Positive Commutators and the Spectrum of Pauli-Fierz Hamiltonian of Atoms and Molecules

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Abstract

In this paper we study the energy spectrum of the Pauli-Fierz Hamiltonian generating the dynamics of nonrelativistic electrons bound to static nuclei and interacting with the quantized radiation field. We show that, for sufficiently small values of the elementary electric charge, and under weaker conditions than those required in [3], the spectrum of this Hamiltonian is absolutely continuous, except possibly in small neighbourhoods of the ground state energy and the ionization thresholds. In particular, it is shown that (for a large range of energies) there are no stable excited eigenstates. The method used to prove these results relies on the positivity of the commutator between the Hamiltonian and a suitably modified dilatation generator on photon Fock space.

1 Introduction

In this paper we extend the method of positive commutators to a family of Hamiltonians related to the Pauli-Fierz Hamiltonian describing nonrelativistic electrons bound to static nuclei and interacting with the quantized electromagnetic field, subject to an ultraviolet cut-off. This is a standard Hamiltonian of quantum electrodynamics of nonrelativistic particles. Let e and m be the electron charge and mass and $\alpha := \frac{e^2}{\hbar c}$, the fine-structure constant. The physical value of α is approximately $\frac{1}{137}$, however, in this paper it is considered as a small dimensionless parameter. In dimensionless units in which the energy, photon wave vector, particle coordinate, particle charge and particle mass are measured in units of $mc^2\alpha^2$, $\alpha\frac{me^2}{\hbar^2}$, $\frac{\hbar^2}{me^2}$, $e(\alpha^{3/2}K)^{-1}$ and m, respectively (here K is an ultraviolet cut-off defined below), the Pauli-Fierz Hamiltonian for a system of N charged particles (typically electrons) is given by

$$H(e) \;=\; \sum_{j=1}^{N} \frac{1}{2m_j}\Big(p_j - e_j A(x_j)\Big)^2 + V(x)\otimes \mathbf{1}_f + \mathbf{1}_{\text{part}} \otimes H_f\,, \tag{1.1}$$

where $e := (e_1, \ldots, e_N)$, e_j is the electric charge, m_j the mass, x_j the position (-operator), and $p_j := -i\nabla_j$ the momentum operator of the j^{th} particle, for $j = 1, \ldots, N$; moreover $x := (x_1, \ldots, x_N)$. The operator $K^{1/2}A(y)$ is the quantized electromagnetic vector potential, cut-off at large wave vectors, at the point y in physical space $\mathbb{R}^3$. It is assumed to satisfy the Coulomb gauge condition, $(\nabla \cdot A)(y) = 0$. The operator $V(x)$ originates in a properly rescaled electrostatic (scalar) potential of the charged particles (electrons) in the Coulomb field of static charges (nuclei) (see [2]). Finally, H_f is the usual Hamiltonian of the noninteracting, quantized electromagnetic field. The operators $A(y)$, $y \in \mathbb{R}^3$, and H_f are densely defined, self-adjoint operators on the usual Fock space, $\mathcal{H}_f$, of the quantized electromagnetic field (the photon Fock space), and $V(x)$ is a multiplication operator on the particle Hilbert space, $\mathcal{H}_{\text{part}}$, which is given by (a subspace of prescribed symmetry character of) $L^2(\mathbb{R}^{3N})$, with $\mathbb{R}^{3N}$ the configuration space of the charged particles. The Hilbert space of the entire system constisting of the charged particles and an arbitrary number of photons is given by the tensor product space $\mathcal{H}_{\text{part}} \otimes \mathcal{H}_f$. One can prove without much difficulty (see, e.g., [8, 9]) that $H(e)$ is a densely defined, self-adoint operator on $\mathcal{H}_{\text{part}} \otimes \mathcal{H}_f$, whose energy spectrum is bounded below by a finite constant (depending on the positions of the nuclei and their electric charges). A proof can be based, either on diamagnetic type inequalities or on constructing the semigroup $\exp(-tH(e))$, for $t \geq 0$, with the help of path-integrals.

It should be noted that, for simplicity, we have set the magnetic moments of the charged particles to zero. (Otherwise, the Hamiltonian $H(e)$ would contain an additional term describing the Zeeman energies of magnetic moments in the ultraviolet cut-off, quantized electromagnetic field. This term would complicate our analysis slightly.)

For $|e| := \sum_{j=1}^{N} |e_j|$ sufficiently small, we shall construct a suitable modification of the (2^{nd} -quantized) generator of dilatations on the photon Fock space, with the property that its commutator with the Hamiltonian $H(e)$ is positive, provided that we restrict the energy to small neighbourhoods of the eigenvalues of the particle Hamiltonian,

$$H_{\text{part}} \;=\; \sum_{j=1}^{N} \frac{1}{2m_j} p_j^2 + V(x)\,, \tag{1.2}$$

corresponding to excited states of the atom or molecule. This result has the following implications: In the vicinity of the eigenvalues of H_{part} corresponding to excited eigenstates,

- $H(e)$ has no eigenvalues;
- the spectrum of $H(e)$ is purely absolutely continuous;
- $H(e)$ satisfies the *limiting absorption principle.*

Implication (i) is derived from the basic positive-commutator estimate via a virial theorem, while (ii) and (iii) follow from that estimate with the help of a slight extension of Kato-Mourre theory presented in this paper. The limiting absorption principle represents a first step towards analyzing properties of the time evolution of a quantum mechanical system.

The results announced in the abstract follow from (i) and (ii) above, together with similar (but simpler) results in Section IV of [3]. Results similar to (i) and (ii) above (but of somewhat more detailed nature), were first obtained, under *stronger* hypotheses, in [2, 3, 4]; (see remarks after Theorem 3.1). If the quantized electromagnetic field is not only cut off in the ultraviolet, but also in the infrared (at small wave vectors), e.g., by introducing a small photon mass, results similar to ours have previously been established in [22, 10, 12, 11]. Furthermore, in [12], commutator estimates were derived that inspired, in part, our findings. Parallel results for sufficiently high temperatures (here the temperature leads to an effective infrared cut-off) were obtained in [15,16].

Commutator methods were introduced in [24, 18], further developed in [19] and turned into a deep theory in [20]. In [20, 21, 23, 26] they were shown to yield a powerful tool in analyzing spectral properties of Hamiltonians of quantum-mechanical systems and in studying their time evolution. The present paper is inspired by these earlier discoveries and should be viewed as a step towards understanding the time evolution of systems of photons interacting with nonrelativistic, quantum-mechanical matter.

2 The Hamiltonian of Nonrelativistic QED

As announced, we study systems of nonrelativistic, quantum-mechanical, charged particles interacting with the quantized electromagnetic field, The dynamics of such systems is described by the Hamiltonian $H(e)$ introduced in (1.1). The potential energy $V(x)$ is assumed to satisfy standard Kato-type conditions specified below. The Hamiltonian H_f of the non-interacting, quantized electromagnetic field can be expressed in terms of standard photon creation- and annihilation operators, $a^*(k)$ and $a(k)$, as follows:

$$H_f \;=\; \int \omega(k)\, a^*(k)\cdot a(k)\, d^3k\,, \tag{2.1}$$

where $\omega = \omega(k) = |k|$ is the energy of a photon with wave vector k. The creation- and annihilation operators $a^*(k)$ and $a(k)$ are transverse, vector-valued, operator-valued distributions on $\mathcal{H}_f$ satisfying $k\cdot a^*(k) = k\cdot a(k) = 0$ and $a(k)\Omega = 0$, for all $k \in \mathbb{R}^3$, where Ω is the *vacuum* (zero-photon) *vector* in $\mathcal{H}_f$. Furthermore, these operators satisfy the canonical commutation relations

$$[\, a_i^{\#}(k)\,,\, a_j^{\#}(k)\,] \;=\; 0\,, \qquad [\, a_i(k)\,,\, a_j^*(k)\,] \;=\; \Big(\delta_{ij} \;-\; \frac{k_i k_j'}{|k|^2}\Big)\, \delta(k-k')\,, \tag{2.2}$$

where $a_i^{\#}$ is the i^{th} component of $a^{\#}$ (in the plane perpendicular to k), and $a^{\#} = a$ or a^*.

The cut-off electromagnetic vector potential $A(y)$, $y \in \mathbb{R}^3$, is the densely defined self-adjoint operator on $\mathcal{H}_f$ given by

$$A(y) \;=\; \int \Big(e^{-iky} \otimes a^*(k) \;+\; e^{iky} \otimes a(k) \Big) \frac{\kappa(k)}{\sqrt{\omega(k)}} d^3k\,, \tag{2.3}$$

where κ is a real function on $\mathbb{R}^3$ of rapid decrease, as $|k| \to \infty$. It describes the ultraviolet cut-off and is necessary for $A(y)$ to be densely defined and self-adjoint, for every $y \in \mathbb{R}^3$. We assume it lives on a scale K, i.e., it is of the form $\kappa(k) = K^{-1/2}\kappa_0(k/K)$, where κ_0 is a fixed function. The particular form of κ_0 is irrelevant for our analysis. All that is required are certain bounds on κ_0 and its derivatives.

It is convenient to forget the origin of the vector potential $A(y)$ and consider a slighty generalized form of it given by

$$A(y) \;=\; \int \Big(G_y(k) \otimes a^*(k) \;+\; \overline{G}_y(k) \otimes a(k) \Big) d^3k \,, \tag{2.4}$$

where the function $G_x(k)$ is assumed to satisfy a variety of conditions (depending on the problem we study), the most important one being

$$\sup_x \left\{ \int \frac{1}{\omega(k)} \, |G_x(k)|^2 \, d^3k \right\} \;<\; \infty \,. \tag{2.5}$$

This condition guarantees that, for $|e|$ small enough, the operator $H(e)$ is bounded below and self-adjoint on the domain of $H(e=0)$ (see [5]).

We recall that we neglect the Zeeman term,

$$-\sum \mu_i \, S_i \cdot B(x_i) \,, \tag{2.6}$$

describing the interaction energy of the interaction energy of the magnetic moments $\mu_i \, S_i$, where S_i is the spin operator of the i^{th} particle, with the magnetic field $B(y) = \mathrm{curl}\, A(y)$.

In order to simplify notation and exposition, we demonstrate our approach on the model of a particle system interacting with a massless scalar field, instead of the vector potential. The Hamiltonian for such a model is given by

$$H \;=\; H_{\rm part} \otimes \mathbf{1}_f + \mathbf{1}_{\rm part} \otimes H_f + gI \,, \tag{2.7}$$

acting on $\mathcal{H}_{\rm part} \otimes \mathcal{F}$, where the Hilbert space $\mathcal{H}_{\rm part}$ is the same as before, $\mathcal{F}$ is the Fock space of scalar fields generated by $L^2(\mathbb{R}^3)$, $H_{\rm part}$ is given in (1.2) and is a particle (atomic) Hamiltonian, acting on $\mathcal{H}_{\rm part}$, and H_f is a scalar field Hamiltonian on $\mathcal{F}$ given, similarly to (2.1), by

$$H_f \;=\; \int \omega(k) \, a^*(k) \, a(k) \, d^3k \,, \tag{2.8}$$

with $\omega = \omega(k) = |k|$, as above. Finally, the interaction term I is defined by

$$\begin{aligned} I \;\; &:= \;\; \int \Big(G_x(k) \otimes a^*(k) \;+\; \overline{G}_x(k) \otimes a(k) \Big) \, d^3k \\ &= \;\; a^*(G_x) + a(G_x) \,, \end{aligned} \tag{2.9}$$

where $x = (x_1, \ldots, x_N) \in \mathbb{R}^{3N}$, and where $G_x(k)$ is required to satisfy (2.5) (we use the same notation for coupling functions as in the vector case). The operators $a^*(k)$ and $a(k)$

are creation- and annihilation operators of a scalar quantum field acting on $\mathcal{F}$. They obey the canonical commutation relations, $[a^{\#}(k), a^{\#}(k')] = 0$, $[a(k), a^*(k')] = \delta(k-k')$, and $a(k)\Omega = 0$, for all $k, k' \in \mathbb{R}^3$, where Ω is the vacuum vector in $\mathcal{F}$. (For brevity we continue to refer to the scalar field as *photon field.*) Note that for a scalar field the coupling to matter cannot be "minimal", i.e., it cannot be described by replacing the momentum operator by a covariant derivative.

The simplified model contains all the difficulties of the vector model, but the infrared problem becomes visible in its pure form, unencumbered by vector notation and other inessential particulars. In (2.9), it is straightforward to also include terms quadratic in a and a^*. We do not pursue this in order not to muddle the key ideas underlying our methods.

