi_\infty$$

where χ_{R_0} is the characteristic function of the ball $\{y \in \mathbb{R}^3 : |y| < R_0\}$.

Proof of Step 1. The properties of the Hamiltonians that are relevant, are shared by $H_{N-N'}$ and $H^0_{N'}$. So it suffices to prove existence of φ_0. Let $H_0 := H_{N-N'}$ and $E_0 := E_{N-N'}$ for short. Let χ_P be the operator of multiplication with $\chi(|X|/P)$ on $\mathcal{H}_{N-N'}$ where $\chi \in C^\infty(\mathbb{R}_+)$, $\chi(t) = 1$ for $t \leq 1$, $\chi(t) = 0$ for $t \geq 2$ and $0 \leq \chi \leq 1$. Let j_R be the operator of multiplication with $\chi(|y|/R)$ on $L^2(\mathbb{R}^3, dk)$. Existence of φ_0 with property (i) and (ii) follows from the fact that $\mathcal{D}_{N-N'}$ is a form core of H_0, the argument (11), and Lemma 8. If we now show that

$$\begin{aligned} \langle \chi_P\varphi_0, (H_0 - E_0)\chi_P\varphi_0\rangle &\overset{P\to\infty}{\longrightarrow} \langle \varphi_0, (H_0 - E_0)\varphi_0\rangle && (12) \\ \langle \Gamma(j_R)\chi_P\varphi_0, (H_0 - E_0)\Gamma(j_R)\chi_P\varphi_0\rangle &\overset{R\to\infty}{\longrightarrow} \langle \chi_P\varphi_0, (H_0 - E_0)\chi_P\varphi_0\rangle && (13) \end{aligned}$$

then (iii), and (iv) will follow, because, by the strong convergence $\chi_P \to 1$ and $\Gamma(j_R) \to 1$ the norm $\|\Gamma(j_R)\chi_P\varphi_0\|$ is close to 1 for large P and large R.

Properties (12) and (13) follow from

$$\begin{aligned} \lim_{P\to\infty} [H_0, \chi_P]\varphi_0 &= 0 && (14) \\ \lim_{R\to\infty} (N_f + 1)^{-1/2}[H_0, \Gamma(j_R)]\chi_P\varphi_0 &= 0 && (15) \end{aligned}$$

(to be proven shortly) by commuting the operators χ_P and $\Gamma(j_R)$ through $H_0 - E_0$ and using (ii) and that $s - \lim_{P\to\infty} \chi_P^2 = 1$ and $s - \lim_{R\to\infty} \Gamma(j_R)^2 = 1$. Note that $\Gamma(j_R)\chi_P\mathcal{D}_{N-N'} \subset \mathcal{D}_{N-N'}$.

Equation (14) follows from

$$[H_0, \chi_P] = \sum_{j=1}^{N-N'} (-2i)\nabla_{x_j}\chi_P \cdot (p_j + A(x_j)) - \Delta_{x_j}\chi_P$$

using $\nabla_{x_j}\chi_P = O(P^{-1})$, $\Delta_{x_j}\chi_P = O(P^{-2})$ and Lemma 8.

To prove (15) we write the commutator as

$$\begin{aligned} [H_0, \Gamma(j_R)] = \sum_{i=1}^{N-N'} \Big\{ &(p_i + A(x_i))[A(x_i), \Gamma(j_R)] + [A(x_i), \Gamma(j_R)](p_i + A(x_i)) \\ &+ [\sigma_i \cdot B(x_i), \Gamma(j_R)] + [H_f, \Gamma(j_R)] \Big\} \end{aligned} \qquad (16)$$

