An Infrared-Finite Algorithm for Rayleigh Scattering Amplitudes, and Bohr's Frequency Condition

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Abstract

In this paper, we rigorously justify Bohr's frequency condition in atomic spectroscopy. Moreover, we construct an algorithm enabling us to calculate the transition amplitudes for Rayleigh scattering of light at an atom, up to a remainder term of arbitrarily high order in the finestructure constant. Our algorithm is constructive and circumvents the infrared divergences that invalidate standard perturbation theory.

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I Description of the Problem and Summary of Main Results

In this paper, we present a mathematical justification of Bohr's frequency condition in atomic spectroscopy. Since the physical value, $\alpha \cong 1/137$, of the finestructure constant is very small, it suffices to expand scattering amplitudes for Rayleigh scattering of light at an atom to leading order in α in order to reach a precise understanding of Bohr's frequency condition. We accomplish more than that: We provide a constructive algorithm enabling us to calculate the scattering amplitudes up to (finite) remainder terms of arbitrarily high order in the finestructure constant. For two reasons, this is a non-trivial result. The rate of convergence of the interpolating electromagnetic field to the asymptotic field crucially enters the control of the Duhamel expansion of propagators appearing in reduction formulae for the scattering matrix elements. It is therefore not obvious, a priori, that one can construct an algorithm to determine these matrix elements to arbitrarily high order in α. Infrared divergences invalidate a straightforward Taylor expansion of the groundstate and the groundstate energy. Since the scattering amplitudes for Rayleigh scattering depend on the atomic groundstate and the groundstate energy, it is thus far from obvious how to calculate these amplitudes to arbitrarily high order in α. The convergence to the asymptotic field is sufficiently rapid (faster than any inverse power of time t) to allow for a complete control of the expansion of the propagator in powers of α, provided some technical subtleties, connected to the vector nature of the interaction in QED, are properly taken into account. The expansion of the groundstate is a more delicate issue. In fact, we require an iterative construction (see [1], [2]), based on a multiscale analysis, to remove an infrared cut-off in photon momentum space in our construction of the atomic groundstate. As a result of our analysis, we have a mathematical tool to calculate contributions to the scattering amplitudes up to finite remainder terms of arbitrarily high order in α. Because of the infrared features of the theory, naive perturbation theory is infrared divergent at some finite order in α. But if the finestructure constant were not as small as it is in nature experimental data could only be reproduced accurately by the theory if radiative corrections of very high order in α were taken into account. We therefore construct an algorithm to calculate such corrections.

In the following, an atom is described as a quantum-mechanical bound state consisting of a static, positively charged, pointlike nucleus surrounded by electrons. The electrons are described as nonrelativistic, pointlike quantum-mechanical particles with electric charge $-e$ and spin $\frac{1}{2}$, as originally proposed by Pauli. They are bound to the nucleus by the electrostatic Coulomb force, and they interact with the transverse soft modes of the quantized electromagnetic field. We eliminate ultraviolet divergences by imposing an ultraviolet cutoff on the interaction term.

To keep our exposition as simple as possible, we consider a hydrogen atom consisting of a single, static proton of charge e accompanied by only one electron. The spin of the electron then turns out to be an inessential complication. We neglect the coupling of the magnetic moment of the electron to the quantized magnetic field. It is, however, not difficult to include the Zeeman term in our analysis. Throughout our paper we follow the notation and conventions of [1]. Next, we recall the mathematical definition of our model system.