Throughout the paper, we assume that

$H_{\text{part}} = H^*_{\text{part}}$ *on the domain of* $\sum_{j=1}^{N} \frac{1}{2m_j} p_j^2$ *and has several isolated eigenvalues of finite multiplicity,* $E_0, E_1, \ldots,$ *below the bottom,* Σ, *of its essential spectrum:*

$$E_0 < E_1 < \cdots < \Sigma.$$

This assumption is satisfied for a large class of potentials including many-body Coulomb potentials (see e.g. [25]).

The Hamiltonian $H(e)$ defined in (1.1) is self-adjoint under the above assumption on the potential $V(x)$ and under assumption (2.5) on the coupling function G_x. This is proven by using diamagnetic-type inequalities or by considering the semigroup $e^{-H(e)t}$. It was shown in [3] that for $|e| = \sum |e_j|$ sufficiently small, it is self-adjoint on the domain $D(H(e)) = D(H(0))$. The self-adjointness of the Hamiltonian H, defined in (2.7)–(2.9), on the domain $D(H) = D(H_0)$, for g sufficiently small, follows from a result of a result of [3] (see Eqn (4.10) of Section 4).

In what follows, $E_\Delta(H)$ stands for the spectral projection function of a self-adjoint operator H associated with an interval Δ, while $\chi_{\lambda\in\Omega}$, for the characteristic function of a set Ω (thus $E_\Delta(H) = \chi_{H\in\Delta}$). Below, we make use of the following exponential decay estimate proven in [3]: If $\phi \in C_0^\infty$, with $\text{supp}\phi \subset \left(-\infty, \Sigma - g^2 \sup_x \int \frac{|G_x|^2}{\omega}\right)$, then

$$\|e^{\alpha|x|}\phi(H)\| \leq C_\alpha , \tag{2.10}$$

for α sufficiently small $\left(\alpha < \Sigma - \sup \text{supp}\phi - g^2 \sup_x \int \frac{|G_x|^2}{\omega}\right)$. Since the operators H_f and

$[H, x]$ are H-bounded, Eqn 2.10 implies that

$$\|\langle x\rangle^M \otimes (H_f + 1)\phi(H)\| < \infty \text{ for any } M \geq 0\,. \tag{2.11}$$

3 Results

First we formulate the restrictions on the coupling functions $G_x = G_x(k)$ used in this paper:

$$\sup_x \left\{ \int \frac{|G_x(k)|^2}{\omega(k)}\, d^3k \;+\; \langle x\rangle^{-M} \int \frac{\left|(k\cdot\nabla_k)G_x(k)\right|^2}{\omega(k)}\, d^3k \right\} < \infty. \tag{3.1}$$

and

$$\sup_x \langle x\rangle^{-M} \sum_{n=1}^{2} \int (1 + \omega(k)^{-1})|(k\cdot\nabla)^n G_x(k)|^2 d^3k < \infty \tag{3.2}$$

for some $M \geq 0$.

In order to simplify somewhat the technical part of the paper we assume that

$$\sup_{x,k} \langle k\rangle^2 \langle x\rangle^{-M} |(\hat{k}\cdot\nabla_k)^n G_x(k)| < \infty\ , \tag{3.3}$$

where $\hat{k} = k\cdot|k|^{-1}$, for some $M \geq 0$ and for $n = 0, 1$, and that

$$g(\rho) := \sup_x \left(\int_{\omega\leq\rho} \frac{|G_x|^2}{\omega} \right)^{1/2} \leq C\rho^{1/2}\,. \tag{3.4}$$

Let E^i and ψ^{is}_{part}, $s = 1, \ldots, m_i$, be the eigenvalues and corresponding eigenfunctions of H_{part}, where $i = 0, 1, \ldots,$ and $E^0 < E^1 < \ldots$. For $i, j \geq 0$, we assume that $\int_{|k|=\omega} (A_{ij})^* A_{ij} dS_\omega$ is continuous in ω and vanishes at $\omega = 0$. Here A_{ij} are the $m_i \times m_j$ matrices with the entries $g\langle\psi^{i\ell}_{\text{part}}, G_x\psi^{jr}_{\text{part}}\rangle$, in the case of the Hamiltonian H, and $\langle\psi^{i\ell}_{\text{part}}, \sum_{a=1}^{N} \frac{e_a}{m_a} p_a^\perp G_{x_a}\psi^{jr}_{\text{part}}\rangle$, $p^\perp = p - (p\cdot\hat{k})\hat{k}$, with $\hat{k} = \frac{k}{|k|}$ (the projection of p onto the plane, $k^\perp$, perpendicular to k), in the case of the Hamiltonian $H(e)$, $\ell = 1, \ldots, m_i$ and $r = 1, \ldots, m_j$, and dS_ω is the area element on the sphere $\{k \in \mathbb{R}^3 \mid |k| = \omega\}$. For $j \geq 1$ (i.e., for excited states ψ^{js}_{part}), we define the self-adjoint matrix $,_j$ by

$$,_j \;=\; \sum_{i:E^i<E^j} \int (A_{ij})^* A_{ij}\, \delta(\omega - E^{ji})\, d^3k, \tag{3.5}$$

where $E^{ji} = E^j - E^i$. The eigenvalues of this matrix are the resonance widths to second order in the coupling constant, associated with the eigenvalue E^j, what is known in quantum mechanics as Fermi's Golden Rule. We assume that

$$\delta_j \;=\; \liminf_{|\lambda|\to 0}(\lambda^{-2},\, {}_j) \;>\; 0\,, \tag{3.6}$$

where $\lambda = g$ in the case of the Hamiltonian H and $|e| = \max_i |e_i|$, in the case of the Hamiltonian $H(e)$.

The main result of this paper is the following theorem.

Theorem 3.1 *Assume (3.1)-(3.4) and (3.6). Let $j \geq 1$. Then for $|e|$ sufficiently small, the spectrum of $H(e)$ in any interval containing E^j, but not containing any other part of the spectrum of $H_{\rm part}$, and whose distance to $\operatorname{spec} H_{\rm part} \cap (-\infty, E^j)$ is $\gg |e|$, is purely absolutely continuous. Moreover, in such an interval, $H(e)$ has the local decay property (formulated below). A similar statement, but with $|e|$ replaced by g, holds for H.*

The first statement of the theorem was proved in [2, 3, 4] under additional assumptions of analyticity of G_x and $\int \sup_x \frac{|G_x|^2}{\omega^{1+\beta}} < \infty$ for some $\beta > 0$, which is a stronger condition in the infrared region, $k \to 0$, than the one we require in this paper.

Next, we formulate the local decay property mentioned in Theorem 3.1. To this end, we introduce the anti-self-adjoint operator

$$-A \;=\; \mathbf{1}_{\rm part} \otimes \frac{1}{2}\int a^*(k)\Big(k\cdot\nabla_k + \nabla_k\cdot k\Big)a(k)\, d^3k\,. \tag{3.7}$$

This operator is a second quantization of the generator of dilatations in the one-photon momentum space, i.e., of $\frac{1}{2}(k\cdot\nabla_k + \nabla_k\cdot k)$. In what follows, whenever no danger of confusion arises, we omit the trivial factors $\mathbf{1}_{\rm part}\otimes$ and $\otimes\mathbf{1}_f$. We say that H has the *local decay property* in a spectral interval Δ (with respect to an operator A), if the following estimate holds

$$\int_{-\infty}^{\infty} \left\| \langle A\rangle^{-\alpha}\, e^{-iHt}\psi \right\|^2 dt \;\leq\; C_\alpha \,\|\psi\|^2\,, \tag{3.8}$$

for any $\alpha > 1/2$ and any $\psi \in \operatorname{Ran}\chi_{H\in\Delta}$. (In fact, a slightly stronger property, the limiting absorption principle with Hölder constant $\theta < \alpha - \frac{1}{2}$, holds in our case.)

Theorem 3.1 follows from a positive commutator estimate derived below (Theorem 5.2) and from the Kato-Mourre theory mentioned in the introduction and expounded upon in Section 5. We prove only the part of Theorem 3.1 concerning the operator H. The corresponding part for the operator $H(e)$, given in (1.1), is proven in exactly the same way, using some simple additional estimates related to the quadratic part $\sum \frac{e_j^2}{2m_j} A(x_j)^2$ of the perturbation $H(e) - H(0)$.

We note that absolute continuity of the spectrum and the local decay property outside of $O(g^2)$- (resp. $O(|e|^2)$-) neighbourhoods of the eigenvalues and thresholds of $H_{\rm part}$ has been proven in [3].

Remark 3.2 *The requirement that g is small is not completely satisfactory, since if we, remembering the origin of G_x in (2.3), take $G_x(k) = \frac{\kappa(k)}{\sqrt{\omega(k)}} e^{-ik\cdot x}$ and $\kappa(k) = K^{-1/2}\kappa_0(k/K)$, then*

$$\langle x\rangle^{-2} \int \frac{|k\cdot\nabla_k G_x(k)|^2}{\omega(k)} d^3k = O(K^2) \tag{3.9}$$

for large K. However, the operator $\langle x\rangle^{-M/2} k\cdot\nabla_k$ in conditions (3.1)–(3.2) on the coupling function $G_x(k)$ can be replaced by the operator $k\cdot\nabla_k - x\cdot\nabla_x$. This is done by replacing in our analysis the key operator A, given in (3.7), by the operator

$$\begin{aligned} -A' &= \mathbf{1}_{\rm part} \otimes \frac{1}{2} \int a^*(k)(k\cdot\nabla_k + \nabla_k\cdot k)a(k)d^3k \\ &\quad -\Big[\frac{1}{2}(x\cdot\nabla_x + \nabla_x\cdot x)\otimes \mathbf{1}_f\Big]. \end{aligned} \tag{3.10}$$

Given standard additional conditions on $V(x)$ (see e.g. [6, 13]), most of the analysis given below goes without a change. The advantage of the modified conditions on G_x is in the fact that they do not require the ultraviolet cut-off K to be small in the case of interest: $G_x(k) = \frac{\kappa(k)}{\sqrt{\omega(k)}} e^{-ik\cdot x}$ with $\kappa(k) = K^{-\frac{1}{2}}\kappa_0(k/K)$. Indeed, in this case, e.g.

$$\sup_x \int \frac{|(k\cdot\nabla_k - x\cdot\nabla_x)G_x(k)|^2}{\omega(k)} d^3k = O(1) \tag{3.11}$$

instead of (3.9). Moreover, if, abstracting properties of $G_x(k) = \frac{\kappa(k)}{\sqrt{\omega(k)}} e^{-ik\cdot x}$, we assume that G_x satisfies

$$\sum_{n=0}^{1} \sup_x \int \frac{|(k\cdot\nabla_k - x\cdot\nabla_x)^n G_x(k)|^2}{\omega(k)} d^3k < \infty, \tag{3.12}$$

instead of (3.1), and a corresponding relation replacing (3.2), then the analysis presented in Section 5 below simplifies considerably (see also Remark 5.7).

In what follows we *absorb the paremeter g into the coupling function $G_x(k)$.*

4 Relative Bounds on the Interaction

In this section we collect some elementary bounds needed for the proof of Theorem 3.1. In what follows, by $H_f^{-1/2}$ we always understand $H_f^{-1/2}\overline{P}_\Omega$, where $\overline{P}_\Omega$ is the projection onto the orthogonal complement of the vacuum state Ω in Fock space.

