Mourre Estimate and Spectral Theory for the Standard Model of Non-Relativistic QED

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Abstract

For a model of atoms and molecules made from static nuclei and non-relativistic electrons coupled to the quantized radiation field (the standard model of non-relativistic QED), we prove a Mourre estimate and a limiting absorption principle in a neighborhood of the ground state energy. As corollaries we derive local decay estimates for the photon dynamics, and we prove absence of (excited) eigenvalues and absolute continuity of the energy spectrum near the ground state energy, a region of the spectrum not understood in previous investigations.

The conjugate operator in our Mourre estimate is the second quantized generator of dilatations on Fock space.

1 Introduction

According to Bohr's well known picture, an atom or molecule has only a discrete set of stationary states (bound states) at low energies and a continuum of states at energies above the ionization threshold. Electrons can jump from a stationary state to another such state at lower energy by emitting photons. These radiative transitions tend to render excited states unstable,

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i.e., convert them into resonances. Exceptions are the *ground state* and, in some cases, excited states that remain stable for reasons of symmetry (e.g. ortho-helium). In *non-relativistic QED*, the instability of excited states finds its mathematical expression in the migration of eigenvalues to the lower complex half-plane (second Riemannian sheet for a weighted resolvent) as the interaction between electrons and photons is turned on. Indeed, the spectrum of the Hamiltonian becomes purely *absolutely continuous* in a neighborhood of the unperturbed excited eigenvalues [7, 5]. The ground state, however, remains stable [4, 5, 16]. The methods used to analyze the spectrum near unperturbed excited eigenvalues have either failed [7], or not been pushed far enough [5], to yield information on the spectrum of the interacting Hamiltonian in a neighborhood of the ground state energy. The purpose of this paper is to close this gap. We establish a Mourre estimate and a corresponding limiting absorption principle for a spectral interval at the infimum of the energy spectrum. It follows that the spectrum is purely absolutely continuous above the ground state energy. As a corollary we prove local decay estimates for the photon dynamics.

In non-relativistic QED (regularized in the ultraviolet), the Hamiltonian, H, of an atom or molecule with static nuclei with is a self-adjoint operator on the tensor product, $\mathcal{H} := \mathcal{H}_{\text{part}} \otimes \mathcal{F}$, of the electronic Hilbert space $\mathcal{H}_{\text{part}} = \wedge_{i=1}^{N} L^2(\mathbb{R}^3; \mathbb{C}^2)$ and the symmetric (bosonic) Fock space $\mathcal{F}$ over $L^2(\mathbb{R}^3, \mathbb{C}^2; dk)$. It is given by

$$H = \sum_{i=1}^{N} (-i\nabla_{x_i} + \alpha^{3/2} A(\alpha x_i))^2 + V + H_f, \tag{1}$$

where N is the number of electrons and $\alpha > 0$ is the fine structure constant. The variable $x_i \in \mathbb{R}^3$ denotes the position of the ith electron, and V is the operator of multiplication by $V(x_1, \ldots, x_N)$, the potential energy due to the interaction of the electrons and the nuclei through their electrostatic fields. In our units, $V(x_1, \ldots, x_N)$ is independent of α and given by

$$V(x_1, \ldots, x_N) = -\sum_{i=1}^{N} \sum_{l=1}^{M} \frac{Z_l}{|x_i - R_l|} + \sum_{i<j} \frac{1}{|x_i - x_j|}.$$

The operator H_f accounts for the energy of the transversal modes of the electromagnetic field, and $A(x)$ is the quantized vector potential in the Coulomb gauge with an ultraviolet cutoff. In terms of creation- and annihilation operators, $a_\lambda^*(k)$ and $a_\lambda(k)$, these operators are

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

and

$$A(x) = \sum_{\lambda=1,2} \int d^3k \frac{\kappa(k)}{|k|^{1/2}} \varepsilon_\lambda(k) \Big\{ e^{ik\cdot x} a_\lambda(k) + e^{-ik\cdot x} a_\lambda^*(k) \Big\}, \tag{2}$$

where $\lambda \in \{1, 2\}$ labels the two possible photon polarizations perpendicular to $k \in \mathbb{R}^3$. The corresponding polarization vectors are denoted by $\varepsilon_\lambda(k)$; they are normalized and orthogonal to each other. Thus, for each $x \in \mathbb{R}^3$, $A(x) = (A_1(x), A_2(x), A_3(x))$ is a triple of operators on the Fock space $\mathcal{F}$. The real-valued function κ is an ultraviolet cutoff and serves to make the components of $A(x)$ densely defined self-adjoint operators. We assume that κ belongs to the Schwartz space, although much less smoothness and decay suffice. We emphasize that no infrared cutoff is used; that is, (physically relevant) choices of κ, with

$$\kappa(0) \neq 0 \tag{3}$$

are allowed. The spectral analysis of H for such choices of κ is the main concern of this paper. Under the simplifying assumption that $|\kappa(k)| \leq |k|^\beta$, for some $\beta > 0$, the analysis is easier and some of our results are already known for β sufficiently large; see the brief review at the end of this introduction.

The spectrum of H is the half-line $[E, \infty)$, with $E = \inf \sigma(H)$. The end point E is an eigenvalue if $N - 1 < \sum_l Z_j$ [6, 16, 19], but the rest of the spectrum is expected to be purely absolutely continuous (with possible exception as explained above). For a large interval between E and the threshold, Σ, of ionization, absolute continuity has been proven in [7, 6]; but the nature of the spectrum in small neighborhoods of E and Σ has not been analyzed. There are further results on absolute continuity of the spectrum for simplified variants of H, and we shall comment on them below. Our main goal, in this paper, is to analyze the spectrum of H in a neighborhood of E. Under the assumption that $e_1 = \inf \sigma(H_{\text{part}})$ is a simple and isolated eigenvalue of $H_{\text{part}} = -\sum_{i=1}^N \Delta_{x_i} + V$, we show that $\sigma(H)$ is purely absolutely continuous in $(E, E + e_{\text{gap}}/2)$, where $e_{\text{gap}} = e_2 - e_1$ and e_2 is the first point in the spectrum of H_{part} above e_1. It follows, in particular, that H has no eigenvalues near E other than E, and, as a byproduct of our proofs, a local decay estimate is obtained for the photon dynamics.

Our approach to the spectral analysis of H is based on Conjugate Operator Theory in its standard form with a *self-adjoint* conjugate operator. Our choice for the conjugate operator, B, is the second quantized dilatation generator on Fock space, that is,

$$B = \mathrm{d}\Gamma(b), \qquad b = \frac{1}{2}(k \cdot y + y \cdot k), \tag{4}$$

where $y = i\nabla_k$ denotes the "position operator" for photons. The hypotheses of conjugate operator theory are a regularity assumption on H and a positive commutator estimate, called *Mourre estimate*. Concerning the first assumption we show that $s \mapsto e^{-iBs} f(H) e^{iBs} \psi$ is twice continuously differentiable, for all $\psi \in \mathcal{H}$ and for all f of class C_0^∞ on the interval $(-\infty, \Sigma)$ below the ionization threshold Σ. Our Mourre estimate says that, if α is small enough, then

$$E_\Delta(H - E)[H, iB]E_\Delta(H - E) \geq \frac{\sigma}{10} E_\Delta(H - E), \tag{5}$$

for arbitrary $\sigma \leq e_{\text{gap}}/2$ and $\Delta = [\sigma/3, 2\sigma/3]$. As a result we obtain all the standard consequences of conjugate operator theory on the interval $(E, E + e_{\text{gap}}/2)$ [21], in particular, absence of eigenvalues (Virial Theorem), absolute continuity of the spectrum, existence of the boundary values

$$\langle B\rangle^{-s}(H-\lambda\pm i0)^{-1}\langle B\rangle^{-s} \tag{6}$$

for $\lambda \in (E, E+e_{\rm gap}/3)$, $s\in(1/2,1)$ (Limiting Absorption Principle), and their Hölder continuity of degree $s-1/2$ with respect to λ. This Hölder continuity implies the following local decay estimate: if $f\in\mathbb{C}_0^\infty(\mathbb{R})$ with $\mathrm{supp}(f)\subset(E,E+e_{\rm gap}/3)$, then

$$\|\langle B\rangle^{-s}e^{-iHt}f(H)\langle B\rangle^{-s}\| = O(\frac{1}{t^{s-1/2}}),\qquad (t\to\infty),$$

which is a statement about the growth of $\langle B\rangle := (1+B^2)^{1/2}$ under the time evolution of states in the range of $f(H)\langle B\rangle^{-s}$. Such estimates are useful in scattering theory. See [13] for a discussion of this point.

The idea to use conjugate operator theory with (4) as the conjugate operator is not new and has been used for instance in [7]. It is based on the property that

$$[H_f, iB] = H_f$$

and that H_f is positive on the orthogonal complement of the vacuum sector. There is an obvious problem, however, with the implementation of this idea that discouraged people from using it in the analysis of the spectrum close to E: if $\alpha^{3/2}W = H-(H_{\rm part}+H_f)$ denotes the interaction part of H, then

$$[H, iB] = H_f + \alpha^{3/2}[W, iB], \tag{7}$$

and the commutator $[W, iB]$ has *no definite sign*. It can be compensated for by part of the field energy H_f so that $H_f+\alpha^{3/2}[W,iB]$ becomes positive, but only so on spectral subspaces corresponding to energy intervals separated from E by a distance of order α^3 [7]. For fixed $\alpha>0$ no positive commutator, and thus no information on the spectrum is obtained near $E=\inf\sigma(H)$. For this reason, Hübner and Spohn and, later, Skibsted, Dereziński and Jakšić, and Georgescu et al. chose the operator

$$\hat{B} = \frac{1}{2}\mathrm{d}\Gamma(\hat{k}\cdot y + y\cdot\hat{k}),\qquad \hat{k} = \frac{k}{|k|},$$

or a variant thereof, as conjugate operator; see [18, 22, 9, 14]. It has the advantage that, formally, $[H_f, i\hat{B}] = N$, the number operator, which is bounded below by the identity operator on the orthogonal complement of the vacuum sector. It follows that $[H, i\hat{B}] \geq \frac{1}{2}N$, for $\alpha>0$ small enough, and one may hope to prove absolute continuity of the energy spectrum all the way down to $\inf\sigma(H)$. The drawback of $\hat{B}$ is that it is only symmetric, but not self-adjoint, and hence not admissible as a conjugate operator. Therefore Skibsted, and, later, Georgescu, Gérard, and Møller developed suitable extensions of conjugate operator theory that allow for non-selfajoint conjugate operators [22, 14]. Skibsted applied his conjugate operator theory to (1) and obtained absolute continuity of the energy spectrum away from thresholds and eigenvalues under an *infrared* (IR) regularization, but not for (3). For the spectral results of Georgescu et al. see the review below. Given this background, the *main achievement* of the present paper is the discovery of the Mourre estimate (5). We now sketch the main elements of its proof.

1. As an auxiliary operator we introduce an IR-cutoff Hamiltonian H_σ in which the interaction of electrons with photons of energy $\omega \leq \sigma$ is turned off. It follows that H_σ is of the form

$$H_\sigma = H^\sigma \otimes 1 + 1 \otimes H_{f,\sigma},$$

with respect to $\mathcal{H} = \mathcal{H}^\sigma \otimes \mathcal{F}_\sigma$, where $\mathcal{F}_\sigma$ is the symmetric Fock space over $L^2(|k| \leq \sigma; \mathbb{C}^2)$ and $H_{f,\sigma}$ is $\mathrm{d}\Gamma(\omega)$ restricted to $\mathcal{F}_\sigma$. We show that the reduced Hamiltonian H^σ does not have spectrum in the interval $(E_\sigma, E_\sigma + \sigma)$ above the ground state energy $E_\sigma = \inf \sigma(H_\sigma) = \inf \sigma(H^\sigma)$. It follows that, for any $\Delta \subset (0, \sigma)$,

$$E_\Delta(H_\sigma - E_\sigma) = P^\sigma \otimes E_\Delta(H_{f,\sigma}), \tag{8}$$

where P^σ is the ground state projection of H^σ.

2. We split B into two pieces $B = B_\sigma + B^\sigma$ where B_σ and B^σ are the second quantizations of the generators associated with the vector fields $\eta_\sigma^2(k)k$ and $\eta^\sigma(k)^2 k$, respectively. Here $\eta_\sigma, \eta^\sigma \in C^\infty(\mathbb{R}^3)$ is a partition of unity, $\eta_\sigma^2 + (\eta^\sigma)^2 = 1$, with $\eta_\sigma(k) = 1$ for $|k| \leq 2\sigma$ and $\eta^\sigma(k) = 1$ for $|k| \geq 4\sigma$. It follows that $B^\sigma = B^\sigma \otimes 1$ with respect to $\mathcal{H} = \mathcal{H}^\sigma \otimes \mathcal{F}_\sigma$, and that $[H, B^\sigma] = [H^\sigma, B^\sigma] \otimes 1$. Thus (8) and the virial theorem, $P^\sigma [H^\sigma, B^\sigma] P^\sigma = 0$, imply that

$$E_\Delta(H_\sigma - E_\sigma)[H, iB^\sigma] E_\Delta(H_\sigma - E_\sigma) = 0. \tag{9}$$

3. The first key estimate in our proof of (5) is the operator inequality

$$E_\Delta(H_\sigma - E_\sigma)[H, iB_\sigma] E_\Delta(H_\sigma - E_\sigma) \geq \frac{\sigma}{8} E_\Delta(H_\sigma - E_\sigma) \tag{10}$$

valid for the interval $\Delta = [\sigma/3, 2\sigma/3]$ and $\alpha \ll 1$, with α independent of σ. This inequality follows from

$$[H_f, iB_\sigma] = \mathrm{d}\Gamma(\eta_\sigma^2 \omega) \geq H_{f,\sigma} \tag{11}$$

and from

$$E_\Delta(H_\sigma - E_\sigma)[\alpha^{3/2} H_f + \alpha^{3/2} W, iB_\sigma] E_\Delta(H_\sigma - E_\sigma) \geq O(\alpha^{3/2}\sigma). \tag{12}$$

Indeed, by writing $H_f = (1 - \alpha^{3/2}) H_f + \alpha^{3/2} H_f$, combining (11) and (12), and using (8) we obtain

$$E_\Delta(H_\sigma - E_\sigma)[H, iB_\sigma] E_\Delta(H_\sigma - E_\sigma) \geq \big((1 - \alpha^{3/2}) \inf \Delta + O(\alpha^{3/2}\sigma)\big) E_\Delta(H_\sigma - E_\sigma). \tag{13}$$

For $\Delta = [\sigma/3, 2\sigma/3]$ and α small enough this proves (10).

4. The second key estimate in our proof of (5) is the norm bound

$$\|f_\Delta(H-E) - f_\Delta(H_\sigma - E_\sigma)\| = O(\alpha^{3/2}\sigma) \tag{14}$$

valid for smoothed characteristic functions f_Δ of the interval $\Delta = [\sigma/3, 2\sigma/3]$. The Mourre estimate (5) follows from (9), (10), from $B = B_\sigma + B^\sigma$ and from (14) if $\alpha \ll 1$, with α independent of σ.

We conclude this introduction with a review of previous work closely related to this paper. Absolute continuity of (part of) the spectrum of Hamiltonians of the form (1), or caricatures thereof, was previously established in [18, 2, 22, 14, 4, 6, 7]. Arai considers the explicitly solvable case of a harmonically bound particle coupled to the quantized radiation field in the dipole approximation. Hübner and Spohn study the spin-boson model with massive bosons or with a photon number cutoff imposed. Their work inspired [22] and [14], where better results were obtained: Skibsted analyzed (1) and assumed that $|\kappa(k)| \leq |k|^{5/2}$, while, in [14], $|\kappa(k)| \leq |k|^\beta$, with $\beta > 1/2$, is sufficient for a Nelson-type model with scalar bosons; (see Section 2 of the present article). The main achievement of [14] is that no bound on the coupling strength is required. Papers [6] and [7] do not introduce an infrared regularization but establish the spectral properties mentioned above only away from $O(\alpha^3)$-neighborhoods of the particle ground state energy and the ionization threshold.

2 Non-relativistic Matter and Scalar Bosons

To illustrate the main ideas on which this work is based we first derive results for a simplified model of matter and radiation with only one electron and scalar bosons, rather than transversal photons. We suppress proofs of technical details that are similar and easier than the corresponding proofs of results on non-relativistic QED, in the next section.

The Hamiltonian, in this section, is the operator

$$H = H_{\text{part}} \otimes 1 + 1 \otimes H_f + g\phi(G) \tag{15}$$

on the Hilbert space $L^2(\mathbb{R}^3) \otimes \mathcal{F}$, with $\mathcal{F}$ being the symmetric Fock space over $L^2(\mathbb{R}^3; dk)$. We assume that $H_{\text{part}} = -\Delta + V$, where V denotes the operator of multiplication with a real-valued function $V \in L^2_{loc}(\mathbb{R}^3)$ that is Δ-bounded with bound zero. Moreover we assume that $e_1 = \inf \sigma(H_{\text{part}})$ is an isolated simple eigenvalue. The number $e_2 > e_1$ denotes the first point in the spectrum of H_{part} above e_1 and $e_{\text{gap}} = e_2 - e_1$. The parameter $g \geq 0$ measures the strength of interaction between the electron and the bosons.

