On one photon scattering in non-relativistic qed

David G. Hasler*

Institute for Mathematics, University of Jena
Jena, DE

Abstract

We consider scattering of a single photon by an atom or a molecule in the framework of non-relativistic qed, and we express the scattering matrix for one photon scattering as a boundary value of the resolvent.

1 Introduction

Rayleigh scattering describes the scattering of light by bound particles much smaller than the wavelength of the radiation. We study such a process in the framework of non-relativistic qed. Non-relativistic qed is a mathematical rigorous model describing low energy aspects of the quantized electromagnetic field interacting with non-relativistic quantum mechanical matter [39]. Mathematical aspects of Rayleigh scattering has been intensively studied for this and related models [14, 19, 20, 15, 26, 17, 13]. Existence of asymptotic creation and annihilation operators as well as asymptotic completeness has been established.

We define the scattering matrix as the inner product of asymptotically incoming photon states with asymptotically outgoing photon states. Physically, the scattering matrix describes the emission and absorption of photons by an atom or molecule. It can be used for example to determine the absorption spectrum, observe Bohr’s frequency condition, and to detect properties of resonances. More specifically, we consider in this paper the one photon scattering matrix and relate it to boundary values of the resolvent. The resulting expression resembles a special case of a LSZ reduction formula [35, 10] obtained in [3 (III.13)] after performing a formal time integration. The relation which we obtain, can be

*E-mail: david.hasler@uni-jena.de
used to calculate expansions of the one photon scattering matrix using well established results about the ground state, resonance states, and boundary values of the resolvent [4, 5, 11, 30, 24, 28, 29]. We note that an analogous relation has been obtained for the spin boson model, where the leading order expansion has been studied in connection with resonances [7, 8]. For the hydrogen atom with a spinless electron expansions of the scattering matrix have been studied in [3] using the LSZ reduction formalism combined with iterated perturbation theory. In the present paper we provide a different approach, which gives an explicit relation of the scattering matrix to boundary values of the resolvent. Thus it can be used to relate resonance eigenvalues to singularities of the scattering matrix.

To prove our result we make several assumptions, which have been established in the literature in various situations. We assume the existence of a ground state, the existence of wave operators, and regularity properties of boundary values of the resolvent. In Section 2 we introduce the model and state the main result. The proofs are given in Section 3. In Section 4 we verify the Hypotheses about boundary values of the resolvent for explicit models.

The idea of the proof of the main result is as follows. First we define the asymptotic creation and annihilation operators. Then we express the asymptotic creation operators using Cook’s method as an integral over the current, which is formulated in Lemma 3.1 cf. 3. Using this identity we relate matrix elements of the current with one particle scattering states and the ground state to the T-matrix, which is stated in Proposition 3.2. The T-matrix, defined in (2.19), is given as a matrix element of boundary values of the resolvent. The method can be viewed as a generalization of one particle scattering in quantum mechanics, cf. 15, 43, and is analogous to the corresponding relation obtained in [8] for the spin boson model. To show Proposition 3.2 we use an Abelian limit to integrate out the time evolution by means of the following identity for a self-adjoint operator $A$

$$\int_0^\infty e^{-it(A-i\epsilon)}dt = \frac{-i}{A-i\epsilon},$$

which is understood as a strong Riemann-integral and $\epsilon > 0$ is a regularization. Then we use a pull-through formula, cf. (3.16), and assumptions about boundary values of the resolvent to take the limit $\epsilon \downarrow 0$. We then use once more the integral representation of the asymptotic creation operators, Lemma 3.1, their relation to the T-matrix, Proposition 3.2, and the canonical commutation relations, which are satisfied by the asymptotic creation and annihilation operators [19, Theorem 4]. Combining these results with assumed regularity properties about boundary values of the resolvent, we can interchange integrals and relate the scattering matrix to the boundary value of the resolvent.
In Section 4, we verify the assumed regularity properties using analytic dilation \cite{9,46}. In particular, we combine a result about exponential decay of analytic extensions of the ground state \cite{31} with estimates of analytic dilations of the resolvent \cite{5,30}.

We note that in contrast to an analogous result for the simpler spin boson model with a mild infrared regularization \cite{8}, we have to deal with the electronic degrees of freedom, which are described by an infinite dimensional space. Furthermore, we do not impose any infrared regularization. In \cite{8} a multiscale analysis was central to the prove of the result. In the present paper we, a priori, do not need such an analysis. The emphasis of our proof is to isolate abstract hypotheses which are needed for the main result. Moreover, we show that these hypotheses can be verified using that the ground is dilation analytic and has spatial exponential decay \cite{31}. A result which is involved to show, but is of interest of its own. Nevertheless, we believe that the hypotheses made in the present paper could alternatively be established using more accessible methods such as Mourre theory \cite{37}. Moreover, we want to mention that the ideas of the proof of the present paper have been applied to the related Nelson model \cite{36}.

2 Model and Statement of Result

Let $\mathfrak{h}$ be a Hilbert space. We denote the Bosonic Fock space over $\mathfrak{h}$ by $\mathcal{F}(\mathfrak{h})$. We define $\mathfrak{h}^{\otimes n} := \bigotimes_{j=1}^{n} \mathfrak{h}$ for $n \in \mathbb{N}$ and set $\mathfrak{h}^{\otimes 0} = \mathbb{C}$. Let $\mathfrak{S}_n$ denote the permutation group of $\{1, \ldots, n\}$. For $\sigma \in \mathfrak{S}_n$ we define a linear operator, also denoted by $\sigma$, on basis elements of $\mathfrak{h}^{\otimes n}$ by

$$\sigma(\varphi_1 \otimes \varphi_2 \otimes \cdots \otimes \varphi_n) = \varphi_{\sigma(1)} \otimes \varphi_{\sigma(2)} \otimes \cdots \otimes \varphi_{\sigma(n)},$$

extend it first linearly and then by taking the closure to a bounded operator on $\mathfrak{h}^{\otimes n}$. Define $S_n = \frac{1}{n!} \sum_{\sigma \in \mathfrak{S}_n} \sigma$ and $S_0 = 1$. The Fock space is defined by

$$\mathcal{F}(\mathfrak{h}) := \bigoplus_{n=0}^{\infty} \mathcal{F}_n(\mathfrak{h}), \quad \mathcal{F}_n(\mathfrak{h}) := S_n(\mathfrak{h}^{\otimes n}).$$

For $h \in \mathfrak{h}$ the creation operator, $a^*(h)$, is defined on elements $\eta \in \mathcal{F}_n(\mathfrak{h})$ by

$$a^*(h)\eta = (n + 1)^{1/2} S_{n+1}(h \otimes \eta),$$

and extends linearly to a densely defined closed linear operator in $\mathcal{F}(\mathfrak{h})$. Its adjoint, $a(h)$, is called the annihilation operator. It follows from the definition that the operators $a^*(h)$ and $a(h)$ obey the usual canonical commutation relations (CCR)

$$[a(g), a^*(h)] = \langle g, h \rangle, \quad [a^#(g), a^#(h)] = 0,$$
here \( \langle g, h \rangle \) denotes the inner product in \( \mathfrak{h} \) and \( a^\#(\cdot) \) stands for either \( a^*(\cdot) \) or \( a(\cdot) \). We define the Bosonic field operator by

\[
\phi(h) = \frac{1}{\sqrt{2}}(a(h) + a^*(h))^\dagger,
\]

where \( (\cdot)^\dagger \) stands for the operator closure. In this paper we consider photons, i.e., relativistic transversally polarized Bosons, and choose henceforth

\[
\mathfrak{h} = L^2(\mathbb{R} \times \mathbb{Z}_2) \cong L^2(\mathbb{R}^3, \mathbb{C}^2).
\]

Let \( \omega(k) = |k| \). The operator of multiplication by \( | \cdot | \) shall be denoted by \( \omega \) as well. The operator \( H_f \) in \( \mathcal{F}(\mathfrak{h}) \) is defined by

\[
H_f|_{\mathcal{F}_n(\mathfrak{h})} = \sum_{j=1}^{n} \left( \mathbf{1}^{\otimes(j-1)} \otimes \omega \otimes \mathbf{1}^{\otimes(n-j-1)} \right)
\]

and linearly extends to a self-adjoint operator in \( \mathcal{F}(\mathfrak{h}) \). The Hilbert space of \( N \in \mathbb{N} \) non-relativistic particles is assumed to be

\[
\mathcal{H}_{at} := L^2_\#((\mathbb{R}^3 \times \mathbb{Z}_{2s+1})^N),
\]

where \( s \in \{0, 1/2\} \) denotes the spin of the non-relativistic particles, \( L^2_\# \) stands for the subspace of either symmetric or antisymmetric elements with respect to interchange of particle coordinates, c.f., \( \{A.5\} \). We shall denote the spacial particle coordinates by \( x_j, j = 1, \ldots, N \). The Laplacian on \( \mathbb{R}^{3N} \) is written as usual by the symbol \( \Delta \). The potential describing the forces acting on the non-relativistic particles is denoted by \( V \). We assume that \( V \in L^2_{loc}(\mathbb{R}^{3N}) \), that \( V \) is symmetric with respect to permutations of particle coordinates, and that \( V_- := \max(0, -V) \) satisfies the following relative form bound. For all \( \epsilon > 0 \) there exists a constant \( C_\epsilon \) such that

\[
V_- \leq \epsilon(\Delta) + C_\epsilon.
\]

By \( S_j \) we shall denote the spin operator of the \( j \)-th particle. If \( s = 0 \), then \( S_j = 0 \), and if \( s = 1/2 \), then

\[
(S_j)_l = \mathbf{1}^{\otimes(j-1)} \otimes \frac{1}{2} \sigma_l \otimes \mathbf{1}^{\otimes(N-j-1)}, \quad l = 1, 2, 3,
\]

with \( \sigma_1, \sigma_2, \sigma_3 \) denoting the Pauli matrices. The Hilbert space of the total system is

\[
\mathcal{H} := \mathcal{H}_{at} \otimes \mathcal{F}(\mathfrak{h})
\].
To describe the interaction we introduce the following weighted $L^2$-space. For $h \in L^2(\mathbb{R}^3; \mathbb{C}^2) \cong L^2(\mathbb{R}^3 \times \mathbb{Z}_2)$ we define

$$
\|h\|_\omega := \left( \sum_{\lambda=1,2} \int |h(k, \lambda)|^2 \left( 1 + |k|^{-1} \right) dk \right)^{1/2}
$$

and

$$
h_\omega := L^2_\omega(\mathbb{R}^3 \times \mathbb{Z}_2) := \{h \in L^2(\mathbb{R}^3 \times \mathbb{Z}_2) : \|h\|_\omega < \infty\}.
$$

The interaction between non-relativistic particles and the quantized field is described by the quantized vector potential in Coulomb gauge and the quantized magnetic field, which are defined by

$$A_l(x) = \phi(G_{x,l}) \quad \text{and} \quad B_l(x) = \phi(J_{x,l}), \quad x \in \mathbb{R}^3, \quad l = 1, 2, 3,$$

respectively, where

$$
G_{x,l}(k, \lambda) = \frac{1}{(2\pi)^{3/2}} \frac{\kappa(k)}{\sqrt{|k|}} \varepsilon_l(k, \lambda) e^{-ik \cdot x},
$$

$$
J_{x,l}(k, \lambda) = \frac{1}{(2\pi)^{3/2}} \frac{\kappa(k)}{\sqrt{|k|}} [(i k) \wedge \varepsilon(k, \lambda)] e^{-ik \cdot x},
$$

$k \in \mathbb{R}^3 \setminus \{0\}$, and $\lambda \in \mathbb{Z}_2$. Here, $\varepsilon(k, 1), \varepsilon(k, 2) \in \mathbb{R}^3$ are the polarization vectors. We assume that they only depend on $k/|k|$, for $k \in \mathbb{R}^3 \setminus \{0\}$, that $(k/|k|, \varepsilon(k, 1), \varepsilon(k, 2))$ forms an orthonormal basis in $\mathbb{R}^3$, and that they are measurable functions of their arguments. Moreover, we assume that $\kappa$ is a measurable function from $\mathbb{R}^3$ to $\mathbb{C}$ such that (or more precisely for its canonical extension $\kappa(k, \lambda) = \kappa(k)$)

$$
\omega^{-1/2} \kappa \in L^2_\omega(\mathbb{R}^3 \times \mathbb{Z}_2) \quad \text{and if } s = 1/2, \text{ also } \omega^{1/2} \kappa \in L^2_\omega(\mathbb{R}^3 \times \mathbb{Z}_2). \quad (2.3)
$$