Lemma 4.1 *(Relative bounds)*

$$\|a(f)\psi\|_{\text{Fock}} \;\le\; \left(\int \frac{|f|^2}{\omega}\right)^{1/2} \left\|(H_f)^{1/2}\psi\right\|_{\text{Fock}} \tag{4.1}$$

and

$$\|a^*(f)\psi\|^2_{\text{Fock}} \;\le\; \left(\int \frac{|f|^2}{\omega}\right) \left\|(H_f)^{1/2}\psi\right\|^2_{\text{Fock}} + \left(\int |f|^2\right) \|\psi\|^2_{\text{Fock}} . \tag{4.2}$$

Proof: We drop the subindex "Fock" in the proof. By Schwarz' inequality we have

$$\|a(f)\psi\| \;\le\; \int |f(k)|\,\|a(k)\psi\| \;\le\; \left(\int \frac{|f|^2}{\omega}\right)^{1/2} \left(\int \omega(k)\,\|a(k)\psi\|^2\right)^{1/2} . \tag{4.3}$$

Thanks to

$$\int \omega(k)\,\|a(k)\psi\|^2 \;=\; \langle\psi,\, H_f\psi\rangle \;, \tag{4.4}$$

this implies (4.1). Inequality (4.2) follows from

$$a(f)a^*(f) \;=\; a^*(f)a(f) \,+\, \langle f,\, f\rangle \mathbf{1} \,, \tag{4.5}$$

$\langle\psi,\, a^*(f)a(f)\psi\rangle = \|a(f)\psi\|^2$ and (4.1). ∎

We rewrite bound (4.1) as

$$\left\|a(f)\, H_f^{-1/2}\right\|_{\text{Fock}} \;\le\; \left(\int \frac{|f|^2}{\omega}\right)^{1/2} , \tag{4.6}$$

$$\left\|H_f^{-1/2}\, a^*(f)\right\|_{\text{Fock}} \;\le\; \left(\int \frac{|f|^2}{\omega}\right)^{1/2} . \tag{4.7}$$

These two bounds are equivalent, since the expressions under the norm signs are adjoint to each other. Moreover, (4.1) implies that

$$\pm\langle a^*(f) + a(f)\rangle_\psi \;\le\; 2\left(\int \frac{|f|^2}{\omega}\right)^{1/2} \left\|H_f^{1/2}\psi\right\| \cdot \|\psi\| \,, \tag{4.8}$$

which yields

$$\pm\Big(a^*(f) + a(f)\Big) \;\le\; \alpha H_f \,+\, \frac{1}{\alpha}\int \frac{|f|^2}{\omega} \,, \tag{4.9}$$

for any $\alpha > 0$. Furthermore, inequalities (4.1) and (4.2) imply

$$\left\| \left(a^*(f) + a(f)\right)\psi \right\| \leq \left(\int |f|^2\right)^{1/2} \|\psi\| + 2\left(\int \frac{|f|^2}{\omega}\right)^{1/2} \left\|H_f^{1/2}\psi\right\|. \tag{4.10}$$

Eqn. (4.9) implies that I is H_f form-bounded with relative bound zero, provided (2.5) holds, while Eqn. (4.10) implies that I is $H_f^{1/2}$-bounded with relative bound $2\sup_x\left(\int \frac{|G_x|^2}{\omega}\right)^{1/2}$, provided (2.5) holds. The latter of these two statements implies that, if (2.5) is satisfied, then H is self-adjoint on the domain of H_f.

To develop more refined bounds we need Pull-through formulae (see [2, 3])

$$a(k)g(H_f) = g(H_f + \omega(k))a(k) \tag{4.11}$$

and

$$g(H_f)a^*(k) = a^*(k)g(H_f + \omega), \tag{4.12}$$

valid for any piecewise continuous and bounded function g. (These formulae follow from the following commutation relation

$$a(k)H_f = (H_f + \omega(k))a(k) \tag{4.13}$$

and its adjoint.)

Now if $\psi = \chi_{H_f \leq \rho}\psi$, then

$$\begin{aligned} \|a(k)\psi\|_{\text{Fock}} &= \|\chi_{H_f+\omega(k)\leq\rho}a(k)\psi\|_{\text{Fock}} \\ &\leq \chi_{\omega(k)\leq\rho}\|a(k)\psi\|_{\text{Fock}} . \end{aligned} \tag{4.14}$$

Using this in (4.3) we obtain instead of (4.1) (or (4.6))

$$\int |f(k)|\|a(k)\chi_{H_f\leq\rho}\|_{\text{Fock}} \leq \left(\int_{\omega\leq\rho} \frac{|f|^2}{\omega}\right)^{1/2} \cdot \rho^{1/2} . \tag{4.15}$$

These estimates can be extended to products of several annihilation or creation operators. Namely, relation (4.11) and a property of characteristic functions imply that

$$\left(\prod_1^m a(k_j)\right)\chi_{H_f\leq\rho} = \prod_1^m \left(a(k_j)\chi_{H_f\leq\rho}\right) . \tag{4.16}$$

Applying estimate (4.15) to each factor on the r.h.s., we find

$$\int \prod{}^{\otimes} |f_j| \|(\prod_1^m a(k_j))\chi_{H_f\leq\rho}\| \leq \prod_1^m \left(\int_{\omega\leq\rho} \frac{|f_j|^2}{\omega}\right)^{1/2} \rho^{m/2} \tag{4.17}$$

and similarly for certain operators:

$$\int \prod^{\otimes} |f_j| \|\chi_{H_f \le \rho}(\prod_1^m a(k_j))\| \le \prod_1^m \left(\int_{\omega \le \rho} \frac{|f_j|^2}{\omega} \right)^{1/2} \rho^{m/2} . \tag{4.18}$$

5 Positive Commutators

In this section we formulate our key technical result. In the following, when we speak of a communtator of two, in general unbounded, operators, H and A, we understand that $D(H) \cap D(A)$ is dense, and $[H, A]$ is defined first as a form on $D(H) \cap D(A)$ and then extended to a bounded or unbounded operator.

We fix $j \ge 1$ once and for all. Let $P_{\text{part}} = P^j_{\text{part}}$ be the orthogonal projection onto the eigenspace of H_{part} corresponding to the eigenvalue E^j. For a fixed energy scale ρ, we define the projection operator

$$P \;=\; P_{\text{part}} \otimes \chi_{H_f \le \rho} \tag{5.1}$$

and $\overline{P} = \mathbf{1} - P$. We define a family of operators

$$A_V \;=\; A + \overline{P} V P - P V^* \overline{P} , \tag{5.2}$$

where A is the second quantized dilatation generator defined in (3.7), and

$$V \;=\; \theta \overline{R}_\varepsilon^2 I , \qquad \overline{R}_\varepsilon \;=\; R_\varepsilon \overline{P} , \tag{5.3}$$

for positive constants θ and ε to be chosen below, where

$$R_\varepsilon \;=\; \left[(H_0 - E^j)^2 + \varepsilon^2 \right]^{-1/2} . \tag{5.4}$$

Note that $\varepsilon R_\varepsilon^2 \to \delta(H_0 - E^j)$, as $\varepsilon \to 0$. We note also that A_V depends on four parameters, g, ε, θ and ρ.

Lemma 5.1 *The commutator $[H, A_V]$ can be defined as a quadratic form on the dense set $D(H_0) \cap D(A)$ and can be extended from there to a $(\langle x \rangle^M \otimes H_f)$-bounded operator. Moreover, for any $\phi \in C_0^\infty$ with $\operatorname{supp} \phi \subset \left(-\infty, \Sigma - \sup_x \int \frac{|G_x|^2}{\omega} \right)$ the operator*

$$\phi(H)[H, A_V] \textit{ is bounded.} \tag{5.5}$$

Proof: The first statement of the lemma follows from the relations $D(H) = D(H_0)$ and $D(A_V) = D(A)$. The second of these two relations is due to the fact that the operator $A_V - A$ is bounded.

To prove the second statement we observe that, by a direct computation, $e^{\theta A}$, $\theta \in \mathbb{R}$, maps $D(H) = D(H_0)$ into itself and therefore, in a sense of quadratic forms,

$$[H, A] = \frac{\partial}{\partial\theta}\Big|_{\theta=0} H_\theta, \tag{5.6}$$

where $H_\theta = e^{-\theta A} H e^{\theta A}$. A direct computation (see Eqn (5.18) below) and Lemma 4.1 show that the r.h.s. of this equality is a $(\langle x\rangle^M \otimes H_f)$-bounded operator. Hence $[H, A]$ extends to a $(\langle x\rangle^M \otimes H_f)$-bounded operator. Furthermore, due to definition (5.1)–(5.4), $A_V - A$ is a bounded operator mapping $\mathcal{H} = \mathcal{H}_{\text{part}} \otimes \mathcal{F}$ into $D(H)$, so $[H, A_V - A]$ is well defined. As can be easily shown, it is a bounded operator. Hence $[H, A_V]$ extends to a $(\langle x\rangle^M \otimes H_f)$-bounded operator. Finally, the third statement follows from the second one and estimate (2.11). ∎

Observe that it is not hard to show that the operator $[H, A_V]$ is self-adjoint. Hence taking adjoints in (5.5) once concludes that also the operator

$$[H, A_V]\phi(H) \text{ is bounded.} \tag{5.7}$$

Let Δ be an energy interval containing E^j but no other parts of the spectrum of H_{part}, and let

$$\theta_1 \;=\; \inf\Delta \;-\; \sup\Big\{\sigma(H_{\text{part}}) \cap (-\infty, \inf\Delta)\Big\} \;>\; 0\,, \tag{5.8}$$

i.e., the distance, θ_1, of $\inf\Delta$ to the part of the spectrum of H_{part} below Δ is assumed to be positive. The key technical result of this paper is

Theorem 5.2 *Assume that Conditions (3.1)-(3.4) and (3.6) hold, and let, for simplicity, the parameters* ε, θ, *and* ρ *in (5.1)–(5.4) satisfy the inequalities* $\varepsilon \le \rho \le \theta_1$ *and* $\varepsilon \le \theta$. *If* γ_j *is the smallest eigenvalue of* Γ_j *and* $\alpha = O\left(\varepsilon\theta^{-1} + \theta\varepsilon\rho^{-2} + \theta_1^{-1}\theta\rho^2\varepsilon^{-2} + \theta g^2\varepsilon^{-2}\rho^{-1} + g\right) + o_\varepsilon(1)$, *then*

$$E_\Delta(H)\,[H, A_V]\,E_\Delta(H) \;\ge\; \frac{\theta(2-\alpha)\,\gamma_j}{\varepsilon}\,E_\Delta(H)^2\,. \tag{5.9}$$

(Here $o_\varepsilon(1) \to 0$, *as* $\varepsilon \to 0$, *and* Γ_j *is the matrix introduced in (3.5).)*

This theorem is proven in Section 7.

Since $g \ll \theta_1$, we can pick the parameters ε, θ and ρ in (5.1)–(5.4) satisfying the inequalities

$$\sqrt{\frac{\theta}{\theta_1}}\rho \ll \varepsilon \ll \theta \ , \qquad \theta\varepsilon \ll \rho^2 \leq \theta_1^2 \ , \tag{5.10}$$

and

$$g \ll \theta^{-1/2}\varepsilon\rho^{1/2} \ . \tag{5.11}$$

Then the parameter α in (5.9) is much smaller than 1 and therefore the r.h.s. is strictly positive on $\operatorname{Ran} E_\Delta(H)$. In what follows we assume that conditions (5.10)–(5.11) are satisfied.

Before proceeding any further we derive the most important consequence of this theorem—the instability of the eigenvalue E^j.

Theorem 5.3 *(Virial theorem) Let the conditions of Theorem 5.2 be satisfied. If* ψ *is an eigenfunction of the operator* H *with an eigenvalue* $E < \Sigma - \sup_x \int \frac{|G_x|^2}{\omega}$, *then* ψ *is in the domain of* $[H, A_V]$ *and*

$$\langle \psi, [H, A_V]\psi \rangle = 0. \tag{5.12}$$

Consequently, in view of Theorem 5.2, H *has no eigenvalues in any interval* Δ *containing only one eigenvalue of* H_{part} *and satisfying* $\theta_1 \gg g^2$ *with* θ_1 *defined in (5.8).*

Proof: Let $g_1 \in C_0^\infty(\mathbb{R})$, be real, be supported in $(-\infty, \Sigma - \sup_x \int \frac{|G_x|^2}{\omega})$ and satisfy $g_1(E) = 1$. Then $g_1(H)\psi = \psi$, so (5.12) is equivalent to the relation

$$\langle \psi, [g(H), A_V]\psi \rangle = 0 \ , \tag{5.13}$$

where $g(\lambda) := (\lambda - E)g_1(\lambda)$. Note $g(H)\psi = 0$. Since we do not know whether $\psi \in D(A_V)$, we must understand the commutator on the l.h.s. of (5.13) as an operator resulting once the commutation is performed. Now we claim that

$$[A, g(H)] \text{ is bounded} \ . \tag{5.14}$$

Indeed, let $\bar{g} \in C_0^\infty$ be s.t. $\bar{g}g = g$ and $\operatorname{supp}\bar{g} \subset \left(-\infty, \Sigma - \sup_x \int \frac{|G_x|^2}{\omega}\right)$. The proof of (5.14) will follow from the following formula

$$\begin{aligned}[A, g(H)] = &\int d\tilde{g}(z)(z - H)^{-1}[A, H]\bar{g}(H)(z - H)^{-1} \\ &+ \int d\tilde{\bar{g}}(z)(z - H)^{-1}g(H)[A, H](z - H)^{-1} \ ,\end{aligned} \tag{5.15}$$

understood in the sense of quadratic forms on $D(A)$. Here we use the notation and definitions of Appendix B of [14]. Indeed, the l.h.s. is defined as a quadratic form on $D(A)$ by $\langle\psi,[A,g(H)]\psi\rangle = 2\mathrm{Re}\langle g(H)\psi, A\psi\rangle$, while the r.h.s. represents a bounded operator in virtue of (5.5) and (5.7) and with $V=0$ and estimates (B.6) of [14] on $\tilde{g}$ and $\tilde{\bar{g}}$.