The Hilbert space of pure state vectors is given by

$$\mathcal{H} \; := \; \mathcal{H}_{el} \otimes \mathcal{F} \, , \tag{I.1}$$

where $\mathcal{H}_{el} = L^2(\mathbb{R}^3)$ is the Hilbert space appropriate to describe states of a single electron (neglecting its spin), and $\mathcal{F}$ is the Fock space used to describe the states of the transverse modes of the quantized electromagnetic field, i.e., the *photons*. More explicitly,

$$\mathcal{F} \; := \; \bigoplus_{N=0}^{\infty} \mathcal{F}^{(N)} \, , \qquad \mathcal{F}^{(0)} = \mathbb{C} \, \Omega \, , \tag{I.2}$$

where Ω is the vacuum vector (i.e., the state of the electromagnetic field without any excited field modes), and

$$\mathcal{F}^{(N)} \; := \; \mathcal{S}_N \bigotimes_{j=1}^{N} \mathfrak{h} \, , \qquad N \geq 1 \, , \tag{I.3}$$

where the Hilbert space, $\mathfrak{h}$, of state vectors of a single photon is given by

$$\mathfrak{h} \; := \; L^2[\mathbb{R}^3 \times \mathbb{Z}_2]. \tag{I.4}$$

In (I.4), $\mathbb{R}^3$ is the photon momentum space, and $\mathbb{Z}_2$ accounts for the two independent transverse polarizations, or helicities, of a photon. In Eq. (I.3), $\mathcal{S}_N$ denotes the orthogonal projection onto the subspace of $\bigotimes_{j=1}^{N} \mathfrak{h}$ of totally symmetric N-photon wave functions, in accordance with the fact that photons satisfy Bose-Einstein statistics. Thus, $\mathcal{F}^{(N)}$ is the subspace of $\mathcal{F}$ of state vectors of configurations of exactly N photons. It is convenient to represent the Hilbert space $\mathcal{H}$ as the space of square-integrable wave functions on electron position space, $\mathbb{R}^3$, with values in the photon Fock space $\mathcal{F}$, i.e.,

$$\mathcal{H} \; \cong \; L^2\Big[\mathbb{R}^3 \, ; \, \mathcal{F}\Big] \, . \tag{I.5}$$

The dynamics of the system is generated by the Hamiltonian

$$H \ := \ \Big(- i\vec{\nabla}_{\vec{x}} + \alpha^{3/2}\vec{A}(\alpha\vec{x})\Big)^2 \ - \ V(x) \ + \ \check{H} \, . \tag{I.6}$$

Here, $\vec{\nabla}_{\vec{x}}$ denotes the gradient with respect to the electron position variable $\vec{x} \in \mathbb{R}^3$, $\alpha \cong 1/137$ is the finestructure constant, $\vec{A}(\vec{x})$ denotes the vector potential of the transverse modes of the quantized electromagnetic field in the *Coulomb gauge*,

$$\vec{\nabla}_{\vec{x}} \cdot \vec{A}(\vec{x}) \ = \ 0 \, , \tag{I.7}$$

and with an ultraviolet cutoff imposed on the high-frequency modes, V is the Coulomb potential of electrostatic attraction of the electron to the nucleus. A general class of potentials, V, for which our analysis can be carried out, is characterized in the following hypothesis. We define the atomic Hamiltonian, H_{el}, by

$$H_{el} := -\Delta_{\vec{x}} - V(\vec{x}), \tag{I.8}$$

where $\Delta_{\vec{x}}$ is the Laplacian.

Hypothesis 1. *The form domain of V includes the form domain,* $\mathrm{H}^1(\mathbb{R}^3)$*, of the Laplacian $-\Delta$, and, for any $\varepsilon > 0$, there exists a constant $b_\varepsilon < \infty$, such that*

$$\pm V \ \le \ \varepsilon\,(-\Delta) \ + \ b_\varepsilon \cdot \mathbf{1} \tag{I.9}$$

on $\mathrm{H}^1(\mathbb{R}^3)$*. Moreover, $\lim_{|x|\to\infty} V(x) = 0$, and*

$$\begin{array}{l} e_{el} := \inf\sigma(H_{el}) < 0 \textit{ is an isolated eigenvalue of multiplicity} \\ \quad \textit{one, with corresponding normalized eigenvector } \varphi_{el} \in \mathcal{H}_{el}. \end{array} \tag{I.10}$$