Physically, the function $\kappa$ is used as an ultraviolet cutoff and incorporates the coupling strength (Eq. (2.3) holds for example if $\kappa(k) = e1_{|k|<\Lambda}$ with $e \in \mathbb{R}$ the electric charge and $\Lambda \in (0, \infty)$ an ultraviolet cutoff). The Hamiltonian of the total system is given by

$$H = \sum_{j=1}^N \{(p_j + A(x_j))^2 + \mu S_j \cdot B(x_j)\} + V \otimes 1 + 1 \otimes H_t, \quad (2.4)$$

where $\mu \in \mathbb{R}$ (the value for the standard model of non-relativistic qed is $\mu = 2$) and $p_j = -i \partial_{x_j}$. In (2.4) and henceforth, we adopt the convention that for a vector of operators $T = (T_1, T_2, T_3)$ we write $T^2$ for $T \cdot T$. Furthermore, for notational compactness we shall suppress the tensor product in the notation of operators, if it is clear from the context on
which factor an operator acts. The definition (2.4) yields a priori a symmetric operator on a suitable dense subspace, $C$, of $H$ which we choose to be equal to the linear span of the set
\[ \{ f \otimes \eta : f \in C^\infty, \eta \in S_n(C_c^\infty(\mathbb{R}^3 \times \mathbb{Z}_2)^{\otimes n}), n \in \mathbb{N}_0 \}. \]
Using assumptions (2.2) and (2.3) it follows from Lemma A.2, in the appendix, that the operator is bounded from below. This allows to define a self-adjoint operator by means of the Friedrichs extension, see for example [41, Theorem X.23]. Henceforth we shall denote by $H$ this self-adjoint extension. We assume that $H$ is essentially self-adjoint on $C$ and that
\[ \mathcal{D}(H) \subset \mathcal{D}((-\Delta + H_t)^{1/2}), \quad (2.5) \]
where the right hand side denotes the natural domain of $(-\Delta + H_t)^{1/2}$. For a closed linear operator $T$ in a Hilbert space we shall denote by $\sigma(T)$ its spectrum and by $\rho(T)$ its resolvent set. Let
\[ \begin{align*}
E_{gs} &= \inf \sigma(H).
\end{align*} \]

**Remark 2.1.** We note that if $V$ is infinitesimally bounded with respect to $-\Delta$, which is the case for Coulomb potentials, then the assumptions on $V$ are satisfied. Clearly, (2.2) holds. Furthermore, $H$ is essentially self-adjoint on $C$ and the domain of $H$ is equal to $\mathcal{D}(-\Delta + H_t)$, the natural domain of $-\Delta + H_t$, [32, 27], and hence (2.5) is satisfied.

Introducing annihilation operators, $a(k, \lambda)$, as distributions defined in Equation (A.7) in the appendix, we can write in the sense of forms on a dense subspace (e.g. finite linear combinations of finite tensor products of compactly supported smooth functions) the quantized vector potential and magnetic field as
\begin{align*}
A(x) &= \frac{1}{(2\pi)^{3/2}} \sum_{\lambda=1,2} \int \frac{\varepsilon(k, \lambda)}{\sqrt{2|k|}} \{ \kappa(k) e^{ik \cdot x} a(k, \lambda) + \kappa(k) e^{-ik \cdot x} a^*(k, \lambda) \} dk, \quad (2.6) \\
B(x) &= \frac{1}{(2\pi)^{3/2}} \sum_{\lambda=1,2} \int \frac{i k \wedge \varepsilon(k, \lambda)}{\sqrt{2|k|}} \{ \kappa(k) e^{ik \cdot x} a(k, \lambda) - \kappa(k) e^{-ik \cdot x} a^*(k, \lambda) \} dk, \quad (2.7)
\end{align*}
respectively, and the field energy as
\[ H_f = \sum_{\lambda=1,2} \int |k| a^*(k, \lambda) a(k, \lambda) dk. \quad (2.8) \]
Here, $a^*(k, \lambda)$ denotes the formal adjoint of $a(k, \lambda)$ and the integrals (2.6)–(2.8) are understood in the weak sense.

To state the main result, we shall introduce several hypotheses. It has been shown in the literature that these assumptions hold true in various situations.
**Hypothesis A.** The number $E_{gs}$ is an eigenvalue of $H$, i.e., the operator $H$ has a square integrable ground state.

Assuming Hypothesis (A) we will denote by $\psi_{gs}$ a normalized eigenvector with eigenvalue $E_{gs}$.

**Remark 2.2.** For small coupling, i.e., $\|\omega^{-1/2}\kappa\|_\omega$ and $\|\omega^{1/2}\kappa\|_\omega$ small, the existence of ground states has been established in [4]. For large coupling existence has been shown in [25], where it is assumed that $\kappa(k) = e_1|k| \leq \Lambda$ with $e \in \mathbb{R}$ and $\Lambda \in [0, \infty)$ arbitrary.

Let us now introduce the so called asymptotic creation and annihilation operators. They are defined for $h \in \mathfrak{h}$ on vectors $\psi \in \mathcal{H}$ by

$$a^\#_{\text{in}}(h)\psi = \lim_{t \to \pm \infty} e^{iHt}e^{-iHt}a^\#(h)e^{iHt}e^{-iHt}\psi, \quad (2.9)$$

provided the limit exists. One refers to $a^\#_{\text{in}}$ and $a^\#_{\text{out}}$ as an incoming and outgoing asymptotic operator, and (2.9) is called an incoming and outgoing state, respectively. We note that as a consequence of the definitions it is straightforward to see that for $h \in \mathfrak{h}$

$$e^{-iHt}a^\#(h)e^{iHt} = a^\#(e^{-i\omega t}h). \quad (2.10)$$

Furthermore, we shall assume the following hypothesis.

**Hypothesis B.** There exists an $E > E_{gs}$, such that for all $g, h \in \mathfrak{h}_\omega$ the following holds.

(i) For $\varphi \in \mathcal{H}$ with $\varphi = 1_{H \leq E}\varphi$ the limits

$$a^\#_{\text{in}}(h)\varphi = \lim_{t \to \pm \infty} e^{iHt}e^{-iHt}a^\#(h)e^{iHt}e^{-iHt}\varphi$$

exist. Furthermore, there exists a constant $C > 0$ such that for all $f \in \mathfrak{h}_\omega$

$$\|a^\#_{\text{in}}(f)1_{H \leq E}\| \leq C\|f\|_\omega. \quad (2.11)$$

(ii) The canonical commutation relations

$$[a_{\text{in}}(g), a_{\text{in}}^\#(h)] = \langle g, h \rangle \quad \text{and} \quad [a_{\text{in}}^\#(g), a_{\text{in}}^\#(h)] = 0$$

hold true, in form-sense, on $1_{H \leq E}\mathcal{H}$. If $\psi \in 1_{H = E_{gs}}\mathcal{H}$, then

$$a_{\text{in}}(g)\psi = 0. \quad (2.12)$$
Remark 2.3. We note that Hypothesis \[ \Theta \] has been shown in [19, Theorem 4] in the spinless case. There it was assumed that \( \kappa \) has compact support and that the potential \( V \) is given as a sum of one body and two body potentials. Specifically, we note that from the assertion of Theorem 4 in [19] Eq. (2.12) follows first for \( g \in \mathfrak{h}_\omega \) with \( m := \inf \{ |k| : g(k) \neq 0 \} > 0 \), since \( a_{in}(g) \text{Ran}_{1,H=E_{gs}} \subset \text{Ran}_{1,H \leq E_{gs} - m} = \{0\} \), where the inclusion holds by Part (iv) of Theorem 4 in [19]. Then (2.12) extends to all \( g \in \mathfrak{h}_\omega \) in view of [19, Eq. (39) in Theorem 4].

To formulate the main result, we define the following commutators, which are related to the electric current, see for example [3]. Calculating a commutator we find for \( \psi \in \mathcal{C} \) and \( h \in \mathfrak{h} \), that

\[
\sum_j \left[ (p_j + A(x_j))^2 + \mu S_j \cdot B(x_j), a^*(h) \right] \psi = -\sum_{\lambda=1,2} \int_{\mathbb{R}^3} h(k,\lambda)D_1(k,\lambda)\psi dk, \tag{2.13}
\]

(using \( k \cdot \varepsilon(k,\lambda) = 0 \)) where we defined for \( k \in \mathbb{R}^3 \setminus \{0\} \) and \( \lambda \in \mathbb{Z}_2 \) the following operator in \( \mathcal{H} \)

\[
D_1(k,\lambda) := \frac{1}{(2\pi)^{3/2}} \sum_{j=1}^N \left\{ 2 \frac{\varepsilon(k,\lambda)}{2|k|} \kappa(k)e^{ik \cdot x_j} \cdot (p_j + A(x_j)) + \mu S_j \cdot \frac{ik \wedge \varepsilon(k,\lambda)}{\sqrt{2|k|}} \kappa(k)e^{ik \cdot x_j} \right\} \tag{2.14}
\]

with domain \( \mathcal{D}((-\Delta + H)^{1/2}) \). Here we understand the right hand side of (2.13) as a Bochner integral, cf. [48, 16, 2]. Explicitly, it follows from (2.14) that for all \( \psi \in \mathcal{D}((-\Delta + H_t)^{1/2}) \) there exists a constant \( C \) such that for almost all \( (k,\lambda) \in \mathbb{R}^3 \times \mathbb{Z}_2 \)

\[
\| h(k,\lambda)D_1(k,\lambda)\psi \| = \| h(k,\lambda) \| \| D_1(k,\lambda)\psi \| \\
\leq C\| h(k,\lambda) \| \| \kappa(k) \| \sum_{j=1}^N \left( \| (p_j + A(x))\psi \| + |k|\| \psi \| \right). \tag{2.15}
\]

Since the right hand side is bounded in view of the elementary inequalities in Lemma A.1 we see from (2.3) that (2.15) is an \( L^1 \)-function of \( (k,\lambda) \), and so the right hand side of (2.13) converges for all \( \psi \in \mathcal{D}((-\Delta + H_t)^{1/2}) \) as a Bochner integral in \( L^1(\mathbb{R}^3 \times \mathbb{Z}_2; \mathcal{H}) \), cf. [48, V.5, Theorem 1] or [16, Appendix E.3, Theorem 8]. Note that weak measurability follows directly from the assumptions about \( h \) and \( \kappa \) and hence strong measurability is granted by the separability of \( \mathcal{H} \), cf. [10, Theorem IV.22]. Taking a second commutator, we find for \( h \in \mathfrak{h} \) and \( \psi \in \mathcal{C} \) that

\[
[a(h), D_1(k,\lambda)]\psi = \sum_{N'=1,2} \int_{\mathbb{R}^3} h(k',\lambda')D_2(k,\lambda,k',\lambda')\psi dk', \tag{2.16}
\]
where we defined for \( k, k' \in \mathbb{R}^3 \setminus \{0\} \) and \( \lambda, \lambda' \in \mathbb{Z}_2 \) the following bounded operator in \( \mathcal{H}_{at} \)

\[
D_2(k, \lambda, k', \lambda') := \frac{2}{(2\pi)^3} \sum_{j=1}^{N} e^{i(k-k') \cdot x_j} \kappa(k) \kappa(k') \frac{\varepsilon(k, \lambda) \cdot \varepsilon(k', \lambda')}{\sqrt{|k|} \sqrt{|k'|}}.
\]

Again we understand (2.16) as a Bochner integral in \( L^1(\mathbb{R}^3 \times \mathbb{Z}_2; \mathcal{H}) \), that is for all \( (k, \lambda) \in \mathbb{R}^3 \times \mathbb{Z}_2 \) and \( \psi \in \mathcal{H} \) the map

\[
(k', \lambda') \mapsto h(k', \lambda') D_2(k, \lambda, k', \lambda') \psi
\]

is an element of \( L^1(\mathbb{R}^3 \times \mathbb{Z}_2; \mathcal{H}) \).