Thus it suffices to prove the representation above. To this end we use the formula

$$\partial_\theta|_{\theta=0}\langle\psi, e^{-\theta A}g(H)e^{\theta A}\psi\rangle = \partial_\theta|_{\theta=0}\langle\psi, e^{-\theta A}g(H)e^{\theta A}\bar{g}(H)\psi\rangle$$
$$+\partial_\theta|_{\theta=0}\langle\psi, g(H)e^{-\theta A}\bar{g}(H)e^{\theta A}\psi\rangle\ . \tag{5.16}$$

It suffices to consider one of the terms on the r.h.s., say the first one. To this end we use the Helffer-Sjöstrand formula

$$g(H) = \int d\tilde{g}(z)(z-H)^{-1}$$

(see [14]) to obtain

$$\partial_\theta|_{\theta=0}\langle\psi, e^{-\theta A}g(H)e^{\theta A}\bar{g}(H)\psi\rangle = \partial_\theta|_{\theta=0}\int d\tilde{g}(z)\langle\psi,(z-H_\theta)^{-1}\bar{g}(H)\psi\rangle\ , \tag{5.17}$$

where, recall, $H_\theta = e^{-\theta A}He^{\theta A}$ and is given by an explicit formula

$$H_\theta = H_{\text{part}}\otimes\mathbf{1}_f + \mathbf{1}_{\text{part}}\otimes e^{-\theta}H_f + I_\theta$$

with $I_\theta = a^*(G_{x,\theta}) + a(G_{x,\theta})$, $G_{x,\theta}(k) = e^{-\frac{3\theta}{2}}G_x(e^{-\theta}k)$.

It is not difficult to see that the operator function $(z-H_\theta)^{-1}\bar{g}(H)$ is differentiable in θ at $\theta=0$: due to (5.7) with $V=0$,

$$\frac{1}{\theta}[(z-H_\theta)^{-1}-(z-H)^{-1}]\bar{g}(H) = (z-H_\theta)^{-1}\frac{1}{\theta}(H_\theta-H)\bar{g}(H)(z-H)^{-1}$$
$$\to (z-H)^{-1}[H,A]\bar{g}(H)(z-H)^{-1}$$

as $\theta\to 0$, in the operator norm. Taking this into account and taking the θ-derivative under the sign of integral in (5.17) we arrive at

$$\partial_\theta|_{\theta=0}\langle\psi, e^{-\theta A}g(H)e^{\theta A}\bar{g}(H)\psi\rangle = \int d\tilde{g}(z)\langle\psi,(z-H)^{-1}[A,H]\bar{g}(H)(z-H)^{-1}\psi\rangle\ .$$

The last equation together with a similar equation for the second term in (5.16) yields (5.15). As was already mentioned Eqn (5.15) together with Eqns (5.5) and (5.7) for $V=0$ yields (5.14).

Eqn (5.14) implies that $[A_V, g(H)]$ is also bounded.

In order to write the l.h.s. of (5.13) as a quadratic form, which is what we ultimately need for the proof, we proceed in a standard way by approximating it as follows

$$\langle\psi, [g(H), A_V]\psi\rangle = \lim_{\lambda\uparrow\infty} \langle\psi_\lambda, [g(H), A_V]\psi_\lambda\rangle,$$

where $\psi_\lambda = R_\lambda\psi$, $R_\lambda = i\lambda(i\lambda + A)^{-1}$. (Note that $\psi_\lambda \to \psi$ as $\lambda \to \infty$.) Since $\psi_\lambda \in D(A) = D(A_V)$ we can write

$$\langle\psi_\lambda, [g(H), A_V]\psi_\lambda\rangle = 2\mathrm{Re}\langle g(H)\psi_\lambda, A_V\psi_\lambda\rangle.$$

Since $g(H)\psi = 0$ and $[g(H), R_\lambda] = i\lambda(i\lambda + A)^{-1}[A, g(H)](i\lambda + A)^{-1}$ (in a sense of quadratic forms), we have

$$g(H)\psi_\lambda = R_\lambda[A, g(H)](i\lambda + A)^{-1}\psi.$$

Hence, since (5.14), $\|R_\lambda\| \leq 1$ and $\|(i\lambda + A)^{-1}\psi\| \leq \frac{1}{\lambda}\|\psi\|$, we have

$$\|g(H)\psi_\lambda\| \leq \frac{1}{\lambda}\|[A, g(H)]\|\|\psi\|.$$

Consequently,

$$\langle\psi_\lambda, [g(H), A_V]\psi_\lambda\rangle \ \to \ 0$$

as $\lambda \to \infty$, so (5.12) follows. ∎

To deduce the statements of Theorem 3.1, about absolute continuity and local decay, from Theorem 5.2, we use an abstract Kato-Mourre theory. A standard variant of this theory (see, e.g., [1, 6, 13, 20, 23]) requires H-boundedness of the commutators $[A_V, H]$ and $\big[A_V, [A_V, H]\big]$. In our case, these commutators are not H-bounded for two reasons.

First, under Condition (3.1), $[A, H]$ and $\big[A, [A, H]\big]$ are H-bounded only for $M = 0$, where M is the exponent appearing in (3.1). This follows from the straightforward computation (justified in the proof of Lemma 5.5 below)

$$\mathrm{ad}_A^n(H) = H_f + a^*((k\cdot\nabla_k + \frac{3}{2})^n G_x) + a((k\cdot\nabla_k + \frac{3}{2})^n G_x)\,, \tag{5.18}$$

where we used the standard notation $\mathrm{ad}_A(H) = [H, A]$ (see, however, Remarks 3.2 and 5.7).

The second reason is that the second part of the operator A_V (see Eqns (5.2)–(5.4)) contains the projection $\chi_{H_f\leq\rho}$, entering in the definition of P, and this operator, not being differentiable in H_f, has a very singular commutator with the dilatation generator A (or any other operator not commuting with H_f).

To remedy the first problem, we weaken the conditions used in Mourre theory (see Lemmata 5.5 and 5.6 below).

We go around the second problem by replacing A_V by a smooth version, as follows. In definition (5.2)–(5.4) of the operator A_V, we replace the projection P by the projection P_s, where

$$P_s \;=\; P_{\text{part}} \otimes \chi_{H_f \le s\rho} \; . \tag{5.19}$$

Thus, we just vary the photon energy scale a little. Denote the resulting operator by $A_{V,s}$. Let μ be a non-negative function supported in the interval $[1,2]$ and satisfying $\int \mu = 1$. Define

$$A_V^{(av)} := \int \mu(s)\; A_{V,s}\; ds\; . \tag{5.20}$$

The next two lemmas establish the desired properties of $A_V^{(av)}$.

Lemma 5.4 *Theorem 5.2 holds if we replace A_V by $A_V^{(av)}$.*

Proof: Inequalities (5.10)–(5.11) still hold true if we replace ρ by $s\rho$ with $1 \le s \le 2$. Hence (5.9) holds after A_V is replaced by $A_{V,s}$, for $1 \le s \le 2$. Since $\mu \ge 0$ and $\int \mu = 1$, this implies (5.9) with A_V replaced by $A_V^{(av)}$. ∎

Lemma 5.5 *Let $\phi \in C_0^\infty$ and $\text{supp}\phi \subset \left(-\infty, \Sigma - \sup_x \int \frac{|G_x|^2}{\omega}\right)$, where $\Sigma = \inf \sigma_{\text{cont}}(H_{\text{part}})$. Then the operators $[A_V^{(av)}, H]\phi(H)$ and $[A_V^{(av)}, [A_V^{(av)}, H]]\phi(H)$ are bounded.*

Proof: The boundedness of the first commutator follows from Lemma 5.1 (see also the sentence after Eqn (5.23)). To show the boundedness of the second commutator we write $A_V^{(av)} = A + Q$, where

$$Q := \int (\overline{P}_s V P_s - P_s V^* \overline{P}_s)\mu(s) ds\; . \tag{5.21}$$

We consider first the operator A and make sense of the formal computation (5.18). The case $n = 1$ was justified in the proof of Lemma 5.1. So we consider the case $n = 2$. Due to (5.14)

$$\phi(H):\; D(A) \to D(A). \tag{5.22}$$

Hence, due to (5.7), the commutator $[[H,A],A]$ is defined as a quadratic form on $\phi(H)D(A)$. The fact that $e^{\theta A}$, $\theta \in \mathbb{R}$, preserves $D(H) = D(H_0)$ and a simple computation shows that

$$\left.\frac{d^2}{d\theta^2}\right|_{\theta=0} H_\theta = [[H,A],A],$$

where, recall, $H_\theta := e^{-\theta A} H e^{\theta A}$, in a sense of quadratic forms. The l.h.s. of this equality can be evaluated explicitly: it is exactly the r.h.s. of (5.18). Applying Eqn. (4.10), with $f := \langle x\rangle^{-M}(k\cdot\nabla_k + \frac{3}{2})^n G_x$, to (5.18) and observing that Condition (3.1) guarantees that $\sup_x(\|f\| + \|\omega^{-1/2} f\|)$ is finite, we conclude that the operators $\mathrm{ad}_A^n(H)\langle x\rangle^{-M}$ are H_f-bounded for $n = 1, 2$. Hence, due to Eqn. (2.10),

$$\mathrm{ad}_A^n(H)\phi(H) \text{ are bounded for } n = 1, 2\,. \tag{5.23}$$

(Again, Q is a bounded operator, and Eqns. (5.2)–(5.4) show that so are the operators $H\cdot Q$ and $Q\cdot H$. Hence $[A_V^{(av)}, H]\phi(H)$ is bounded as was also shown above.)

Now we write

$$\begin{aligned} \Big[[H, A_V^{(av)}], A_V^{(av)}\Big] &= \Big[[H, A], A\Big] + \Big[[H, A], Q\Big] \\ &\quad + \Big[[H, Q], A\Big] + \Big[[H, Q], Q\Big]\,. \end{aligned} \tag{5.24}$$

By Eqn (5.23) and since Q and $[H, Q]$ are bounded, the first two terms and the last term on the r.h.s. of (5.24), multiplied by $\phi(H)$ on both sides, are bounded.