The field energy H_f and the interaction term $g\phi(G)$ are given in terms of creation and annihilation operators $a^*(k)$ and $a(k)$, as

$$H_f = \int \omega(k) a^*(k) a(k)\, d^3k, \qquad \omega(k) = |k|,$$

and

$$\phi(G) = \int \left\{ G(k)^* \otimes a(k) + G(k) \otimes a^*(k) \right\} d^3k,$$

where, for each $k \in \mathbb{R}^3$, $G(k)$ is a multiplication operator given by a function $x \mapsto G_x(k)$ on the electronic Hilbert space $L^2(\mathbb{R}^3; dx)$. We assume that $G_x(k)$ is twice continuously differentiable with respect to k and that

$$\sup_{x\in\mathbb{R}^3} \int \left| \langle x\rangle^{-n} |k|^n \partial_{|k|}^n G_x(k) \right|^2 (|k|^{-1}+1) d^3k < \infty \tag{16}$$

for $n \in \{0, 1, 2\}$, where $\langle x\rangle = (1+x^2)^{1/2}$. Moreover, we assume that

$$|G_x(k)| \leq |k|^\mu, \qquad \text{for } |k| \leq 2e_{\text{gap}} \tag{17}$$

$$\langle x\rangle^{-1}|k| \left| \frac{\partial}{\partial|k|} G_x(k) \right| \leq |k|^\mu, \qquad \text{for } |k| \leq 2e_{\text{gap}}, \tag{18}$$

uniformly in $x \in \mathbb{R}^3$, for a suitably chosen $\mu \in \mathbb{R}$. The main theorem of this section holds for $\mu \geq 1/2$.

Assumption (16) with $n = 0$ implies that $\phi(G)$ is H_0-bounded, $H_0 = H_{\text{part}} \otimes 1 + 1 \otimes H_f$, with relative bound zero. It follows from the Kato-Rellich Theorem, that H is self-adjoint on the domain of H_0, essentially self-adjoint on any core of H_0, and bounded from below. We use $E = \inf \sigma(H)$ to denote the lowest point of the spectrum of H and Σ to denote the ionization threshold

$$\Sigma = \lim_{R\to\infty} \left(\inf_{\varphi\in D_R,\, \|\varphi\|=1} \langle\varphi, H\varphi\rangle \right), \tag{19}$$

where $D_R := \{\varphi \in D(H) | \chi(|x| \leq R)\varphi = 0\}$.

Our conjugate operator is the second quantized dilatation generator

$$B = \mathrm{d}\Gamma(b), \qquad b = \frac{1}{2}(k\cdot y + y \cdot k) \tag{20}$$

where $y = i\nabla_k$. By the methods of Section 4 one can show, using (16), that H is locally of class $C^2(B)$ on $\Omega := (-\infty, \Sigma)$. That is, the mapping

$$s \mapsto e^{-iBs} f(H) e^{iBs} \varphi \tag{21}$$

is twice continuously differentiable, for every $\varphi \in \mathcal{H}$ and every $f \in C_0^\infty(\Omega)$. This makes the conjugate operator theory in the variant of Sahbani [21] applicable, and, in particular, it allows one to define the commutator $[H, iB]$ as a sesquilinear form on $\cup_K E_K(H)\mathcal{H}$, the union being taken over all compact subsets K of Ω.

We are now ready to state our main results on the Hamiltonian (15).

Theorem 1 (Mourre estimate). *Suppose that Hypotheses* (16)*,* (17)*, and* (18) *hold with* $\mu \geq 1/2$*. If* $g \ll 1$ *and* $\sigma \leq e_{\text{gap}}/2$ *then*

$$E_\Delta(H-E)[H, iB]E_\Delta(H-E) \geq \frac{\sigma}{10} E_\Delta(H-E),$$

where $\Delta = [\sigma/3, 2\sigma/3]$.

This theorem verifies the second hypothesis of Conjugate Operator Theory, see Section B of the appendix, and it has all the standard implications of this theory: In $(E, E + e_{\text{gap}}/3)$, the spectrum of H is absolutely continuous, the boundary values $\langle B\rangle^{-s}(H - \lambda \pm i0)\langle B\rangle^{-s}$ are Hölder continuous of degree $s - 1/2$, and $\langle B\rangle^{-s}e^{-iHt}f(H)\langle B\rangle^{-s} = O(t^{1/2-s})$, for $f \in C_0^\infty(E, E + e_{\text{gap}}/3)$ and $s \in (1/2, 1)$; see Theorems 31, 32, and 33. For the more important standard model of nonrelativistic QED, these properties are spelled out explicitly in the next section.

The proof of Theorem 1 depends, of course, on an explicit expression for the commutator $[H, iB]$. By Lemma 37 and an analog of Proposition 18, we know that for $f \in C_0^\infty(E, E+e_{\text{gap}}/3)$

$$
\begin{aligned}
f(H)[H, iB]f(H) &= \lim_{s\to 0} f(H)\left[H, \frac{e^{iBs} - 1}{s}\right] f(H) \\
&= f(H)\big(\mathrm{d}\Gamma(\omega) - g\phi(ibG_x)\big)f(H), \qquad (22)
\end{aligned}
$$

where the limit is taken in the strong operator topology. Therefore we may identify $[H, iB]$ with the operator $\big(\mathrm{d}\Gamma(\omega) - g\phi(ibG_x)\big)$, which is defined on $D(|x|) \cap D(H_f)$. One of our main tools for estimating (22) from below is an infrared cutoff Hamiltonian H_σ, σ as in Theorem 1, whose spectral subspaces for energies close to $\inf \sigma(H_\sigma)$ are explicitly known (see Lemma 2). A second key tool is the decomposition of B into two pieces, B_σ and B^σ. We now define these operators along with some other auxiliary operators and Hilbert spaces. As a general rule, we will place the index σ downstairs if only *low-energy* photons are involved, and upstairs for *high-energy* photons. The fact that this rule does not cover all cases should not lead to any confusion.

Let $\chi_0, \chi_\infty \in C^\infty(\mathbb{R}, [0, 1])$, with $\chi_0 = 1$ on $(-\infty, 1]$, $\chi_\infty = 1$ on $[2, \infty)$, and $\chi_0^2 + \chi_\infty^2 \equiv 1$. For a given $\sigma > 0$, we define $\chi_\sigma(k) = \chi_0(|k|/\sigma)$, $\chi^\sigma(k) = \chi_\infty(|k|/\sigma)$, $\tilde{\chi}^\sigma(k) = 1 - \chi_\sigma(k)$, and a Hamiltonian H_σ by

$$H_\sigma = H_{\text{part}} \otimes 1 + 1 \otimes H_f + g\phi(\tilde{\chi}^\sigma G). \qquad (23)$$

Let $\mathcal{F}_\sigma$ and $\mathcal{F}^\sigma$ denote the bosonic Fock spaces over $L^2(|k| < \sigma)$ and $L^2(|k| \geq \sigma)$, respectively, and let $\mathcal{H}^\sigma = L^2(\mathbb{R}^3) \otimes \mathcal{F}^\sigma$. Then $\mathcal{H}$ is isomorphic to $\mathcal{H}^\sigma \otimes \mathcal{F}_\sigma$, and, in the sense of this isomorphism,

$$H_\sigma = H^\sigma \otimes 1 + 1 \otimes H_{f,\sigma}. \qquad (24)$$

Here $H^\sigma = H_\sigma \restriction \mathcal{H}^\sigma$ and $H_{f,\sigma} = H_f \restriction \mathcal{F}_\sigma$.

Next, we split the operator B into two pieces depending on σ. To this end we define new cutoff functions $\eta_\sigma = \chi_{2\sigma}$, $\eta^\sigma = \chi^{2\sigma}$ and cut-off dilatation generators $b_\sigma = \eta_\sigma b \eta_\sigma$, $b^\sigma = \eta^\sigma b \eta^\sigma$. Since $\eta_\sigma^2 + (\eta^\sigma)^2 \equiv 1$ and $[\eta_\sigma, [\eta_\sigma, b]] = 0 = [\eta^\sigma, [\eta^\sigma, b]]$ it follows from the IMS-formula that $b = b_\sigma + b^\sigma$. Let $B_\sigma = \mathrm{d}\Gamma(b_\sigma)$ and $B^\sigma = \mathrm{d}\Gamma(b^\sigma)$. Then

$$B = B_\sigma + B^\sigma.$$

An analog of Theorem 16 implies that H is locally of class $C^2(B)$, $C^2(B_\sigma)$ and $C^2(B^\sigma)$ on $(-\infty, \Sigma)$. Since $E \le e_1$ and $\Sigma \ge e_2 - \Lambda g^2$, by Equation (44), we have that $\Sigma - E \ge (2/3)e_{\text{gap}}$, for g sufficiently small. It follows that $(-\infty, \Sigma) \supset (-\infty, E + 2/3e_{\text{gap}})$ and hence, arguing as in (22), that

$$[H, iB_\sigma] = \mathrm{d}\Gamma(\eta_\sigma^2\omega) - g\phi(ib_\sigma G_x), \tag{25}$$

$$[H, iB^\sigma] = \mathrm{d}\Gamma((\eta^\sigma)^2\omega) - g\phi(ib^\sigma G_x), \tag{26}$$

in the sense of quadratic forms on the range of $\chi(H \le E + e_{\text{gap}}/2)$. Equally, H^σ is of class $C^1(B^\sigma)$ and

$$[H^\sigma, iB^\sigma] = \mathrm{d}\Gamma((\eta^\sigma)^2\omega) - g\phi(ib^\sigma\tilde{\chi}^\sigma G_x) \tag{27}$$

on $\chi(H^\sigma \le E + e_{\text{gap}}/2)\mathcal{H}^\sigma$.

As a last piece of preparation we introduce smooth versions of the energy cutoffs $E_\Delta(H-E)$ and $E_\Delta(H_\sigma - E_\sigma)$. We choose $f \in C_0^\infty(\mathbb{R}; [0,1])$ with $f = 1$ on $[1/3, 2/3]$ and $\operatorname{supp}(f) \subset [1/4, 3/4]$, so that $f_\Delta(s) := f(s/\sigma)$ is a smoothed characteristic function of the interval $\Delta = [\sigma/3, 2\sigma/3]$. We define

$$F_\Delta = f_\Delta(H - E), \qquad F_{\Delta,\sigma} = f_\Delta(H_\sigma - E_\sigma). \tag{28}$$

Lemma 2. *Suppose that Hypothesis* (16) *holds. If $g \ll 1$ and $\sigma \le e_{\text{gap}}/2$, then*

$$F_{\Delta,\sigma} = P^\sigma \otimes f_\Delta(H_{f,\sigma}), \qquad \textit{w.r.t. } \mathcal{H} = \mathcal{H}^\sigma \otimes \mathcal{F}_\sigma, \tag{29}$$

where P^σ denotes the ground state projection of H^σ.

Proof. For g sufficiently small, depending on $e_2 - e_1 - \sigma$, the operator H^σ has the gap $(E_\sigma, E_\sigma + \sigma)$ in the spectrum above $E_\sigma = \inf \sigma(H^\sigma)$ by Theorem 23 of [11] (see also Appendix A, Theorem 26). Since the support of f_Δ is a subset of $(0, \sigma)$, the assertion of the lemma follows. □

Proposition 3. *Suppose that Hypothesis* (16) *holds, and let $[H, iB^\sigma]$ be defined by* (26). *If $g \ll 1$ and $\sigma \le e_{\text{gap}}/2$, then*

$$F_{\Delta,\sigma}[H, iB^\sigma]F_{\Delta,\sigma} = 0.$$

Proof. From $\eta^\sigma\chi_\sigma = 0$ and $\chi_\sigma + \tilde{\chi}^\sigma = 1$ it follows that $b^\sigma = b^\sigma\tilde{\chi}^\sigma$. Comparing (26) with (27) we see that $[H, iB^\sigma] = [H^\sigma, iB^\sigma] \otimes 1$ with respect to $\mathcal{H} = \mathcal{H}^\sigma \otimes \mathcal{F}_\sigma$. The proposition now follows from Lemma 2 and the Virial Theorem $P^\sigma[H^\sigma, iB^\sigma]P^\sigma = 0$, Proposition 34. □

Proposition 4. *Suppose that Hypotheses* (16), (17), *and* (18) *hold, and let $[H, iB_\sigma]$ be defined by* (25). *If $g \ll 1$ and $\sigma \le e_{\text{gap}}/2$, then*

$$\begin{aligned} F_{\Delta,\sigma}[H, iB_\sigma]F_{\Delta,\sigma} &\ge \Big[(1-g)\sigma/4 - Cg\sigma^{2\mu+2}\Big]F_{\Delta,\sigma}^2 \\ &\ge (\sigma/8)F_{\Delta,\sigma}^2, \end{aligned}$$

where $\mu \geq -1/2$ is assumed in the second inequality and C is independent of g and σ.

Remark. The fact that this Proposition only assumes that $\mu \geq -1/2$, unlike Theorem 1, will be important in our analysis of QED in the next section.

Proof. We write

$$\mathrm{d}\Gamma(\eta_\sigma^2\omega) - g\phi(ib_\sigma G_x) = (1-g)\mathrm{d}\Gamma(\eta_\sigma^2\omega) + g\Big[\mathrm{d}\Gamma(\eta_\sigma^2\omega) - \phi(ib_\sigma G_x)\Big]$$

and first estimate the term in brackets from below. Using that $\mathrm{d}\Gamma(\eta_\sigma^2\omega)$ is quadratic in $\eta_\sigma a^\#(k)$ while $\phi(ib_\sigma G_x)$ is linear, we complete the square and find

$$\begin{aligned} \mathrm{d}\Gamma(\eta_\sigma^2\omega) - \phi(ib_\sigma G_x) &\geq -\int_{|k|\leq 4\sigma} \frac{|b\eta_\sigma G_x|^2}{\omega}\, d^3k \\ &\geq -\mathrm{const}\ \langle x\rangle^2 \sigma^{2\mu+2}, \end{aligned}$$

because $|b\eta_\sigma| \leq$ const, $|G_x(k)| \leq |k|^\mu$, and $|bG_x(k)| \leq \mathrm{const}\langle x\rangle |k|^\mu$ for $|k| \leq 4\sigma \leq 2e_{\mathrm{gap}}$, by assumptions (17) and (18). This proves that

$$\mathrm{d}\Gamma(\eta_\sigma^2\omega) - g\phi(ib_\sigma G_x) \geq (1-g)\mathrm{d}\Gamma(\eta_\sigma^2\omega) - \mathrm{const}\ g\langle x\rangle^2\sigma^{2\mu+2}. \tag{30}$$

It remains to estimate $F_{\Delta,\sigma}\mathrm{d}\Gamma(\eta_\sigma^2\omega)F_{\Delta,\sigma}$ from below and $F_{\Delta,\sigma}\langle x^2\rangle F_{\Delta,\sigma}$ from above. Using that $F_{\Delta,\sigma} = P^\sigma \otimes f_\Delta(H_{f,\sigma})$, by Lemma 2, and

$$\mathrm{d}\Gamma(\eta_\sigma^2\omega) \geq H_{f,\sigma}, \qquad f_\Delta(H_{f,\sigma})H_{f,\sigma}f_\Delta(H_{f,\sigma}) \geq \frac{\sigma}{4} f_\Delta^2(H_{f,\sigma}),$$

we obtain

$$F_{\Delta,\sigma}\mathrm{d}\Gamma(\eta_\sigma^2\omega)F_{\Delta,\sigma} \geq \frac{\sigma}{4}F_{\Delta,\sigma}^2. \tag{31}$$

Furthermore, by Lemma 6,

$$\sup_{\sigma>0} \|x^2 E_{[0,\sigma]}(H_\sigma - E_\sigma)\| < \infty. \tag{32}$$

Since $E_{[0,\sigma]}(H_\sigma - E_\sigma)F_{\Delta,\sigma} = F_{\Delta,\sigma}$ the proposition follows from (30), (31), and (32). □

Proposition 5. *Suppose Hypotheses* (16), (17) *and* (18) *hold with $\mu \geq -1/2$. Then there exists a constant C_μ, such that*

$$\big\|f_\Delta(H-E) - f_\Delta(H_\sigma - E_\sigma)\big\| \leq gC_\mu\sigma^{\min\{\mu+1/2,\,2\mu\}}$$

for all $g \leq 1$ and $\sigma \leq e_{\mathrm{gap}}/2$.

Remark. Our proof of Theorem 1 requires that $\big\|f_\Delta(H-E) - f_\Delta(H_\sigma - E_\sigma)\big\| = O(\sigma)$. To achieve this using Proposition 5, we are forced to assume that $\mu \geq 1/2$.

Proof. Let $j \in C_0^\infty([0,1],\mathbb{R})$ with $j=1$ on $[1/4,3/4]$ and $\mathrm{supp}(j) \subset [1/5,4/5]$. Let $j_\Delta(s) = j(s/\sigma)$, so that $f_\Delta j_\Delta = f_\Delta$, and let $J_\Delta = j_\Delta(H-E)$ and $J_{\Delta,\sigma} = j_\Delta(H_\sigma - E_\sigma)$. We will show that, for $\mu \geq -1/2$,

$$\|F_\Delta - F_{\Delta,\sigma}\| \leq C_1 g\sigma^\mu \tag{33}$$

$$\|(F_\Delta - F_{\Delta,\sigma})J_{\Delta,\sigma}\| \leq C_2 g\sigma^{\mu+1/2}, \tag{34}$$

and, likewise, with F and J interchanged, where the constants C_1, C_2 depend on μ but not on g or σ. These estimates prove the proposition, because

$$\begin{aligned} F_\Delta - F_{\Delta,\sigma} &= F_\Delta J_\Delta - F_{\Delta,\sigma}J_{\Delta,\sigma} \\ &= F_{\Delta,\sigma}(J_\Delta - J_{\Delta,\sigma}) + (F_\Delta - F_{\Delta,\sigma})J_{\Delta,\sigma} + (F_{\Delta,\sigma} - F_\Delta)(J_\Delta - J_{\Delta,\sigma}). \end{aligned}$$

To prove (33) and (34) we use the functional calculus based on the representation

$$f(s) = \int \mathrm{d}\tilde{f}(z)\frac{1}{z-s}, \qquad \mathrm{d}\tilde{f}(z) := -\frac{1}{\pi}\frac{\partial \tilde{f}}{\partial \bar{z}}(z)dxdy, \tag{35}$$

for an almost analytic extension $\tilde{f}$ of f that satisfies $|\partial_{\bar{z}}\tilde{f}(x+iy)| \leq \text{const } y^2$ [8]. From (28) and (35) we obtain

$$F_\Delta - F_{\Delta,\sigma} = \sigma^{-1}\int \mathrm{d}\tilde{f}(z)\frac{1}{(z-[H-E]/\sigma)}(H - H_\sigma - E + E_\sigma)\frac{1}{(z-[H_\sigma - E_\sigma]/\sigma)} \tag{36}$$

where, by Lemma 8,

$$|E - E_\sigma| = O(g^2\sigma^{2\mu+2}). \tag{37}$$

Hence the contribution of $E - E_\sigma$ to (36) is $O(g^2\sigma^{2\mu+1})$, which, for $\mu \geq -1/2$, may be neglected for both (33) and (34). By Lemma 22 and Hypothesis (17)

$$\begin{aligned} \|(H-H_\sigma)(H_f+1)^{-1/2}\| &= g\|\phi(\chi_\sigma G_x)(H_f+1)^{-1/2}\| \\ &\leq 2g\sup_x \|\chi_\sigma G_x\|_\omega \leq 2g\left(\frac{4^{\mu+2}}{\mu+1}\pi\right)\sigma^{\mu+1}, \end{aligned} \tag{38}$$

while

$$\left\|(H_f+1)^{1/2}(z-[H_\sigma - E_\sigma]/\sigma)^{-1}\right\| \leq \text{const}\frac{\sqrt{1+|z|}}{|y|} \tag{39}$$

by an analog of Lemma 23. Since $\sqrt{1+|z|}/|y|$ is integrable with respect to $|\partial_{\bar{z}}\tilde{f}|dxdy$, bound (33) follows from (36), (37), (38), and (39).