Next we formulate a hypothesis about boundary values of the resolvent.

**Hypothesis C.** Hypothesis \([\mathcal{A}] \) holds and \( S \subset \mathbb{R}^3 \setminus \{0\} \) is a set such that for all \( \lambda, \lambda' \in \mathbb{Z}_2 \) and \( k, k' \in S \) the boundary value of the resolvent

\[
\langle D_1(k, \lambda) \psi_{gs}, (H - E_{gs} - \omega(k') - i\eta) + D_1(k', \lambda') \psi_{gs} \rangle
\]

exists. For every compact \( S_0 \subset S \) there exists an \( \varepsilon_0 > 0 \) such that for all \( k \in S \) and \( \lambda, \lambda' \in \mathbb{Z}_2 \)

\[
\sup_{k' \in S_0, \eta \in (0, \varepsilon_0)} |\langle D_1(k, \lambda) \psi_{gs}, (H - E_{gs} - \omega(k') - i\eta) + D_1(k', \lambda') \psi_{gs} \rangle| < \infty.
\]

If there exits a ground state, \( k, k' \in \mathbb{R}^3 \setminus \{0\} \), and the limit (2.17) exists, then we can define

\[
T(k, \lambda, k', \lambda') := -\langle (H + \omega(k')) - E_{gs} \rangle^{-1} D_1(k', \lambda') \psi_{gs}, D_1(k, \lambda) \psi_{gs} \rangle + \langle D_2(k, \lambda, k', \lambda') \psi_{gs}, \psi_{gs} \rangle,
\]

which shall be called \( T \)-matrix. Note that the \( T \)-matrix depends on the choice of the ground state, in case where the ground state energy is degenerate. We need one more Hypothesis.

**Hypothesis D.** Hypothesis \([\mathcal{C}] \) holds for \( S \subset \mathbb{R}^3 \setminus \{0\} \). The \( T \)-matrix (2.19) is bounded for \( k, k' \) in any compact subset of \( S \). As a function on \( (S \times \mathbb{Z}_2)^2 \) the \( T \)-matrix depends for each \( k \in S \) continuously on \( |k'| \) for \( k' \in S \). (c.f. Definition (2.1) below).
Definition 2.4. Let $S \subset \mathbb{R}^3$ and $f : x \mapsto f(x)$ be a function on $S$. We say that $f(x)$ depends continuously (differentiably) on $|x|$ if for each $s \in \mathbb{R}^3$ with $|s| = 1$ the map $r \mapsto f(rs)$ is a continuous (differentiable) function on the set $\{r \in [0, \infty) : rs \in S\}$.

In Section 4 we verify Hypothesis D and C for an atom with dilation analytic coupling by means of dilation analyticity [9, 46]. We only need that there exists a ground state which is dilation analytic and whose analytic extension decays exponentially. For atoms with spinless “electrons” this assumption has been verified [31], see also [38, 12, 42, 44, 24, 28] for related results. Furthermore we use existence and regularity of analytically dilated resolvents, which have been shown for atoms in [33, 4, 5, 30, 1]. We believe that alternatively one could use Mourre’s commutator method [37] to verify Hypothesis D and C. This theory has been applied to the standard model of non-relativistic qed or related models by various authors [6, 22, 21, 11], see also [8] and references therein, where it has been applied for a related purpose. Specifically, using the limiting absorption principles proven in these references together with the existence of an exponentially decaying ground state [4, 25, 23].

Theorem 2.5. Suppose Hypotheses B and D hold for a set $S \subset \mathbb{R}^3 \setminus \{0\}$. Then for $f, h \in C_c(\mathbb{R}^3)^2$ we have

$$\langle a^*_\text{out}(f)\psi_{gs}, a^*_\text{in}(h)\psi_{gs} \rangle - \langle f, h \rangle = -2\pi i \sum_{\lambda, \lambda' = 1, 2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} f(k, \lambda) \delta(\omega(k) - \omega(k')) h(k', \lambda') T(k, \lambda, k', \lambda') dk' dk.$$ (2.20)

Remark 2.6. Let us comment on the notation used in Theorem 2.5.

(a) For a set $S \subset \mathbb{R}^d$ we shall denote by $C_c(S)$ the set of all continuous functions $f : S \to \mathbb{C}$ with compact support. Without mention we shall use the canonical isomorphism $C_c(S)^2 \cong \{f : S \times \mathbb{Z}_2 \to \mathbb{C} : f(\cdot, \lambda) \in C_c(S), \lambda = 1, 2\}$.

(b) For $t > 0$ the expression $\delta(t - \cdot)$ is defined as a point measure on $(0, \infty)$ at $t$ with mass one. Explicitly, for $f \in C_c(\mathbb{R}^3 \setminus \{0\})$ and $t > 0$ we define

$$\int_{\mathbb{R}^3} \delta(t - |x|) f(x) dx := \int_{S_2} \int_0^\infty \delta(t - r) f(r\omega) r^2 dr dS(\omega) = \int_{S_2} f(t\omega) t^2 dS(\omega),$$

where $dS$ denotes the measure on $S_2 := \{x \in \mathbb{R}^3 : |x| = 1\}$. The integral (2.20) is understood as an iterated integral, where we first integrate with respect to $k'$ according to the displayed equation just above and then with respect to $k$.
Remark 2.7. We note that a relation similar to (2.20) has been shown in [8] for the spin boson model. In contrast to the spin boson model there is in non-relativistic qed an additional term in the $T$-matrix, which comes from the quadratic expressions of the field operators in the Hamiltonian.

Remark 2.8. Relation (2.20) can be used as a starting point for calculations of the one photon scattering matrix. A procedure to control the scattering amplitude for arbitrary photon processes up to remainder terms of arbitrarily high order in the coupling constant has been carried out in [3], using a type of iterated perturbation theory. In that paper a relation of the scattering amplitude to Bohr’s frequency condition was established. In contrast to [3] the abstract relation (2.20) allows to use expansions which have already been established in the literature. In this regard we note that analytic expansions of the ground state have been established in [24, 28, 29, 31]. Moreover, expansions of boundary values of resolvents have been obtained in the literature, see [4, 5, 44, 30] and references therein.

3 Proofs

The basic idea of the proof is to integrate out the time evolution using the spectral theorem together with an Abelian limit. For this we shall use the following representation of the asymptotic creation operator, which is obtained by means of Cook’s method.

Lemma 3.1. Suppose Hypothesis B holds for some $E > E_{gs}$. Then for $\psi = 1_{H \leq E} \psi$ and $h \in L^2_\omega (\mathbb{R}^3; \mathbb{C}^2)$

$$a_{\text{out}}^* (h) \psi = a^* (h) \psi + i \int_0^{\pm \infty} \sum_{\lambda=1,2} \int_{\mathbb{R}^3} h(k, \lambda) e^{i u (H - \omega(k))} D_1 (k, \lambda) e^{-i H u} \psi dk du,$$

(3.1)

where the first integral over $k$ converges as an integral in $L^1 (\mathbb{R}^3 \times \mathbb{Z}_2; \mathcal{H})$ and the second integral with respect to $u$ converges in the sense of Riemann integrals with respect to the norm topology in $\mathcal{H}$.

We note that the relation in Lemma 3.1 is formally equivalent to the relations given in [3] (II.7),(II.8),(II.12),(II.17)]. The following proof of Lemma 3.1 is based on Hypothesis B.

Proof. Let $\psi = 1_{H \leq E} \psi$ and $h \in \mathfrak{h}$. The convergence of the $k$ integral in (3.1) follows from the following estimate analogous to (2.15). Using $\|(H + i) e^{-i H u} \psi\| \leq (\max \{|E_{gs}|, |E|\} + \|H^\dagger \| \cdot \|e^{-i H u} \psi\|)$.
Indeed, for \( v \in \mathbb{R}, \) and show that the map by the spectral theorem for self-adjoint operators. First, we assume in addition (Theorem 5.9) we see that there exists a constant \( C \) such that for almost all \((k, \lambda) \in \mathbb{R}^3 \times \mathbb{Z}_2\)

\[
|h(k, \lambda)e^{iu(H-\omega(k))}D_1(k, \lambda)e^{-iHu}\psi| = |h(k, \lambda)D_1(k, \lambda)e^{-iHu}\psi| \leq C|\partial H(k, \lambda)| \sum_{j=1}^N (\|p_j + A(x)(-\Delta + H + 1)^{-1/2}\| + |k|) \|\psi\|.
\]

Now (3.3) is by (2.3) an \( L^1 \)-function of \((k, \lambda)\). It follows that the integral

\[
\sum_{\lambda=1,2} \int_{\mathbb{R}^3} h(k, \lambda) [e^{iu(H-\omega(k))}D_1(k, \lambda)e^{-iHu}] \psi dk
\]

exists as a Bochner integral.

Next we show (3.1) using a type of Cook’s argument. Thus let \( h \in \mathfrak{h}_\omega \). We first claim that the map

\[
\eta_h : \mathbb{R} \rightarrow \mathcal{H}, \quad u \mapsto \eta_h(u) := [e^{iuH}a^*(e^{-i\omega u}h)e^{-iHu}] \psi
\]

is differentiable with respect to the norm topology in \( \mathcal{H} \). For this, observe that \( u \mapsto e^{-iHu}\psi \) as well as \( u \mapsto e^{-iHu}H\psi \) are continuously differentiable since \( \psi \in \text{Ran} 1_{H \leq E} \), as can be seen by the spectral theorem for self-adjoint operators. First, we assume in addition \( \omega h \in \mathfrak{h}_\omega \) and show that the map \( \mathbb{R} \mapsto \mathcal{H} \) given by \( u \mapsto \xi(u) := a^*(e^{-i\omega u}h)e^{-iHu}\psi \) is differentiable. Indeed, for \( v \in \mathbb{R} \setminus \{0\} \)

\[
\frac{1}{v} (\xi(u + v) - \xi(u)) = \frac{1}{v} \left( a^*(e^{-i\omega(u+v)}h) - a^*(e^{-i\omega u}h) \right) (H + i)^{-1} e^{-iHu}(H + i)\psi
\]

\[+ a^*(e^{-i\omega(u+v)}h)(H + i)^{-1} \frac{1}{v} (e^{-iH(u+v)}(H + i)\psi - e^{-iH}(H + i)\psi)
\]

\[\rightarrow a^*(-i\omega e^{-i\omega u}h)e^{-iHu}\psi + a^*(e^{-i\omega u}h)e^{-iH}(H + i)\psi = \xi'(u)
\]

where the convergence follows using (3.2) and Lemma A.1 as well as the differentiability of \( u \mapsto e^{-iH}(H + i)\psi \), just discussed. Thus \( u \mapsto \xi(u) \) is an \( \mathcal{H} \)-valued differentiable function. Since moreover \( \xi(u) \in \mathcal{D}(H) \), by Lemma A.3 it follows from

\[
v^{-1}(e^{iH(u+v)}\xi(u) + v^{-1}(e^{iH(u+v)} - e^{iHu})\xi(u) + e^{iH(u+v)}v^{-1}(\xi(u) + v) - \xi(u))
\]

\[\rightarrow e^{iHu}(iH\xi(u) + \xi'(u)).\]
that $e^{iHu}\xi(u)$ is a differentiable function with derivative $e^{iHu}(iH\xi(u) + \xi'(u))$. We now conclude using (3.6) that the function in (3.5) is for $h \in \mathfrak{h}_\omega$ with $\omega h \in \mathfrak{h}_\omega$ differentiable with derivative

$$
\frac{d}{du} \eta_h(u) = \frac{d}{du} \left[ e^{iuH} a^*(e^{-i\omega h}) e^{-iHu} \right] \psi
$$

(3.7)

$$
e^{iuH} \left( [iH, a^*(e^{-i\omega h})] + a^*(-i\omega e^{-i\omega h}) \right) e^{-iHu} \psi
$$

$$
= e^{iuH} \left[ i \sum_{j=1}^{N} \left\{ (p_j + A(x_j))^2 + \mu S_j \cdot B(x_j) \right\} , a^*(e^{-i\omega h}) \right] e^{-iHu} \psi
$$

$$
= e^{iuH} \left\{ \frac{i}{(2\pi)^{3/2}} \sum_{j=1}^{N} \left\{ \sum_{\lambda=1,2} \int_{\mathbb{R}^3} 2 \frac{\varepsilon(k, \lambda)}{\sqrt{2|k|}} \kappa(k)e^{ik \cdot x_j} h(k, \lambda) e^{-i\omega(k)u} dk \cdot (p_j + A(x_j)) \right\}
$$

$$
+ \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \mu S_j : \frac{i \kappa(k) e^{ik \cdot x_j} h(k, \lambda) e^{-i\omega(k)u} dk}{\sqrt{2|k|}} \right\} e^{-iHu} \psi, \quad (3.8)
$$

where in the third line we used the basic relation $[H_t, a^*(f)] \subseteq a^*(\omega f)$ and in the fourth line we used the canonical commutation relations. Now observe from the explicit expression that (3.8) depends continuously on $u$ for all $h \in \mathfrak{h}_\omega$. It now follows from a standard limiting argument, that the function (3.5) is for all $h \in \mathfrak{h}_\omega$ continuously differentiable in $u$ with derivative given by (3.8) (for $h_n = 1_{|\cdot| \leq n}h$, we see from (3.2) that $\eta_{h_n}(u) \to \eta_h(u)$ for each $u \in \mathbb{R}$ and the derivatives $\eta'_{h_n}$ converges uniformly on compact sets in view of (3.8)).