It remains to show that $\Big[[H, Q], A\Big]$, the third term on the r.h.s. of (5.24), times $\phi(H)$, is bounded. To this end, we want to use the Jacobi identity and rewrite this term as

$$\Big[[Q\,,\,H]\,,\,A\Big] \;=\; \Big[[A\,,\,Q]\,,\,H\Big] \;+\; \Big[Q\,,\,[A\,,\,H]\Big]\,. \tag{5.25}$$

To demonstrate this identity we prove it first for A replaced by the bounded operator $A_\lambda := A\cdot i\lambda(i\lambda + A)^{-1}$ and then take the limit $\lambda\to\infty$ for the quadratic forms. Now we demonstrate that $[A\,,\,Q]$ and $H\cdot[A, Q]$ are bounded. We write

$$[A\,,\,Q] \;=\; \theta(S \,+\, S^*)\,,$$

where

$$S \;=\; \Big[\,A\,,\,\int \mu(s)\,\overline{P}_s R_\varepsilon^2 I P_s\,\Big]\,.$$

We present S in the form

$$\begin{aligned} S &= \frac{d}{d\theta}\int \mu(s)\, e^{\theta A}\,\overline{P}_s\, R_\varepsilon^2\, I\, P_s\, e^{-\theta A}\, ds\Big|_{\theta=0} \\ &= \frac{d}{d\theta}\int \mu(s)\,\overline{P}_{se^{-\theta}}\, R_{\varepsilon,\theta}^2\, I_\theta\, P_{se^{-\theta}}\, ds\Big|_{\theta=0}\,, \end{aligned}$$

where $R_{\varepsilon,\theta} = e^{\theta A} R_\varepsilon e^{-\theta A}$, etc., and where we have used that $e^{\theta A} H_f e^{-\theta A} = e^\theta H_f$. Therefore

$$e^{\theta A}\, P_s\, e^{-\theta A} \;=\; P_{se^{-\theta}}\,.$$

Next, using Leibnitz' rule, we rewrite this relation as

$$\begin{aligned} S \;=\; & \int \mu(s)\, \overline{P}_s\, [A, R_\varepsilon^2]\, \overline{P}_s\, I\, P_s\, ds \;+\; \int \mu(s)\, \overline{P}_s\, R_\varepsilon^2\, [A, I]\, P_s\, ds \\ & + \int \mu(s)\, \frac{d}{d\theta}\Big(\overline{P}_{se^{-\theta}}\, R_\varepsilon^2\, I\, P_{se^{-\theta}} \Big)\, ds \Big|_{\theta=0}\,. \end{aligned}$$

Since $[A, H_0]$ and $[A, I]\langle x\rangle^{-M}$ are H_f-bounded, the first two terms on the r.h.s. are bounded. The last term on the r.h.s. can be rewritten as

$$-\int s\, \mu(s)\, \frac{d}{ds}\Big(\overline{P}_s\, R_\varepsilon^2\, I\, P_s \Big)\, ds \;=\; \int \frac{d(s\,\mu(s))}{ds}\, \overline{P}_s\, R_\varepsilon^2\, I\, P_s\, ds\,,$$

which shows that it is bounded, as well. Thus we proved that $[A, Q]$ is bounded. Using the above analysis and Eqns. (4.1) and (4.2), one shows that $H \cdot [A, Q]$ is bounded as well. Consequently, $[[A, Q], H]$ is bounded. Next, since $[A, H]$ is $(\langle x\rangle^M \otimes H_f)$-bounded and $Q(H_f + i)$ is bounded, remembering Eqn (2.10) and commuting $\langle x\rangle^{-M}$ through Q, if necessary, we conclude that $[Q, [A, H]]$ is bounded. Thus by identity (5.25), the boundedness of $[[Q, H], A]$ follows, which completes the proof of the lemma. ∎

In the next lemma, we slightly weaken the standard hypotheses of Mourre theory (see, e.g., [1, 6, 13, 20, 23]), in order to accommodate our situation (see Lemma 5.5).

Lemma 5.6 *Let H and iA be two self-adjoint operators, defined on the same Hilbert space, and let $\Delta \Subset \Delta' \subset\subset \mathbb{R}$ be intervals such that for any real $\phi \in C_0^\infty(\Delta')$, the operators $[H, A]$ and $[[H, A], A]$, defined originally as quadratic forms on the domains $D(H) \cap D(A)$ and $\phi(H)D(A)$, extend to unbounded operators satisfying*

$$[H, A]\phi(H) \text{ and } \phi(H)[[H, A], A]\phi(H) \text{ are bounded,} \tag{5.26}$$

$$\phi(H)[H, A]\phi(H) \geq \theta\phi(H)^2, \text{ for some } \theta > 0. \tag{5.27}$$

Then the spectrum of H in Δ is absolutely continuous and H has the local decay property in Δ with respect to the operator A.

The proof of this lemma follows, by now standard, arguments of [20, 23, 6]. For the reader's convenience it is given in Appendix A. (For a different proof see [15].)

Proof of Theorem 3.1: By Lemma 5.4, we have a positive commutator estimate as in (5.9), but with $A_V^{(av)}$ replacing A_V,

$$E_\Delta(H)\,[H, A_V^{(av)}]\,E_\Delta(H) \;\geq\; \frac{\theta(2-\alpha)\,\gamma_j}{\varepsilon}\,E_\Delta(H)^2\,, \tag{5.28}$$

and by Lemma 5.5, we know that, for any $\phi \in C_0^\infty$ with $\mathrm{supp}\phi \subset \left(-\infty, \Sigma - \sup_x \int \frac{|G_x|^2}{\omega}\right)$, the operators $[A_V^{(av)}, H]\phi(H)$ and $[A_V^{(av)}, [A_V^{(av)}, H]]\phi(H)$ are bounded. Thus Lemma 5.6 implies that the spectrum of H in Δ is absolutely continuous and that the local decay property holds w.r.t. $A_V^{(av)}$. To pass to the local decay property w.r.t. the operator A, it suffices to observe that, due to (4.10), Q is a bounded operator and therefore $\langle A\rangle^{-\alpha}\cdot\langle A_V^{(av)}\rangle^{\alpha} \leq \mathrm{const}$, for $\alpha > 0$. ∎

Remark 5.7 *The arguments presented above can be simplified if we use, from the beginning, the operator (3.10) instead of (3.7). Indeed, under assumptions which generalize the case of interest —* $G_x(k) = g\frac{\kappa(k)}{\sqrt{\omega(k)}}e^{-ik\cdot x}$ *— (see Remark 3.2), the coupling functions arising in the commutators* $[H, A']$ *and* $[[H, A'], A']$ *do not grow in* x *and therefore do not require* $\phi(H)$ *for bounding them.*

6 Positivity of the Truncated Commutator

Before tackling the proof of Theorem 5.2 head on, we go part of the way by proving the positivity of a simpler commutator. Namely, let

$$\overline{B}_{0,\Delta} \;=\; \overline{P}_\Delta\, B_0\, \overline{P}_\Delta\,, \tag{6.1}$$

where

$$B_0 \;=\; [\,H\,,\,A\,] \tag{6.2}$$

and

$$\overline{P}_\Delta \;=\; \overline{P}\,E_\Delta(H_0)\,. \tag{6.3}$$

Recall that Δ is an energy interval containing E^j but disjoint from the rest of the spectrum of H_{part}. The main result of this section is the following lemma.

Lemma 6.1 *Assume* $g^2 \ll \rho \leq \theta_1$. *Then*

$$\overline{B}_{0,\Delta} \;\geq\; \frac{1}{2}H_f\,\overline{P}_\Delta \;\geq\; \frac{1}{2}\rho\,\overline{P}_\Delta\,, \tag{6.4}$$

and, if in addition $3|z| \leq \rho$ *, then*

$$\left\| \, |\overline{B}_{0,\Delta} - z|^{-1/2} \, \overline{P}_\Delta \, \psi \right\| \;\leq\; 2 \left\| H_f^{-1/2} \, \overline{P}_\Delta \, \psi \right\|, \tag{6.5}$$

where $|A| := \sqrt{A^* A}$ *, for a closed operator* A *.*

Proof: We begin with a computation. For B_0 as in (6.2), we have by (5.15) with $n = 1$

$$B_0 \;=\; H_f \,+\, \widetilde{I}\,, \tag{6.6}$$

where $\widetilde{I} \;=\; a^*(\widetilde{G}_x) + a(\widetilde{G}_x)$, and

$$\widetilde{G}_x(k) \;:=\; k \cdot \nabla_k G_x(k) \;+\; \frac{3}{2} G_x(k)\,. \tag{6.7}$$

Inequality (4.9) with $\alpha = 1/4$ and $f = \widetilde{G}_x$ yields

$$\pm \widetilde{I} \;\leq\; \frac{1}{4} H_f \;+\; 4 \int \frac{|\widetilde{G}_x|^2}{\omega} \tag{6.8}$$

which implies

$$B_0 \;\geq\; \frac{3}{4} H_f \;-\; 4 \int \frac{|\widetilde{G}_x|^2}{\omega}\,. \tag{6.9}$$

Since $H_f \geq 0$, inequality (2.10) implies that

$$\left\| \langle x \rangle^M \, E_\Delta(H_0) \right\| \;\leq\; C_M \,, \tag{6.10}$$

for any $M < \infty$, provided $\sup\,\Delta < \inf \operatorname{cont\,spec} H_{\text{part}} - \sup_x \int \frac{|G_x|^2}{\omega}$. The last two inequalities imply that

$$\overline{B}_{0,\Delta} \;\geq\; \Big(\frac{3}{4} H_f \;-\; C g^2 \Big) \overline{P}_\Delta \,. \tag{6.11}$$

Next, definition (5.1) yields that

$$\overline{P} \;=\; \overline{P}_{\text{part}} \otimes \mathbf{1} \;+\; P_{\text{part}} \otimes \chi_{H_f \geq \rho}\,. \tag{6.12}$$

Since, by energy conservation,

$$\overline{P}_{\text{part}} \; E_\Delta(H_0) \;=\; \sum_{i:\, E^i < E^j} P^i_{\text{part}} \; E_\Delta(H_f + E^i)\,, \tag{6.13}$$

we have that

$$H_f \, \overline{P}_{\text{part}} \, E_\Delta(H_0) \;\geq\; \theta_1 \, \overline{P}_{\text{part}} \, E_\Delta(H_0)\,, \tag{6.14}$$

where θ_1 is given in (5.8). This yields

$$H_f\,\overline{P}_\Delta \;\geq\; \min(\theta_1,\rho)\,\overline{P}_\Delta \;=\; \rho\,\overline{P}_\Delta\,, \tag{6.15}$$

which, together with (6.11) and the condition $g^2 \ll \rho$, implies (6.4).

The proof of (6.5) is based on the following identity,

$$\left(\overline{B}_{0,\Delta} - z\right)^{-1} \;=\; H_f^{-1/2}\left(\mathbf{1} + K\right)^{-1} H_f^{-1/2}\,, \tag{6.16}$$

where

$$K \;=\; H_f^{-1/2}\,\overline{P}_\Delta\,(\widetilde{I} - z)\,\overline{P}_\Delta\,H_f^{-1/2}\,. \tag{6.17}$$

It suffices to prove that for $g^2 \ll \rho$,

$$\|K\| \;\leq\; \frac{1}{2}\,, \tag{6.18}$$

which would imply (6.5). To prove the latter inequality, we write $K \;=\; K_0 + K_1$, where

$$K_0 \;=\; -z\,H_f^{-1}\,\overline{P}_\Delta^2 \tag{6.19}$$

and

$$K_1 \;=\; H_f^{-1/2}\,\overline{P}_\Delta\,\widetilde{I}\,\overline{P}_\Delta\,H_f^{-1/2}\,. \tag{6.20}$$

Since $|z| \leq \rho/3$, we have that $\|K_0\| \leq 1/3$, due to (6.4). Next, using (6.7), inequality (4.6) with $f = \widetilde{G}_x$, and inequality (6.10) again, we arrive at

$$K_1 \;=\; H_f^{-1/2}\,\overline{P}_\Delta\,O(g) \;+\; O(g)\,\overline{P}_\Delta\,H_f^{-1/2}\,, \tag{6.21}$$

which, together with (6.15), yields that $\|K_1\| \;=\; O(\rho^{-1/2}g)$. Since $g^2 \ll \rho$ and since $\|K_0\| \leq 1/3$, this implies (6.18) which in turn yields (6.5). ∎

Now we boost this proposition to a more complicated result. Let

$$B_V \;:=\; [\,H\,,\,A_V\,] \quad \text{and} \quad \overline{B}_{V,\Delta} \;:=\; \overline{P}_\Delta\,B_V\,\overline{P}_\Delta\,. \tag{6.22}$$

Lemma 6.2 *Assume* $g^2 \ll \rho \leq \theta_1$ *and* $g \ll \varepsilon^{3/4}\rho^{1/2}$. *Then*

$$\overline{B}_{V,\Delta} \;\geq\; \frac{1}{2}\,H_f\,\overline{P}_\Delta \;\geq\; \frac{1}{2}\,\rho\,\overline{P}_\Delta\,, \tag{6.23}$$

and, if in addition $3|z| \leq \rho$, *then*

$$\left\|\,|\overline{B}_{V,\Delta} - z|^{-1/2}\,\overline{P}_\Delta\,\psi\,\right\| \;\leq\; 2\left\|\,H_f^{-1/2}\,\overline{P}_\Delta\,\psi\,\right\|. \tag{6.24}$$

Proof: By the definition of A_V, we have

$$\overline{B}_{V,\Delta} \;=\; \overline{B}_{0,\Delta} \;-\; E\,, \tag{6.25}$$

where, since $\overline{P}_\Delta P = P\overline{P}_\Delta = 0$,

$$\begin{aligned} E &= -\overline{P}_\Delta \left[I\,,\, \overline{P} V P - P V^* \overline{P} \right] \overline{P}_\Delta \\ &= \overline{P}_\Delta \, I \, P \, V^* \overline{P}_\Delta \;+\; h.c. \\ &= \theta \, \overline{P}_\Delta \, I \, P \, I \, R_\varepsilon^2 \, \overline{P}_\Delta \;+\; h.c.\,. \end{aligned} \tag{6.26}$$