By (36) and (37), with obvious notations for the resolvents,

$$(F_\Delta - F_{\Delta,\sigma})J_{\Delta,\sigma} = \sigma^{-1}\int \mathrm{d}\tilde{f}(z)R(z)(H-H_\sigma)J_{\Delta,\sigma}R_\sigma(z) + O(g^2\sigma^{2\mu+1}). \tag{40}$$

Lemma 7 and Lemma 28 yield

$$\begin{aligned} \|(H-H_\sigma)J_{\Delta,\sigma}\| &= g\|\phi(\chi_\sigma G_x)J_{\Delta,\sigma}\| \\ &\leq 2g\|a(\chi_\sigma G_x)J_{\Delta,\sigma}\| + g\|\chi_\sigma G_x\| \\ &\leq C_\mu g(\sigma^{2\mu+2}+\sigma^{\mu+3/2}). \end{aligned}$$

Combined with (40) this proves (34). □

Proof of Theorem 1. Since $(\eta^\sigma)^2+\eta_\sigma^2=1$ and $b_\sigma+b^\sigma=b$, it follows from (25) and (26) that $\mathrm{d}\Gamma(\omega)-g\phi(ibG_x)=[H,iB_\sigma]+[H,iB^\sigma]$. Thus Propositions 3 and 4 imply that

$$F_{\Delta,\sigma}\big(\mathrm{d}\Gamma(\omega)-g\phi(ibG_x)\big)F_{\Delta,\sigma}\geq\frac{\sigma}{8}F_{\Delta,\sigma}^2.$$

We next replace $F_{\Delta,\sigma}$ by F_Δ, using Proposition 5 with $\mu\geq 1/2$ and noticing that $(\mathrm{d}\Gamma(\omega)-g\phi(ibG_x))F_{\Delta,\sigma}$ and $F_\Delta(\mathrm{d}\Gamma(\omega)-g\phi(ibG_x))$ are bounded, uniformly in σ. Since, by (22), $(\mathrm{d}\Gamma(\omega)-g\phi(ibG_x))=[H,iB]$ on the range of F_Δ we arrive at

$$F_\Delta[H,iB]F_\Delta\geq\frac{\sigma}{8}F_\Delta^2+O(g\sigma).$$

After multiplying this operator inequality from both sides with $E_\Delta(H-E)$, the theorem follows. □

Ground state properties and localization of the electron

In this section we collect some technical auxiliaries for the proof of Theorem 1.

Lemma 6. *Suppose that Hypothesis* (16) *holds. Then for every $\lambda<e_2$ there exists a constant $g_\lambda>0$ such that for all $n\in\mathbb{N}$*

$$\sup_{\sigma>0,\,g\leq g_\lambda}\||x|^n E_\lambda(H_\sigma)\|<\infty.$$

Proof. From Theorem 1 of [15] we know that $\|e^{\varepsilon|x|}E_\lambda(H_\sigma)\|<\infty$ if $\lambda+\varepsilon^2<\Sigma_\sigma$, where Σ_σ is the ionization threshold of H_σ. From the proof of that theorem we see that

$$\sup_{\sigma>0,\,g\leq g_\lambda}\|e^{\varepsilon|x|}E_\lambda(H_\sigma)\|<\infty,$$

provided $R>0$ and $\delta>0$ can be found such that

$$\Sigma_{\sigma,R}:=\inf_{\varphi\in D_R,\,\|\varphi\|=1}\langle\varphi,H_\sigma\varphi\rangle\geq\lambda+\varepsilon^2+\delta+\frac{\tilde{C}}{R^2} \tag{41}$$

uniformly in $\sigma>0$ and $g\leq g_\lambda$. Here $\tilde{C}$ is a constant that is independent of H_σ. It remains to prove (41). To this end we note that, by a standard estimate,

$$H_\sigma\geq H_{\mathrm{part}}\otimes 1-g^2\Lambda \tag{42}$$

where $\Lambda = \sup_x \int |G_x(k)|^2/|k|\, dk < \infty$ due to Hypothesis (16), and, moreover, that

$$\inf_{\varphi \in D_R,\, \|\varphi\|=1} \langle \varphi, H_{\rm part} \otimes 1\varphi \rangle \geq \inf \sigma_{\rm ess}(H_{\rm part}) + o(1), \qquad (R \to \infty), \tag{43}$$

by Persson's characterization of $\inf \sigma(H_{\rm part})$; see, e.g., [15]. Since $\inf \sigma_{\rm ess}(H_{\rm part}) \geq e_2$ we conclude from (42), (43), and the definition of $\Sigma_{\sigma,R}$, that

$$\Sigma_{\sigma,R} \geq e_2 + o(1) - g^2\Lambda, \tag{44}$$

with $o(1) \to 0$, as $R \to \infty$, uniformly in σ, g. Since $e_2 > \lambda$ we may indeed find $\varepsilon, \delta, R, g_\lambda > 0$ so that (41) holds for all $\sigma > 0$ and all $g \leq g_\lambda$. □

The following two Lemmas assume the existence of a ground state for H_σ, $\sigma \geq 0$. This assumption is justified under our assumptions on $H_{\rm part}$ if $\mu > -1/2$, at least for g sufficiently small (see, e.g.,[23]).

Lemma 7. *Let Hypotheses* (16) *and* (17) *be satisfied and suppose that $\varphi \in \mathcal{H}$ is a normalized ground state of H_σ, where $\sigma \geq 0$, $g \geq 0$, and $H_{\sigma=0} := H$. Then*

$$\|a(k)\varphi\| \leq g|k|^{\mu-1}, \qquad \textit{for } |k| \leq 2e_{\rm gap}.$$

Proof. Use the usual pull through trick (see the proof of Lemma 29) and assumption (17). □

Lemma 8. *Let Hypotheses* (16) *and* (17) *with $\mu > -1$ be satisfied, suppose that $\sigma \leq e_{\rm gap}$, $g \geq 0$, and that $E = \inf \sigma(H)$ and $E_\sigma = \inf \sigma(H_\sigma)$ are eigenvalues of H and H_σ, respectively. Then there exists a constant C_μ such that*

$$|E - E_\sigma| \leq C_\mu g^2 \sigma^{2\mu+2}.$$

Proof. Let φ and φ_σ be normalized ground state vectors of H and H_σ respectively. Then by Rayleigh-Ritz

$$E_\sigma - E \leq \langle \varphi, (H_\sigma - H)\varphi \rangle \tag{45}$$

$$E - E_\sigma \leq \langle \varphi_\sigma, (H - H_\sigma)\varphi_\sigma \rangle. \tag{46}$$

From (45), Hypothesis (17), and Lemma 7 it follows that

$$\begin{aligned} E_\sigma - E &\leq -g\langle \varphi, \phi(\chi_\sigma G_x)\varphi \rangle \leq 2g\|a(\chi_\sigma G_x)\varphi\|\|\varphi\| \\ &\leq 2g \int_{|k|\leq 2\sigma} |G_x(k)|\|a(k)\varphi\|\, d^3k \leq \left(\frac{4^{\mu+2}}{\mu+1}\pi\right) g^2\sigma^{2\mu+2}. \end{aligned}$$

The corresponding estimate for $E - E_\sigma$ is a copy of the one above with φ replaced by φ_σ. □

3 Non-relativistic Matter and Quantized Radiation

We now come to the main part of this paper, the spectral analysis of atoms and molecules in the standard model of non-relativistic QED. The methods and results of this section are analogous to the ones presented in the previous section for matter and scalar bosons. For notational simplicity again a one-electron model is presented and spin is neglected; our analysis can easily be extended to many-electron systems with spin.

The Hilbert space of our systems is the tensor product

$$\mathcal{H} = L^2(\mathbb{R}^3, dx) \otimes \mathcal{F},$$

where $\mathcal{F}$ denotes the bosonic Fock space over $L^2(\mathbb{R}^3; \mathbb{C}^2)$. The Hamiltonian $H : D(H) \subset \mathcal{H} \to \mathcal{H}$ is given by

$$H = \Pi^2 + V + H_f, \qquad \Pi = -i\nabla_x + \alpha^{3/2} A(\alpha x) \tag{47}$$

where V, as in the previous section, denotes multiplication with a real-valued function $V \in L^2_{\text{loc}}(\mathbb{R}^3)$. We assume that V is $\Delta-$bounded with relative bound zero and that $e_1 = \inf \sigma(-\Delta + V)$ is an isolated eigenvalue with multiplicity one. The first point in $\sigma(-\Delta + V)$ above e_1 is denoted by e_2 and $e_{\text{gap}} := e_2 - e_1$. The field energy H_f and the quantized vector potential have already been introduced, formally, in the introduction. More proper definitions are $H_f := \mathrm{d}\Gamma(\omega)$, the second quantization of multiplication with $\omega(k) = |k|$, and $A_j(\alpha x) = a(G_{x,j}) + a^*(G_{x,j})$ where

$$G_x(k, \lambda) := \frac{\kappa(k)}{\sqrt{|k|}} \varepsilon_\lambda(k) e^{-i\alpha x \cdot k},$$

and $\varepsilon_\lambda(k)$, $\lambda \in \{1, 2\}$, are two polarization vectors that, for each $k \neq 0$, are perpendicular to k and to one another. We assume that $\varepsilon_\lambda(k) = \varepsilon_\lambda(k/|k|)$. The ultraviolet cutoff $\kappa : \mathbb{R}^3 \to \mathbb{C}$ is assumed to be a Schwartz-function that depends on $|k|$ only. It follows that

$$|G_x(k, \lambda) - G_0(k, \lambda)| \;\leq\; \alpha |k|^{1/2} |x| |\kappa(k)| \tag{48}$$

$$|k| \left| \frac{\partial}{\partial |k|} G_x(k, \lambda) \right| \;\leq\; \alpha \langle x \rangle |k|^{-1/2} f(k) \tag{49}$$

with some Schwartz-function function f that depends on κ and $\nabla \kappa$.

The Hamiltonian (47) is self-adjoint on $D(H) = D(-\Delta + H_f)$ and bounded from below [17]. We use $E = \inf \sigma(H)$ to denote the least point of the spectrum of H and Σ to denote the ionization threshold. On the set $\Omega := (-\infty, \Sigma)$ the operator H is locally of class $C^2(B)$, where B denotes the second quantized dilatation generator (20); see Section 4. The remarks in the previous section concerning this property apply here as well. Thus we are prepared to state the main results of this paper.

Theorem 9. *Suppose that $\alpha \ll 1$. Then for any $\sigma \le e_{\rm gap}/2$*

$$E_\Delta(H-E)[H,iB]E_\Delta(H-E) \ge \frac{\sigma}{10}E_\Delta(H-E),$$

where $\Delta = [\sigma/3, 2\sigma/3]$.

Given Theorem 9, the remark preceding it, and the fact that, by Lemma 24, $\Sigma \ge E + e_{\rm gap}/3$ for α small enough, we see that both Hypotheses of Conjugate Operator Theory (Appendix B) are satisfied for $\Omega = (E, E + e_{\rm gap}/3)$. This implies that the consequences, Theorems 32 and Theorem 33, of the general theory hold for the system under investigation, and, thus, it proves Theorem 10 and Theorem 11 below. Alternatively, the first part of Theorem 10 can also be derived from Theorem 9 using Theorem A.1 of [7].

Theorem 10 (Limiting absorption principle). *Let $\alpha \ll 1$. Then for every $s > 1/2$ and all $\varphi, \psi \in \mathcal{H}$ the limits*

$$\lim_{\varepsilon\to 0}\langle \varphi, \langle B\rangle^{-s}(H-\lambda \pm i\varepsilon)^{-1}\langle B\rangle^{-s}\psi\rangle \tag{50}$$

exist uniformly in λ in any compact subset of $(E, E+e_{\rm gap}/3)$. For $s \in (1/2, 1)$ the map

$$\lambda \mapsto \langle B\rangle^{-s}(H-\lambda \pm i0)^{-1}\langle B\rangle^{-s} \tag{51}$$

is (locally) Hölder continuous of degree $s - 1/2$ in $(E, E + e_{\rm gap}/3)$.

As a corollary from the finiteness of (50) one can show that $\langle B\rangle^{-s}f(H)(H-z)^{-1}f(H)\langle B\rangle^{-s}$ is bounded on $\mathbb{C}_\pm$ for all $f \in C_0^\infty(\mathbb{R})$ with support in $(E, E + e_{\rm gap}/3)$. This implies H-smoothness of $\langle B\rangle^{-s}f(H)$ and *local decay*

$$\int_{\mathbb{R}} \|\langle B\rangle^{-s}f(H)e^{-iHt}\varphi\|^2 dt \le C\|\varphi\|^2.$$

See [20], Theorem XIII.25 and its Corollary. From the Hölder continuity of (51) we obtain in addition a pointwise decay in time (c.f. Theorem 33).

Theorem 11. *Let $\alpha \ll 1$ and suppose $s \in (1/2, 1)$ and $f \in C_0^\infty(\mathbb{R})$ with $\operatorname{supp}(f) \subset (E, E + e_{\rm gap}/3)$. Then*

$$\|\langle B\rangle^{-s}e^{-iHt}f(H)\langle B\rangle^{-s}\| = O(\frac{1}{t^{s-1/2}}), \qquad (t\to\infty).$$

3.1 Proof of the Mourre estimate

This section describes the main steps of the proof of Theorem 9. Technical auxiliaries such as the existence of a spectral gap, soft boson bounds, and the localization of the electron are collected in Appendix A. We follow closely the line of arguments in the proof of Theorem 1, and we take over many notations of the previous section. This applies in particular to $\chi_\sigma, \chi^\sigma, \tilde{\chi}^\sigma$, b, b_σ, b^σ, and B, B_σ, B^σ. To simplify notations we set

$$\int dk := \sum_{\lambda=1,2} \int d^3k$$

and we suppress the index λ in $a_\lambda(k)$, $a^*_\lambda(k)$, and $G_x(k,\lambda)$.

The IR-cutoff Hamitonian, corresponding to (23), is now given by

$$H_\sigma = (p + \alpha^{3/2} A^\sigma(\alpha x))^2 + V + H_f \tag{52}$$

where $p = -i\nabla_x$ and $A^\sigma(\alpha x) = \phi(\tilde{\chi}^\sigma G_x)$. Again we have that

$$H_\sigma = H^\sigma \otimes 1 + 1 \otimes H_{f,\sigma}$$

with respect to $\mathcal{H} = \mathcal{H}^\sigma \otimes \mathcal{F}_\sigma$. By Theorem 16, the Hamiltonian H is locally of class $C^2(B)$, $C^2(B_\sigma)$ and $C^2(B^\sigma)$ on $(-\infty, \Sigma)$. By Lemma 37 and Proposition 18,

$$[H, iB] = \mathrm{d}\Gamma(\omega) - \alpha^{3/2}\phi(ibG_x)\cdot\Pi - \alpha^{3/2}\Pi\cdot\phi(ibG_x) \tag{53}$$

$$[H, iB_\sigma] = \mathrm{d}\Gamma(\eta_\sigma^2\omega) - \alpha^{3/2}\phi(ib_\sigma G_x)\cdot\Pi - \alpha^{3/2}\Pi\cdot\phi(ib_\sigma G_x) \tag{54}$$

$$[H, iB^\sigma] = \mathrm{d}\Gamma((\eta^\sigma)^2\omega) - \alpha^{3/2}\phi(ib^\sigma G_x)\cdot\Pi - \alpha^{3/2}\Pi\cdot\phi(ib^\sigma G_x) \tag{55}$$

in the sense of quadratic forms on the range of $\chi(H \le E + e_{\mathrm{gap}}/2)$, if $\alpha \ll 1$. Also H^σ is of class $C^1(B^\sigma)$ and

$$[H^\sigma, iB^\sigma] = \mathrm{d}\Gamma((\eta^\sigma)^2\omega) - \alpha^{3/2}\phi(ib^\sigma\tilde{\chi}^\sigma G_x)\cdot\Pi - \alpha^{3/2}\Pi\cdot\phi(ib^\sigma\tilde{\chi}^\sigma G_x) \tag{56}$$

Let $f_\Delta \in C_0^\infty(\mathbb{R})$ be defined as in Section 2, and let $F_\Delta := f_\Delta(H-E)$, $F_{\Delta,\sigma} := f_\Delta(H_\sigma - E_\sigma)$, as in the previous section.

Lemma 12. *If $\alpha \ll 1$ and $\sigma \le e_{\mathrm{gap}}/2$, then*

$$F_{\Delta,\sigma} = P^\sigma \otimes f_\Delta(H_{f,\sigma}), \qquad \text{w.r.t. } \mathcal{H} = \mathcal{H}^\sigma \otimes \mathcal{F}_\sigma,$$

where P^σ denotes the ground state projection of H^σ.