Next we use the definition of $D_1$ given in (2.13) and the convergence of the Bochner-integral justified by (3.3) to see that

$$
(3.8) = e^{iuH} \sum_{\lambda=1,2} \int_{\mathbb{R}^3} h(k, \lambda) e^{-i\omega(k)} D_1(k, \lambda) e^{-iHu} \psi dk, \quad (3.9)
$$

where equality can be seen by calculating for both sides the inner product with elements of the dense subset $C$ (using elementary properties of Bochner-integrals, cf. [48, V.5, Corollary 2] or [16, Appendix E.3, Theorem 8]) and interchanging integrals with respect to the integration variables $k$ and $x = (x_1, ..., x_N)$ by means of Fubini (in the l.h.s. one calculates first the $k$-integral and then the $x$-integral and in the r.h.s. in the reversed order). By continuity of $e^{iuH}$ it follows again from the convergence of the Bochner integral, established by means of (3.3) (using elementary properties of Bochner-integrals [48, V.5.}
Corollary 2] or [2, Theorem 2.11 (iii)] that for all \( h \in \mathfrak{h}_\omega \)

\[
e^{iuH} \sum_{\lambda=1,2} \int_{\mathbb{R}^3} h(k, \lambda)e^{-iu(k)}D_1(k, \lambda)e^{-iHu}\psi dk
= \sum_{\lambda=1,2} \int_{\mathbb{R}^3} h(k, \lambda)e^{iu(H-\omega(k))}D_1(k, \lambda)e^{-iHu}\psi dk.
\]

(3.10)

Finally, to show (3.1) we will use the definition of the asymptotic creation and annihilation operators (2.9) and (2.10). Thus

\[
a_{\text{out}} a_{\text{in}}(h) = \lim_{t \to \pm \infty} e^{iHt} a_{\text{out}}(e^{-i\omega t}h)e^{-iHt}\psi
= a_{\text{in}}(h)\psi + i \int_{ \mathbb{R}^3 } \frac{d}{du} \left[ e^{iHt} a_{\text{out}}(e^{-i\omega u}h)e^{-iHt} \right] \psi du
= a_{\text{in}}(h)\psi + i \int_{ \mathbb{R}^3 } \frac{d}{du} \sum_{\lambda=1,2} \int_{\mathbb{R}^3} h(k, \lambda)e^{iu(H-\omega(k))}D_1(k, \lambda)e^{-iHu}\psi dk du,
\]

(3.11)

where for the first identity we used the existence of the asymptotic creation operators, i.e., Hypothesis B (i), for the second identity we used the fundamental theorem of calculus and the continuity of the derivative in \( u \) (i.e. (3.8)), and in the last identity we used (3.9) and (3.10). Thus (3.11) shows the desired identity. We note that instead of using Hypothesis B (i) one could use a stationary phase estimate and a density argument to show the integrability at infinity with respect to \( u \) directly, cf. [19, Proposition 3, Theorem 4] or [3, Lemma II.1].

\[\square\]

**Proposition 3.2.** Suppose Hypothesis B holds for some \( E > E_{gs} \) and that Hypothesis C holds for some \( S \subset \mathbb{R}^3 \setminus \{0\} \). Then for all \( k \in S, \lambda \in \mathbb{Z}_2 \), and \( h \in C_c(S)^2 \)

\[
\langle D_1(k, \lambda)\psi_{gs}, a_{\text{in}}^*(h)\psi_{gs}\rangle = \sum_{\lambda'=1,2} \int_{\mathbb{R}^3} T(k, \lambda, k', \lambda') h(k', \lambda')dk'
\]

Proof. To simplify notation we write \( K = (k, \lambda), K' = (k', \lambda') \), and

\[
\int \cdots dK = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \cdots dk.
\]

(3.12)

To calculate the right argument of the inner product we use Lemma 3.1 and find after the substitution \( u \mapsto -u \)

\[
a_{\text{in}}^*(h)\psi_{gs} = a^*(h)\psi_{gs} - i \int_{0}^{\infty} \int_{\mathbb{R}^3} h(K')e^{-iu(H-\omega(k')-E_{gs})}D_1(K')\psi_{gs}dK' du.
\]

(3.13)
Next we want to evaluate the integral in (3.13) with respect to $u$. For this, we first observe that for a self-adjoint operator $A$, we have by the spectral theorem the following identity
\[
\int_0^T e^{-it(A-i\epsilon)}dt = \frac{1}{-i(A-i\epsilon)}(e^{-iT(A-i\epsilon)} - 1), \quad (\epsilon > 0)
\]
where the integral is understood with respect to the strong operator topology as a Riemann-integral. Taking the limit $T \to \infty$, again in the strong operator topology, gives
\[
\int_0^\infty e^{-it(A-i\epsilon)}dt = \frac{-i}{A-i\epsilon}.
\] (3.14)
Let us apply $\langle D_1(K)\psi_{gs}, \cdot \rangle$ to the integral in (3.13). Using that strong convergence implies weak convergence and elementary properties of Bochner-integrals [18, V.5, Corollary 2] (see also [16, Appendix E.3, Theorem 8]) we obtain the following integral. We rewrite this integral using an Abelian limit, see Proposition B.1 (where the required existence of the limit follows from the existence of the limit of the improper integral in (3.13)), we then use (3.14) to evaluate the integral in (3.13) with respect to $u$. This gives for all $k \neq 0$
\[
\left< D_1(K)\psi_{gs}, \int_0^\infty \left( \int h(K'), e^{-iu(H-\omega(k')-E_{gs})} D_1(K')\psi_{gs}dK' \right) du \right>
\]
\[
= \int_0^\infty \left( \int h(K') \left< D_1(K)\psi_{gs}, e^{-iu(H-\omega(k')-E_{gs})} D_1(K')\psi_{gs} \right> dK' \right) du
\]
\[
= \lim_{t \to \infty} \int_0^t \left( \int h(K') \left< D_1(K)\psi_{gs}, e^{-iu(H-\omega(k')-E_{gs})} D_1(K')\psi_{gs} \right> dK' \right) du
\]
\[
= \lim_{\epsilon \to 0} \int_0^\infty e^{-iu} \left( \int h(K') \left< D_1(K)\psi_{gs}, e^{-iu(H-\omega(k')-E_{gs}-i\epsilon)} D_1(K')\psi_{gs} \right> dK' \right) du
\]
\[
= \lim_{\epsilon \to 0} \int_0^\infty \left( \int h(K') \left< D_1(K)\psi_{gs}, e^{-iu(H-\omega(k')-E_{gs}-i\epsilon)} D_1(K')\psi_{gs} \right> dK' \right) du
\]
\[
= -i \lim_{\epsilon \to 0} \int h(K') \left< D_1(K)\psi_{gs}, (H - \omega(k') - E_{gs} - i\epsilon)^{-1} D_1(K')\psi_{gs} \right> dK'
\]
\[
= -i \int h(K') \left< D_1(K)\psi_{gs}, (H - \omega(k') - E_{gs} - i0_+)^{-1} D_1(K')\psi_{gs} \right> dK',
\] (3.15)
where we first used Fubini in the second to last line, which is justified since the integrand satisfies the bound
\[
\left| h(K') \left< D_1(K)\psi_{gs}, e^{-iu(H-\omega(k')-E_{gs}-i\epsilon)} D_1(K')\psi_{gs} \right> \right| \leq |h(K')| \left\| D_1(K)\psi_{gs} \right\| \left\| D_1(K')\psi_{gs} \right\| e^{-\epsilon u}
\]
so it is integrable with respect to $K'$ (by (2.3) and (2.15)) as well as trivially with respect to $u$, and we then used (3.14) in the second to last line. In the last line of (3.15) we used dominated convergence, which is justified by (2.18) of Hypothesis C.
Next, we shall also use a pull-through resolvent identity, which states that for almost all $k' \neq 0$
\[
a(k', \lambda)\psi_{gs} = -(H + \omega(k') - E_{gs})^{-1}D_1(k', \lambda')^*\psi_{gs},
\]
for a proof see for example [13]. Using identity (3.13), inserting (3.15), and calculating an elementary commutator, we find
\[
\langle D_1(K)\psi_{gs}, a^*(h)\psi_{gs} \rangle = \langle D_1(K)\psi_{gs}, a^*(h)\psi_{gs} \rangle \\
- i \int_0^\infty \int h(K') \left( D_1(K)\psi_{gs}, e^{-iu(H-\omega(k')-E_{gs})}D_1(K')\psi_{gs} \right) dK' du \\
= \langle [a(h), D_1(K)]\psi_{gs}, \psi_{gs} \rangle + \langle a(h)\psi_{gs}, D_1(K)^*\psi_{gs} \rangle \\
- \int h(K') \left( D_1(K)\psi_{gs}, (H - \omega(k') - E_{gs} - i0^+)^{-1}D_1(K')\psi_{gs} \right) dK' \\
= \int h(K') \left( \langle D_2(K', K')\psi_{gs}, \psi_{gs} \rangle \\
- \langle (H + \omega(k') - E_{gs})^{-1}D_1(K')^*\psi_{gs}, D_1(K)^*\psi_{gs} \rangle \\
- \langle D_1(K)\psi_{gs}, (H - \omega(k') - E_{gs} - i0^+)^{-1}D_1(K')\psi_{gs} \rangle \right) dK' \\
= \int h(K')T(K, K')dK',
\]
where in the second to last line we used the definition of $D_2$ given in (2.16) and (3.16). In the last line we used the definition of the $T$-matrix, (2.19).