Using that $H_f = \mathrm{d}\Gamma(|k|)$, the last term in (16) restricted to $\otimes_s^n L^2(\mathbb{R}^3)$ is given by $[H_f, \Gamma(j_R)] = \sum_{l=1}^n j_R \otimes \ldots \otimes [|k|, j_R] \ldots \otimes j_R$, the commutator being the lth factor. Since $\|[|k|, j_R]\| = O(R^{-1})$ it follows that $\|(N+1)^{-1/2}[H_f, \Gamma(j_R)](N+1)^{-1/2}\| = O(R^{-1})$, and hence, by (ii), that the contribution due to H_f is of order R^{-1}. To deal with the first two terms in (16) note that, by (19) and (20),

$$[A(x_i), \Gamma(j_R)] = a^*((1 - j_R)G_{x_i})\Gamma(j_R) - \Gamma(j_R)a((1 - j_R)G_{x_i})$$

where

$$\|a^\sharp((j_R-1)G_{x_i})\chi_P(N+1)^{-1/2}\| \le \sup_{|x_i|\le 2P} \|(j_R-1)G_{x_i}\| \to 0, \qquad \text{as} \quad R\to\infty.$$

It follows that the terms in (16) which are quadratic in $A(x_i)$ give vanishing contributions, as the factors $A(x_i)$ outside the commutators can be controlled by $(N+1)^{-1/2}$. To show that the terms with an operator p_i vanish in the limit $R\to\infty$ it suffices to add to the above arguments that $p_i[A(x_i),\Gamma(j_R)] = [A(x_i),\Gamma(j_R)]p_i$ because p_i commutes with $A(x_i)$ and $\Gamma(j_R)$, that $p_i\chi_P = \chi_P p_i - i\nabla_i\chi_P$ and that $\|p_i\varphi_0\| < \infty$ by Lemma 8. The term involving $B(x_i)$ is dealt with similarly.

Step 2. Let ε, φ_0, and φ_∞ be as in Step 1. Pick R_0 so large that, with χ_{R_0} is as in Step 1 (iv), $\varphi_0 = \Gamma(\chi_{R_0})\varphi_0$, $\varphi_\infty = \Gamma(\chi_{R_0})\varphi_\infty$, $\varphi_0(X_{N-N'}) = 0$ if $|X_{N-N'}| > R_0$ and $\varphi_\infty(X_{N'}) = 0$ if $|X_{N'}| > R_0$. Let $R \ge R_0$ and pick a vector $d\in\mathbb{R}^3$ with $|d| = 3$. Let $T_R : \mathcal{H}_{N-N'} \to \mathcal{H}_{N-N'}$ be the translation

$$T_R = \exp\left(-iRd\cdot\Big\{\sum_{i=1}^{N'} p_i + P_f\Big\}\right)$$

where $P_f = \mathrm{d}\Gamma(k)$ is the total momentum operator of the photons. Then

$$\begin{aligned}\left\langle T_R\varphi_\infty, H^0_{N'}T_R\varphi_\infty\right\rangle &= \left\langle \varphi_\infty, H^0_{N'}\varphi_\infty\right\rangle,\\ \psi_R := I(\varphi_0\otimes T_R\varphi_\infty) &\in \mathcal{D}_{N,2R}.\end{aligned}$$

Step 3. If $R\ge R_0$ then $\|\psi_R\| = 1$ and

$$\langle\psi_R, H_N\psi_R\rangle = \langle\varphi_0, H_{N-N'}\varphi_0\rangle + \left\langle\varphi_\infty, H^0_{N'}\varphi_\infty\right\rangle + o(R^0), \quad R\to\infty.$$

In particular $\Sigma_R(H_N) \le E_{N-N'} + E^0_{N'} + 2\varepsilon$ for all R, which proves the theorem.