We claim that

$$\|E\| \;\leq\; C\theta g^2 \varepsilon^{-3/2}\,. \tag{6.27}$$

Indeed, since $I = a^*(G_x) + a(G_x)$, estimates (4.6) and (4.7) imply that

$$\|\overline{P}_\Delta I P\| \;\leq\; Cg\,. \tag{6.28}$$

It remains to estimate the operator $PI\overline{R}_\varepsilon^2$. It is shown in Lemma 6.4 below that $\|PI\overline{R}_\varepsilon\| \leq cg\varepsilon^{-1/2}$. The last two estimates and the inequality $\|R_\varepsilon\| \leq \varepsilon^{-1}$ imply (6.27). The latter estimate together with (6.25) and (6.4) implies (6.23). Eqn. (6.24) is proven similarly to (6.5). ∎

Remark 6.3 *It suffices to prove an appropriate H_f-form bound on E, rather than the norm bound, Eqn (6.27). The former bound would improve our final estimates.*

Lemma 6.4 *We have*

$$\|PI\overline{R}_\varepsilon\| \leq Cg\varepsilon^{-1/2}\,. \tag{6.29}$$

Proof: We write

$$(\overline{R}_\varepsilon IP)^*(\overline{R}_\varepsilon IP) = PI\overline{R}_\varepsilon^2 IP \tag{6.30}$$

Next, we analyze the operator $I\overline{R}_\varepsilon^2 I$ restricted to $\mathrm{Ran}\,\chi_{H_f \leq \rho}$. To this end we need the Pull-through formulae (see (4.11) - (4.12))

$$a(k)\,\overline{R}_\varepsilon \;=\; \overline{R}_{\varepsilon,\omega(k)}\, a(k)\,, \tag{6.31}$$

$$\overline{R}_\varepsilon \, a^*(k) \;=\; a^*(k)\, \overline{R}_{\varepsilon,\omega(k)}\,, \tag{6.32}$$

where

$$\overline{R}_{\varepsilon,\omega} \;=\; \overline{R}_\varepsilon|_{H_f \to H_f + \varepsilon}\,. \tag{6.33}$$

Recalling (2.9) and pulling, in $I\overline{R}_\varepsilon^2 I = \Big(a^*(G_x) + a(G_x)\Big)\overline{R}_\varepsilon^2\Big(a^*(G_x) + a(G_x)\Big)$, the a 's to the right and the a^* 's to the left with the help of the Pull-through formulae (6.31) and (6.32), we obtain

$$I\,\overline{R}_\varepsilon^2\,I \;=\; M \;+\; L\,, \tag{6.34}$$

where

$$M \;=\; \int \overline{G_x}(k)\,\overline{R}^2_{\varepsilon,\omega(k)}\,G_x(k)\,d^3k \tag{6.35}$$

and, with $\omega_i = \omega(k_i)$,

$$\begin{aligned} L \;&=\; a^*(G_x)\,\overline{R}_\varepsilon^2\,a(G_x) \;+\; \iint \overline{G_x}(k_1)\,a^*(k_2)\,\overline{R}^2_{\varepsilon,\omega_1+\omega_2}\,a(k_1)\,G_x(k_2)d^3k_1d^3k_2 \\ &\quad+\; \int \overline{G_x}(k)\,\overline{R}^2_{\varepsilon,\omega(k)}\,a(k)\,a(G_x)d^3k \;+\; \text{adjoint}\,. \end{aligned} \tag{6.36}$$

Using that $\|\overline{R}_{\varepsilon,\omega}\| \le \varepsilon^{-1}$, we estimate the latter operator by

$$\begin{aligned} \Big\|\,\chi_{H_f\le\rho}\,L\,\chi_{H_f\le\rho}\Big\| \;&\le\; 2\varepsilon^{-2}\iint |G_x(k_1)G_x(k_2)|\;\|a(k_1)a(k_2)\chi_{H_f\le\rho}\| \\ &\quad+2\left(\varepsilon^{-1}\int |G_x(k)|\;\|a(k)\chi_{H_f\le\rho}\|\right)^2\,. \end{aligned} \tag{6.37}$$

Applying inequalities (4.17) and (4.18) to the r.h.s., we arrive at

$$\Big\|\,\chi_{H_f\le\rho}\,L\,\chi_{H_f\le\rho}\Big\| \;\le\; 4\varepsilon^{-2}\rho g(\rho)^2\,, \tag{6.38}$$

where, recall, $g(\rho) := \sup_x \left(\int_{\omega\le\rho} \frac{|G_x|^2}{\omega}\right)^{1/2}$. Since by our restrictions $g(\rho) \le Cg\sqrt{\rho}$, this in turn yields that, on $\operatorname{Ran}\chi_{H_f\le\rho}$,

$$I\,\overline{R}_\varepsilon^2\,I \;=\; M \;+\; O(\varepsilon^{-2}g^2\rho^2)\,. \tag{6.39}$$

Now it is not hard to convince oneself that

$$\|M\| \le Cg^2\varepsilon^{-1}\,. \tag{6.40}$$

Indeed, remembering expression (6.12) for $\overline{P}$, one can represent M as a sum of terms of the form

$$\int_0^\infty \frac{f_i(\omega)d\omega}{(\omega + H_f - E^{ji})^2 + \varepsilon^2},$$

where $f_i(\omega)$ are bounded by Cg^2 (in fact, decaying at ∞), continuous functions. Instituting the change of variable as $\omega \to \lambda = \varepsilon^{-1}(\omega + H_f - E^{ji})$, one shows easily that each integral is bounded by $Cg^2\varepsilon^{-1}$.

Estimates (6.30), (6.39) and (6.40) and the condition $\rho^2 \le \varepsilon$ imply (6.29). ∎

7 Proof of Theorem 5.2

First we estimate from below the following operator

$$B_{V,\Delta} \ := \ E_\Delta(H_0)\,[\,H\,,\,A_V\,]\,E_\Delta(H_0). \tag{7.1}$$

Using the definition of A_V (see Eqn. (5.2)), we write $B_{V,\Delta}$ as

$$B_{V,\Delta} \ = \ \overline{B}_{V,\Delta} \ + \ P_\Delta\, C^*\, \overline{P}_\Delta \ + \ \overline{P}_\Delta\, C\, P_\Delta \ + \ P_\Delta\, F\, P_\Delta\,, \tag{7.2}$$

where, in accordance with (5.2), (6.2), (6.3) and (6.22),

$$P_\Delta \ = \ P\,E_\Delta(H_0)\,, \tag{7.3}$$

$$C \ = \ [\,H - E^j\,,\,V] \ + \ B_0\,, \tag{7.4}$$

$$F \ = \ B_0 \ + \ V^*\,\overline{P}\,I \ + \ I\,\overline{P}\,V\,. \tag{7.5}$$

Here we used that, in virtue of the definition of V, we may identify $V \equiv \overline{P} V P$.

The key to the proof is the following inequality which follows from an application of the Feshbach projection method (a derivation is given in Appendix B):

$$\lambda_0 \ \geq \ \inf\ \mathrm{spec}\Big\{\mathcal{E} \restriction \mathrm{Ran}\, P_\Delta\Big\}\,, \tag{7.6}$$

where

$$\lambda_0 \ = \ \inf\ \mathrm{spec}\Big\{B_{V,\Delta} \restriction \mathrm{Ran}\, E_\Delta(H_0)\Big\} \tag{7.7}$$

and

$$\mathcal{E} \ = \ F \ - \ C^*\left(\overline{B}_{V,\Delta} - \lambda_0\right)^{-1} C\,. \tag{7.8}$$

We may assume here that $3\lambda_0 \leq \rho$; otherwise Theorem 5.2 follows readily from conditions (5.10)–(5.11) on the parameters. With this assumption, Lemma 6.2 is applicable and yields that $\left(\overline{B}_{V,\Delta} - \lambda_0\right)^{-1}$ is bounded on $\mathrm{Ran}\,\overline{P}_\Delta$. Hence (7.8) is well-defined.

Our task is to estimate $\mathcal{E}$ on $\mathrm{Ran}\,P_\Delta$ from below. The first term on the r.h.s. of (7.8) can be easily analyzed. Due to (5.3),

$$V^*\,\overline{P}\,I \ + \ I\,\overline{P}\,V \ = \ 2\theta\, I\, \overline{R}_\varepsilon^2\, I\,. \tag{7.9}$$

Next, Eqns. (6.6)–(6.10) imply that

$$P_\Delta\, B_0\, P_\Delta \ \geq \ \left(\frac{3}{4}\, H_f \ - \ C g^2\right) P_\Delta \ \geq \ -C g^2\, P_\Delta\,. \tag{7.10}$$

Hence, on $\operatorname{Ran} P_\Delta$

$$F \;\geq\; 2\theta\, I\,\overline{R}_\varepsilon^2\, I - Cg^2\,. \tag{7.11}$$

Next, we estimate from above the operator

$$G \;:=\; C^* \left(\overline{B}_{V,\Delta} - \lambda_0\right)^{-1} C\,, \tag{7.12}$$

on $\operatorname{Ran} P_\Delta$. A large part of the remainder of this section is devoted to this estimate.

As mentioned after Eqn. (7.8), Lemma 6.2 is applicable to (7.12). It yields

$$|\langle G\rangle_\psi| \;\leq\; 2\left\| H_f^{-1/2}\,\overline{P}_\Delta\, C\,\psi\right\|^2. \tag{7.13}$$

From now on, we assume that $\psi \in \operatorname{Ran} P$, which implies that $\overline{P}_\Delta\psi = 0$. This relation, the definition of C (Eqn. (7.4)), and Eqn. (6.6) imply that

$$\left\| H_f^{-1/2}\,\overline{P}_\Delta\, C\,\psi\right\| \;\leq\; \left\| H_f^{-1/2}\,\overline{P}_\Delta\, \widetilde{I}\,\psi\right\| \;+\; \left\| H_f^{-1/2}\,\overline{P}_\Delta\,[H - E^j\,,\, V]\,\psi\right\|, \tag{7.14}$$

where $V = \overline{P}VP = \theta\,\overline{R}_\varepsilon^2 IP$. To estimate the first term on the r.h.s. of (7.14), we use that $\widetilde{I} = a^*(\widetilde{G}_x) + a(\widetilde{G}_x)$ (see Eqn. (6.7)) and Eqns. (6.3) and (6.4), to obtain

$$\begin{aligned}\left\| H_f^{-1/2}\,\overline{P}_\Delta\, \widetilde{I}\,\psi\right\| \;&\leq\; \left\|\langle x\rangle^M\, E_\Delta(H_0)\right\|\cdot\left(\left\|\langle x\rangle^{-M} H_f^{-1/2}\, a^*(\widetilde{G}_x)\right\|\cdot\|\psi\|\right.\\ &\quad\left. +\;\rho^{-1/2}\left\|\langle x\rangle^{-M}\, a(\widetilde{G}_x)\, H_f^{-1/2}\right\|\left\|H_f^{1/2}\psi\right\|\right).\end{aligned} \tag{7.15}$$

Since $\left\|\langle x\rangle^M E_\Delta(H_0)\right\| \leq C_M$ and $\left\|H_f^{1/2}\psi\right\|$ is bounded by $\rho^{1/2}\|\psi\|$, we obtain from (4.6)-(4.7) that

$$\left\| H_f^{-1/2}\,\overline{P}_\Delta\, \widetilde{I}\psi\right\| \;\leq\; C\, g\|\psi\|\,. \tag{7.16}$$

It remains to estimate the second term on the r.h.s. of (7.14). Using the properties of P , $\overline{P}_\Delta$, and $H - E^j = (H_0 - E^j) + I$, we obtain that

$$H_f^{-1/2}\,\overline{P}_\Delta\,[H - E^j\,,\, V]\,P = \theta\sum_1^4 A_i \tag{7.17}$$

where

$$A_1 \;:=\; H_f^{-1/2}\overline{P}_\Delta(H_0 - E^j)\overline{R}_\varepsilon^2 IP\,, \tag{7.18}$$

$$A_2 \;:=\; -H_f^{-1/2}\overline{P}_\Delta\overline{R}_\varepsilon^2 IPH_f\,, \tag{7.19}$$

$$A_3 \;:=\; -H_f^{-1/2}\overline{P}_\Delta\overline{R}_\varepsilon^2 IPIP \tag{7.20}$$

and

$$A_4 \; := \; H_f^{-1/2}\overline{P}_\Delta I\overline{R}_\varepsilon^2 IP\,. \tag{7.21}$$