Lemma 3.3. Suppose Hypothesis $B$ holds for $E > E_{gs}$. Then for $\varphi = 1_{H\leq E}\varphi$ and $f \in L^2_{\mathbb{C}}(\mathbb{R}^3; \mathbb{C})$ we have for all $t \in \mathbb{R}$
\[
e^{iHt}a_{in}^*(f)\varphi = a_{in}^*(e^{i\omega t}f)e^{iHt}\varphi.
\]

Proof. For $\psi \in 1_{H\leq E}\mathcal{H}$ we find using (2.9), (2.10), and Hypothesis $B$ (i)
\[
e^{-iHt}a_{in}^*(e^{i\omega t}f)e^{iHt}\psi = e^{-iHt} \lim_{u \to -\infty} e^{iHu}e^{-iHt}\psi \\
= \lim_{u \to -\infty} e^{iH(u-t)}e^{-iHt}\psi \\
= a_{in}^*(f)\psi.
\]
Multiplying both sides with $e^{iHt}$ yields the claimed identity.
Proof of Theorem 2.5. From Lemma 3.1 we see that for the ground state $\psi_{gs}$ of $H$ with ground state energy $E_{gs}$ we find

$$a_{out}^*(f) \psi_{gs} - a_{in}^*(f) \psi_{gs} = i \int_{-\infty}^{\infty} \sum_{\lambda = 1,2} \int_{\mathbb{R}^3} f(k, \lambda) e^{i\lambda k} e^{i\lambda(k - E_{gs})} D_1(k, \lambda) \psi_{gs} dk du. \quad (3.18)$$

We shall use notation (3.12). Using Hypothesis [B] (ii), (3.18) together with the continuity if the inner product, Proposition [B.1] and elementary properties of Bochner-integrals, [48] V.5. Corollary 2], we find

$$L := \langle a_{out}^*(f) \psi_{gs}, a_{in}^*(g) \psi_{gs} \rangle - \langle f, g \rangle$$

$$= \langle (a_{out}^*(f) - a_{in}^*(f)) \psi_{gs}, a_{in}^*(g) \psi_{gs} \rangle + \langle a_{in}^*(f) \psi_{gs}, a_{in}^*(g) \psi_{gs} \rangle - \langle f, g \rangle$$

$$= -i \lim_{\epsilon \to 0} \int_{-\infty}^{\infty} e^{-\epsilon|u|} \int f(K) e^{i\lambda(k - E_{gs})} D_1(K) \psi_{gs} dK, a_{in}^*(g) \psi_{gs} \rangle \rangle dK$$

$$= -i \lim_{\epsilon \to 0} \int_{-\infty}^{\infty} e^{-\epsilon|u|} \int f(K) \langle D_1(K) \psi_{gs}, e^{-i\lambda(k - E_{gs})} a_{in}^*(g) \psi_{gs} \rangle \rangle dK $$

Now using first Lemma [3.3] and then Proposition [3.2] we obtain

$$iL = \lim_{\epsilon \to 0} \int_{-\infty}^{\infty} e^{-\epsilon|u|} \int \overline{f(K)} \langle D_1(K) \psi_{gs}, e^{-i\lambda(k - E_{gs})} a_{in}^*(g) \psi_{gs} \rangle \rangle dK$$

$$= \lim_{\epsilon \to 0} \int_{-\infty}^{\infty} e^{-\epsilon|u|} \int \overline{f(K)} e^{i\lambda(k - E_{gs})} \langle D_1(K) \psi_{gs}, a_{in}^*(g) \psi_{gs} \rangle \rangle dK$$

$$= \lim_{\epsilon \to 0} \int_{-\infty}^{\infty} e^{-\epsilon|u|} \int \overline{f(K)} g(K') e^{i\lambda(k - E_{gs})} T(K, K') dK' dK$$

$$= \lim_{\epsilon \to 0} \int \int \overline{f(K)} g(K') \int_{-\infty}^{\infty} e^{-\epsilon|u|} e^{i\lambda(k - E_{gs})} T(K, K') dK' dK$$

$$= \lim_{\epsilon \to 0} \int \int \overline{f(K)} g(K') \frac{2\epsilon}{\epsilon^2 + (\lambda(k) - \lambda(k'))^2} T(K, K') dK' dK$$

$$= 2\pi \int \int \overline{f(K)} g(K') \delta(\lambda(k') - \lambda(k)) T(K, K') dK' dK,$$

where in the fourth line we used Fubini (which is justified by the boundedness assumptions in Hypotheses [C] and [D]). In the last equality we integrated by Hypothesis [D] first over $|k'|$ and then use dominated convergence for the $k$-integration to take the limit $\epsilon \downarrow 0$ into the integral.
4 Verification of the Hypothesis

In this section we show, in Theorem 4.5, that Hypothesis D (and thus Hypothesis C) holds for an atom for small but nontrivial coupling in an energy interval, for which a Fermi’s golden rule condition holds. We make the following additional assumptions on the potential \( V \), which are assumed to hold throughout this section. Let

\[
V(x_1, ..., x_N) = V_C(x_1, ..., x_N) := -\sum_{j=1}^{N} \frac{Z\alpha}{|x_j|} + \sum_{i<j}^{N} \frac{\alpha}{|x_j - x_i|},
\]

with \( Z = N \) and \( \alpha > 0 \). Let \( \mathcal{H}_{at} = L^2_\alpha((\mathbb{R}^3 \times \mathbb{Z}_{2s+1})^N) \) be given as the antisymmetric subspace. Then it follows that the spectrum of \( \mathcal{H}_{at} = -\Delta + V_C \) has the structure

\[
\sigma(\mathcal{H}_{at}) = \{E_{at,j} : j = 0, ..., M\} \cup [\Sigma_{at}, \infty), \tag{4.1}
\]

where \( \Sigma := \inf \sigma_{ess}(\mathcal{H}_{at}), M \in \{1, 3, ...\} \cup \{\infty\}, (E_{at,j})_{j=1, ..., M} \) is strictly monotone, and \( E_{at,j} < \Sigma \), see [12] and references therein. For \( \theta \in \mathbb{R}, \psi \in \mathcal{H}_{at} \) and \( h \in \mathfrak{h} \) we define the transformations

\[
U_{el}(\theta)\psi(x_1, s_1, ..., x_N, s_N) = e^{\frac{\theta}{2}N}\psi(e^{\theta}x_1, s_1, ..., e^{\theta}x_N, s_N), \quad x_j \in \mathbb{R}^3, s_j \in \{1, 2s + 1\}
\]

\[
U_{ph}(\theta)h(k, \lambda) = e^{\frac{\theta}{2}N}h(e^{-\theta}k, \lambda), \quad (k, \lambda) \in \mathbb{R}^3 \times \mathbb{Z}_2.
\]

Note that it is straightforward to see that these transformations are unitary. Let \( \Gamma(U_{ph}) \) denote the bounded linear operator on \( \mathcal{F}(\mathfrak{h}) \) such that \( \Gamma(U_{ph})|_{\mathcal{F}_n(\mathfrak{h})} = \bigotimes_{j=1}^{n} U_{ph} \). We define \( U(\theta) = U_{el} \otimes \Gamma(U_{ph}) \). As an immediate consequence of the definitions one finds

\[
U(\theta)x_jU(\theta)^{-1} = e^{\theta}x_j, \quad U(\theta)p_jU(\theta)^{-1} = e^{-\theta}p_j, \quad U(\theta)H_fU(\theta)^{-1} = e^{\theta}H_f.
\]

For the Hamiltonian \( H \), given in (2.4), we define for \( \theta \in \mathbb{R} \)

\[
H(\theta) = U(\theta)HU(\theta)^{-1}.
\]

A straightforward calculation shows that

\[
H(\theta) = \sum_{j=1}^{N} \{ (e^{-\theta}p_j + A_\theta(x_j))^2 + \mu S_j \cdot B_\theta(x_j) \} + e^{-\theta}V_C \otimes 1 + e^{-\theta}1 \otimes H_f, \tag{4.2}
\]

where we defined

\[
A_{\theta,l}(x) := \phi(G_{x,l,\theta}), \quad B_{\theta,l} := \phi(J_{x,l,\theta}), \quad x \in \mathbb{R}^3, \quad l = 1, 2, 3,
\]
with
\[
G_{x,l,\theta}(k, \lambda) := \frac{e^{-\theta} \kappa(e^{-\theta} k)}{(2\pi)^{3/2} \sqrt{|k|}} \varepsilon_l(k, \lambda) e^{-ik \cdot x},
\]
\[
J_{x,l,\theta}(k, \lambda) := \frac{e^{-\theta} \kappa(e^{-\theta} k)}{(2\pi)^{3/2} \sqrt{|k|}} [(-ie^{-\theta} k) \wedge \varepsilon_l(k, \lambda)] e^{-ik \cdot x},
\]
for \( k \in \mathbb{R}^3 \setminus \{0\} \) and \( \lambda \in \mathbb{Z}_2 \). We assume that the coupling function is of the form
\[
\kappa(k) = g \tilde{\kappa}(|k|), \quad k \in \mathbb{R}^3,
\]  
(4.3)
with \( g \in \mathbb{R} \), called minimal coupling constant, and with \( \tilde{\kappa} : (0, \infty) \to \mathbb{R} \) a positive function, which satisfies \( \tilde{\kappa}(r) \to a \) as \( r \to \infty \) for some \( a \in [0, \infty) \), and has an analytic continuation to a cone, \( \{re^{i\varphi} : r > 0, -\tilde{\theta}_0 < \varphi < \tilde{\theta}_0 \} \) for some \( \tilde{\theta}_0 > 0 \), around the positive real axis, which is bounded and decays faster than any inverse polynomial, e.g. \( \tilde{\kappa}(r) = \exp(-r^4) \). The Hamiltonian \( H(\theta) \) is self-adjoint on the domain \( \mathcal{D}(-\Delta + H_f) \) for any \( \theta \in \mathbb{R} \), see Remark 2.1. For \( a \in \mathbb{C} \) and \( r \geq 0 \) we define \( D_r(a) := \{ z \in \mathbb{C} : |z - a| < r \} \) and \( D_r := D_r(0) \).

The following lemma collects a elementary facts, which can be shown using elementary estimates. A proof can be found for example in [5, Lemma 1.1,Corollary 1.4] or [31].

**Lemma 4.1.** Suppose \( V = V_C \) and (4.3). Let \( \theta_0 \in (0, \min\{\tilde{\theta}_0, \pi/4\}) \). Then the following holds.

(a) There exists a \( g_0 > 0 \) such that for all \( g \in (-g_0, g_0) \) the mapping \( \theta \mapsto H(\theta) \) has an analytic continuation to \( D_{\theta_0} \). The resulting analytic continuation is an analytic family of type (A) with common domain of the operators \( \mathcal{D}(-\Delta + H_f) \).

(b) The maps \( \theta \mapsto A_{\theta}(x_j)(-\Delta + H_f + 1)^{-1/2} \) and \( \theta \mapsto (-\Delta + H_f + 1)^{-1/2} A_{\theta}(x_j)|_{\mathcal{D}((H_f+1)^{1/2})} \) are analytic functions on \( D_{\theta_0} \).

(c) Let \( W_{g}(\theta) := \sum_{j=1}^{N} \{ A_{\theta}(x_j) \cdot e^{-\theta} p_j + e^{-\theta} p_j \cdot A_{\theta}(x_j) + A_{\theta}(x_j)^2 + \mu S_j \cdot B_{\theta}(x_j) \} \). There exists a constant \( C \) such that for all \( \theta \in D_{\theta_0} \) and \( g \in \mathbb{R} \)
\[
\|W_{g}(\theta)(-\Delta + H_f + 1)^{-1}\| \leq C|g|(1 + |g|).
\]

Henceforth, we shall denote by \( H(\theta) \) the analytic continuation to a neighborhood of zero granted by Part (a) of Lemma 4.1.
Lemma 4.2. Suppose $V = V_C$ and (1.3). Let $\theta_0 \in (0, \min\{\theta_0, \pi/4\})$ and $x \in \mathbb{R}$. Then there exists a $y > 0$ and a $g_0 > 0$ such that

$$x + iy \in \rho(H(\theta))$$

(4.4)

for all $\theta \in D_{\theta_0}$ with $\Im \theta \leq 0$ and $g \in (-g_0, g_0)$.

Proof. We devide the proof into steps.