In equation (I.6), $\check{H}$ is the Hamiltonian of the quantized, free electromagnetic field. This operator is given by

$$\check{H} \ := \ \sum_{\lambda=\pm} \int d^3k \; a^*(\vec{k},\lambda)\,|\vec{k}|\,a(\vec{k},\lambda) \, , \tag{I.11}$$

where $a^*(\vec{k},\lambda)$ and $a(\vec{k},\lambda)$ are the usual photon creation- and annihilation operators obeying the canonical commutation relations

$$[a^*(\vec{k},\lambda)\, , \, a^*(\vec{k}',\lambda')] \ = \ [a(\vec{k},\lambda)\, , \, a(\vec{k}',\lambda')] \ = \ 0 \, , \tag{I.12}$$

$$[a(\vec{k},\lambda)\, , \, a^*(\vec{k}',\lambda')] \ = \ \delta_{\lambda\lambda'}\,\delta(\vec{k}-\vec{k}') \, , \tag{I.13}$$

$$a(\vec{k},\lambda)\,\Omega \ = \ 0 \, , \tag{I.14}$$

for all $\vec{k},\vec{k}' \in \mathbb{R}^3$ and $\lambda,\lambda' \in \mathbb{Z}_2 \equiv \{\pm\}$.

The vector potential in the Coulomb gauge is given by

$$\vec{A}(\vec{x}) \;:= \tag{I.15}$$
$$\frac{1}{(2\pi)^{3/2}} \sum_{\lambda=\pm} \int \frac{d^3k}{\sqrt{2\,|\vec{k}|}} \Lambda(\vec{k}) \left\{ \vec{\varepsilon}(\vec{k},\lambda) e^{-i\vec{k}\cdot\vec{x}} a^*(\vec{k},\lambda) \;+\; \vec{\varepsilon}(\vec{k},\lambda)^* e^{i\vec{k}\cdot\vec{x}} a(\vec{k},\lambda) \right\},$$

where $\Lambda(\vec{k})$ is the characteristic function of the ball $\{\vec{k} \in \mathbb{R}^3 \,|\, |\vec{k}| \leq \kappa\}$ (or a nonnegative, smooth approximation thereof), and $\vec{\varepsilon}(\vec{k},+)$, $\vec{\varepsilon}(\vec{k},-)$ are photon polarization vectors, i.e., two unit vectors in $\mathbb{C} \otimes \mathbb{R}^3$ satisfying

$$\vec{\varepsilon}(\vec{k},\lambda)^* \cdot \vec{\varepsilon}(\vec{k},\mu) \;=\; \delta_{\lambda\mu}\,, \qquad \vec{k} \cdot \vec{\varepsilon}(\vec{k},\lambda) \;=\; 0\,, \tag{I.16}$$

for $\lambda, \mu = \pm$. The equation $\vec{k} \cdot \vec{\varepsilon}(\vec{k},\lambda) = 0$ expresses the Coulomb gauge condition.

The function $\Lambda(\vec{k})$ ensures that modes of the electromagnetic field corresponding to wave vectors $\vec{k}$ with $|\vec{k}| \geq \kappa$ do not interact with the electron; i.e., Λ is an *ultraviolet cutoff* that will be kept fixed throughout our analysis.

Next, we recall some well known properties of the Hamiltonian H and of its spectrum used in the following sections. For sufficiently small values of α, the Hamiltonian H is selfadjoint on its domain, $\mathcal{D}(H) = \mathcal{D}(H_0)$, where $\mathcal{D}(H_0)$ is the domain of the selfadjoint operator

$$H_0 \;:=\; -\Delta_{\vec{x}} \;-\; V(x) \;+\; \check{H}\,. \tag{I.17}$$

The operator H is bounded from below, and the infimum of the spectrum is a non-degenerate eigenvalue, the groundstate energy, E_{gs}, corresponding to a unique eigenvector, ϕ_{gs}. There is an ionization threshold Σ, $\Sigma > E_{gs}$, above which the spectrum is absolutely continuous and the electron is not bound to the nucleus, anymore. For an analysis of resonances corresponding to the eigenstates of the Hamiltonian H_0 with energy in the interval (E_{gs}, Σ), we refer the reader to [4] and references given there.