Proof. By Theorem 26 of Appendix A, H^σ has the gap $(E_\sigma, E_\sigma + \sigma)$ in its spectrum if $\alpha \ll 1$. Since the support of f_Δ is a subset of $(0,\sigma)$, the assertion follows. □

Proposition 13. *Let $[H, iB^\sigma]$ be defined by (55). If $\alpha \ll 1$ and $\sigma \le e_{\mathrm{gap}}/2$, then*

$$F_{\Delta,\sigma}[H, iB^\sigma]F_{\Delta,\sigma} = 0.$$

Proof. The proof is a copy of the proof of Proposition 3: From $b^\sigma = b^\sigma\tilde{\chi}^\sigma$, Equations (55) and (56) it follows that $[H, iB^\sigma] = [H^\sigma, iB^\sigma] \otimes 1$ with respect to $\mathcal{H} = \mathcal{H}^\sigma \otimes \mathcal{F}_\sigma$. The statement now follows from Lemma 2 and the Virial Theorem $P^\sigma[H^\sigma, iB^\sigma]P^\sigma = 0$, Proposition 34. □

Proposition 14. *Let* $[H, iB_\sigma]$ *be defined by* (54). *If* $\alpha \ll 1$ *and* $\sigma \le e_{\rm gap}/2$, *then*

$$F_{\Delta,\sigma}[H, iB_\sigma]F_{\Delta,\sigma} \ge \frac{\sigma}{8} F^2_{\Delta,\sigma}.$$

Proof. On the right hand side of (54) we move the creation operators $a^*(ib_\sigma G_x)$ to the left of Π and the annihilation operators $a(ib_\sigma G_x)$ to the right of Π. Since

$$\sum_{j=1}^{3} \Big([\Pi_j, a^*(ib_\sigma G_{x,j})] + [a(ib_\sigma G_{x,j}), \Pi_j] \Big) = 0$$

we arrive at

$$[H, iB_\sigma] = \mathrm{d}\Gamma(\eta_\sigma^2 \omega) - 2\alpha^{3/2} a^*(ib_\sigma G_x)\cdot \Pi - 2\alpha^{3/2}\Pi \cdot a(ib_\sigma G_x). \tag{57}$$

Next, we estimate (57) from below using only the fraction $2\alpha^{3/2}\mathrm{d}\Gamma(\eta_\sigma^2\omega)$ of $\mathrm{d}\Gamma(\eta_\sigma^2\omega)$ at first. By completing the square we get, using (48) and (49),

$$\begin{aligned}
&\mathrm{d}\Gamma(\chi_\sigma^2\omega) - a^*(ib_\sigma G_x)\cdot\Pi - \Pi\cdot a(ib_\sigma G_x)\\
&= \int \omega \Big[\chi_\sigma a^* - \omega^{-1}\Pi\cdot \big(ib\chi_\sigma G_x\big)^*\Big]\Big[\chi_\sigma a - \omega^{-1}(ib\chi_\sigma G_x)\cdot\Pi\Big]\, dk\\
&\quad - \sum_{n,m=1}^{3}\int \Pi_n \frac{(b\chi_\sigma G_{x,n})^*(b\chi_\sigma G_{x,m})}{\omega}\Pi_m\, dk\\
&\ge -\mathrm{const}\ \sigma \sum_{n=1}^{3} \Pi_n \langle x\rangle^2 \Pi_n.
\end{aligned} \tag{58}$$

From (57) and (58) it follows that

$$[H, iB_\sigma] \ge (1-2\alpha^{3/2})\mathrm{d}\Gamma(\eta_\sigma^2\omega) - \mathrm{const}\ \alpha^{3/2}\sigma \sum_n \Pi_n\langle x\rangle^2\Pi_n.$$

This estimate and Lemma 12 imply the statement of the proposition along the line of arguments following estimate (30) in the proof of Proposition 4. Note that $\langle x\rangle \Pi E_{[0,\sigma]}(H_\sigma - E_\sigma)$ is bounded uniformly in σ, thanks to Lemmas 25 and 23. □

Proposition 15. *There exists a constant* C *such that for* $\alpha \ll 1$ *and* $\sigma \le e_{\rm gap}/2$,

$$\big\| f_\Delta(H-E) - f_\Delta(H_\sigma - E_\sigma)\big\| \le C\alpha^{3/2}\sigma.$$

Proof. The idea is to apply a Pauli-Fierz transformation $H_{(\sigma)} = U_\sigma H U_\sigma^*$ affecting only the photons with $|k| \le \sigma$, so that $H_{(\sigma)} - H_\sigma$ has an improved IR behavior corresponding to $\mu = 1/2$. Then we can proceed as in the proof of Lemma 5, Section 2. Let

$$U_\sigma = \exp(i\alpha^{3/2} x\cdot A_\sigma(0)), \qquad A_\sigma(\alpha x) := \phi(\chi_\sigma G_x).$$

Then

$$\begin{aligned} H_{(\sigma)} &:= U_\sigma H U_\sigma^* \\ &= \Big(p + \alpha^{3/2} A^{(\sigma)}(\alpha x)\Big)^2 + V + H_f + \alpha^{3/2} x \cdot E_\sigma(0) + \frac{2}{3}\alpha^3 x^2 \|\chi_\sigma \kappa\|^2 \end{aligned}$$

where

$$\begin{aligned} A^{(\sigma)}(\alpha x) &:= A(\alpha x) - A_\sigma(0) \\ E_\sigma(0) &:= -i[H_f, A_\sigma(0)]. \end{aligned}$$

We compute, dropping the argument αx temporarily,

$$\begin{aligned} H_{(\sigma)} - H_\sigma = 2\alpha^{3/2} p \cdot (A^{(\sigma)} - A^\sigma) \\ + \alpha^3 (A^{(\sigma)} + A^\sigma) \cdot (A^{(\sigma)} - A^\sigma) \\ + \alpha^{3/2} x \cdot E_\sigma(0) + \frac{2}{3}\alpha^3 x^2 \|\chi_\sigma \kappa\|^2, \end{aligned} \tag{59}$$

where $(A^{(\sigma)})^2 - (A^\sigma)^2 = (A^{(\sigma)} + A^\sigma) \cdot (A^{(\sigma)} - A^\sigma)$ was used. Based on the equations

$$A^{(\sigma)}(\alpha x) - A^\sigma(\alpha x) = A_\sigma(\alpha x) - A_\sigma(0) = \phi(\chi_\sigma(G_x - G_0)) \tag{60}$$

$$x \cdot E_\sigma(0) = \phi(i\omega \chi_\sigma G_0 \cdot x), \tag{61}$$

estimate (48), and Proposition 5, with $\mu = 1/2$, we expect that

$$\|F_{\Delta,(\sigma)} - F_{\Delta,\sigma}\| = O(\alpha^{3/2}\sigma), \tag{62}$$

where $F_{\Delta,(\sigma)} = f_\Delta(H_{(\sigma)} - E) = U_\sigma F_\Delta U_\sigma^*$. Suppose (62) holds true, and moreover that

$$\|(U_\sigma^* - 1) F_{\Delta,\sigma}\| = O(\alpha^{3/2}\sigma); \tag{63}$$

then the proposition will follow from

$$\begin{aligned} F_\Delta - F_{\Delta,\sigma} &= U_\sigma^* F_{\Delta,(\sigma)} U_\sigma - F_{\Delta,\sigma} \\ &= (U_\sigma^* - 1) F_{\Delta,\sigma} + U_\sigma^* F_{\Delta,\sigma}(U_\sigma - 1) + U_\sigma^* \Big(F_{\Delta,(\sigma)} - F_{\Delta,\sigma}\Big) U_\sigma. \end{aligned}$$

It thus remains to prove (62) and (63). We begin with (63). By the spectral theorem

$$\begin{aligned} \|(U_\sigma^* - 1) F_{\Delta,\sigma}\| &\leq \|\alpha^{3/2} x \cdot A_\sigma(0) F_{\Delta,\sigma}\| \\ &= \alpha^{3/2} \|x \cdot \phi(\chi_\sigma G_0) F_{\Delta,\sigma}\| \\ &\leq 2\alpha^{3/2} \|x \cdot a(\chi_\sigma G_0) F_{\Delta,\sigma}\| + \alpha^{3/2} \|\chi_\sigma G_0\| \cdot \|x F_{\Delta,\sigma}\|. \end{aligned}$$

The second term is of order $\alpha^{3/2}\sigma$ as $\sigma \to 0$, because, by assumption on G_0, $\|\chi_\sigma G_0\| = O(\sigma)$, and because $\sup_{\sigma>0} \|x F_{\Delta,\sigma}\| < \infty$ by Lemma 25. The first term is of order $\alpha^{3/2}\sigma$ as well, by Lemma 28 and Lemma 29 . To prove (62) it suffices to show that

$$\|F_{\Delta,(\sigma)} - F_{\Delta,\sigma}\| = O(\alpha^{3/2}\sigma^{1/2}), \tag{64}$$

$$\|(F_{\Delta,(\sigma)} - F_{\Delta,\sigma}) J_{\Delta,\sigma}\| = O(\alpha^{3/2}\sigma), \tag{65}$$

as we have seen in the proof of Proposition 5. Here the operators $J_{\Delta,\sigma}$, $J_{\Delta,(\sigma)}$, and J_Δ are defined in terms of j_Δ like $F_{\Delta,\sigma}$, $F_{\Delta,(\sigma)}$, and F_Δ are defined through f_Δ, the function j_Δ being given in the proof of Proposition 5. The equations (64) and (65), with F and J interchanged, hold likewise. We begin with the proof of (65). By the functional calculus

$$\begin{aligned}&(F_{\Delta,(\sigma)} - F_{\Delta,\sigma})J_{\Delta,\sigma}\\ &\qquad = \sigma^{-1}\int \mathrm{d}\tilde{f}(z)\frac{1}{z-(H_{(\sigma)}-E)/\sigma}\Big(H_{(\sigma)} - H_\sigma - E + E_\sigma\Big)J_{\Delta,\sigma}\frac{1}{z-(H_\sigma - E_\sigma)/\sigma}. \quad (66)\end{aligned}$$

Since, by Lemma 30, $|E - E_\sigma| = O(\alpha^{3/2}\sigma^2)$, it remains to estimate the contributions of the various terms due to $H_{(\sigma)} - H_\sigma$ as given by (59). To begin with, we note that

$$\|(A^{(\sigma)} - A^\sigma)J_{\Delta,\sigma}\| = O(\alpha\sigma^2) \qquad (67)$$

$$\|x\cdot E_\sigma(0)J_{\Delta,\sigma}\| = O(\sigma^2). \qquad (68)$$

This follows from (60), (61), (48), Lemma 28 and Lemma 29, as far as the annihilation operators in (67) and (68) are concerned. For the term due to the creation operator in (67) we use

$$\|a^*(\chi_\sigma(G_x - G_0))J_{\Delta,\sigma}\| \le \|a(\chi_\sigma(G_x - G_0))J_{\Delta,\sigma}\| + \Big\|\|\chi_\sigma(G_x - G_0)\|\, J_{\Delta,\sigma}\Big\|$$

and $\|\chi_\sigma(G_x - G_0)\| = O(|x|\alpha\sigma^2)$, as well as $\sup_{\sigma>0}\||x|J_{\Delta,\sigma}\| < \infty$. The operators p and $A^{(\sigma)} + A^\sigma$ stemming from the first and second terms of (59) are combined with the first resolvent of (66): using $U_\sigma^* p U_\sigma = p + \alpha^{3/2}A_\sigma(0)$ and Lemma 23 we obtain

$$\begin{aligned}\|(z-(H_{(\sigma)}-E)/\sigma)^{-1}p\| &= \|(z-(H-E)/\sigma)^{-1}(p+\alpha^{3/2}A_\sigma(0))\|\\ &\le \text{const}\frac{\sqrt{1+|z|}}{|y|}\end{aligned}$$

which is integrable with respect to $\mathrm{d}\tilde{f}(z)$. This proves that the first, second and third terms of (59) give contributions to (66) of order $\alpha^{5/2}\sigma$, $\alpha^4\sigma$, and $\alpha^{3/2}\sigma$, respectively. Since $\|\chi_\sigma\kappa\|^2 = O(\sigma^3)$, (65) follows.

The proof of (64) is more involved than the corresponding estimate in the scalar case, due to factors of x. We begin with

$$\begin{aligned}F_{\Delta,(\sigma)} - F_{\Delta,\sigma} &= F_{\Delta,(\sigma)}J_{\Delta,(\sigma)} - F_{\Delta,\sigma}J_{\Delta,\sigma}\\ &= (F_{\Delta,(\sigma)} - F_{\Delta,\sigma})J_{\Delta,\sigma} + F_{\Delta,(\sigma)}(J_{\Delta,(\sigma)} - J_{\Delta,\sigma})\end{aligned}$$

The first term is of order $\alpha^{3/2}\sigma$ by (65). The second one can be written as

$$\sigma^{-1}\int d\tilde{f}(z)R_{(\sigma)}(z)F_{\Delta,(\sigma)}\Big(H_{(\sigma)} - H_\sigma - E + E_\sigma\Big)R_\sigma(z), \qquad (69)$$

with obvious notations for the resolvents. We recall that, by Lemma 30, $|E-E_\sigma| = O(\alpha^{3/2}\sigma^2)$. As in the proof of (65) we need to estimate the contributions due to the four terms of $H_{(\sigma)} - H_\sigma$ given by (59). We do this exemplarily for the second one and begin with the estimate

$$\begin{aligned} &\|F_{\Delta,(\sigma)}(A^{(\sigma)} + A^\sigma)\cdot(A^{(\sigma)} - A^\sigma)R_\sigma(z)\| \\ \leq\ & \|F_{\Delta,(\sigma)}\langle x\rangle(A^{(\sigma)} + A^\sigma)\|\|\langle x\rangle^{-1}(A^{(\sigma)} - A^\sigma)(H_f+1)^{-1/2}\|\|(H_f+1)^{1/2}R_\sigma(z)\| \end{aligned} \tag{70}$$

For the second factor of (70) we use

$$\begin{aligned} \|\langle x\rangle^{-1}(A^{(\sigma)} - A^\sigma)(H_f+1)^{-1/2}\| &= \|\langle x\rangle^{-1}\phi(\chi_\sigma(G_x - G_0))(H_f+1)^{-1/2}\| \\ &\leq \sup_x \langle x\rangle^{-1}\|\chi_\sigma(G_x - G_0)\|_\omega \\ &= O(\alpha\sigma^{3/2}), \end{aligned}$$

which is of the desired order. In the first factor of (70) we use that U_σ commutes with $\langle x\rangle$, $A^{(\sigma)}$, and A^σ, as well as Lemma 22, Lemma 23 and Lemma 25. We obtain the bound

$$\begin{aligned} \|F_{\Delta,(\sigma)}\langle x\rangle(A^{(\sigma)} + A^\sigma)\| &= \|F_\Delta\langle x\rangle(A^{(\sigma)} + A^\sigma)\| \\ &\leq \|F_\Delta\langle x\rangle(H_f+1)^{1/2}\|\|(H_f+1)^{-1/2}(A^{(\sigma)} + A^\sigma)\| \\ &\leq \text{const}\ \|F_\Delta(\langle x\rangle^2 + H_f + 1)\| < \infty. \end{aligned}$$

Finally, for the last factor of (70), Lemma 23 implies the bound

$$\|(H_f+1)^{1/2}R_\sigma(z)\| \leq \text{const}\frac{\sqrt{1+|z|}}{|y|},$$

which is integrable with respect to $\mathrm{d}\tilde{f}(z)$. In a similar way the contributions of the other terms of (59) are estimated. It follows that (69) is of order $O(\alpha^{3/2}\sigma^{1/2})$ which proves (64). This completes the proof of Proposition 15. □

Proof of Theorem 9. Since $(\eta^\sigma)^2 + \eta_\sigma^2 = 1$ and $b_\sigma + b^\sigma = b$, it follows from (54) and (55) that $C := \mathrm{d}\Gamma(\omega) - \alpha^{3/2}\phi(ibG_x)\cdot\Pi - \alpha^{3/2}\Pi\cdot\phi(ibG_x) = [H, iB_\sigma] + [H, iB^\sigma]$. Thus Propositions 13 and 14 imply that

$$F_{\Delta,\sigma}CF_{\Delta,\sigma} \geq \frac{\sigma}{8}F_{\Delta,\sigma}^2.$$

We next replace $F_{\Delta,\sigma}$ by F_Δ, using Proposition 15 and noticing that $CF_{\Delta,\sigma}$ and $F_\Delta C$ are bounded, uniformly in σ. Since, by (53), $C = [H, iB]$ on the range of F_Δ we arrive at

$$F_\Delta[H, iB]F_\Delta \geq \frac{\sigma}{8}F_\Delta^2 + O(g\sigma).$$

After multiplying this operator inequality from both sides with $E_\Delta(H-E)$, the theorem follows. □

4 Local regularity of H with respect to B

The purpose of this section is to prove that H is locally of class $C^2(B)$ in $(-\infty, \Sigma)$, where Σ is the ionization threshold of H, and B is any of the three operators $\mathrm{d}\Gamma(b), \mathrm{d}\Gamma(b_\sigma), \mathrm{d}\Gamma(b^\sigma)$ defined in Section 3. Some background on the concept of local regularity of a Hamiltonian with respect to a conjugate operator and basic criteria for this property to hold are collected in Appendix B. To prove a result that covers the three aforementioned operators we consider a class of operators B that contains all of them and is defined as follows.

Let $k \mapsto v(k)$ be a C^∞-vector field on $\mathbb{R}^3$ of the form $v(k) = h(|k|)k$ where $h \in C^\infty(\mathbb{R})$ such that $s^n \partial^n h(s)$ is bounded for $n \in \{0, 1, 2\}$. It follows

$$|v(k)| \leq \beta|k|, \qquad \text{for all } k \in \mathbb{R}^3, \tag{71}$$

for some $\beta > 0$, and that partial derivatives of v times a Schwartz-function, such as κ, are bounded. We remark that the assumption that v is parallel to k is not needed if a representation of H free of polarization vectors is chosen.