Step 1: Since $V_C$ is infinitesimally $-\Delta$ bounded [H1], we have

$$\lim_{y \to \infty} \|V_C(-\Delta - iy)^{-1}\| = 0.$$  

(4.5)

Step 2: Let $x \in \mathbb{R}$ and $y_0 = \sqrt{x^2 + 1}$. Then

$$\sup_{\theta \in D_{\theta_0}, y \geq y_0, \Im \theta \leq 0} \sup_{\Delta \leq \epsilon} \|(-\Delta - iy)(-e^{-2\theta} \Delta + e^{-\theta} H_f - x - iy)^{-1}\| < \infty,$$

(4.6)

$$\sup_{\theta \in D_{\theta_0}, y \geq y_0, \Im \theta \leq 0} \|(-\Delta + H_f + 1)(-e^{-2\theta} \Delta + e^{-\theta} H_f - x - iy)^{-1}\| < \infty.$$

These bounds follow from the bounds (4.6)–(4.8) below and the triangle inequality. Let $\theta \in D_{\theta_0}$ with $\Im \theta \leq 0$. Then using the spectral theorem and $\Im(e^{-2\theta} r + e^{-\theta} s + x) \leq 0$ for $r, s \in [0, \infty)$, we obtain for $y \geq y_0$ the following estimates. We estimate

$$\|y(-e^{-2\theta} \Delta + e^{-\theta} H_f - x - iy)^{-1}\|$$

(4.6)

$$= \sup_{r, s \geq 0} \left| \frac{y}{e^{-2\theta} r + e^{-\theta} s - x - iy} \right| \leq \frac{y}{\Im(e^{-2\theta} r + e^{-\theta} s + x) - y} \leq \frac{y}{y} = 1,$$

and

$$\left\| -\Delta(-e^{-2\theta} \Delta + e^{-\theta} H_f - x - iy)^{-1} \right\| = \sup_{r, s \geq 0} \frac{r}{|e^{-2\theta} r + e^{-\theta} s - x - iy|}$$

(4.7)

$$\leq \sup_{r, s \geq 0} \frac{r}{\frac{1}{2}(\Re(e^{-2\theta} r + e^{-\theta} s + x)^2 + y^2)^{1/2}} \leq \sup_{r, s \geq 0} \frac{\frac{1}{2} |\Re(e^{-2\theta} r + e^{-\theta} s)|^2 + y^2 - x^2|^{1/2}}{\sqrt{2}e^{2\theta_0}}.
$$

where in the second inequality we used $(u + v)^2 \geq \frac{1}{2} u^2 - v^2$. An analogous estimate as (4.7) (interchanging the roles of $s$ and $r$) gives

$$\left\| H_f(-e^{-2\theta} \Delta + e^{-\theta} H_f - x - iy)^{-1} \right\| = \sup_{r, s \geq 0} \frac{s}{|e^{-2\theta} r + e^{-\theta} s - x - iy|} \leq \frac{\sqrt{2}e^{\theta_0}}{\cos(\theta_0)}.$$  

(4.8)

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Step 3: It follows from Lemma 4.1 (c) and Step 1 and Step 2, that there exists a \( g_0 > 0 \) and a \( y > 0 \) such that for all \( \theta \in D_{\theta_0} \) with \( \text{Im} \theta \leq 0 \) and \( g \in (-g_0, g_0) \) we have
\[
\|(e^{-\theta}V_C + W_g(\theta))(-e^{-2\theta} \Delta + e^{-\theta}H_f - x - iy)^{-1}\| \leq 1/2. \tag{4.9}
\]
It follows using a Neumann expansion for the operator
\[
H(\theta) - x - iy = (-e^{-2\theta} \Delta + e^{-\theta}H_f - x - iy) + (e^{-\theta}V_C + W_g(\theta))
\]
that \( x + iy \in \rho(H(\theta)) \) for all \( \theta \in D_{\theta_0} \) with \( \text{Im} \theta \leq 0 \) and \( g \in (-g_0, g_0) \).

For \( x \in \mathbb{R}^n \) we write \( \langle x \rangle = (1 + x^2)^{1/2} \). The proof of Theorem 4.5, below, is based on the following nontrivial result, which is stated in the following Hypothesis.

**Hypothesis E.** The ground state \( \psi_{gs} \) of \( H \) has the following properties. There exist positive \( \beta > 0 \) and \( \theta_0 > 0 \) such that
\begin{enumerate}
    \item \( \theta \mapsto \psi_{gs,\theta} := U(\theta)\psi_{gs} \) has an \( \mathcal{H} \)-valued analytic extension for \( \theta \) into \( D_{\theta_0} \),
    \item \( \|e^{\beta(\cdot)}\psi_{gs,\theta}\| \) is uniformly bounded on \( D_{\theta_0} \).
\end{enumerate}

**Remark 4.3.** We will use the following simple consequence of Hypothesis E that \( \theta \mapsto e^{\beta(\cdot)}\psi_{gs,\theta} \) is an \( \mathcal{H} \)-valued analytic function. This follows as an application of the abstract result in Lemma C.1.

Let us now introduce notation to formulate Fermi’s golden rule condition. Let \( P_{at,j} = 1\{E_{at,j}\}(H_{at}) \), where \( 1_A(x) := 1 \) if \( x \in A \) and otherwise \( 1_A(x) = 0 \). Define for \( k \in \mathbb{R}^3 \setminus \{0\} \) and \( \lambda \in \mathbb{Z}_2 \) the operator
\[
w(k, \lambda) := \sum_{j=1}^N \{2G_{x_j}(k, \lambda) \cdot p_j + \mu S_j \cdot J_{x_j}(k, \lambda)\}
\]
in \( \mathcal{H}_{at} \) on the domain \( D((-\Delta)^{1/2}) \) and the linear map
\[
Z_j := \lim_{\epsilon \downarrow 0} \sum_{\lambda=1,2} \int_{\mathbb{R}^3} P_{at,j}w(k, \lambda)P_{at,j}^* \left( \mathcal{P}_{at,j}H_{at} - E_{at,j} + |k| - i\epsilon \right)^{-1} \mathcal{P}_{at,j}w(k, \lambda)^* P_{at,j} dk + \sum_{\lambda=1,2} \int_{\mathbb{R}^3} P_{at,j}w(k, \lambda)P_{at,j}w(k, \mu)^* P_{at,j} \frac{dk}{|k|}, \tag{4.10}
\]
where \( \mathcal{P}_{at,j} = 1_{\mathcal{H}_{at}} - P_{at,j} \). We say that a Fermi’s golden Rule condition holds for the \( j \)-the eigenvalue, \( E_j \), if
\[
\text{Im} Z_j > 0. \tag{4.11}
\]
Let us state the following theorem, which follows directly from the results in [5, 30]. To formulate it, we define

$$\delta_j := \text{dist} \left( E_{at,j}, \sigma(H) \setminus \{ E_{at,j} \} \right)$$

(4.12)

and

$$\mathcal{A}(E, \delta, c) := (E - \delta/2, E + \delta/2) + i[-cg^2, \infty).$$

(4.13)

Figure 1: Illustration of the situation in Theorem 4.4, where the putative spectrum of $H(\theta)$ is indicated with blue.

**Theorem 4.4.** Suppose $V = V_C$ and (4.3). Let $\theta_0 \in (0, \min\{\tilde{\theta}_0, \pi/4\})$ and $j \in \{1, ..., N\}$. Assume $\text{Im}Z_j > 0$. Suppose $\theta = i\vartheta$ with $\vartheta \in (0, \min\{\theta_0, \pi/4\})$. Then there exist $c_j > 0$ and $g_0 > 0$ such that for all $g \in \mathbb{R}$ with $0 < |g| < g_0$

$$\mathcal{A}(E_{at,j}, \delta_j, c_j) \subset \rho(H(\theta)),$$

in particular the interval $[E_{at,j} - \delta_j/2, E_{at,j} + \delta/2]$ is contained in the resolvent set $\rho(H(\theta))$, and there exists a constant $C_j$ such that for any $z \in \mathcal{A}(E_{at,j}, \delta_j, c_j)$ we have

$$\|H_g(\theta) - z\|^{-1} \leq C_j.$$

**Proof.** The theorem follows directly from [30] Corollary 8 (or [5] Theorem 3.2) which needs an additional non-degeneracy condition) by observing that the set given there contains for some $c_j > 0$ the set $\mathcal{A}(E_{at,j}, \delta_j, c_j)$ for all small nonzero $|g|$. The result [30] Corollary 8 is formulated for electrons with spin $s = 1/2$, but the proof carries over to the spinless case $s = 0$ (by dropping the additional term which couples to the spin). The main idea of the proof of [30] Corollary 8 is to consider $H(\theta)|_{g=0}$ and to use a perturbation expansion in $g$. More explicitly, one studies a so called Feshbach projection with respect to an energy interval around $E_j$ and uses Fermi’s golden rule condition. \[\square\]
We are now ready to prove the main theorem of this section.

**Theorem 4.5.** Suppose $V = V_C$, \((4.3)\) and that Hypothesis \([\mathcal{H}]\) holds. Let $j \in \{1,...,M\}$. Suppose $\Im Z_j > 0$. Then there exists a $g_0 > 0$ such that for all real $g$ with $0 < |g| < g_0$ Hypothesis \([\mathcal{H}]\) holds for the Hamiltonian $H$ and the set

$$S_j = \{k \in \mathbb{R}^3 \setminus \{0\} : E_{at,j} - E_{gs} - \delta_j/2 < \omega(k) < E_{at,j} - E_{gs} + \delta_j/2\}.$$  

In fact, the $T$-matrix is for $k,k' \in S$ a $C^\infty$-function of $|k|$ and $|k'|$.

For the proof of Theorem 4.5 we will use the following interpolation result.

**Lemma 4.6.** Suppose $V = V_C$ and \((4.3)\). Let $\theta_0 \in (0,\min\{\tilde{\theta}_0, \pi/4\})$ and let $g_0 > 0$ be such that the assertions of Lemma \([4.1]\) hold. Let $|g| < g_0$ and let $U \subset D_{\theta_0} \times \mathbb{C}$ be an open set such that $(H(\theta) - z)^{-1}$ is an analytic bounded operator valued function of $(\theta, z) \in U$. Then for each $(\theta, z) \in U$ the closure of the operator

$$(-\Delta + H_f + 1)^{1/2}(H(\theta) - z)^{-1}(-\Delta + H_f + 1)^{1/2} \quad (4.14)$$

is bounded and depends analytically on $(\theta, z)$ in $U$.

**Proof.** First we show that the operators $(H(\theta) - z)^{-1}(-\Delta + H_f + 1)$ with domain $\mathcal{C}$ depend continuously on $(\theta, z) \in U$, w.r.t. the operator norm topology. For this let $(\theta', z') \in U$. Since $H(\theta)$ is an analytic family of type (A), by Lemma \([4.1]\) it follows that

$$T_0(\theta) := (H(\theta') - z')^{-1}(H(\theta') - H(\theta))$$

is a bounded operator the domain $\mathcal{D}(-\Delta + H_f)$ and $\lim_{\theta \to \theta'} T_0(\theta) = 0$ (see for example \([31]\) VII. §2 (2.4))). Thus for $(\theta, z)$ sufficiently close to $(\theta', z')$ we obtain from a Neumann expansion the following identity on $\mathcal{C}$

$$(H(\theta) - z)^{-1}(-\Delta + H_f + 1)$$

$$(H(\theta) - z)^{-1}(H(\theta) - z')^{-1}(-\Delta + H_f + 1) + (1 + (z - z')(H(\theta) - z)^{-1}((H(\theta') - z')^{-1}(H(\theta') - H(\theta)))^{-1}(-\Delta + H_f + 1)$$

$$(1 + (z - z')(H(\theta) - z)^{-1}) \sum_{n=0}^\infty T_0(z)^n (H(\theta') - z')^{-1}(-\Delta + H_f + 1). \quad (4.15)$$

Continuity of \((4.15)\) in $(\theta, z)$ now follows, since $(H(\theta') - z')^{-1}(-\Delta + H_f + 1)$ is bounded (for the latter observe that $H(\theta')$ is a closed operator with the same domain as the closed operator $-\Delta + H_f$, c.f. \([47]\) Theorem 5.9)). Likewise one shows that $(-\Delta + H_f +
1) \( (H(\theta) - z)^{-1} \) is a bounded operator depending continuously on \((\theta, z)\). It now follows from interpolation, explicitly Lemma [C.2] that (4.14) extends to a bounded operator with norm uniformly bounded on compact subsets of \( U \). Since \( \langle \phi_1, (4.14) \phi_2 \rangle \) is by assumption for \( \phi_1, \phi_2 \in \mathcal{D}(-\Delta + H_f) \) analytic on \( U \) (see e.g. [12] Theorem XII.7) the analyticity of the closure of (4.14) now follows, because weak analyticity implies strong analyticity, cf. Lemma [C.1].