Proof of Step 3. By construction of φ_0 and $T_R\varphi_\infty$ the photons in these states have disjoint support if $R\ge R_0$. Therefore

$$\begin{aligned}\langle\psi_R,\psi_R\rangle &= \langle I(\varphi_0\otimes T_R\varphi_\infty), I(\varphi_0\otimes T_R\varphi_\infty)\rangle\\ &= \langle\varphi_0\otimes T_R\varphi_\infty, \varphi_0\otimes T_R\varphi_\infty\rangle\\ &= \langle\varphi_0,\varphi_0\rangle\langle\varphi_\infty,\varphi_\infty\rangle = 1.\end{aligned}$$

In the following this property of I, that it acts like an isometry on product states with photons supported in $\{|y|\le R_0\}$ and $\{|y-Rd|\le R_0\}$ respectively, will be used repeatedly and tacitly.

Writing $H_f = \sum_{\lambda=1,2}\int |k| a^*_\lambda(k)a_\lambda(k)d^3k$ and using (21) one gets

$$\begin{aligned}\left\langle\psi_R, H_f\psi_R\right\rangle &= \left\langle\varphi_0, H_f\varphi_0\right\rangle + \left\langle T_R\varphi_\infty, H_f T_R\varphi_\infty\right\rangle\\ &\quad +2\,\mathrm{Re}\sum_{\lambda=1,2}\int |k|\,\langle a_\lambda(k)\varphi_0,\varphi_0\rangle\,\langle\varphi_\infty, a_\lambda(k)\varphi_\infty\rangle\, e^{iRd\cdot k}d^3k\end{aligned}$$

where $T_R^* a(k) T_R = e^{iRd\cdot k} a(k)$ was also used. The third term converges to zero as $R \to \infty$ by the Riemann-Lebesgue Theorem because the integrand is in $L^1(\mathbb{R}^3, \mathbb{C}^2)$.

Since the distance of the electrons described by $T_R\varphi_\infty$ to the origin and to the electrons in φ_0 is bounded below by $3R - 3R_0$, we have, by assumption (H2), that

$$\langle \psi_R, V_N \psi_R \rangle = \langle \varphi_0, V_{N-N'}\varphi_0 \rangle + \sum_{i<j} \left\langle T_R\varphi_\infty, w(x_i - x_j) T_R \varphi_\infty \right\rangle + o(R^0), \qquad (R \to \infty),$$

as desired. Next we compare

$$\sum_{j=1}^{N} \left\langle \psi_R, (p_j + A(x_j))^2 \psi_R \right\rangle$$

with

$$\sum_{j \le N-N'} \left\langle \varphi_0, (p_j + A(x_j))^2 \varphi_0 \right\rangle + \sum_{j > N-N'} \left\langle T_R\varphi_\infty, (p_j + A(x_j))^2 T_R\varphi_\infty \right\rangle .$$

To this end we write $A(x_j) = a(G_{x_j}) + a^*(G_{x_j})$ and use that

$$\begin{aligned} (p_j + A(x_j))^2 &= p_j^2 + 2p_j \cdot a(G_{x_j}) + 2a^*(G_{x_j}) \cdot p_j \\ &\quad + a(G_{x_j})^2 + a^*(G_{x_j})^2 + 2a^*(G_{x_j}) a(G_{x_j}) + \|G_{x_j}\|^2. \end{aligned}$$

Let $j \le N - N'$, then using (21) and again disjointness of the supports of the photons in φ_0 and $T_R\varphi_\infty$, one finds that

$$\begin{aligned} \left\langle \psi_R, (p_j + A(x_j))^2 \psi_R \right\rangle &= \left\langle \varphi_0, (p_j + A(x_j))^2 \varphi_0 \right\rangle \\ &\quad + 2 \left\langle \varphi_0 \otimes T_R\varphi_\infty, p_j\varphi_0 \otimes a(G_{x_j}) T_R\varphi_\infty \right\rangle \ + \ \text{h.c.} \\ &\quad + 2 \left\langle \varphi_0 \otimes T_R\varphi_\infty, a(G_{x_j})\varphi_0 \otimes a(G_{x_j}) T_R\varphi_\infty \right\rangle \ + \ \text{h.c.} \\ &\quad + \left\langle \varphi_0 \otimes T_R\varphi_\infty, \varphi_0 \otimes a(G_{x_j})^2 T_R\varphi_\infty \right\rangle \ + \ \text{h.c.} \\ &\quad + \left\langle a(G_{x_j})\varphi_0 \otimes T_R\varphi_\infty, \varphi_0 \otimes a(G_{x_j}) T_R\varphi_\infty \right\rangle \ + \ \text{h.c.} \\ &\quad + \left\langle \varphi_0 \otimes a(G_{x_j}) T_R\varphi_\infty, \varphi_0 \otimes a(G_{x_j}) T_R\varphi_\infty \right\rangle . \end{aligned}$$