Let $\phi_s : \mathbb{R}^3 \to \mathbb{R}^3$ be the flow generated by v, that is,

$$\frac{d}{ds}\phi_s(k) = v(\phi_s(k)), \qquad \phi_0(k) = k. \tag{72}$$

Then $\phi_s(k)$ is of class C^∞ with respect to s and k, and by Gronwall's lemma and (71)

$$e^{-\beta|s|}|k| \leq |\phi_s(k)| \leq e^{\beta|s|}|k|, \qquad \text{for } s \in \mathbb{R}. \tag{73}$$

Induced by the flow ϕ_s on $\mathbb{R}^3$ there is a one-parameter group of unitary transformations on $L^2(\mathbb{R}^3)$ defined by

$$f_s(k) = f(\phi_s(k))\sqrt{\det D\phi_s(k)}. \tag{74}$$

Since these transformations leave $C_0^\infty(\mathbb{R}^3)$ invariant, their generator b is essentially self-adjoint on this space. From $bf = id/ds\, f_s|_{s=0}$ we obtain

$$b = \frac{1}{2}(v \cdot y + y \cdot v) \tag{75}$$

where $y = i\nabla_k$. Let $B = \mathrm{d}\Gamma(b)$. The main result of this section is:

Theorem 16. *Let H be the Hamiltonian defined by* (47) *and let Σ be its ionization threshold. Under the assumptions above on the vector-field v, the operator H is locally of class $C^2(B)$ in $\Omega = (-\infty, \Sigma)$ for all values of α.*

The proof, of course, depends on the explicit knowledge of the unitary group generated by B, and in particular on the formulas

$$e^{-iBs}H_f e^{iBs} = \mathrm{d}\Gamma(e^{-ibs}\omega e^{ibs}) = \mathrm{d}\Gamma(\omega \circ \phi_s) \tag{76}$$

$$e^{-iBs}A(x)e^{iBs} = \phi(e^{-ibs}G_x) = \phi(G_{x,s}) \tag{77}$$

with $G_{x,s}$ given by (74). Another essential ingredient is that, by [15], Theorem 1,

$$\|\langle x\rangle^2 f(H)\| < \infty \tag{78}$$

for every $f \in C_0^\infty(\Omega)$. We begin with four auxiliary results, Propositions 17, 18, 19, and 20.

Proposition 17. *(a) For all $s \in \mathbb{R}$, $e^{iBs}D(H_f) \subset D(H_f)$ and*

$$\|H_f e^{iBs}(H_f+1)^{-1}\| \le e^{\beta|s|}$$

(b) For all $s \in \mathbb{R}$, $e^{iBs}D(H) \subset D(H)$ and

$$\|He^{iBs}(H+i)^{-1}\| \le \text{const } e^{\beta|s|}$$

Proof. From $e^{-iBs}H_f e^{iBs} = \mathrm{d}\Gamma(e^{-ibs}\omega) = \mathrm{d}\Gamma(\omega\circ\phi_s)$ and (73) it follows that

$$\|H_f e^{iBs}\varphi\| = \|\mathrm{d}\Gamma(\omega\circ\phi_s)\varphi\| \le e^{\beta|s|}\|H_f\varphi\|$$

for all $\varphi \in \mathcal{F}_0(C_0^\infty)$, which is a core of H_f. This proves, first, that $e^{iBs}D(H_f) \subset D(H_f)$, and next, that the estimate above extends to $D(H_f)$, proving (a).

The Hamiltonian H is self-adjoint on the domain of $H^{(0)} = -\Delta + H_f$. Therefore the operators $H^{(0)}(H+i)^{-1}$ and $H(H^{(0)}+i)^{-1}$ are bounded and it suffices to prove (b) for $H^{(0)}$ in place of H. The subspace $D(\Delta)\otimes D(H_f)$ is a core of $H^{(0)}$. By (a) it is invariant w.r. to e^{iBs} and

$$\|H^{(0)}e^{iBs}\varphi\| \le \|\Delta\varphi\| + \|H_f\varphi\|e^{\beta|s|} \le \sqrt{2}e^{\beta|s|}\|H^{(0)}\varphi\|$$

As in the proof of (a), it now follows that $e^{iBs}D(H^{(0)}) \subset D(H^{(0)})$ and then the estimate above extends to $D(H^{(0)})$. □

Let $B_s := (e^{iBs}-1)/is$. Then, by Proposition 17, $[B_s, H]$ is well defined, as a linear operator on $D(H)$. The main ingredients for the proof of Theorem 16 are Propositions 18 and 20 below.

Proposition 18. *(a) For all $\varphi \in D(H)$*

$$i\lim_{s\to 0}\langle x\rangle^{-1}[H,B_s]\varphi = \langle x\rangle^{-1}\Big(\mathrm{d}\Gamma(\nabla\omega\cdot v) - \alpha^{3/2}\phi(ibG_x)\cdot\Pi - \Pi\cdot\phi(ibG_x)\alpha^{3/2}\Big)\varphi.$$

(b)

$$\sup_{0<|s|\le 1}\|\langle x\rangle^{-1}[B_s,H](H+i)^{-1}\| < \infty.$$

Proof. Part (b) follows from (a) and the uniform boundedness principle. Part (a) is equivalent to the limit

$$i\lim_{s\to 0}\langle x\rangle^{-1}\frac{1}{s}\left(e^{-iBs}He^{iBs} - H\right)\varphi$$

being equal to the expression on the right hand side of (a). By (76), for all $\varphi \in D(H_f)$

$$\lim_{s\to 0} \frac{1}{s}\left(e^{-iBs}H_f e^{iBs} - H_f\right)\varphi = \lim_{s\to 0}\frac{1}{s}\mathrm{d}\Gamma(\omega\circ\phi_s - \omega)\varphi = \mathrm{d}\Gamma(\nabla\omega\cdot v)\varphi,$$

where the last step is easily established using Lebesgue's dominated convergence Theorem. The necessary dominants are obtained from $|s^{-1}(\omega\circ\phi_s - \omega)| \le |s|^{-1}(e^{\beta|s|}-1)\omega$, by (73), and from the assumption $\varphi \in D(\mathrm{d}\Gamma(\omega))$.

It remains to consider the contribution due to $H_{\mathrm{int}} := 2\alpha^{3/2}A(\alpha x)\cdot p + \alpha^3 A(\alpha x)^2$. Let $\Delta G_{x,s} := G_{x,s} - G_x$. By (77),

$$\begin{aligned} & e^{-iBs}H_{\mathrm{int}}e^{iBs} - H_{\mathrm{int}} \\ &= 2\alpha^{3/2}\phi(\Delta G_{x,s})\cdot p + \alpha^3\phi(\Delta G_{x,s})\cdot\phi(G_x) + \alpha^3\phi(G_{x,s})\cdot\phi(\Delta G_{x,s}), \end{aligned} \tag{79}$$

a sum of three operators, each of which contains $\Delta G_{x,s}$. By Lemma 21 at the end of this section, for each $x \in \mathbb{R}^3$

$$\frac{1}{s}\Delta G_{x,s} = \frac{1}{s}\left(G_{x,s} - G_x\right) \to -ibG_x, \qquad (s\to 0) \tag{80}$$

in the norm $\|\cdot\|_\omega$ of $L_\omega(\mathbb{R}^3)$ (see Appendix A), and

$$\sup_{x\in\mathbb{R}^3}\langle x\rangle^{-1}\|bG_x\|_\omega < \infty \tag{81}$$

by the assumptions on G_x. Since the operators $p(H_f+1)^{1/2}(H+i)^{-1}$ and $H_f(H+i)^{-1}$ are bounded by Lemma 22 and since, by Lemma 23, $\|\phi(f)(H_f+1)^{-1/2}\| \le \|f\|_\omega$ and $\|\phi(f)\phi(g)(H_f+1)^{-1}\| \le 8\|f\|_\omega\|g\|_\omega$ for all $f, g \in L^2(\mathbb{R}^3)$, it follows from (79), (80), and (81) that

$$\begin{aligned} & \lim_{s\to 0}\langle x\rangle^{-1}\frac{1}{s}\left(e^{-iBs}H_{\mathrm{int}}e^{iBs} - H_{\mathrm{int}}\right)\varphi \\ &= \Big(2\alpha^{3/2}\phi(-ibG_x)\cdot p + \alpha^3\phi(-ibG_x)\cdot\phi(G_x) + \alpha^3\phi(G_x)\cdot\phi(-ibG_x)\Big)\varphi \\ &= -\alpha^{3/2}\Big(\phi(ibG_x)\cdot\Pi + \Pi\cdot\phi(ibG_x)\Big)\varphi \end{aligned}$$

for all $\varphi \in D(H)$. □

Proposition 19. *For all $f \in C_0^\infty(\Omega)$,*

$$\sup_{0<|s|\le 1}\|[B_s, f(H)]\| < \infty.$$

Remark. By Proposition 35 this Proposition implies that $f(H)$ is of class $C^1(B)$ for all $f \in C_0^\infty(\Omega)$, that is, H is locally of class $C^1(B)$ in Ω.

Proof. Let $F = f(H)$ and let $\mathrm{ad}_{B_s}(F) = [B_s, F]$. If $g \in C_0^\infty(\Omega)$ is such that $g \equiv 1$ on $\mathrm{supp}(f)$ and $G = g(H)$, then $F = GF$ and hence

$$\mathrm{ad}_{B_s}(F) = G\,\mathrm{ad}_{B_s}(F) + \mathrm{ad}_{B_s}(G)F.$$

The norm of $\mathrm{ad}_{B_s}(G)F$ is equal to the norm of its adjoint which is $-F^*\mathrm{ad}_{B_{-s}}(G^*)$ where $F^* = \bar{f}(H)$ and $G^* = \bar{g}(H)$. It therefore suffices to prove that

$$\sup_{0<|s|\leq 1} \|G\mathrm{ad}_{B_s}(F)\| < \infty \tag{82}$$

for all $f, g \in C_0^\infty(\Omega)$. To this end we use the representation $f(H) = \int \mathrm{d}\tilde{f}(z)R(z)$ where $R(z) = (z-H)^{-1}$ and $\tilde{f}$ is an almost analytic extension of f with $|\partial_{\bar{z}}\tilde{f}(x+iy)| \leq \mathrm{const}|y|^2$, c.f. (35). It follows that

$$G\mathrm{ad}_{B_s}(F) = \int \mathrm{d}\tilde{f}(z)R(z)G[B_s, H]R(z),$$

which is well-defined by Proposition 17, part (b). Upon writing $[B_s, H] = \langle x\rangle\langle x\rangle^{-1}[B_s, H]R(i)(i-H)$ we can estimate the norm of the resulting expression for $G\mathrm{ad}_{B_s}(F)$ with $0 < |s| \leq 1$, by

$$\|G\mathrm{ad}_{B_s}(F)\| \leq \sup_{0<|s|\leq 1} \|\langle x\rangle^{-1}[B_s, H]R(i)\|\|g(H)\langle x\rangle\| \int |\mathrm{d}\tilde{f}(z)|\|R(z)\|\|(i-H)R(z)\|.$$

Since

$$\|(i-H)R(z)\| \leq \mathrm{const}\left(1 + \frac{1}{|\operatorname{Im}(z)|}\right), \tag{83}$$

the integral is finite by choice of $\tilde{f}$. The factors in front of the integral are finite by Proposition 18 and by (78). □

Proposition 20.

$$\sup_{0<|s|\leq 1} \|\langle x\rangle^{-2}[B_s[B_s, H]](H+i)^{-1}\| < \infty.$$

Proof. By Definition of H,

$$\begin{aligned} [B_s, [B_s, H]] &= [B_s, [B_s, H_f]] + \alpha^{3/2}[B_s, [B_s, p \cdot \phi(G_x)]] \\ &\quad + \alpha^3[B_s, [B_s, \phi(G_x)^2]]. \end{aligned}$$

We estimate the contributions of these terms one by one in Steps 1-3 below. As a preparation we note that

$$\mathrm{ad}_{B_s} = ie^{iBs}\frac{1}{s}(W(s)-1) \tag{84}$$

$$\mathrm{ad}_{B_s}^2 = -e^{2iBs}\frac{1}{s^2}(W(s)-1)^2 = -e^{2iBs}\frac{1}{s^2}\big(W(2s) - 2W(s) + W(0)\big), \tag{85}$$

Where $W(s)$ maps an operator T to $e^{-iBs}Te^{iBs}$. In view of Equations (76), (77), we will need that for every twice differentiable function $f : [0, 2s] \to \mathbb{C}$

$$\frac{1}{s^2}|f(2s) - 2f(s) + f(0)| \leq \sup_{|t|\leq 2|s|} |f''(t)|. \tag{86}$$

Step 1.

$$\sup_{|s|\leq 1} \|\mathrm{ad}^2_{B_s}(H_f)(H_f+1)^{-1}\| < \infty.$$

By (85) and (76)

$$\mathrm{ad}^2_{B_s}(H_f) = -e^{2iBs}\frac{1}{s^2}\mathrm{d}\Gamma(\omega\circ\phi_{2s} - 2\omega\circ\phi_s + \omega). \tag{87}$$

Thus in view of (86) we estimate the second derivative of $s \mapsto \omega\circ\phi_s(k) = |\phi_s(k)|$. For $k \neq 0$,

$$\begin{aligned}\frac{\partial^2}{\partial s^2}|\phi_s(k)| &= -\frac{1}{|\phi_s(k)|}\langle\phi_s(k), v(\phi_s(k))\rangle^2 + \frac{v(\phi_s(k))}{|\phi_s(k)|}\\ &\quad + \frac{1}{|\phi_s(k)|}\sum_{i,j}\phi_s(k)_i v_{i,j}(\phi_s(k))\phi_s(k)_j.\end{aligned}$$

By assumption on v, $v_{i,j} \in L^\infty$ and $|v(\phi_s(k))| \leq \beta|\phi_s(k)| \leq e^{\beta|s|}|k|$. It follows that

$$\frac{1}{s^2}\big|\big(\omega\circ\phi_{2s} - 2\omega\circ\phi_s + \omega\big)(k)\big| \leq \text{const } e^{\beta|s|}\omega(k),$$

which implies

$$\left\|\frac{1}{s^2}\mathrm{d}\Gamma(\omega\circ\phi_{2s} - 2\omega\circ\phi_s + \omega)(H_f+1)^{-1}\right\| \leq \text{const } e^{\beta|s|}.$$

By (87) this establishes Step 1.

Step 2.

$$\sup_{|s|\leq 1}\sup_{x\in\mathbb{R}^3}\langle x\rangle^{-2}\|\mathrm{ad}^2_{B_s}(\phi(G_x)\cdot p)(H+i)^{-1}\| < \infty.$$

Since $p(H_f+1)^{1/2}(H+i)^{-1}$ is bounded, it suffices to show that

$$\sup_{|s|\leq 1,\, x}\langle x\rangle^{-2}\|\mathrm{ad}^2_{B_s}(\phi(G_x))(H_f+1)^{-1/2}\| < \infty. \tag{88}$$

By Equation (77)

$$\frac{1}{s^2}(W(s)-1)^2(\phi(G_x)) = \frac{1}{s^2}\phi(G_{x,2s} - 2G_{x,s} + G_x), \tag{89}$$

and by (86)

$$\begin{aligned}&\langle x\rangle^{-2}\frac{1}{s^2}\left\|\phi(G_{x,2s} - 2G_{x,s} + G_x)(H_f+1)^{-1/2}\right\|\\ \leq\ &\langle x\rangle^{-2}\frac{1}{s^2}\|G_{x,2s} - 2G_{x,s} + G_x\|_\omega \ \leq\ \langle x\rangle^{-2}\left\|\frac{\partial^2}{\partial s^2}G_{x,s}\right\|_\omega\end{aligned}$$

For $k \neq 0$ the function $s \mapsto G_{x,s}(k)$ is arbitrarily often differentiable by assumption on v and

$$-i\frac{\partial}{\partial s}G_{x,s}(k) = (v\cdot\nabla_k G_x)_s(k) + \frac{1}{2}(\mathrm{div}(v)G_x)_s(k) \tag{90}$$

$$-\frac{\partial^2}{\partial s^2}G_{x,s}(k) = \big((v\cdot\nabla_k)^2 G_x\big)_s(k) + (\mathrm{div}(v)v\cdot\nabla_k G_x)_s \tag{91}$$

$$+\frac{1}{2}\sum_{i,j}\big((v_i\partial_i\partial_j v_j)G_x\big)_s + \frac{1}{4}\big(\mathrm{div}(v)^2 G_x\big)_s. \tag{92}$$

By part (a) of Lemma 21 below, it suffices to estimate the L^2_ω-norm of these four contributions with $s = 0$. By our assumptions on v, $\mathrm{div}(v)$ and $v_i\partial_i\partial_j v_j$ are bounded functions. This and the bound $\|G_x\| \leq \|G_0\|_\omega < \infty$ account for the contributions of (92), and for the factor $\mathrm{div}(v)$ in front of the second term of (91). It remains to show that the L^2_ω-norms of

$$\langle x\rangle^{-1}(v\cdot\nabla_k)G_x \quad \text{and} \quad \langle x\rangle^{-2}(v\cdot\nabla_k)^2 G_x$$

are bounded uniformly in x. But this is easily seen by applying $v\cdot\nabla_k$ to each factor of $G_x(k,\lambda) = \varepsilon_\lambda(k)e^{-ik\cdot x}\kappa(k)|k|^{-1/2}$ and using that $v\cdot\nabla\varepsilon_\lambda(k) = 0$, $v\cdot\nabla e^{-ik\cdot x} = -iv\cdot x e^{-ik\cdot x}$ and that $v\cdot\nabla|k|^{-1/2}$ is again of order $|k|^{-1/2}$ by assumption on v.