**Proof of Theorem 4.5.** First observe that by Hypothesis [E] there exists a ground state. First we show Hypothesis [C] for the set \( S_j \). For fixed \( k \in \mathbb{R}^3 \setminus \{0\} \) we consider the dilation of the operator \( D_1(k, \lambda) \) for \( \theta \in \mathbb{R} \)

\[
D_1(k, \lambda; \theta) := U(\theta)D_1(k, \lambda)U(\theta)^{-1}
\]

\[
= \frac{1}{(2\pi)^3/2} \sum_{l=1}^{N} \left\{ (e^{-\theta} p_l + A_\theta(x_l)) \cdot \frac{2\varepsilon(k, \lambda)}{\sqrt{2|k|}} e^{ik \cdot e^\theta x_l} + \mu S_l \cdot \frac{ik \wedge \varepsilon(k, \lambda)}{\sqrt{2|k|}} e^{ik \cdot e^\theta x_l} \right\},
\]

(note we interchanged the factors of the first term on the right hand side, which is justified by \( \varepsilon(k, \lambda) \cdot k = 0 \)). Now choose \( \theta_0 \in (0, \min\{\tilde{\theta}_0, \pi/4\}) \) such that the assertions of Lemma [4.1] Lemma [4.2] for \( x = E_{at,j} \), and Hypothesis [E] hold for some \( g_0 > 0 \) and \( \beta > 0 \). By possibly making \( \theta_0 > 0 \) smaller, we can assume without loss that

\[
\theta_0 < \frac{\beta e^{-\pi/4}}{E_{at,j} - E_{gs} + \delta_j/2} = \frac{\beta e^{-\pi/4}}{\sup\{\|k\|: k \in S_j\}}.
\]

(4.16)

It follows from (4.16) that for \( k \in S_j \)

\[
|\text{Re}(ik \cdot e^\theta x_l)| = e^{\text{Re}\theta} |\sin(\text{Im}\theta)||k||x| \leq e^{\pi/4} \theta_0 |k||x| < \beta |x|, \quad l = 1, \ldots, N.
\]

(4.17)

It follows with \( X := (p^2 + H_f + 1) \) that for \( k \in S_j \)

\[
X^{-1/2} D_1(k, \lambda; \theta) \psi_{gs, \theta}
\]

\[
= \frac{1}{(2\pi)^3/2} \sum_{l=1}^{N} 2X^{-1/2}(e^{-\theta} p_l + A_\theta(x_l)) \cdot \frac{\varepsilon(k, \lambda)}{\sqrt{2|k|}} e^{ik \cdot e^\theta x_l} e^{-\beta |x|} e^{\beta |x|} \psi_{gs, \theta}
\]

\[
+ X^{-1/2} \sum_{l=1}^{N} \mu S_l \cdot \frac{ik \wedge \varepsilon(k, \lambda)}{\sqrt{2|k|}} e^{ik \cdot e^\theta x_l} e^{-\beta |x|} e^{\beta |x|} \psi_{gs, \theta}
\]

is an \( \mathcal{H} \)-valued analytic function of \( \theta \) on \( D_{\theta_0} \) as a consequence of Lemma [4.1] Remark [4.3] to Hypothesis [E] and inequality (4.17).

Now we observe for any \( z \in \mathbb{C} \) with \( \text{Im} z > 0 \) that for \( \theta \in \mathbb{R} \) and \( k, k' \in \mathbb{R}^3 \setminus \{0\} \)

\[
\langle D_1(k, \lambda) \psi_{gs, \theta}, (H - z)^{-1} D_1(k', \lambda') \psi_{gs, \theta} \rangle
\]

\[
= \langle D_1(k, \lambda; \theta) \psi_{gs, \theta}, (H(\theta) - z)^{-1} D_1(k, \lambda; \theta) \psi_{gs, \theta} \rangle
\]

\[
= \langle X^{-1/2} D_1(k, \lambda; \theta) \psi_{gs, \theta}, X^{1/2}(H(\theta) - z)^{-1} X^{1/2} X^{-1/2} D_1(k', \lambda'; \theta) \psi_{gs, \theta} \rangle,
\]

(4.19)
where we used the unitarity of dilation and a trivial insertion of the identity $1 = X^{1/2} X^{-1/2}$.

Next we consider an analytic continuation of (4.19). First, for fixed spectral parameter $z$ in the complex upper half plane we extend $\theta$ into the complex lower half plane, and then, for fixed $\theta$ in the lower half plane we extend the spectral parameter $z$ from the complex upper half plane across the real axis into the complex lower half plane. By Lemma 4.2 we can choose $y \in (0, \infty)$ sufficiently large such that $E_{\omega, j} + iy \in \rho(H(\theta))$ for all $g \in (-g_0, g_0)$ and $\theta \in D_{\theta_0}$ with $\text{Im} \theta \geq 0$. Thus it follows that for $z = z_0 := E_{\omega, j} + iy$ the right hand side of (4.19) is complex differentiable in points $\theta \in D_{\theta_0}$ with $\text{Im} \theta \geq 0$, by the analyticity of (4.18) and the analyticity of $X^{1/2}(H(\theta) - z_0)^{-1}X^{1/2}$, which in turn holds by Lemma 4.6. Since the left hand side of (4.19) does not depend on $\theta$ we conclude by analytic continuation that for $\vartheta \in (0, \theta_0)$ and $z = z_0$

$$\langle D_1(k, \lambda)\psi_{g_0}, (H - z)^{-1}D_1(k', \lambda')\psi_{g_0} \rangle \quad (4.20)$$

$$= \langle X^{-1/2}D_1(k, \lambda; i\vartheta)\psi_{g_0,i\vartheta}, X^{1/2}(H(i\vartheta) - z)^{-1}X^{1/2}X^{-1/2}D_1(k', \lambda; i\vartheta)\psi_{g_0,i\vartheta} \rangle.$$

Now fix $\vartheta \in (0, \theta_0)$. Since $H$ is self-adjoint the left hand side of (4.20) is analytic in $z$ on the upper half complex plane. By Theorem 4.4 there exists a $c_j > 0$ and a $g_1 \in (0, \theta_0)$ such that

$$\mathcal{A}(E_j, \delta_j, c_j) \subset \rho(H(i\vartheta)) \quad (4.21)$$

for $0 < |g| < g_1$. Thus the right hand side of (4.20) is an analytic function of $z \in \mathcal{A}(E_j, \delta_j, c_j)$. Since (4.20) holds for $z = z_0$ and $z_0 \in \mathcal{A}(E_j, \delta_j, c_j)$ we conclude that the left hand side of (4.20) has an analytic continuation to $z \in \mathcal{A}(E_j, \delta_j, c_j)$, and that this analytic continuation satisfies for $0 < |g| < g_1$ and all $z \in \mathcal{A}(E_j, \delta_j, c_j)$ the identity

$$\langle D_1(k, \lambda)\psi_{g_0}, (H - z)^{-1}D_1(k', \lambda')\psi_{g_0} \rangle \quad (4.22)$$

$$= \langle X^{-1/2}D_1(k, \lambda; i\vartheta)\psi_{g_0,i\vartheta}, X^{1/2}(H(i\vartheta) - z)^{-1}X^{1/2}X^{-1/2}D_1(k', \lambda; i\vartheta)\psi_{g_0,i\vartheta} \rangle.$$

Since $k' \in S_j$ implies $E_{g_0} + |k'| \in \mathcal{A}(E_j, \delta_j, c_j)$, we see from (4.21) by inserting $z = E_{g_0} + |k'|$ into (4.22) that Hypothesis C holds.

Next we show regularity of (4.19) in $|k|$ and $|k'|$. Let $k \in S_j$ and $k' \in \mathbb{R}^3 \setminus \{0\}$. By what we showed we can evaluate (4.22) at the point $z = E_{g_0} + \omega(k') \in \mathcal{A}(E_j, \delta_j, c_j)$ and find

$$\langle D_1(k, \lambda)\psi_{g_0}, (H - E_{g_0} - \omega(k'))^{-1}D_1(k', \lambda')\psi_{g_0} \rangle \quad (4.23)$$

$$= \langle X^{-1/2}D_1(k, \lambda; i\vartheta)\psi_{g_0,i\vartheta}, X^{1/2}(H(i\vartheta) - E_{g_0} - \omega(k'))^{-1}X^{1/2}X^{-1/2}D_1(k', \lambda; i\vartheta)\psi_{g_0,i\vartheta} \rangle.$$
First observe that the vector given in (4.18) is for any \( \theta \in D_{\theta_0} \) arbitrary many times differentiable in \(|k|\) for \( k \neq 0 \) (as a \( \mathcal{H} \)-valued differentiable function), since \( k \mapsto e^{ik \cdot x_{j} e^{-\beta |x|}} \) is for \( k \in S_j \) a \( C^{\infty} \)-map into the bounded operators on \( \mathcal{H} \), cf. (4.17). Clearly, \( k \mapsto \omega(k) \) is on \( S_j \) a \( C^{\infty} \)-map and the resolvent is an analytic and hence \( C^{\infty} \)-function of its spectral parameter. We thus conclude that the right hand side of (4.23) is infinitely often differentiable as a function of \(|k'|\) for \( k' \in S_j \). Similarly (but simpler as it does not involve derivatives with respect to the spectral parameter of the resolvent), one shows for \( k' \in \mathbb{R}^3 \setminus \{0\} \) the \( C^{\infty} \)-differentiability as a function of \(|k|\). The treatment of the second term in (2.19) is similar but simpler. Indeed, the resolvent map is always evaluated in the resolvent set, so no analytic dilation is necessary. Finally, that the last term in (2.19), i.e.,

\[
\langle \psi_{gs}, D_2(k, \lambda, k', \lambda') \psi_{gs} \rangle
\]

\[
= \left\langle \psi_{gs}, \frac{2}{(2\pi)^3} \sum_{l=1}^{N} e^{i(k-k') \cdot x_l} \frac{1}{k(k')^2} \frac{e \cdot (k, \lambda)}{\sqrt{2|k|}} \frac{\varepsilon(k, \lambda)}{\sqrt{2|k'|}} \psi_{gs} \right\rangle
\]

is infinitely differentiable as a function of \(|k|\) and \(|k'|\) for \( k, k' \in \mathbb{R}^3 \setminus \{0\} \) follows easily by dominated convergence and the exponential decay of \( \psi_{gs} \). This shows Proposition 4.5.

By collecting the results of this section and combining them with Theorem 2.5 we obtain the following result, recalling the notation introduced in (4.1), (4.10), and (4.12).

**Theorem 4.7.** Suppose \( V = V_C \), (4.3) and that Hypotheses \( B \) and \( E \) hold. Let \( j \in \{1, \ldots, M\} \). If \( \text{Im} Z_j > 0 \), then there exists a \( g_0 > 0 \) such that for \( 0 < |g| < g_0 \) the following holds for the set

\[
S_j = \{ k \in \mathbb{R}^3 \setminus \{0\} : E_{at,j} - E_{gs} - \delta_j/2 < \omega(k) < E_{at,j} - E_{gs} + \delta_j/2 \}.
\]

For \( f, h \in C_c(S_j)^2 \) we have

\[
\langle a_{out}^*(f) \psi_{gs}, a_{in}^*(h) \psi_{gs} \rangle - \langle f, h \rangle = -2\pi i \sum_{\lambda, \lambda'} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \delta(\omega(k) - \omega(k')) h(k', \lambda') T(k, \lambda, k', \lambda') dk' dk.
\]

**Remark 4.8.** Hypothesis \( E \) has been verified in [31] for \( V = V_C \), (4.3), spinless “electrons” and small values of the coupling constant \( g \) in case the atomic Hamiltonian has a nondegenerate ground state (which is known to be the case for the Hydrogen atom).

**Remark 4.9.** We note that Hypothesis \( B \) has been shown in [19, Theorem 4] in the spinless case. The result in [19] was proven for models, for which \( V = V_C \) holds, but with
the additional assumption that $\tilde{\kappa}$ vanishes outside a compact set. There is no obvious reason why the result in [19] as well as its proof do not carry over to situations where $\tilde{\kappa}$ is merely exponentially decaying (as was noted by one of the authors). In particular, given that in [20] an analogous result was shown for the related Nelson model, where only exponential falloff for the coupling function was assumed.

**Remark 4.10.** For the hydrogen atom $V = V_C$ with $Z = N = 1$ and (4.3), with the physically natural assumption $\lim_{r \to 0} \tilde{\kappa}(r) = 1$, we believe that for any $j \geq 2$ and $\alpha > 0$ sufficiently small Fermi’s golden rule condition $\text{Im} Z_j > 0$ holds. Explicitly, this should follow by means of the scaling $U_{el}(\xi)(-\Delta - \alpha |x|^{-1})U_{el}^{-1}(\xi) = \alpha^2(-\Delta - |x|^{-1})$, with $\xi = -\ln \alpha$, from an expansion in $\alpha$ around $0$ and the explicit calculation in [30, Theorem B.1].