Next, we summarize the organization and the main results of this paper.

In Section II, we construct asymptotic electromagnetic field operators applied to vectors in the spectral subspace,

$$\mathcal{H}_{\Sigma-\delta} := \chi(H < \Sigma - \delta)\mathcal{H}, \tag{I.18}$$

of the Hamiltonian corresponding to energies below $\Sigma - \delta$ where Σ is the ionization threshold and $\delta > 0$ is arbitrarily small. We exploit the fact that, in such states, the electron is exponentially well localized near the nucleus, which yields an estimate of the rate of convergence of the interpolating field operators to the asymptotic field operators.

In Section III, we rigorously establish general *reduction formulae* (see [5]) for the S-matrix elements of Rayleigh scattering in our model, i.e., for the matrix elements

$$S_{\alpha}^{m',m}(\{\vec{f}_i\},\{\vec{h}_j\}) := \Big(\prod_{i=1}^{m'} \vec{A}^{out}[\vec{f}_i]\phi_{gs}, \prod_{j=1}^{m} \vec{A}^{in}[\vec{h}_j]\phi_{gs}\Big) \tag{I.19}$$

where the asymptotic states, on the right side of (I.19), are constructed in Section II and are assumed to belong to $\mathcal{H}_{\Sigma-\delta}$. The vector-valued functions $\{\vec{f}_i\}_{i=1}^{m'}$ and $\{\vec{h}_j\}_{j=1}^{m}$ in (I.19) are solutions of the free wave equation whose Fourier transforms are smooth and vanish at the origin of momentum space. The reduction process amounts to expressing the scalar product (I.19) in terms of integrals of expectation values of time-ordered products of interpolating fields. A precise formulation of our result is given in Proposition III.2; (see Section III).

In Section IV, starting from the general expressions in Proposition III.2, we develop a modified reduction procedure useful to calculate the $S-$matrix elements (I.19), up to a remainder of arbitrarily high order in α. Our algorithm for calculating the matrix elements (I.19) uses, as an ingredient, the infrared-finite algorithm developed in [1], [2], for the construction and re-expansion of the groundstate ϕ_{gs} and the groundstate energy E_{gs}. In Section IV.2, we provide a rather detailed outline of the re-expansion procedure for ϕ_{gs} and E_{gs} that enables us to circumvent infrared divergences appearing in standard perturbation theory. Our analysis culminates in the following results for the connected parts of the $S-$matrix elements $S_{\alpha}^{m',m}(\{\vec{f}_i\},\{\vec{h}_j\})$.

Main Result

For $\alpha \leq \bar{\alpha}$, with $\bar{\alpha} \equiv \bar{\alpha}_N$ small enough and N-dependent, the S-matrix elements $S_{\alpha}^{m',m}(\{\vec{f}_i\},\{\vec{h}_j\})$, with $(f_i, h_j) = 0$, have expansions of the form

$$S_{\alpha}^{m',m}(\{\vec{f}_i\},\{\vec{h}_j\})^{conn} = \sum_{\ell=6}^{2N} S_{l}^{m',m}(\{\vec{f}_i\},\{\vec{h}_j\};\alpha)\alpha^{\frac{\ell}{2}} \ + \ o(\alpha^N) \tag{I.20}$$

with

$$\lim_{\alpha\to 0} \alpha^{\delta}|S_{l}^{m',m}(\{\vec{f}_i\},\{\vec{h}_j\};\alpha)| = 0 \qquad , \quad \textit{for arbitrary} \quad \delta > 0, \tag{I.21}$$

for $N = 3, 4, 5, \ldots$. The coefficients $S_{l}^{m',m}(\{\vec{f}_i\},\{\vec{h}_j\};\alpha)$ are computable in terms of finitely many convergent integrals, for arbitrary $l < \infty$ (with $l \geq 6$).