To estimate the first of these terms we use the expression $\overline{P}_\Delta$ (Eqns (6.3) and (6.12)) and the estimate $\|(H_0-E_j)R_\varepsilon\|\le 1$ to obtain

$$\begin{aligned}\|A_1\| \;&\le\; \|H_f^{-1/2}E_\Delta(H_0)\overline{P}_{\text{part}}\|\cdot\|\overline{R}_\varepsilon IP\|\\ &+\; \|P_{\text{part}}\otimes\chi_{H_f\ge\rho}R_\varepsilon\|\cdot\|H_f^{-1/2}IP\|\,.\end{aligned}$$

Now we use that, due to (4.6)–(4.7), $\|PIP\|\le 2g$, $\|PH_f\|\le\rho$,

$$\left\| H_f^{-1/2}\,\chi_{H_f\ge\rho}\,I\,P\right\| \;\le\; \left\|H_f^{-1/2}\,a^*(G_x)\right\| \;+\; \rho^{-1/2}\left\|a(G_x)\,P\right\| \;\le\; 2\,g \tag{7.22}$$

use inequality (6.29) and use the fact that $H_f\ge\theta_1$ on $\mathrm{Ran}(E_\Delta(H_0)\overline{P}_{\text{part}})$ to obtain

$$\|A_1\|\le C\theta_1^{-1/2}\varepsilon^{-1/2}g+2\rho^{-1}g \tag{7.23}$$

Similarly we have

$$\|A_2\|\le C\theta_1^{-1/2}\varepsilon^{-3/2}g\rho+2\rho^{-1}g \tag{7.24}$$

Next using the estimates $\|H_f^{-1/2}\overline{P}_\Delta\|\le 2\rho^{-1/2}$ (see (6.15)), $\|R_\varepsilon\|\le\varepsilon^{-1}$, (6.29) and $\|PIP\|\le g\sqrt{\rho}$, we find

$$\|A_3\|\le\varepsilon^{-3/2}g^2\,.$$

Now taking into account expressions (6.3) and (6.12) for $\overline{P}_\Delta$, we estimate $\|\overline{P}_\Delta H_f^{-1/2}\|\le C\rho^{-1/2}$. Next, using (4.6) and (4.7) we find

$$\begin{aligned}\|\overline{P}_\Delta H_f^{-1/2}I\overline{R}_\varepsilon\| \;&\le\; \|H_f^{-1/2}a^*(G_x)\|\|\overline{R}_\varepsilon\|\\ &+\; \|\overline{P}_\Delta H_f^{-1/2}\|\|a(G_x)\overline{R}_\varepsilon\|\\ &\le\; C(g\cdot\varepsilon^{-1}+\rho^{-1/2}g\varepsilon^{-1})\,.\end{aligned}$$

Finally using (6.29), we obtain

$$\|A_4\|\le C\rho^{-1/2}\varepsilon^{-3/2}g^2\,. \tag{7.25}$$

Collecting the estimates above and remembering (7.17) and remembering that $\varepsilon\le\rho$, we find

$$\|H_f^{-1/2}\overline{P}_\Delta[H-E^j,V]P\|\le C\theta g(\rho^{-1}+\theta_1^{-1/2}\rho\varepsilon^{-3/2}+\rho^{-1/2}\varepsilon^{-3/2}g)\,. \tag{7.26}$$

This together with (7.13), (7.14) and (7.16) gives

$$G \geq -Cg^2(1+\theta^2\rho^{-2}+\theta_1^{-1}\theta^2\rho^2\varepsilon^{-3}+\theta^2\rho^{-1}\varepsilon^{-3}g^2)\,. \tag{7.27}$$

Finally, combining the last inequalities with (7.8), (7.11) and (7.24) yields on $\mathrm{Ran}P_\Delta$

$$\mathcal{E} \geq 2\theta I\overline{R}_\varepsilon^2 I - Cg^2(1+\theta^2\rho^{-2}+\theta_1^{-1}\theta^2\rho^2\varepsilon^{-3}+\theta^2 g^2\varepsilon^{-3}\rho^{-1})\,. \tag{7.28}$$

This estimate together with (6.39) implies that on $\mathrm{Ran}\,P$

$$\mathcal{E} \geq 2\theta M - Cg^2(1+\theta^2\rho^{-2}+\theta^2\rho^2\varepsilon^{-3}+\theta^2 g^2\varepsilon^{-3}\rho^{-1}+\theta\varepsilon^{-2}\rho^{-2})\,. \tag{7.29}$$

Now we analyze the operator PMP. Introducing

$$P_{\mathrm{part}}^{(\leq j)} \;:=\; \sum_{i:\,E^i\leq E^j} P_{\mathrm{part}}^i \quad \text{and} \quad P_{\mathrm{part}}^{(>j)} \;:=\; \mathbf{1}_{\mathrm{part}} \;-\; P_{\mathrm{part}}^{(\leq j)}\,, \tag{7.30}$$

and noting that $(H_{\mathrm{part}}-E^j)\,P_{\mathrm{part}}^{(>j)} \geq \delta P_{\mathrm{part}}^{(>j)}$, for some $\delta>0$, we estimate

$$\left\| PMP \;-\; P\Big(\int \overline{G_x}(k)\,P_{\mathrm{part}}^{(\leq j)}\,\overline{R}_{\varepsilon,\omega(k)}^2\,G_x(k)\,d^3k\Big)P\right\| \leq Cg^2\,. \tag{7.31}$$

This relation can be rewritten as

$$PMP \;=\; \sum_{i:\,E^i\leq E^j}\int f_{ij}(\omega)\Big[(H_f+\omega-E^{ji})^2+\varepsilon^2\Big]^{-1}d\omega P \;+\; O(g^2)\,, \tag{7.32}$$

where $E^{ji} := E^j - E^i$ and $f_{ij}(\omega) = \int\limits_{|k|=\omega}(A_{ij})^*A_{ij}dS_\omega$ with the matrices A_{ij} defined in the paragraph preceeding Eqn (3.5). Now using the change of the variables formula and the mean value theorem we find

$$\begin{aligned} & \int f_{ij}(\omega)[(H_f+\omega-E^{ji})^2+\varepsilon^2]d\omega \\ = & \int f_{ij}(\alpha-H_f)[(\alpha-E^{ji})^2+\varepsilon^2]d\alpha \\ = & \int f_{ij}(\alpha)[(\alpha-E^{ji})^2+\varepsilon^2]^{-1}d\alpha + R\,, \end{aligned}$$

where

$$R = \int_0^1\int f_{ij}'(\alpha-sH_f)[(\alpha-E^{ji})^2+\varepsilon^2]^{-1}d\alpha ds H_f\,.$$

Since the functions f_{ij} have, by the assumptions on $G_x(k)$, bounded derivatives, we obtain that

$$RP = O\left(\frac{g^2\rho}{\varepsilon}\right)\,. \tag{7.33}$$

Using this together with Eqn (7.32) and with the fact that $f_{ij}(\omega)$ vanish at $\omega = 0$ and remembering the definition of Γ_i (see Eqn (3.5)) yields on $\mathrm{Ran} P$

$$M \;=\; \frac{\Gamma_j}{\varepsilon} \cdot \Big[1 + o_\varepsilon(1) + O(\rho)\Big] + O(g^2)\,, \tag{7.34}$$

where $o_\varepsilon(1)$ stands for a function of ε vanishing as $\varepsilon \to 0$.

Eqn (7.34) inserted into (7.29) yields

$$\mathcal{E} \geq \frac{\theta \Gamma_j}{\varepsilon}[2 - o_\varepsilon(1) - O(\rho)] - O(g^2)[1 + \theta^2\rho^{-2} + \theta_1^{-1}\theta^2\rho^2\varepsilon^{-3} + \theta^2 g^2 \varepsilon^{-3}\rho^{-1} + \theta\varepsilon^{-2}\rho^2]\,. \tag{7.35}$$

Since $\Gamma_j \geq \delta_j g^2$ with δ_j positive and independent of g and since $\rho \geq \varepsilon$, we may write (7.35) on $\mathrm{Ran}\, P_\Delta$ as

$$\mathcal{E} \;\geq\; \frac{\theta\, \Gamma_j\, (2 - \alpha_1)}{\varepsilon}\,, \tag{7.36}$$

where

$$\alpha_1 \;=\; O\Big(\frac{\varepsilon}{\theta} + \frac{\theta\varepsilon}{\rho^2} + \frac{\theta\rho^2}{\varepsilon^2\theta_1} + \frac{\theta g^2}{\rho\varepsilon^2} + \frac{\rho^2}{\varepsilon}\Big) + o_\varepsilon(1) \;<\; 2\,. \tag{7.37}$$

This together with (7.6)–(7.8) (see also the paragraph after Eqn. (7.8)) implies

$$B_{V,\Delta} \;\geq\; \frac{\theta\, \gamma_j\, (2 - \alpha_1)}{\varepsilon}\, E_\Delta(H_0)^2\,, \tag{7.38}$$

where, we recall, γ_j is the smallest eigenvalue of Γ_j.

Now we derive (5.9) from (7.38). Let $\Delta \subset\subset \Delta'$ and pick a smooth function h supported in Δ' and equal to 1 on Δ. Moreover, we denote $\overline{E}_\Delta(\lambda) = 1 - E_\Delta(\lambda)$. We use the estimate

$$\Big\| \Big(h(H) - h(H_0)\Big)(H_0 + i)^{1/2} \Big\| \;\leq\; C\, g/|\Delta|\,, \tag{7.39}$$

which can be easily derived using operator calculus (see, e.g., [14]) and (4.6)–(4.7). Recalling that $B_{V,\Delta} = E_\Delta(H_0)\, B_V\, E_\Delta(H_0)$ and $B_V = [H, A_V]$, we may write

$$E_\Delta(H)\, B_V\, E_\Delta(H) \;=\; E_\Delta(H) B_{V,\Delta'} E_\Delta(H) \;+\; S \;+\; T\,, \tag{7.40}$$

where

$$S \;=\; E_\Delta(H)\overline{E}_{\Delta'}(H_0)\, B_V\, E_{\Delta'}(H_0) E_\Delta(H) \;\;+\;\; \text{adjoint}\,,$$

and

$$T \;=\; E_\Delta(H)\overline{E}_{\Delta'}(H_0)\, B_V\, \overline{E}_{\Delta'}(H_0) E_\Delta(H)\,.$$

Writing $E_\Delta(H)\overline{E}_{\Delta'}(H_0)$ as $E_\Delta(H)(h(H) - h(H_0)) \cdot \overline{E}_{\Delta'}(H_0)$ and using Eqn (7.39) we obtain

$$E_\Delta(H)\overline{E}_{\Delta'}(H_0) \;=\; E_\Delta(H) O(g) \tag{$*$}$$

and similarly for the adjoint operator. The latter estimate implies that

$$T = E_\Delta(H) O(g^2) E_\Delta(H). \tag{7.41}$$

Next, we write

$$B_V \;=\; [H_0, A] + U,$$

where $U := [H_0, \overline{P}VP - PV^*\overline{P}] + [I, A_V]$ and use that $[H_0, A] = H_f$ and therefore commutes with $E_{\Delta'}(H_0)$ so that

$$S \;=\; E_\Delta(H)\overline{E}_{\Delta'}(H_0) U E_{\Delta'}(H_0) E_\Delta(H) + \text{h.c.}\;\;.$$

Again Eqns (6.29) and $(*)$, together with elementary estimates similar to those performed above imply that

$$S \;=\; E_\Delta(H) O(\theta\varepsilon^{-3/2} g^2 \rho) E_\Delta(H)\,. \tag{7.42}$$

Combining estimates (7.40)–(7.42), we obtain

$$E_\Delta(H) B_V E_\Delta(H) \;\geq\; E_\Delta(H)(B_{V,\Delta} - C\theta\varepsilon^{-3/2} g^2\rho) E_\Delta(H)\,.$$

Now using inequalities (7.38) and (7.39) we arrive at

$$E_\Delta(H) B_V E_\Delta(H) \;\geq\; \Big[\frac{\theta\gamma_j(2-\alpha_1)}{\varepsilon}(1 - O(g)) - C\theta\varepsilon^{-3/2} g^2\rho\Big] E_\Delta(H)^2\,.$$

It is not hard now to identify this inequality with (5.19). ∎

A Proof of Lemma 5.6

Both statements of Lemma 5.6 follow in a standard way (see [25], Theorems XIII.23 and XIII.25) from the following result (cf. Theorem 4.9 of [6] and Theorem 7.1 of [23]).