All terms except the first one vanish in the limit $R \to \infty$. In fact,

$$\begin{aligned} a(G_{x_j}) T_R \varphi_\infty &= T_R a(G_{x_j - Rd}) \Gamma(\chi_{R_0}) \varphi_\infty \\ &= T_R \Gamma(\chi_{R_0}) a(\chi_{R_0} G_{x_j - Rd}) \varphi_\infty, \end{aligned}$$

and since $|x_j| \le R_0$ if $\varphi_0(x_1, \dots, x_{N-N'}) \neq 0$, we can multiply this in all the above terms with $\chi_{R_0}(x_j)$. But then, by Equation (18) and with $G_\lambda(k) = |k|^{-1/2} \varepsilon_\lambda(k) \chi_\Lambda(k)$

$$\|\chi_{R_0}(x_j) a(\chi_{R_0} G_{x_j - Rd})(N_f + 1)^{-1/2}\|^2 \le \sup_{|x_j| \le R_0} \sum_{\lambda=1,2} \int_{|y| \le R_0} |\hat{G}_\lambda(x_j - Rd - y)|^2 dy \to 0 \qquad (R \to \infty). \tag{17}$$

The case where $j > N - N'$ is dealt with similarly. The only difference is that then $|x_j - Rd| \leq R_0$ in the support of $T_R\varphi_\infty$ and the photons in φ_0 have support in $|y| \leq R_0$. Hence (17) will be replaced by

$$\|\chi_{R_0}(x_j - Rd)a(\chi_{R_0}G_{x_j})(N_f+1)^{-1/2}\|^2 \leq \sup_{|x_j - Rd| \leq R_0} \sum_{\lambda=1,2} \int_{|y|\leq R_0} |\hat{G}_\lambda(x_j - y)|^2 dy \to 0 \qquad (R \to \infty).$$

The terms involving $B(x_i)$ are dealt with similarly. □

A Important Estimates

Lemma 7. *For all $\Lambda \geq 0$, $\varepsilon > 0$ and all $x \in \mathbb{R}^3$,*

$$\begin{aligned} A(x)^2 &\leq 32\pi\Lambda(H_f + \Lambda/4), \\ \pm\sigma \cdot B(x) &\leq \varepsilon H_f + \frac{8\pi}{\varepsilon}\Lambda^3. \end{aligned}$$

For the proof see [7]. This lemma holds equally for $A_\mu(x)$ and $B_\mu(x)$ with $\mu > 0$.

Lemma 8. *Let $C = 1 + 32\pi\alpha N\Lambda$ and $D = 8\pi\alpha N\Lambda$. Then, for all $\mu \geq 0$,*

$$\sum_{i=1}^N p_i^2 \leq C\left\{\sum_{i=1}^N (p_i + \sqrt{\alpha}A_\mu(x_i))^2 + H_f\right\} + D.$$

Furthermore, if $V_- \leq \varepsilon p^2 + C_\varepsilon$ for all $\varepsilon > 0$, then there exist constants $D(\varepsilon)$, depending on α, g, N, Λ and ε, but not on μ, such that

$$\left\{\sum_{i=1}^N (p_i + \sqrt{\alpha}A_\mu(x_i))^2 + V_+ + H_f\right\} \leq (1+\varepsilon)H_{N,\mu} + D(\varepsilon).$$