The point of Expansion (I.20) is that Eq. (I.21) accounts for the possible appearance of powers of $\ln[1/\alpha]$ ("infrared logarithms"). We expect that infrared logarithms are not an artefact of our algorithm, but are an expression of infrared divergences in naive perturbation theory for the groundstate ϕ_{gs} and the groundstate energy E_{gs}.

In the last section of our paper, Section V, we calculate the scattering amplitude corresponding to a process where an incoming photon excites the atom from the groundstate to an excited (resonance) state, whereupon the atom relaxes to the groundstate by emitting one outgoing photon. As has been known since the birth of quantum electrodynamics, the lowest order contribution to the transition amplitude is significantly different from zero only for photon energies close to the difference of the energy, $\mathcal{E}_n$, of an excited bound state and the groundstate energy, $\mathcal{E}_0$, of H_0. In particular, when the wave functions of the incoming and of the outgoing photon coincide, the imaginary part of the matrix element of the operator $T := i(S - \mathbf{1})$ (where S is the scattering matrix and $\mathbf{1}$ is the identity operator) is not zero, in leading order, only if the photon wave function does not vanish for energies corresponding to $\{\mathcal{E}_n - \mathcal{E}_0\,; n \in \mathbb{N}\}$, $\{\mathcal{E}_n\}$ being the energy levels of the Coulomb system. Only the imaginary part of this matrix element matters in the computation of the total cross section for the given incoming photon state. We provide a recipe to calculate higher order corrections of the scattering amplitudes. Our results represent a rigorous justification of Bohr's frequency condition.

To our knowledge, a mathematically controlled expansion, accurate to an arbitrary order in the finestructure constant α, with a finite remainder term, of the scattering amplitudes for Rayleigh scattering of light at an atom in nonrelativistic QED has not been provided in the literature before. The novelty of our results is that they turn infrared divergences in naive perturbation theory into powers of $\ln[\frac{1}{\alpha}]$.

II Asymptotic fields

Positive energy solutions, f_t, of the free wave equation

$$\vec{\nabla}_{\vec{y}} \cdot \vec{\nabla}_{\vec{y}} f_t(\vec{y}) - \frac{\partial^2 f_t(\vec{y})}{\partial t^2} = 0, \tag{II.1}$$

of fast decay in $|\vec{y}|$, for fixed t, are given by

$$f_t(\vec{y}) := \int \hat{f}(\vec{k}) e^{-i|k|t + i\vec{k}\cdot\vec{y}} \frac{d^3k}{(2\pi)^{3/2}\sqrt{2|k|}} \tag{II.2}$$

with $\hat{f}(\vec{k}) \in C_0^\infty(\mathbb{R}^3 \backslash \{0\})$. We construct a vector of test functions

$$\vec{f}_t(\vec{y}) := \sum_{\lambda=\pm} \int \vec{\varepsilon}(\vec{k},\lambda)^* \hat{f}^\lambda(\vec{k}) e^{-i|k|t + i\vec{k}\cdot\vec{y}} \frac{d^3k}{(2\pi)^{3/2}\sqrt{2|k|}} \tag{II.3}$$

satisfying the wave equation (II.1), with

$$\sum_{\lambda=\pm} \vec{\varepsilon}(\vec{k},\lambda)^* \hat{f}^\lambda(\vec{k}) =: \hat{\vec{f}}(\vec{k}) \in C_0^\infty(\mathbb{R}^3 \backslash \{0\}; \mathbb{C}^3).$$