Step 3.

$$\sup_{|s|\leq 1,\, x} \langle x\rangle^{-2}\|\mathrm{ad}^2_{B_s}(\phi(G_x)^2)(H_f+1)^{-1}\| < \infty.$$

By the Leibniz-rule for ad_{B_s},

$$\begin{aligned} \mathrm{ad}^2_{B_s}(\phi(G_x)^2) &= \mathrm{ad}^2_{B_s}(\phi(G_x))\cdot\phi(G_x) + \phi(G_x)\cdot\mathrm{ad}^2_{B_s}(\varphi(G_x)) \\ &\quad +2\mathrm{ad}_{B_s}(\phi(G_x))\mathrm{ad}_{B_s}(\phi(G_x)). \end{aligned} \tag{93}$$

For the contribution of the first term we have

$$\begin{aligned} &\langle x\rangle^{-2}\|\mathrm{ad}^2_{B_s}(\phi(G_x))\cdot\phi(G_x)(H_f+1)^{-1}\| \\ &\quad \leq \langle x\rangle^{-2}\|\mathrm{ad}^2_{B_s}(\phi(G_x))(H_f+1)^{-1/2}\|\|\phi(G_x)(H_f+1)^{-1/2}\| \end{aligned}$$

which is bounded uniformly in $|s| \leq 1$ and $x \in \mathbb{R}^3$ by (88) in the proof of Step 2. For the second term of (93) we first note that

$$\begin{aligned} \phi(G_x)\mathrm{ad}^2_{B_s}(\phi(G_x)) &= \phi(G_x)e^{2iBs}\frac{1}{s^2}(W(s)-1)^2(\phi(G_x)) \\ &= e^{2iBs}\phi(G_{x,s})\frac{1}{s^2}(W(s)-1)^2(\phi(G_x)) \end{aligned}$$

and hence, by the estimates in Step 2, we obtain a bound similar to the one for the first term of (93) with an additional factor of $e^{2\beta|s|}$ coming from the use of Lemma 21. Finally, by (84) and (77)

$$\mathrm{ad}_{B_s}(\phi(G_x))\mathrm{ad}_{B_s}(\phi(G_x)) = e^{2iBs}\phi\left(\frac{G_{x,2s}-G_{x,s}}{s}\right)\phi\left(\frac{G_{x,s}-G_x}{s}\right)$$

which implies that

$$\langle x\rangle^{-2}\|\mathrm{ad}_{B_s}(\phi(G_x))\mathrm{ad}_{B_s}(\phi(G_x))(H_f+1)^{-1}\| \leq \sup_{|s|\leq 2,\, x\in\mathbb{R}^3}\left(\langle x\rangle^{-1}\|\partial_s G_{x,s}\|_\omega\right)^2.$$

This is finite by (90) and the assumptions on v and G_x. □

Proof of Theorem 16. By Proposition 19 and 36 it suffices to show that

$$\sup_{0<s\leq 1} \|\mathrm{ad}^2_{B_s}(f(H))\| < \infty \tag{94}$$

for all $f \in C_0^\infty(\Omega)$. Let $g \in C_0^\infty(\Omega)$ with $gf = f$ and let $G = g(H)$, $F = f(H)$. Then $F = GF$ and hence

$$\mathrm{ad}^2_{B_s}(F) = \mathrm{ad}^2_{B_s}(GF) = \mathrm{ad}^2_{B_s}(G)F + 2\mathrm{ad}_{B_s}(G)\mathrm{ad}_{B_s}(F) + G\mathrm{ad}^2_{B_s}(F).$$

From Proposition 19 we know that $\sup_{0<s\leq 1} \|\mathrm{ad}_{B_s}(G)\| < \infty$, and similarly with F in place of G. Moreover

$$\Big(\mathrm{ad}^2_{B_s}(G)F\Big)^* = F^*\mathrm{ad}^2_{B_{-s}}(G^*).$$

Thus it suffices to show that for all $g, f \in C_0^\infty(\Omega)$

$$\sup_{0<|s|\leq 1} \|G\mathrm{ad}^2_{B_s}(F)\| < \infty. \tag{95}$$

To this end we use $F = \int \mathrm{d}\tilde{f}(z)R(z)$ with an almost analytic extension $\tilde{f}$ of f such that $|\partial_{\bar{z}}\tilde{f}(x+iy)| \leq \text{const } |y|^4$. We obtain

$$\begin{aligned} G\mathrm{ad}^2_{B_s}(F) &= 2\int \mathrm{d}\tilde{f}(z)R(z)G[B_s,H]R(z)[B_s,H]R(z) && (96)\\ &\quad + \int \mathrm{d}\tilde{f}(z)R(z)G[B_s,[B_s,H]]R(z). && (97)\end{aligned}$$

Since, by (78), $\|G\langle x\rangle^2\| < \infty$ the norm of the second term is bounded uniformly in $s \in \{0 < |s| \leq 1\}$ by Proposition 20. In view of Proposition 18 we rewrite (96) (times 1/2) as

$$\int \mathrm{d}\tilde{f}(z)R(z)G\langle x\rangle[B_s,H]R(z)\langle x\rangle^{-1}[B_s,H]R(z) - \int \mathrm{d}\tilde{f}(z)R(z)G\Big[\langle x\rangle,[B_s,H]R(z)\Big]\langle x\rangle^{-1}[B_s,H]R(z).$$

For the norm of the first integral we get the bound

$$\int |\mathrm{d}\tilde{f}(z)|\|R(z)\|\|G\langle x\rangle^2\|\|\langle x\rangle^{-1}[B_s,H]R(i)\|^2\|(i-H)R(z)\|^2,$$

which is bounded uniformly in s, by Lemma 18, the exponential decay on the range of $G = g(H)$ and by construction of $\tilde{f}$. The norm of the second term is bounded by

$$\int |\mathrm{d}\tilde{f}(z)|\|R(z)\|\,\|g(H)\langle x\rangle\|\,\|\langle x\rangle^{-1}\big[\langle x\rangle,[B_s,H]R(z)\big]\|\,\|\langle x\rangle^{-1}[B_s,H]R(z)\|. \tag{98}$$

The last factor is bounded by $\|(i-H)R(z)\|$, uniformly in $s \in (0,1]$, by Proposition 18. For the term in the third norm we find, using the Jacobi identity and $[B_s,\langle x\rangle] = 0$, that

$$\langle x\rangle^{-1}\big[\langle x\rangle,[B_s,H]R(z)\big] = \langle x\rangle^{-1}\big[B_s,[\langle x\rangle,H]\big]R(z) + \langle x\rangle^{-1}[B_s,H]R(z)[\langle x\rangle,H]R(z) \tag{99}$$

where

$$[\langle x\rangle, H] = 2i\frac{x}{\langle x\rangle}(p+A) + \frac{2}{\langle x\rangle} + \frac{1}{\langle x\rangle^3}. \tag{100}$$

Since (100) is bounded w.r.to H, the norm of the second term of (99), by Proposition 18, is bounded by $\|(i-H)R(z)\|^2$ uniformly in s. As for the first term of (99), in view of (100), its norm is estimated like the norm of $\langle x\rangle^{-1}[B_s, H]R(z)$ in Lemma 18, which leads to a bound of the form const$\|(i-H)R(z)\|$. By (83) and by construction of $\tilde{f}$ it follows that (98) is bounded uniformly in $|s| \in (0,1]$. □

We conclude this section with a lemma used in the proofs of Propositions 18 and 20 above. For the definition of $L^2_\omega(\mathbb{R}^3)$ and its norm see Appendix A.

Lemma 21. *Let $f \mapsto f_s = e^{-ibs}f$ on $L^2_\omega(\mathbb{R}^3)$ be defined by (71), (72) and (74). Then*

(a) The transformation $f \mapsto f_s$ maps $L^2_\omega(\mathbb{R}^3)$ into itself and, for all $s \in \mathbb{R}$,

$$\|f_s\|_\omega \le e^{\beta|s|/2}\|f\|_\omega.$$

(b) The mapping $\mathbb{R} \to L^2_\omega(\mathbb{R}^3)$, $s \mapsto f_s$ is continuous.

(c) For all $f \in L^2_\omega(\mathbb{R}^3)$ with $f \in C^1(\mathbb{R}^3\backslash\{0\})$ and $k \cdot \nabla f, \omega f \in L^2$,

$$L^2_\omega - \lim_{s\to 0}\frac{1}{s}(f_s - f) = v\cdot\nabla f + \frac{1}{2}\mathrm{div}(v)f.$$

Remark. Statement (c) shows, in particular, that $f \in D(b)$ and that $-ibf = v\cdot\nabla f + (1/2)\mathrm{div}(v)f$ for the class of functions f considered there.

Proof. (a) Making the substitution $q = \phi_s(k)$, $dq = \det D\phi_s(k)dk$ and using (73) we get

$$\begin{aligned}\|f_s\|^2 &= \int(|k|^{-1}+1)|f(\phi_s(k))|^2 \det D\phi_s(k)\,dk \\ &= \int(|\phi_{-s}(q)|^{-1}+1)|f(q)|^2\,dq \;\le\; e^{\beta|s|}\|f\|^2_\omega.\end{aligned}$$

(b) For functions $f \in L^2_\omega(\mathbb{R}^3)$ that are continuous and have compact support $\|f_s - f\|_\omega \to 0$ follows from $\lim_{s\to 0} f_s(k) = f(k)$, for all $k \in \mathbb{R}^3$ by an application of Lebesgue's dominated convergence theorem. From here, (b) follows by an approximation argument using (a).

(c) By assumption on f,

$$\tilde{f} := v\cdot\nabla f + \frac{1}{2}\mathrm{div}(v)f \in L^2_\omega(\mathbb{R}^3).$$

Using that

$$f_s(k) - f(k) = \int_0^s \tilde{f}_t(k)\,dt, \qquad k \ne 0$$

and Jensen's inequality we get

$$\begin{aligned}\|s^{-1}(f_s - f) - \tilde{f}\|_\omega^2 &= \int dk(|k|^{-1}+1)\left|\frac{1}{s}\int_0^s [\tilde{f}_t(k) - \tilde{f}(k)]\,dt\right|^2 \\ &\leq \int dk(|k|^{-1}+1)\frac{1}{s}\int_0^s \left|\tilde{f}_t(k) - \tilde{f}(k)\right|^2 dt \\ &= \frac{1}{s}\int_0^s \|\tilde{f}_t - \tilde{f}\|^2 dt\end{aligned}$$

which vanishes in the limit $s \to 0$ by (b). □

A Operator Estimates and Spectrum

Let $L^2_\omega(\mathbb{R}^3, \mathbb{C}^2)$ denote the linear space of measurable functions $f : \mathbb{R}^3 \to \mathbb{C}^2$ with

$$\|f\|_\omega^2 = \sum_{\lambda=1,2}\int |f(k,\lambda)|^2(|k|^{-1}+1)d^3k < \infty.$$

Lemma 22. *For all $f, g \in L^2_\omega(\mathbb{R}^3, \mathbb{C}^2)$*

$$\begin{aligned}\|a^\sharp(f)(H_f+1)^{-1/2}\| &\leq \|f\|_\omega, \\ \|a^\sharp(f)a^\sharp(g)(H_f+1)^{-1}\| &\leq 2\|f\|_\omega\|g\|_\omega,\end{aligned}$$

where $a^\sharp$ may be a creation or an annihilation operator.

The first estimate of Lemma 22 is well known, see e.g., [4]. For a proof of the second one see [10].

Lemma 23 (Operator Estimates). *Let $c_n(\kappa) = \int |\kappa(k)|^2|k|^{n-3}\,d^3k$ for $n \geq 1$. Then*

$$\begin{aligned}&(i) && A(x)^2 \leq 8c_1(\kappa)H_f + 4c_2(\kappa), \\ &(ii) && -\frac{8}{3}c_1(\kappa)\alpha^3p^2 \leq 2p\cdot A(\alpha x)\alpha^{3/2} + H_f, \\ &(iii) && p^2 \leq 2\Pi^2 + 2\alpha^3A(\alpha x)^2.\end{aligned}$$

If $\pm V \leq \varepsilon p^2 + b_\varepsilon$ for all $\varepsilon > 0$, and if $\varepsilon \in (0, 1/2)$ is so small that $16\varepsilon\alpha^3c_1(\kappa) < 1$, then

$$\begin{aligned}&(iv) && \Pi^2 \leq \frac{1}{1-2\varepsilon}(H + b_\varepsilon + 8\varepsilon\alpha^2c_2(\kappa)), \\ &(v) && H_f \leq \frac{1}{1-16\varepsilon\alpha^2c_1(\kappa)}(H + b_\varepsilon + 8\varepsilon\alpha^2c_2(\kappa)), \\ &(vi) && A(x)^2 \leq \frac{8c_1(\kappa)}{1-16\varepsilon\alpha^2c_1(\kappa)}(H + b_\varepsilon + 8\varepsilon\alpha^2c_2(\kappa)) + 4c_2(\kappa).\end{aligned}$$

Proof. Estimate (i) is proved in [16]. (ii) is easily derived by completing the square in creation and annihilation operators, and (iii) follows from $2\alpha^3 p\cdot A(\alpha x) \geq -(1/2)p^2 - 2\alpha^3 A(\alpha x)^2$.

From the assumption on V and statements (i) and (iii) it follows that

$$\begin{aligned} H &\geq \Pi^2 - \varepsilon p^2 - b_\varepsilon + H_f \\ &\geq (1-2\varepsilon)\Pi^2 - 2\varepsilon\alpha^3 A(x)^3 + H_f - b_\varepsilon \\ &\geq (1-2\varepsilon)\Pi^2 + (1-16\varepsilon\alpha^3 c_1(\kappa))H_f - 8\varepsilon\alpha^3 c_2(\kappa) - b_\varepsilon, \end{aligned}$$

which proves (iv) and (v). Statement (vi) follows from (i) and (v). □

Let $E_\sigma = \inf\sigma(H_\sigma)$ and let $\Sigma_\sigma = \lim_{R\to\infty}\Sigma_{\sigma,R}$ be the ionization threshold for H_σ, that is,

$$\Sigma_{\sigma,R} = \inf_{\varphi\in D_R,\, \|\varphi\|=1} \langle\varphi, H_\sigma\varphi\rangle$$

where $D_R = \{\varphi \in D(H_\sigma) | \chi(|x| \leq R)\varphi = 0\}$.

Lemma 24 (Estimates for E_σ and Σ_σ). *With the above definitions*

1. *For all* $\alpha \geq 0$,
$$E_\sigma \leq e_1 + 4c_2(\kappa)\alpha^3.$$

2. *If* $c_1(\kappa)\alpha^3 \leq 1/8$ *then*
$$\Sigma_{\sigma,R} \geq e_2 - o_R(1) - c_1(\kappa)\alpha^3 C, \quad (R\to\infty),$$
where C *and* $o_R(1)$ *depend on properties of* H_{part} *only. In particular*
$$\Sigma_\sigma \geq e_2 - c_1(\kappa)\alpha^3 C$$
uniformly in $\sigma \geq 0$.

Proof. Let ψ_1 be a normalized ground state vector of H_{part}, so that $H_{\text{part}}\psi_1 = e_1\psi_1$, and let $\Omega \in \mathcal{F}$ denote the vacuum. Then

$$\begin{aligned} E_\sigma &\leq \langle\psi_1\otimes\Omega, H_\sigma\psi_1\otimes\Omega\rangle \\ &= e_1 + \alpha^3\langle\psi_1\otimes\Omega, A(\alpha x)^2\psi_1\otimes\Omega\rangle \\ &\leq e_1 + 4c_2(\kappa)\alpha^3 \end{aligned}$$

by Lemma 23. To prove Statement 2 we first estimate H_σ from below in terms of H_{part}. By Lemma 23,

$$\begin{aligned} H_\sigma &= H_{\text{part}} + 2p\cdot A(\alpha x)\alpha^{3/2} + A(\alpha x)^2\alpha^3 + H_f \\ &\geq H_{\text{part}} - \frac{8}{3}c_1(\kappa)\alpha^3 p^2. \end{aligned}$$

Since $p^2 \leq 3(H_{\rm part} + D)$ for some constant D, it follows that

$$H_\sigma \geq H_{\rm part}(1 - 8c_1(\kappa)\alpha^3) - 8c_1(\kappa)D\alpha^3.$$

By Perrson's theorem, $\langle\varphi, (H_{\rm part} \otimes 1)\varphi\rangle \geq e_2 - o_R(1)$, as $R \to \infty$, for normalized $\varphi \in D_R$, with $\|\varphi\| = 1$, and by assumption $1 - 8c_1(\kappa)\alpha^3 \geq 0$. Hence we obtain

$$\begin{aligned} \Sigma_{R,\sigma} &\geq (e_2 - o_R(1))(1 - 8c_1(\kappa)\alpha^3) - 8c_1(\kappa)D\alpha^3 \\ &= e_2 - o_R(1)(1 - 8c_1(\kappa)\alpha^3) - 8c_1(\kappa)\alpha^3(e_2 + D), \end{aligned}$$

which proves the lemma. □

Lemma 25 (Electron localization). *For every $\lambda < e_2$ there exists $\alpha_\lambda > 0$ such that for all $\alpha \leq \alpha_\lambda$ and all $n \in \mathbb{N}$*

$$\sup_{\sigma\geq 0} \||x|^n E_\lambda(H_\sigma)\| < \infty.$$

Proof. From [15, Theorem 1] we know that $\|e^{\varepsilon|x|}E_\lambda(H_\sigma)\| < \infty$ if $\lambda + \varepsilon^2 < \Sigma_\sigma$. Moreover, from the proof of that theorem we see that

$$\sup_{\sigma\geq 0} \|e^{\varepsilon|x|}E_\lambda(H_\sigma)\| < \infty$$

if $R > 0$ and $\delta > 0$ can be found so that

$$\Sigma_{\sigma,R} - \frac{\tilde{C}}{R^2} \geq \lambda + \varepsilon^2 + \delta \tag{101}$$

holds uniformly in σ. Here $\tilde{C}$ is a constant that is independent of the system. Given $\lambda < e_2$, pick $\alpha_\lambda > 0$ so small that $e_2 - c_1(\kappa)\alpha_\lambda^3 C > \lambda$ with C as in Lemma 24. It then follows from Lemma 24 that (101) holds true for some $\delta > 0$ if R is large enough. □

Theorem 26 (Spectral gap). *If $\alpha \ll 1$ then*

$$\sigma(H_\sigma \restriction \mathcal{H}^\sigma) \cap (E_\sigma, E_\sigma + \sigma) = \emptyset$$

for all $\sigma \leq (e_2 - e_1)/2$.