Proof. The first part follows from $p_i^2 \leq 2(p_i + \sqrt{\alpha}A_\mu(x_i))^2 + 2\alpha A_\mu(x_i)^2$ and Lemma 7. The second bound follows from the first and Lemma 7. □

Theorem 9. *Suppose the negative parts v_- and w_- of the external potential v and the two-particle interaction w as functions in $\mathbb{R}^3$ drop off to zero as $|x| \to \infty$. Then for all values of the parameters N, Λ, α, g and $\mu \geq 0$, there exists a functions $f(R)$ and a constant C, depending on these parameters, such that*

$$H_{N,\mu} \geq \tau(H_{N,\mu}) - f(R)(H_{N,\mu} + N_f + C) \qquad \text{on } \mathcal{D}_{N,R}$$

where $\lim_{R\to\infty} f(R) = 0$. Here $\tau(H_{N,\mu}) = \inf_{N'\geq 1}[\inf\sigma(H_{N-N',\mu}) + \inf\sigma(H^0_{N,\mu})]$.

This theorem is a variant of Corollary A.2 in [7] (see also [6]). The positivity of the photon mass in [7] is only needed to estimate N_f in terms of H_N. Thus this theorem holds for positive as well as for vanishing photon mass. The proof is essentially the same as the one in [7].

B Fock Space and Second Quantization

Let $\mathfrak{h}$ be a complex Hilbert space, and let $\otimes_s^n \mathfrak{h}$ denote the symmetric tensor product of n copies of $\mathfrak{h}$. Then the bosonic Fock space over $\mathfrak{h}$:

$$\mathcal{F} = \mathcal{F}(\mathfrak{h}) = \oplus_{n\geq 0} \otimes_s^n \mathfrak{h}$$

is the space of sequences $\varphi = (\varphi_n)_{n\geq 0}$, with $\varphi_0 \in \mathbb{C}$, $\varphi_n \in \otimes_s^n \mathfrak{h}$, and with an inner product defined by

$$\langle \varphi, \psi \rangle := \sum_{n\geq 0} (\varphi_n, \psi_n),$$

where (φ_n, ψ_n) denotes the inner product of $\otimes_s^n \mathfrak{h}$. The vector $\Omega = (1, 0, \ldots) \in \mathcal{F}$ is called the vacuum. By $\mathcal{F}_{\text{fin}} \subset \mathcal{F}$ we denote the dense subspace of vectors φ for which $\varphi_n = 0$, for all but finitely many n. The number operator N_f in $\mathcal{F}$ is defined by $(N_f \varphi)_n = n\varphi_n$.

B.1 Creation- and Annihilation Operators

The creation operator $a^*(h)$, $h \in \mathfrak{h}$, on $\mathcal{F}_{\text{fin}} \subset \mathcal{F}$ is defined by

$$(a^*(h)\varphi)_n = \sqrt{n}\, S_n(h \otimes \varphi_{n-1})$$

where $S_n \in \mathbf{B}(\otimes^n \mathfrak{h})$ denotes the orthogonal projection onto the symmetric subspace $\otimes_s^n \mathfrak{h} \subset \otimes^n \mathfrak{h}$. The annihilation operator $a(h)$ is the adjoint of $a^*(h)$ restricted to $\mathcal{F}_{\text{fin}}$. Creation- and annihilation operators satisfy the canonical commutation relations (CCR)

$$[a(g), a^*(h)] = (g, h), \qquad [a^\sharp(g), a^\sharp(h)] = 0.$$

In particular $[a(h), a^*(h)] = \|h\|^2$. From these definitions it is easy to see that

$$\|a^\sharp(h)(N+1)^{-1/2}\| \leq \|h\|. \tag{18}$$

In the case where $\mathfrak{h} = L^2(\mathbb{R}^3; \mathbb{C}^2)$, the one-photon Hilbert space, the annihilation and creation operators can be expressed in terms of the operator valued distributions $a_\lambda(k)$ and $a_\lambda^*(k)$ by

$$\begin{aligned} a(h) &= \sum_{\lambda=1,2} \int \overline{h_\lambda(k)} a_\lambda(k)\, d^3k \\ a^*(h) &= \sum_{\lambda=1,2} \int h_\lambda(k) a_\lambda^*(k)\, d^3k. \end{aligned}$$