Theorem A.1 *Under the assumptions of Lemma 5.6*

$$\|\langle A\rangle^{-\alpha}(H - z)^{-1}\langle A\rangle^{-\alpha}\| \leq C \tag{A.1}$$

uniformly in $z \in \mathbb{C}^+$ *with* $\mathrm{Re}\, z \in \Delta$, *provided* $\alpha > \frac{1}{2}$.

Proof: Here we prove this theorem for $\alpha = 1$. Its extension to the case of $\alpha > \frac{1}{2}$ is done by repeating the proof of Theorem 7.8 of [23].

Our proof follows closely the proofs of Theorem 4.9 of [6] and Theorem 7.1 of [23]. Let $\Delta \subset\subset \Delta_1 \subset\subset \Delta_2 \subset\subset \Delta'$ and $f \in C_0^\infty(\Delta_2)$, with $f \equiv 1$ on Δ_1 and $f \geq 0$. We use the following notation,

$$M := f(H)[A, H]f(H). \tag{A.2}$$

Note that due to (5.27), $M \geq \theta f(H)^2$ and $M^* = M$. Since $\|(H - i\varepsilon M - z)u\| \geq \mathrm{Im}\langle(-H + i\varepsilon M + z)u, u\rangle/\|u\| \geq \mathrm{Im}\, z\|u\|$ and similarly for the adjoint operator, we have that (see Lemma 4.4(a) of [6] or Lemma 7.3(a) of [23])

$$\text{For } \varepsilon \geq 0 \text{ and } \mathrm{Im}\, z > 0\,,\ H - i\varepsilon M - z \text{ is invertible.} \tag{A.3}$$

Denote $G_\varepsilon(z) = (H - i\varepsilon M - z)^{-1}$. Moreover, we introduce also

$$F_\varepsilon(z) := DG_\varepsilon(z)D \text{ with } D = \langle A\rangle^{-1}.$$

In what follows the argument z is assumed to satisfy, $\mathrm{Re}\, z \in \Delta$, $\mathrm{Im}\, z > 0$; it is fixed and often omitted from the notation. We begin with a series of simple lemmata.

Lemma A.2 *For* $z \in \mathbb{C}^+$ *with* $\mathrm{Re}\, z \in \Delta$, *and* $\varepsilon \geq 0$,

$$\|G_\varepsilon(z)\| \leq C/\varepsilon. \tag{A.4}$$

Proof: Let $f = f(H)$. The relations $\|fG_\varepsilon\varphi\|^2 = \langle G_\varepsilon^* f^2 G_\varepsilon\rangle_\varphi$, $M \geq \theta f^2$ and $\mathrm{Im}\, z \geq 0$ imply

$$\begin{aligned}\|fG_\varepsilon\varphi\|^2 &\leq \frac{1}{2\varepsilon\theta}\langle G_\varepsilon^* 2\varepsilon M G_\varepsilon\rangle_\varphi \\ &\leq \frac{1}{2\varepsilon\theta}\langle G_\varepsilon^*(2\varepsilon M + 2\mathrm{Im}\, z)G_\varepsilon\rangle_\varphi,\end{aligned}$$

where we used the notation $\langle B\rangle_\varphi = \langle\varphi, B\varphi\rangle$. Now, an application of the second resolvent equation yields $\|fG_\varepsilon\varphi\|^2 \leq \frac{1}{2\varepsilon\theta}\langle iG_\varepsilon^* - iG_\varepsilon\rangle_\varphi$, which in turn implies

$$\|fG_\varepsilon\varphi\| \leq \frac{1}{\sqrt{\varepsilon\theta}}|\langle G_\varepsilon\rangle_\varphi|^{1/2} \tag{A.5}$$

and therefore

$$\|fG_\varepsilon\| \leq \frac{1}{\sqrt{\varepsilon\theta}}\|G_\varepsilon\|^{1/2}. \tag{A.6}$$

Next, applying the second resolvent equation to G_ε and G_0 and using that $\|\bar{f}G_0\| < \infty$, thanks to $\mathrm{dist}(z, \mathbb{R}\backslash\Delta_1) > 0$, we find

$$\|\bar{f}G_\varepsilon\| \leq C(1 + \varepsilon\|G_\varepsilon\|), \tag{A.7}$$

where $\bar{f} = \mathbf{1} - f$. This inequality together with (A.6) implies (A.4). ∎

This lemma and its proof have two consequences important for us:

$$\|\bar{f}(H)G_\varepsilon(z)\| \le C, \tag{A.8}$$

uniformly in $\varepsilon > 0$, where $\bar{f}(H) = \mathbf{1} - f(H)$, due to Eqns (A.4) and (A.7); and

$$\|f(H)G_\varepsilon(z)D\| \le C\varepsilon^{-1/2}\|F_\varepsilon(z)\|^{1/2}, \tag{A.9}$$

due to Eqn (A.5) with $\varphi = Du$. The last two equations imply in turn that

$$\|G_\varepsilon(z)D\| \le C(1 + \varepsilon^{-1/2}\|F_\varepsilon(z)\|^{1/2}). \tag{A.10}$$

In what follows we assume that ϕ is a cut-off function satisfying

$$\phi \ge 0, \quad \sqrt{\phi} \in C_0^\infty(\Delta') \quad \text{and} \quad \phi \equiv 1 \text{ on } \Delta_2. \tag{A.11}$$

Next, we introduce the symmetric operator

$$A_\phi := \phi(H)A\phi(H), \tag{A.12}$$

which is well defined in $D(A)$, due to (5.19). Now define $[H, A_\phi]$ as a quadratic form on $D(A) \cap D(H)$. Then

$$[H, A_\phi] = \phi(H)[H, A]\phi(H) \tag{A.13}$$

in a sense of quadratic forms. This relation implies that the operator

$$B_\phi := [H, A_\phi] \text{ is bounded.} \tag{A.14}$$

Lemma A.3 *Let $B := [H, A]$. For any $\psi \in C_0^\infty(\Delta_2)$, the operator*

$$\psi(H)[B, A_\phi]\psi(H) \textit{ is bounded.} \tag{A.15}$$

Here the operator in (A.15) is initially defined in a sense of quadratic forms.

Proof: In the proof below we omit the argument H in $\phi(H)$ and $\psi(H)$. Using that $\psi \cdot \phi = \psi$, we compute as quadratic forms

$$\psi[B, A_\phi]\psi = \psi[B, A]\psi + \psi B[\phi, A]\psi + \psi[\phi, A]B\psi. \tag{A.16}$$

Since, by (5.5), (5.14) and (5.27), ψB, $B\psi$, $[\phi, A]$ and $\psi[B, A]\psi$ are bounded we conclude that the r.h.s. of (A.16) is bounded, so (A.15) follows. ∎

Our last preparatory step is the following

Lemma A.4 *The operator $[M, A_\phi]$ defined initially in a sense of quadratic forms is bounded.*

Proof: Using that $f \cdot \phi = f$ and omitting again the argument H, we compute in a sense of quadratic forms

$$[M, A_\phi] = fB[f, A_\phi] + f[B, A_\phi]f + [f, A_\phi]Bf.$$

Since fB, Bf, $[f, A_\phi] = \phi[f, A]\phi$ and $f[B, A_\phi]f$ are bounded by virtue of (5.26), (5.14) and (A.15), the statement follows. ∎

Now we are ready for a core estimate of this proof.

Lemma A.5 *We have the following estimate*

$$\left\|\frac{dF_\varepsilon(z)}{d\varepsilon}\right\| \leq C(\|F_\varepsilon(z)\| + \varepsilon^{-1/2}\|F_\varepsilon(z)\|^{1/2} + 1). \tag{A.17}$$

Proof: Using the definitions of $G_\varepsilon(z)$ and $F_\varepsilon(z)$, we compute

$$-\frac{dF_\varepsilon}{d\varepsilon} = DG_\varepsilon MG_\varepsilon D.$$

Since $f \cdot \phi = f$, we have that $M = fB_\phi f$. Now we decompose

$$\frac{dF_\varepsilon}{d\varepsilon} = Q_1 + Q_2 + Q_3, \tag{A.18}$$

where

$$Q_1 = DG_\varepsilon \bar{f} B_\phi \bar{f} G_\varepsilon D,$$
$$Q_2 = DG_\varepsilon \bar{f} B_\phi f G_\varepsilon D + DG_\varepsilon f B_\phi \bar{f} G_\varepsilon D,$$
$$Q_3 = -DG_\varepsilon B_\phi G_\varepsilon D.$$

We bound now the Q_j's. Eqns (A.14) and Eqn (A.8) imply

$$\|Q_1\| \leq \|DG_\varepsilon \bar{f}\|^2 \|B_\phi\| \leq C. \tag{A.19}$$

Next, (A.8), (A.9) and (A.14) yield

$$\begin{aligned} \|Q_2\| &\leq 2\|DG_\varepsilon \bar{f}\|\|B\phi\|\|fG_\varepsilon D\| \\ &\leq \tfrac{C}{\sqrt{\varepsilon}}\|F_\varepsilon\|^{1/2}. \end{aligned} \tag{A.20}$$

The term Q_3 is more complicated. We decompose it as

$$-Q_3 = Q_4 + Q_5, \tag{A.21}$$

where

$$Q_4 = DG_\varepsilon[H - i\varepsilon M - z, A_\phi]G_\varepsilon D \tag{$*$}$$

and

$$Q_5 = i\varepsilon DG_\varepsilon[M, A_\phi]G_\varepsilon D.$$

Expanding the commutator in $(*)$, we find

$$Q_4 = DA_\phi G_\varepsilon D - DG_\varepsilon A_\phi D.$$

Hence, due to $\|DA_\phi\| \le C$ and (A.10),

$$\begin{aligned} \|Q_4\| &\le 2\|DA_\phi\|\|G_\varepsilon D\| \\ &\le C(1 + \varepsilon^{-1/2}\|F_\varepsilon\|^{1/2}). \end{aligned} \tag{A.22}$$

Finally, we have due to (A.10) and Lemma A.4

$$\begin{aligned} \|Q_5\| &\le \varepsilon\|DG_\varepsilon\|^2\|[M, A_\phi]\| \\ &\le C(\varepsilon + \|F_\varepsilon\|). \end{aligned} \tag{A.23}$$

Now, Eqns (A.18)–(A.23) imply (A.17). ∎

To complete the proof of Theorem 5.5 we iterate the rough estimate

$$\|F_\varepsilon(z)\| \le \frac{C}{\varepsilon}, \tag{A.24}$$

which follows from (A.4), with the help of differential inequality (A.17). On the first step plugging (A.24) into the r.h.s. of (A.17) we obtain $\left\|\frac{dF_\varepsilon(z)}{d\varepsilon}\right\| \le \frac{C}{\varepsilon}$. Integrating the latter inequality from ε to 1 and using that, due to (A.24), $\|F_1(z)\| \le C$, we find $\|F_\varepsilon(z)\| \le C \log\frac{1}{\varepsilon}$. Plugging the latter estimate into the r.h.s. of (A.17) yields now $\left\|\frac{dF_\varepsilon(z)}{d\varepsilon}\right\| \le C\sqrt{\frac{\log\frac{1}{\varepsilon}}{\varepsilon}}$ which upon the integration from 0 to 1 gives

$$\|F_0(z)\| \le C,$$

uniformly in z, $\operatorname{Im} z > 0$ and $\operatorname{Re} z \in \Delta$, which, in virtue of the definition of $F_\varepsilon(z)$, is equivalent to the statement of Theorem A.1. ∎

B Feshbach Projection Method

Lemma B.1 *Let B be a self-adjoint operator on a Hilbert space $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ and let (in the obvious notation) $B_{22} \geq \theta \, \mathrm{id}_{\mathcal{H}_2}$, $\theta > 0$. Then $\lambda_0 := \inf \operatorname{spec} B$ is either $\geq \theta$ or it satisfies the relation*

$$\lambda_0 \;=\; \inf \operatorname{spec} \Big\{ B_{11} \;-\; B_{12}(B_{22} - \lambda_0)^{-1} B_{21} \Big\} . \tag{B.1}$$

Proof: Let $\lambda_0 < \theta$. The Feshbach projection method implies that $\lambda \in \sigma(B)$ iff

$$\lambda \in \sigma\Big(B_{11} - B_{12}(B_{22} - \lambda)^{-1} B_{21} \Big) \tag{B.2}$$

provided $\lambda < \theta$, which implies (B.1). ∎

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