Remark. Variants of this results are already known [12, 3]. We therefore content ourselves with a proof that is partly formal in the sense that domain questions are ignored.

Proof. From [16] we know that

$$\inf \sigma_{ess}(H_\sigma \restriction \mathcal{H}^\sigma) \geq \min(E_\sigma + \sigma, \Sigma_\sigma).$$

On the other hand, by Lemma 24,

$$\Sigma_\sigma - E_\sigma \geq e_2 - e_1 - \alpha^3(8c_1(\kappa) + 4c_2(\kappa)) \geq \sigma$$

under our assumptions on α and σ. This proves that

$$\inf \sigma_{ess}(H_\sigma \upharpoonright \mathcal{H}^\sigma) \geq E_\sigma + \sigma$$

and it remains to verify that H_σ has no eigenvalues in $(E_\sigma, E_\sigma + \sigma)$. This follows from Proposition 27 and the Virial Theorem. □

The following proposition is part of the proof of Theorem 26.

Proposition 27. *Let* $\tilde{B} = \mathrm{d}\Gamma(\hat{b}) + \alpha^{3/2} x \cdot \phi(i\hat{b}\tilde{\chi}^\sigma G_0)$ *where* $\hat{b} = (\hat{k} \cdot y + y \cdot \hat{k})/2$ *and* $\hat{k} = k/|k|$. *Then for* $\alpha \ll 1$ *and* $\sigma \leq e_{\mathrm{gap}}/2$,

$$E_{(0,\sigma)}(H_\sigma - E_\sigma)[H_\sigma, i\tilde{B}]E_{(0,\sigma)}(H_\sigma - E_\sigma) \geq \frac{1}{2} E_{(0,\sigma)}(H_\sigma - E_\sigma).$$

Remark. The reason for the contribution $\alpha^{3/2} x \cdot \phi(i\hat{b}\tilde{\chi}^\sigma G_0)$ to the operator $\tilde{B}$ is that in Equation (102) it leads to $\phi(i\hat{b}\tilde{\chi}^\sigma \Delta G_x)$ with $\Delta G_x = G_x - G_0$ rather then $\phi(i\hat{b}\tilde{\chi}^\sigma G_x)$.

Proof. Let $\Pi_\sigma = p + \alpha^{3/2} A^\sigma(\alpha x)$ so that $H_\sigma = \Pi_\sigma^2 + V + H_f$. We compute

$$[H_\sigma, i\tilde{B}] = \Pi_\sigma[\Pi_\sigma, i\tilde{B}] + [\Pi_\sigma, i\tilde{B}]\Pi_\sigma + [H_f, i\tilde{B}]$$

where

$$[H_f, i\tilde{B}] = N - \alpha^{3/2} x \cdot \phi(\omega\hat{b}\tilde{\chi}^\sigma G_0)$$

and

$$\begin{aligned} [\Pi_\sigma, i\tilde{B}] &= \left[\Pi_\sigma, i\mathrm{d}\Gamma(\hat{b})\right] + \left[\Pi_\sigma, i\alpha^{3/2} x \cdot \phi(i\hat{b}\tilde{\chi}^\sigma G_0)\right] \\ &= -\alpha^{3/2}\phi(i\hat{b}\tilde{\chi}^\sigma G_x) + \alpha^{3/2}\phi(i\hat{b}\tilde{\chi}^\sigma G_0) - 2\alpha^3 \operatorname{Re}\langle \tilde{\chi}^\sigma G_x, x\hat{b}\tilde{\chi}^\sigma G_0\rangle \\ &= -\alpha^{3/2}\phi(i\hat{b}\tilde{\chi}^\sigma \Delta G_x) - 2\alpha^3 \operatorname{Re}\langle \tilde{\chi}^\sigma G_x, x\hat{b}\tilde{\chi}^\sigma G_0\rangle. \end{aligned} \tag{102}$$

We first show that $[H_\sigma, i\tilde{B}] - N$ between spectral projections $E_{(0,\sigma)}(H_\sigma - E_\sigma)$ is $O(\alpha^{3/2})$ as $\alpha \to 0$. To this end we set $\lambda = (1/4)e_1 + (3/4)e_2$ and prove Steps 1-3 below. Note that, by Lemma 24, $E_\sigma + \sigma \leq \lambda$ for $\sigma \leq e_{\mathrm{gap}}/2$ and $2c_2(\kappa)\alpha^3 \leq e_{\mathrm{gap}}/4$.
Step 1.

$$\sup_{\sigma>0} \|E_\lambda(H_\sigma) x \cdot \phi(\omega\hat{b}\tilde{\chi}^\sigma G_0) E_\lambda(H_\sigma)\| < \infty.$$

One has the estimate

$$\|E_\lambda(H_\sigma) x \cdot \phi(\omega\hat{b}\tilde{\chi}^\sigma G_0) E_\lambda(H_\sigma)\| \leq \|E_\lambda(H_\sigma) x\| \|\omega\hat{b}\tilde{\chi}^\sigma G_0\|_\omega \|(H_f + 1)^{1/2} E_\lambda(H_\sigma)\|$$

where each factor is bounded uniformly in $\sigma > 0$. For the first one this follows from Lemma 25, for the second one from $|\omega\hat{b}\tilde{\chi}^\sigma G_0(k)| = O(|k|^{-1/2})$ and for the third one from $\sup_\sigma \|(H_f + 1)^{1/2}(H_\sigma + 1)^{-1}\| < \infty$, by Lemma 23.

Step 2.

$$\sup_{\sigma>0} \|E_\lambda(H_\sigma)\Pi_\sigma \cdot \phi(i\hat{b}\tilde{\chi}^\sigma \Delta G_x)E_\lambda(H_\sigma)\| < \infty.$$

This time we use

$$\begin{aligned} &\|E_\lambda(H_\sigma)\Pi_\sigma \cdot \phi(i\hat{b}\tilde{\chi}^\sigma \Delta G_x)E_\lambda(H_\sigma)\| \\ \leq\ & \|E_\lambda(H_\sigma)\Pi_\sigma\|\Big(\sup_x \langle x\rangle^{-1}\|\hat{b}\tilde{\chi}^\sigma \Delta G_x\|_\omega\Big)\|\langle x\rangle(H_f+1)^{1/2}E_\lambda(H_\sigma)\|. \end{aligned} \tag{103}$$

Since

$$\begin{aligned} \hat{b}\tilde{\chi}^\sigma \Delta G_x(k,\lambda) &= i\left(\partial_{|k|}+|k|^{-1}\right)\tilde{\chi}^\sigma(e^{-ik\cdot x}-1)\frac{\kappa(k)}{\sqrt{|k|}}\varepsilon_\lambda(k) \\ &= O(\langle x\rangle|k|^{-1/2}), \qquad (k\to 0), \end{aligned}$$

while, as $k \to \infty$, it decays like a Schwartz-function, it follows that

$$\sup_{x,\sigma} \langle x\rangle^{-1}\|\hat{b}\tilde{\chi}^\sigma \Delta G_x\|_\omega < \infty.$$

The first factor of (103) is bounded uniformly in $\sigma > 0$ thanks to Lemma 23, and for the last one we have

$$\|\langle x\rangle(H_f+1)^{1/2}E_\lambda(H_\sigma)\| \leq \|\langle x\rangle^2 E_\lambda(H_\sigma)\| + \|(H_f+1)E_\lambda(H_\sigma)\|,$$

which, by Lemma 25 and Lemma 23, is also bounded uniformly in σ.

Step 3.

$$\sup_\sigma \|E_\lambda(H_\sigma)\Pi_\sigma \cdot \mathrm{Re}\,\langle \tilde{\chi}^\sigma G_x, x\cdot \hat{b}\tilde{\chi}^\sigma G_0\rangle E_\lambda(H_\sigma)\| < \infty.$$

This follows from estimates in the proof of Step 2.

From Steps 1, 2, 3 and $N \geq 1 - P_\Omega$ it follows that

$$E_\lambda(H_\sigma)[H_\sigma, i\tilde{B}]E_\lambda(H_\sigma) \geq E_\lambda(H_\sigma)(1-P_\Omega)E_\lambda(H_\sigma) + O(\alpha^{3/2}). \tag{104}$$

In Steps 4, 5, and 6 below we will show that $E_{(0,\sigma)}(H_\sigma - E_\sigma)P_\Omega E_{(0,\sigma)}(H_\sigma - E_\sigma) = O(\alpha^{3/2})$ as well. Hence the proposition will follow from (104).

Step 4.

$$\|(P_{\mathrm{part}}^\perp \otimes P_\Omega)E_\lambda(H_\sigma)\| = O(\alpha^{3/2}).$$

Let $H^{(0)}$ denote the Hamiltonian H with $\alpha = 0$ and let $f \in C_0^\infty(\mathbb{R})$ with $\mathrm{supp}(f) \subset (-\infty, e_2)$ and $f = 1$ on $[\inf_{\sigma\leq e_{\mathrm{gap}}} E_\sigma, \lambda]$. Then $E_\lambda(H_\sigma) = f(H_\sigma)E_\lambda(H_\sigma)$, $(P_{\mathrm{part}}^\perp \otimes P_\Omega)f(H^{(0)}) = 0$ and

$$f(H_\sigma) - f(H^{(0)}) = \int d\tilde{f}(z)\frac{1}{z-H_\sigma}\left(2\alpha^{3/2}p\cdot A^\sigma(\alpha x) + \alpha^3 A^\sigma(\alpha x)^2\right)\frac{1}{z-H^{(0)}} = O(\alpha^{3/2}).$$

It follows that

$$\begin{aligned} \|(P_{\mathrm{part}}^\perp \otimes P_\Omega)E_\lambda(H_\sigma)\| &= \|(P_{\mathrm{part}}^\perp \otimes P_\Omega)\left[f(H_\sigma) - f(H^{(0)})\right]E_\lambda(H_\sigma)\| \\ &\leq \|f(H_\sigma) - f(H^{(0)})\| = O(\alpha^{3/2}). \end{aligned}$$

Step 5. Let P_σ denote the ground state projection of H_σ. Then

$$\|P_{\rm part}\otimes P_\Omega - P_\sigma\| = O(\alpha^{3/2}).$$

Since $1-P_\Omega \le N^{1/2}$ we have

$$\begin{aligned} 1-P_{\rm part}\otimes P_\Omega &= 1-P_\Omega + P_{\rm part}^\perp\otimes P_\Omega \\ &\le N^{1/2} + P_{\rm part}^\perp\otimes P_\Omega \end{aligned}$$

where $\|(P_{\rm part}^\perp\otimes P_\Omega)P_\sigma\| = O(\alpha^{3/2})$ by Step 4 and $\|N^{1/2}P_\sigma\| = O(\alpha^{3/2})$ by Lemma 29. It follows that $\|(1-P_{\rm part}\otimes P_\Omega)P_\sigma\| = O(\alpha^{3/2})$. Hence, for α small enough, P_σ is of rank one and the assertion of Step 5 follows.

Step 6.

$$E_{(0,\sigma)}(H_\sigma - E_\sigma)(1\otimes P_\Omega)E_{(0,\sigma)}(H_\sigma - E_\sigma) = O(\alpha^{3/2}).$$

Since $P_\sigma E_{(0,\sigma)}(H_\sigma - E_\sigma) = 0$, it follows from Step 4 and Step 5 that

$$\begin{aligned} &\|(1\otimes P_\Omega)E_{(0,\sigma)}(H_\sigma - E_\sigma)\| = \|(1\otimes P_\Omega - P_\sigma)E_{(0,\sigma)}(H_\sigma - E_\sigma)\| \\ &\le \|(P_{\rm part}\otimes P_\Omega - P_\sigma)E_{(0,\sigma)}(H_\sigma - E_\sigma)\| + \|(P_{\rm part}^\perp\otimes P_\Omega)E_{(0,\sigma)}(H_\sigma - E_\sigma)\| \\ &= O(\alpha^{3/2}). \end{aligned}$$

□

The following Lemma is formulated in a way which makes it applicable to the scalar field model of Section 2 as well as to QED.

Lemma 28 (overlap estimates). *Let $P^\sigma\otimes f_\Delta(H_{f,\sigma})$ on $\mathcal{H}^\sigma\otimes\mathcal{F}_\sigma$ be defined as in Section 2 or Section 3.1, and suppose $|\chi_\sigma G_x(k)| = 0$ if $|k|>2\sigma$ while $|\chi_\sigma G_x(k)| \le |k|^\mu$ for some $\mu > -1$ if $|k|\le 2\sigma$. Then*

$$\begin{aligned} \|a(\chi_\sigma G_x)P^\sigma\otimes f_\Delta(H_{f,\sigma})\| &\le \int_{\sigma\le|k|\le 2\sigma} |k|^\mu \|a(k)P^\sigma\|\,dk + C\sigma^{\mu+3/2}, \\ \||x|a(\chi_\sigma G_x)P^\sigma\otimes f_\Delta(H_{f,\sigma})\| &\le \int_{\sigma\le|k|\le 2\sigma} |k|^\mu \||x|a(k)P^\sigma\|\,dk + C\||x|P^\sigma\|\sigma^{\mu+3/2}, \end{aligned}$$

where $C=\sqrt{2\pi/(\mu+1)}$.

Proof. Let $\varphi\in\mathcal{H}^\sigma\otimes\mathcal{F}_\sigma$ with $\|\varphi\|=1$. By assumption on $\chi_\sigma G_x$,

$$\begin{aligned} a(\chi_\sigma G_x)P^\sigma\otimes f_\Delta(H_{f,\sigma})\varphi &= \int_{\sigma\le|k|\le 2\sigma} \chi_\sigma(k)\overline{G_x(k)}a(k)P^\sigma\otimes f(H_{f,\sigma})\varphi\,dk \\ &\quad + \int_{|k|<\sigma} \chi_\sigma(k)\frac{\overline{G_x(k)}}{|k|^{1/2}}P^\sigma\otimes |k|^{1/2}a(k)f(H_{f,\sigma})\varphi\,dk. \end{aligned}$$

Using $|\chi_\sigma G_x(k)| \le |k|^\mu$, $\|f_\Delta(H_{f,\sigma})\| \le 1$, and the Cauchy-Schwarz inequality applied to the second integral

$$\begin{aligned}
&\|a(\chi_\sigma G_x)P^\sigma \otimes f_\Delta(H_{f,\sigma})\varphi\| \\
&\le \int_{\sigma\le|k|\le 2\sigma} |k|^\mu \|a(k)P^\sigma\|\,dk + \left(\int_{|k|\le\sigma} |k|^{2\mu-1}\,dk\right)^{1/2} \|H_{f,\sigma}^{1/2} f(H_{f,\sigma})\varphi\| \\
&\le \int_{\sigma\le|k|\le 2\sigma} |k|^\mu \|a(k)P^\sigma\|\,dk + \left(\frac{2\pi}{\mu+1}\right)^{1/2} \sigma^{\mu+3/2},
\end{aligned}$$

where $\|H_{f,\sigma}^{1/2} f(H_{f,\sigma})\| \le \sigma^{1/2}$ was used in the last step. The proof of the second assertion is a copy of the proof above with P^σ replaced by $|x|P^\sigma$. □

The integrands in Lemma 28 are estimated in the following lemma.

Lemma 29 (ground state photons). *Suppose $H_\sigma P_\sigma = E_\sigma P_\sigma$ where $\sigma \ge 0$, $E_\sigma = \inf\sigma(H_\sigma)$, and P_σ is the ground state projection of H_σ. Here $H_{\sigma=0} = H$. Let $R_\sigma(\omega) = (H_\sigma - E_\sigma + \omega)^{-1}$. Then*

$$\begin{aligned}
(i)\qquad a(k)P_\sigma \;=\; &-i\alpha^{3/2}\Big[1 - \omega R_\sigma(\omega) - 2R_\sigma(\omega)(\Pi_\sigma\cdot k) + \alpha R_\sigma(\omega)k^2\Big] x\cdot G_x(k)^* P_\sigma \\
&-2\alpha^{3/2} R_\sigma(\omega) k\cdot G_{\alpha x}(k)^* P_\sigma.
\end{aligned}$$

There are constants C, D independent of $\sigma, \alpha \in [0,1]$ such that

$$\begin{aligned}
(ii)\quad & \|a(k)P_\sigma\| \le \alpha^{3/2}\frac{C}{|k|^{1/2}}, \\
(iii)\quad & \|xa(k)P_\sigma\| \le \alpha^{3/2}\frac{D}{|k|^{3/2}}.
\end{aligned}$$

Proof. We suppress the subindex σ for notational simplicity. By the usual pull-through trick

$$\begin{aligned}
(H - E + \omega(k))a(k)P &= [H, a(k)]\varphi + \omega(k)a(k)P \\
&= -\alpha^{3/2} 2\Pi\cdot G_x(k)^* P.
\end{aligned}$$

Since $2\Pi = i[H,x] = i[H-E,x]$, and $(H-E)\varphi = 0$ we can rewrite this as

$$\begin{aligned}
i\alpha^{-3/2}a(k)\varphi &= R(\omega)\big[(H-E)x - x(H-E)\big]G_{\alpha x}(k)^* P \\
&= (1-\omega R(\omega))(x\cdot G_x(k)^*)P - R(\omega)x[H, G_{\alpha x}(k)^*]P \qquad (105)
\end{aligned}$$

For the commutator we get

$$\begin{aligned}
[H, G_x(k)^*] &= (\Pi\cdot k)G_x(k)^* + G_{\alpha x}(k)^*(\Pi\cdot k) \\
&= 2(\Pi\cdot k)G_x(k)^* - \alpha k^2 G_x(k)^*
\end{aligned}$$

and hence, using $x(\Pi\cdot k) = (\Pi\cdot k)x + ik$,

$$x[H, G_x(k)^*] = \big[2(\Pi\cdot k) - \alpha k^2\big]x\cdot G_{\alpha x}(k)^* + 2ik\cdot G_x(k)^*. \tag{106}$$

From (105) and (106) we conclude that

$$\begin{aligned} i\alpha^{-3/2}a(k)P &= \big[1-\omega R(\omega) - 2R(\omega)(\Pi\cdot k) + \alpha R(\omega)k^2\big]x\cdot G_x(k)^*P \\ &\quad -2iR(\omega)k\cdot G_x(k)^*P. \end{aligned}$$

(ii) First of all $\sup_{\sigma\geq 0}\|xP\| < \infty$ by Lemma 25 and $|G_x(k)| \leq \text{const}|k|^{-1/2}$ by definition of $G_x(k)$. Since $\|R(\omega)\| \leq |k|^{-1}$ and $\|R(\omega)\Pi\| \leq \text{const}(1+|k|^{-1})$ we find that

$$\Big\|\Big[1-\omega R(\omega) - 2R(\omega)(\Pi\cdot k) + \alpha R(\omega)k^2\Big]\Big\| \leq \text{const} \qquad \text{for } \alpha, |k|\leq 1$$

This proves (ii). To estimate the norm of $xa(k)P$ we use (i) and commute x with all operators in front of P so that we can apply Lemma 25 to the operator x^2P. Since

$$[x, R(\omega)] = -2iR(\omega)\Pi R(\omega)$$

the resulting estimate for $\|xa(k)P\|$ is worse by one power of $|k|$ than our estimate (i) for $\|a(k)P\|$. □

Lemma 30. *There exists a constant C such that*

$$|E - E_\sigma| = C\alpha^{3/2}\sigma^2$$

for all $\sigma \geq 0$ and $\alpha\in[0,1]$.