Setting $G_{x,\lambda}(k) = |k|^{-1/2} \varepsilon_\lambda(k) \chi_{\{|k|\leq\Lambda\}} e^{-ik\cdot x}$ the quantized vector potential $A(x)$ can be defined as $A(x) = a(G_x) + a^*(G_x)$.

B.2 Second Quantization

Suppose b is a bounded operator on $\mathfrak{h}$ and $\|b\| \leq 1$. One then defines an operator $\Gamma(b)$: $\mathcal{F}(\mathfrak{h}) \to \mathcal{F}(\mathfrak{h})$ by

$$\begin{aligned} \Gamma(b)\Omega &= \Omega \\ \Gamma(b)\restriction \otimes_s^n \mathfrak{h} &= b \otimes \ldots \otimes b. \end{aligned}$$

Clearly $\|\Gamma(b)\| \leq 1$. From the definition of $a^*(h)$ it easily follows that

$$\Gamma(b)a^*(h) = a^*(bh)\Gamma(b) \tag{19}$$

$$\Gamma(b)a(b^*h) = a(h)\Gamma(b), \tag{20}$$

and hence that $\Gamma(b)a(h) = a(bh)\Gamma(b)$ if $b^*b = 1$.

If $b : D(b) \subset \mathcal{H} \to \mathcal{H}$ is self-adjoint, then $\mathrm{d}\Gamma(b)$ in $\mathcal{F}(\mathfrak{h})$ is defined by

$$\begin{aligned} \mathrm{d}\Gamma(b)\Omega &= 0 \\ \mathrm{d}\Gamma(b)\restriction \otimes_s^n D(b) &= \sum_{j=1}^{n} (\underbrace{1 \otimes \ldots 1}_{j-1} \otimes b \otimes \underbrace{1 \otimes \ldots 1}_{n-j}) \end{aligned}$$

and by linear extension. $\mathrm{d}\Gamma(b)$ is essentially self-adjoint and, denoting the closure by $\mathrm{d}\Gamma(b)$ as well, $\Gamma(e^{ib}) = e^{i\mathrm{d}\Gamma(b)}$. One example is the number operator $N_f = \mathrm{d}\Gamma(1)$, an other one, for $\mathfrak{h} = L^2(\mathbb{R}^3; \mathbb{C}^2)$ is the field energy

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

B.3 The Identification Operator $I : \mathcal{F} \otimes \mathcal{F} \to \mathcal{F}$

An important role in the proof of Theorem 6 is played by the identification operator $I : \mathcal{F} \otimes \mathcal{F} \to \mathcal{F}$ defined by

$$\begin{aligned} &I(\varphi \otimes \Omega) = \varphi \\ &I\varphi \otimes a^*(h_1) \cdots a^*(h_n)\Omega = a^*(h_1) \cdots a^*(h_n)\varphi, \qquad \varphi \in \mathcal{F}_{\text{fin}}, \end{aligned}$$

and extended by linearity to $\mathcal{F}_{\text{fin}} \otimes \mathcal{F}_{\text{fin}}$. The operator I is unbounded. We need the important commutation relation

$$a(h)I = I(a(h) \otimes 1 + 1 \otimes a(h)), \tag{21}$$

which is in contrast with $a^*(h)I = I(a^*(h) \otimes 1) = I(1 \otimes a^*(h))$.

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