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**A Estimates for creation and annihilation operators**

The following lemma gives elementary estimates of the creation operators in terms of the free field operator.

**Lemma A.1.** For each $n \in \mathbb{N}$ there exists a finite constant $C_n$ such that for all $h_i \in L^2_\omega(\mathbb{R}^3 \times \mathbb{Z}_2)$, $i = 1, \ldots, n$, the inequality

$$\|a^\#(h_1) \cdots a^\#(h_n)(H + 1)^{-n/2}\| \leq C_n \prod_{i=1}^n \|h_i\|_\omega$$

holds.

A proof of Lemma A.1 can be found for example in [19].

**Lemma A.2.** Suppose that (2.2) and (2.3) hold. Then for all $\epsilon > 0$ there exists a constant $D_\epsilon$ such that the following holds in the form sense. We have

$$V_- \leq \epsilon H + D_\epsilon. \quad (A.1)$$

If $s = 1/2$, then in addition

$$|B_l(x_j)| \leq \epsilon H + D_\epsilon, \quad (A.2)$$

for $l = 1, 2, 3$ and $j = 1, \ldots, N$.
Proof. We note that the case \( s = 0 \) has been shown in the proof of Lemma 18 in [19]. We will only show the case \( s = 1/2 \), and thus assume \( s = 1/2 \). For this we use that for any operators \( X \) and \( Y \) in a Hilbert space the following inequality holds in sense of forms

\[
X^*Y + Y^*X \leq X^2 + Y^2, \tag{A.3}
\]

which follows from a simple application of Cauchy’s inequality. For \( \delta > 0 \), we see from (A.3), the trivial operator inequality \( Z^*Z \leq \|Z\|^2 \), and Lemma A.1 that

\[
|B_l(x_j)| \leq \frac{1}{2}\delta B_l(x)^2 + \frac{1}{2}\delta^{-1}
\]

\[
\leq \frac{1}{2}\delta(H_l + 1)^{1/2}(H_l + 1)^{-1/2}B_l(x)^2(H_l + 1)^{-1/2}(H_l + 1)^{1/2} + \frac{1}{2}\delta^{-1}
\]

\[
\leq \frac{1}{2}\delta(H_l + 1)^{1/2}\|B_l(x)(H_l + 1)^{-1/2}\|^2(H_l + 1)^{1/2} + \frac{1}{2}\delta^{-1}
\]

\[
\leq \frac{1}{2}\delta C(H_l + 1) + \frac{1}{2}\delta^{-1},
\]

for some constant \( C \) depending on the norm \( \|J_{x,l}\|_\omega \). Since \( \delta > 0 \) is arbitrary, we see that for any \( \epsilon > 0 \) there is a constant \( E_\epsilon \) such that

\[
|B_l(x_j)| \leq \epsilon H_l + E_\epsilon. \tag{A.4}
\]

Since \( A(x)^2 \leq C(H_l + 1) \), by Lemma [A.1] and

\[
p_j^2 = (p_j - A(x_j) + A(x_j))^2
\]

\[
\leq (p_j - A(x_j))^2 + (p_j - A(x_j)) \cdot A(x_j) + A(x_j) \cdot (p_j - A(x_j)) + A(x_j)^2
\]

\[
\leq 2((p_j + A(x_j))^2 + 2A(x_j)^2),
\]

by (A.3) again, it follows using non-negativity that

\[
\sum_{j=1}^{N} p_j^2 + H_l \leq a(H + V_- - \sum_{j=1}^{N} \mu S_j \cdot B(x_j)) + b
\]

for some \( a, b > 0 \). Combining this with (2.2) and (A.4) it follows that \( \sum_{j=1}^{N} p_j^2 + H_l \) is form bounded with respect to \( H \). This with (2.2) shows (A.1), and with (A.4) it shows (A.2).

For a function \( f : Y^n \to Z \) and \( \sigma \in \mathcal{S}_n \) we define

\[
(\sigma f)(y_1, \ldots, y_n) = f(y_{\sigma(1)}, \ldots, y_{\sigma(n)}), \quad y_j \in Y, \ j = 1, \ldots, n. \tag{A.5}
\]
Fock spaces over $L^2$-spaces can be canonically identified with direct sums of subspaces of $L^2$-spaces over Cartesian products. In the situation of non-relativistic qed we obtain the following identification, see for example [10, Theorem 11.10 (a)],

$$\mathcal{F}_n(h) \cong L^2_\pi((\mathbb{R}^3 \times \mathbb{Z}_2)^n) := \{ \psi \in L^2((\mathbb{R}^3 \times \mathbb{Z}_2)^n) : \sigma \psi = \psi, \ \forall \sigma \in \mathfrak{S}_n \}. \quad (A.6)$$

Thus we can identify $\psi \in \mathcal{F}(h)$ with a sequence $\psi = (\psi_n)_{n \in \mathbb{N}_0}$, where $\psi_n \in L^2_\pi((\mathbb{R}^3 \times \mathbb{Z}_2)^n)$.

We define for $k \in \mathbb{R}^3$ and $\lambda \in \mathbb{Z}_2$ the action of the formal annihilation operator $a(k, \lambda)$ by

$$(a(k, \lambda)\psi)_n(k_1, \lambda_1, ..., k_n, \lambda_n) := (n + 1)^{1/2} \psi_{n+1}(k, \lambda, k_1, \cdot \cdot \cdot, k_n, \lambda_n), \ n \in \mathbb{N}_0, \quad (A.7)$$

which is understood as an identity of measurable functions (note that (A.7) does not necessarily need to define an element of Fock space).

**Lemma A.3.** Let $\psi \in \mathcal{D}(H^2)$. Then $a^*(f)\psi \in \mathcal{D}(H)$ for all $f \in h_\omega$ with $\omega f \in h_\omega$.

**Proof.** For $\psi \in \mathcal{D}(H^2)$ a straightforward calculation shows that for all $\varphi \in \mathcal{C}$

$$\langle H\varphi, a^*(f)\psi \rangle = \langle a(f)H\varphi, \psi \rangle = \langle [a(f), H]\varphi, \psi \rangle + \langle Ha(f)\varphi, \psi \rangle = \langle C\varphi, \psi \rangle + \langle \varphi, a(f)H\psi \rangle,$$

where we introduced the operator

$$C = \sum_{j=1}^{N} \sum_{l=1}^{3} \frac{1}{\sqrt{2}} \left\{ \langle f, G_{x_j,l} \rangle (p_{j,l} + A_l(x_j)) + (p_{j,l} + A_l(x_j)) \langle f, G_{x_j,l} \rangle + \mu S_{j,l} \langle f, J_{x_j,l} \rangle \right\} + a(\omega f)$$

on $\mathcal{C}$. From Lemma [A.1] we see that the domain of the adjoint of $C$ contains the natural domain of $(-\Delta + H_f)^{1/2}$ and so contains the the domain of $\mathcal{D}(H)$, by (2.5). It follows that

$$\langle H\varphi, a^*(f)\psi \rangle = \langle \varphi, C^*\psi \rangle + \langle \varphi, a(f)H\psi \rangle.$$

Since $H$ is by assumption essentially self-adjoint on $\mathcal{C}$, it follows that $a^*(f)\psi \in \mathcal{D}(H)$. \qed

**B  A lemma about Abelian limits**

We will need the following proposition about Abelian limits. Together with its proof it can be found in [13, XI.6, Lemma 5]. For the convenience of the reader, we provide the proof given there.
Proposition B.1. Let $f$ be a bounded measurable function on $[0, \infty)$ and suppose that
\[ \lim_{t \to \infty} \int_0^t f(x) dx = a. \]
Then $\lim_{\epsilon \downarrow 0} \int_0^\infty e^{-\epsilon s} f(s) ds = a$.

Proof. Let $g(t) = \int_0^t f(s) ds$ and $q(\epsilon) = \int_0^\infty e^{-\epsilon s} f(s) ds$. Then $g'(t) = f(t)$, a.e., so integration by parts, change of variables, and $\int_0^\infty e^{-s} ds = 1$ implies that
\[
q(\epsilon) = \int_0^\infty e^{-\epsilon s} g(s) ds = \int_0^\infty e^{-s} g(-1) ds = \int_0^\infty e^{-s} (g(-1) - a) ds + a \\
\to 0 + a \quad (\epsilon \downarrow 0),
\]
where in the last line we used that $g$ is bounded on $\mathbb{R}_+$, $\lim_{t \to \infty} g(t) = a$, and dominated convergence. \qed

C Results from Functional Analysis

We will use the following result which is a version of the well known fact that weak analyticity implies strong analyticity.

Theorem C.1. Let $X$ be a Banach space and $L$ a linear subspace of $X^*$ such that $\|x\| = \sup_{l \in L, \|l\| \leq 1} |l(x)|$ for all $x \in X$. Let $D$ be open and $f : D \to X$ a map such that for all $l \in L$ the composition $l \circ f : D \to \mathbb{C}$ is analytic and $\sup_{z \in K} \sup_{l \in L, \|l\| \leq 1} |l(f(z))| < \infty$ on compact subsets $K$ of $D$. Then $f$ is strongly analytic.

The above theorem follows as a consequence of \cite[III. §1 Theorem 1.37 and Remark 1.38]{3} For convenience of the reader we provide a proof.

Proof. Let $a \in$ and suppose that $\Gamma$ is a circle in $D$ containing $a$, whose interior is contained in $D$. If $l \in L$, then by assumption $l \circ f$ is analytic and so by Cauchy’s formula
\[
l \left( \frac{f(a + h) - f(a)}{h} \right) = \frac{d}{dz} l(f(a)) \\
= \frac{1}{2\pi i} \oint_{\Gamma} \left[ \frac{1}{h} \left( \frac{1}{z - (a + h)} - \frac{1}{z - a} \right) - \frac{1}{(z - a)^2} \right] l(f(z)) dz.
\]
Thus using the triangle inequality we find with $C_\Gamma := \sup_{z \in \Gamma} \sup_{l \in L, \|l\| \leq 1} |l(f(z))|$ that

$$\left| \frac{f(a + h) - f(a)}{h} - \frac{f(a + h') - f(a)}{h'} \right| \leq \frac{1}{2\pi} C_\Gamma \int_{\Gamma} \left( \frac{1}{(z - (a + h))(z - a)} - \frac{1}{(z - a)^2} \right) dS(z),$$

where $dS$ denotes the surface measure of $\Gamma$ as a one dimensional real submanifold of $\mathbb{C} \cong \mathbb{R}^2$. Now the right hand side tends to zero as $h$ and $h'$ tend to zero. It follows by completeness that $\frac{f(a + h) - f(a)}{h}$ converges in $X$, proving that $f$ is strongly analytic.

**Lemma C.2.** Let $A$ be a self-adjoint non-negative operator. Let $B$ be a bounded operator with $\text{Ran} B \subset \mathcal{D}(A)$ such that for some constant $C$ we have

$$\|BA\| \leq C, \quad \|AB\| \leq C.$$

Then $A^{1/2}BA^{1/2} : \mathcal{D}(A) \rightarrow \mathcal{H}$ is a bounded operator with norm bounded by $C$.

**Proof.** We use interpolation. Consider first a regularization of $A$ as follows $A_n = \frac{nA}{n+A}$, $n \in \mathbb{N}$. Then, clearly

$$\|BA_n\| \leq \|BA\|\|(1 + A/n)^{-1}\| \leq \|BA\| \leq C \quad \text{and} \quad \|A_nB\| \leq \|(1 + A/n)^{-1}\||\|AB\| \leq \|AB\| \leq C.$$

It follows from interpolation, see for example [41, Proposition 1 in Appendix to IX.4] which also holds for bounded operators, that for all $n \in \mathbb{N}$

$$\|A_n^{1/2}BA_n^{1/2}\| \leq C.$$

Thus

$$\langle f, A^{1/2}BA^{1/2}g \rangle = \lim_{n \rightarrow \infty} \langle f, A_n^{1/2}BA_n^{1/2}g \rangle$$

for all $f, g \in \mathcal{D}(A)$. We conclude that $A^{1/2}BA^{1/2}$ is bounded by $C$. \hfill $\Box$

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