Proof. Let ψ and ψ_σ be normalized ground states of H and H_σ respectively. Then, by Rayleigh-Ritz,

$$E - E_\sigma \leq \langle\psi_\sigma, (H-H_\sigma)\psi_\sigma\rangle \tag{107}$$

$$E_\sigma - E \leq \langle\psi, (H_\sigma - H)\psi\rangle \tag{108}$$

where $H - H_\sigma = \Pi^2 - \Pi_\sigma^2$ and

$$\begin{aligned} \Pi^2 - \Pi_\sigma^2 &= 2\alpha^{3/2}p\cdot(A(\alpha x) - A^\sigma(\alpha x)) \\ &\quad +\alpha^3[A(\alpha x) + A^\sigma(\alpha x)]\cdot[A(\alpha x) - A^\sigma(\alpha x)]. \end{aligned} \tag{109}$$

To estimate the contribution due to (109) we note that

$$\begin{aligned} [A(\alpha x) + A^\sigma(\alpha x)]\cdot[A(\alpha x) - A^\sigma(\alpha x)] &= [A(\alpha x) + A^\sigma(\alpha x)]\cdot a(\chi_\sigma G_x) \\ &\quad +a^*(\chi_\sigma G_x)\cdot[A(\alpha x) + A^\sigma(\alpha x)] \\ &\quad +2\int |G_x(k)|^2\chi_\sigma^2\,dk. \end{aligned} \tag{110}$$

The last term in (110) is of order σ^2 and from Lemma 29 it follows that

$$\|a(\chi_\sigma G_x)\psi_\sigma\|,\ \|a(\chi_\sigma G_x)\psi\| \leq C\alpha^{3/2}\int_{|k|\leq 2\sigma}|G_x(k)|\frac{1}{\sqrt{|k|}}dk = O(\alpha^{3/2}\sigma^2) \tag{111}$$

Moreover, by Lemma 23,

$$\|p\psi_\sigma\|, \|[A(\alpha x) + A_\sigma(\alpha x)]\psi_\sigma\| \leq \text{const.}$$

It follows that the contributions of (109) to (107) and (108) are of order $\alpha^{3/2}\sigma^2$ and $\alpha^3\sigma^2$. □

B Conjugate Operator Method

In this section we describe the conjugate operator method in the version of Amrein, Boutet de Monvel, Georgescu, and Sahbani [1, 21]. In the paper of Sahbani the theory of Amrein et al. is generalized in a way that is crucial for our paper. For simplicity, we present a weaker form of the results of Sahbani with comparatively stronger assumptions that are satisfied by our Hamiltonians.

The conjugate operator method to analyze the spectrum of a self-adjoint operator $H : D(H) \subset \mathcal{H} \to \mathcal{H}$ assumes the existence of another self-adjoint operator A on $\mathcal{H}$, the conjugate operator, with certain properties. The results below yield information on the spectrum of H in an open subset $\Omega \subset \mathbb{R}$, provided the following assumptions hold:

(i) *H is locally of class $C^2(A)$ in Ω.* This assumption means that the mapping

$$s \mapsto e^{-iAs}f(H)e^{iAs}\varphi$$

is twice continuously differentiable, for all $f \in C_0^\infty(\Omega)$ and all $\varphi \in \mathcal{H}$.

(ii) For every $\lambda \in \Omega$, there exists a neighborhood Δ of λ with $\overline{\Delta} \subset \Omega$, and a constant $a > 0$ such that

$$E_\Delta(H)[H, iA]E_\Delta(H) \geq aE_\Delta(H).$$

Remarks: By (i), the commutator $[H, iA]$ is well defined as a sesquilinear form on the intersection of $D(A)$ and $\cup_K E_K(H)\mathcal{H}$, where the union is taken over all compact subsets K of Ω. By continuity it can be extended to $\cup_K E_K(H)\mathcal{H}$.

The following two theorems follow from Theorems 0.1 and 0.2 in [21] and assumptions (i) and (ii), above.

Theorem 31. *For all $s > 1/2$ and all $\varphi, \psi \in \mathcal{H}$, the limit*

$$\lim_{\varepsilon\to 0+}\langle\varphi, \langle A\rangle^{-s}R(\lambda \pm i\varepsilon)\langle A\rangle^{-s}\psi\rangle$$

exists uniformly for λ in any compact subset of Ω. In particular, the spectrum of H is purely absolutely continuous in Ω.

This theorem allows one to define operators $\langle A\rangle^{-s}R(\lambda\pm i0)\langle A\rangle^{-s}$ in terms of the sesquilinear forms

$$\langle\varphi,\langle A\rangle^{-s}R(\lambda\pm i0)\langle A\rangle^{-s}\psi\rangle=\lim_{\varepsilon\to 0}\langle\varphi,\langle A\rangle^{-s}R(\lambda\pm i\varepsilon)\langle A\rangle^{-s}\psi\rangle.$$

By the uniform boundedness principle these operators are bounded.

Theorem 32. *If* $1/2<s<1$ *then*

$$\lambda\mapsto\langle A\rangle^{-s}R(\lambda\pm i0)\langle A\rangle^{-s}$$

is locally Hölder continuous of degree $s-1/2$ *in* Ω.

Theorem 33. *Suppose* $s\in(1/2,1)$ *and* $f\in C_0^\infty(\Omega)$. *Then*

$$\|\langle A\rangle^{-s}e^{-iHt}f(H)\langle A\rangle^{-s}\|=O\left(\frac{1}{t^{s-1/2}}\right),\qquad(t\to\infty).$$

Proof. For every $f\in C_0^\infty(\mathbb{R})$ and all $\varphi\in\mathcal{H}$

$$e^{-iHt}f(H)\varphi=\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int e^{-i\lambda t}f(\lambda)\,\mathrm{Im}(H-\lambda-i\varepsilon)^{-1}\varphi\,d\lambda \tag{112}$$

by the spectral theorem. Now suppose $f\in C_0^\infty(\Omega)$ and set $F(z)=\pi^{-1}\langle A\rangle^{-s}\,\mathrm{Im}(H-z)^{-1}\langle A\rangle^{-s}$. Then (112) and Theorem 31 imply

$$\langle A\rangle^{-s}e^{-iHt}f(H)\langle A\rangle^{-s}\varphi=\int e^{-i\lambda t}f(\lambda)F(\lambda+i0)\varphi\,d\lambda \tag{113}$$

This equation with $H-\pi/t$ in place of H becomes

$$\langle A\rangle^{-s}e^{-iHt}f(H-\pi/t)\langle A\rangle^{-s}\varphi=-\int e^{-i\lambda t}f(\lambda)F(\lambda+\pi/t+i0)\varphi\,d\lambda. \tag{114}$$

We take the sum of (113) and (114) and use $\|f(H)-f(H-\pi/t)\|=O(t^{-1})$ to get

$$\begin{aligned}&2\|\langle A\rangle^{-s}e^{-iHt}f(H)\langle A\rangle^{-s}\|+O(t^{-1})\\&\quad\le\int|f(\lambda)|\|F(\lambda+i0)-F(\lambda+\pi/t+i0)\|d\lambda=O(1/t^{s-1/2}),\end{aligned}$$

where the Hölder continuity from Theorem 32 was used in the last step. □

For completeness we also include the Virial Theorem (Proposition 3.2 of [21]):

Proposition 34. *If* $\lambda\in\Omega$ *is an eigenvalue of* H *and* $E_{\{\lambda\}}(H)$ *denotes the projection onto the corresponding eigenspace, then*

$$E_{\{\lambda\}}(H)[H,iA]E_{\{\lambda\}}(H)=0.$$

In the remainder of this section we introduce tools that will help us to verify assumption (i). To begin with we recall, from [1, 21], that a bounded operator T on $\mathcal{H}$ is said to be of class $C^k(A)$ if the mapping

$$s \mapsto e^{-iAs} T e^{iAs} \varphi$$

is k times continuously differentiable for every $\varphi \in \mathcal{H}$. The following propositions summarize results in Lemma 6.2.9 and Lemma 6.2.3 of [1].

Proposition 35. *Let T be a bounded operator on $\mathcal{H}$ and let $A = A^* : D(A) \subset \mathcal{H} \to \mathcal{H}$. Then the following are equivalent.*

(i) T is of class $C^1(A)$.

(ii) There is a constant c such that for all $\varphi, \psi \in D(A)$

$$|\langle A\varphi, T\psi\rangle - \langle \varphi, TA\psi\rangle| \le c\|\varphi\|\|\psi\|.$$

(iii) $\liminf_{s\to 0+} \frac{1}{s}\left\|e^{-iAs}Te^{iAs} - T\right\| < \infty.$

Proof. If T is of class $C^1(A)$ then $\sup_{s\neq 0} \|s^{-1}(e^{-iAs}Te^{iAs} - T)\| < \infty$ by the uniform boundedness principle. Thus statement (i) implies statement (iii). To prove the remaining assertions we use that, for all $\varphi, \psi \in D(A)$,

$$\frac{1}{s}\langle \varphi, (e^{-iAs}Te^{iAs} - T)\psi\rangle = \frac{-i}{s}\int_0^s d\tau \Big[\langle e^{iA\tau}A\varphi, Te^{iA\tau}\psi\rangle - \langle e^{iA\tau}\varphi, Te^{iA\tau}A\psi\rangle\Big]. \tag{115}$$

Since the integrand is a continuous function of τ, its value at $\tau = 0$, $\langle A\varphi, T\psi\rangle - \langle \varphi, TA\psi\rangle$, is the limit of 115 as $s \to 0$. It follows that

$$\begin{aligned} |\langle A\varphi, T\psi\rangle - \langle \varphi, TA\psi\rangle| &= \lim_{s\to 0+} s^{-1}|\langle \varphi, (e^{-iAs}Te^{iAs} - T)\psi\rangle| \\ &\le \liminf_{s\to 0+} s^{-1}\|e^{-iAs}Te^{iAs} - T\|\|\varphi\|\|\psi\|. \end{aligned} \tag{116}$$

Therefore (iii) implies (ii).

Next we assume (ii). Then $TD(A) \subset D(A)$ and $[A, T] : D(A) \subset \mathcal{H} \to \mathcal{H}$ has a unique extension to a bounded operator $\mathrm{ad}_A(T)$ on $\mathcal{H}$. The mapping

$$\tau \mapsto e^{-iA\tau}\mathrm{ad}_A(T)e^{iA\tau}\psi$$

is continuous, and hence (115) implies that

$$e^{-iAs}Te^{iAs}\psi - T\psi = -i\int_0^s e^{-iA\tau}\mathrm{ad}_A(T)e^{iA\tau}\psi\, d\tau \tag{117}$$

for each $\psi \in \mathcal{H}$. Since the r.h.s is continuously differentiable in s, so is the l.h.s, and thus $T \in C^1(A)$. □

Let $A_s = (e^{iAs} - 1)/is$, which is a bounded approximation of A. Then

$$\frac{1}{s}\left(e^{-iAs}Te^{iAs} - T\right) = -ie^{-iAs}\mathrm{ad}_{A_s}(T). \tag{118}$$

Hence, by Proposition 35, a bounded operator T is of class $C^1(A)$ if and only if $\liminf_{s\to 0+}\|\mathrm{ad}_{A_s}(T)\| < \infty$. The following proposition gives an analogous characterization of the class $C^2(A)$.

Proposition 36. *Let $A = A^* : D(A) \subset \mathcal{H} \to \mathcal{H}$ and let T be a bounded operator of class $C^1(A)$. Then T is of class $C^2(A)$ if and only if*

$$\liminf_{s\to 0+} \|\mathrm{ad}^2_{A_s}(T)\| < \infty. \tag{119}$$

Remark. This is a special case of [1, Lemma 6.2.3] on the class $C^k(A)$. We include the proof for the convenience of the reader.

Proof. Since T is of class $C^1(A)$ the commutator $[A, T]$ extends to a bounded operator $\mathrm{ad}_A(T)$ on $\mathcal{H}$ and

$$i\frac{d}{ds}e^{-iAs}Te^{iAs}\varphi = e^{-iAs}\mathrm{ad}_A(T)e^{iAs}\varphi \tag{120}$$

for all $\varphi \in \mathcal{H}$. By Proposition 35 the right hand side is continuously differentiable if and only if

$$|\langle A\varphi, \mathrm{ad}_A(T)\psi\rangle - \langle\varphi, \mathrm{ad}_A(T)A\psi\rangle| \le c\|\varphi\|\|\psi\|, \qquad \text{for } \varphi,\psi \in D(A) \tag{121}$$

with some finite constant c. To prove that (121) is equivalent to (119), it is useful to introduce the homomorphism $W(s) : T \mapsto e^{-iAs}Te^{iAs}$ on the algebra of bounded operators. By (117)

$$(W(s) - 1)T = -i\int_0^s \mathrm{d}\tau_1 W(\tau_1)\mathrm{ad}_A(T)$$

and therefore

$$\begin{aligned}\frac{1}{s^2}(W(s)-1)^2 T &= \frac{-i}{s^2}\int_0^s \mathrm{d}\tau_1 (W(s)-1)W(\tau_1)\mathrm{ad}_A(T) \\ &= \frac{-1}{s^2}\int_0^s \mathrm{d}\tau_1 \int_0^s \mathrm{d}\tau_2 W(\tau_1+\tau_2)[A, \mathrm{ad}_A(T)]\end{aligned} \tag{122}$$

in the sense of quadratic forms on $D(A)$, that is,

$$\langle\varphi, W(\tau_1+\tau_2)[A,\mathrm{ad}_A(T)]\psi\rangle := \langle A\varphi, W(\tau_1+\tau_2)\mathrm{ad}_A(T)\psi\rangle - \langle\varphi, W(\tau_1+\tau_2)\mathrm{ad}_A(T)A\psi\rangle$$

for $\varphi,\psi \in D(A)$. Since the right hand side is continuous as a function of $\tau_1 + \tau_2$, it follows from (122), as in the proof of Proposition 35, that

$$\begin{aligned}|\langle A\varphi, \mathrm{ad}_A(T)\psi\rangle - \langle\varphi, \mathrm{ad}_A(T)A\psi\rangle| &= \lim_{s\to 0+}\frac{1}{s^2}|\langle\varphi, (W(s)-1)^2 T\psi\rangle| \\ &\le \liminf_{s\to 0+}\frac{1}{s^2}\|(W(s)-1)^2 T\|\|\varphi\|\|\psi\|.\end{aligned}$$

Since, by (118),

$$\frac{1}{s^2}(W(s)-1)^2 T = -e^{-2iAs}\mathrm{ad}^2_{A_s}(T),$$

condition (119) implies (121). Conversely, by (122) condition (121) implies that $s^{-2}\|(W(s)-1)^2 T\| \le c$ for all $s>0$, which proves (119). □

Lemma 37. *Suppose that H is locally of class $C^1(A)$ in $\Omega \subset \mathbb{R}$ and that $e^{iAs}D(H) \subset D(H)$ for all $s \in \mathbb{R}$. Then, for all $f \in C_0^\infty(\Omega)$ and all $\varphi \in \mathcal{H}$*

$$f(H)[H, iA]f(H)\varphi = \lim_{s\to 0} f(H)\left[H, \frac{e^{iAs}-1}{s}\right] f(H)\varphi.$$

Proof. By Equation 2.2 of [21],

$$f(H)[H, iA]f(H) = [Hf^2(H), iA] - Hf(H)[f(H), iA] - [f(H), iA]Hf(H), \tag{123}$$

where, by assumption, $f(H)$ and $Hf^2(H)$ are of class $C^1(A)$. Since, by (118)

$$[T, iA]\varphi = -i\lim_{s\to 0}\mathrm{ad}_{A_s}(T)\varphi$$

for every bounded operator T of class $C^1(A)$, it follows from (123), the Leibniz-rule for ad_{A_s} and the domain assumption $A_s D(H) \subset D(H)$, that

$$\begin{aligned} & f(H)[H, iA]f(H)\varphi \\ &= -i\lim_{s\to 0}\Big(\mathrm{ad}_{A_s}(Hf^2(H)) - Hf(H)\mathrm{ad}_{A_s}(f(H)) - \mathrm{ad}_{A_s}(f(H))Hf(H)\Big)\varphi \\ &= -i\lim_{s\to 0} f(H)\mathrm{ad}_{A_s}(H)f(H)\varphi. \end{aligned}$$

□

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