An asymptotic vector potential is constructed as an LSZ ($t \to \pm\infty$) limit of interpolating field operators

$$\vec{A}[\vec{f}_t, t] := i \int \Big(\vec{A}(\vec{y},t) \cdot \frac{\partial \vec{f}_t(\vec{y})}{\partial t} - \frac{\partial \vec{A}(\vec{y},t)}{\partial t} \cdot \vec{f}_t(\vec{y}) \Big) d^3y, \tag{II.4}$$

with $\vec{f}_t$ as in (II.3) and

$$\vec{A}(\vec{y},t) := e^{iHt} \vec{A}(\vec{y}) e^{-iHt}. \tag{II.5}$$

If the photon were a massive particle, the smeared field operator (II.4) would converge strongly, as $t \to \infty$, on a dense linear subspace of the Hilbert space of the system. For massless photons, convergence of (II.4) only holds on a subspace of vectors in the Hilbert space whose maximal energy is so small that the propagation speed of the electron is strictly below the speed of light, e.g., on the space $\mathcal{H}_\Sigma$; see [7], [11]. The existence of strong limits of the smeared field operators in Eq. (II.4), as $t \to \pm\infty$, implies the existence of asymptotic creation- and annihilation operators

$$\{a^*_{out/in}(\vec{k},\lambda)\, ,\, a_{out/in}(\vec{k},\mu)\}, \tag{II.6}$$

defined on a dense subspace of $\mathcal{H}_\Sigma$ (see (I.18)) and obeying the canonical commutation relations. In fact, the limits of the operators in (II.4), as $t \to \pm\infty$, correspond to

$$\vec{A}^{out/in}[\vec{f}] = \sum_{\lambda=\pm} \int a^*_{out/in}(\vec{k},\lambda)\hat{f}^\lambda(\vec{k}) d^3k =: a^*_{out/in}(f) \tag{II.7}$$

and, similarly,

$$\vec{A}^{out/in}[-\bar{\vec{f}}] = \sum_{\lambda=\pm} \int a_{out/in}(\vec{k},\lambda)\overline{\hat{f}^\lambda(\vec{k})} d^3k =: a_{out/in}(f). \tag{II.8}$$

Using estimates proven in [7] and in Lemma II.1, below, one can prove that, for $\hat{f}^\lambda(\vec{k}), \hat{h}^\lambda(\vec{k}) \in L_2\Big(\mathbb{R}^3; (1+\frac{1}{|\vec{k}|})^{-1})d^3k\Big)$ the following relations hold in the sense of quadratic forms, on $\mathcal{H}_\Sigma$:
i)

$$[a_{out/in}(f), a^*_{out/in}(h)] = (f,h) = \sum_{\lambda=\pm} \int \overline{\hat{f}^\lambda(\vec{k})}\hat{h}^\lambda(\vec{k}) d^3k \tag{II.9}$$

$$[a_{out/in}(f), a_{out/in}(h)] = [a^*_{out/in}(f), a^*_{out/in}(h)] = 0$$

ii)

$$e^{itH} a^*_{out/in}(h) e^{-itH} = a^*_{out/in}(e^{it\omega}h) \quad , \quad e^{itH} a_{out/in}(h) e^{-itH} = a_{out/in}(e^{-it\omega}h) \tag{II.10}$$

where the Fourier transform of each component of $e^{it\omega}h$ is obtained from the ones of h by multiplying by $e^{it\omega(\vec{k})}$, $\omega(\vec{k}) := |\vec{k}|$.

Since, in this paper, we are interested in Rayleigh scattering, we restrict our attention to the construction of asymptotic states describing an atom below the ionization threshold, Σ. (They have spectral support strictly below the ionization threshold). For such states, the position of the electron remains close to the one of the proton for all times. More precisely, such states exhibit exponential decay in the distance between the electron and the nucleus. This implies that the convergence of (II.4), as time $t \to \pm\infty$, is faster than any inverse power of time t. This implies that when applied to vectors in $\mathcal{H}_{\Sigma-\delta}$ the operators defined in (II.4) converge faster than any inverse power of time t, as $t \to \infty$. This has important consequences for the expansion of Rayleigh scattering amplitudes in the finestructure constant.
In the following, we make use of the field equation

$$\vec{\nabla}_{\vec{y}} \cdot \vec{\nabla}_{\vec{y}} \vec{A}(\vec{y},t) - \frac{\partial^2 \vec{A}(\vec{y},t)}{\partial t^2} = -\vec{J}^{tr}(\vec{y},t), \tag{II.11}$$

where

$$\vec{J}^{tr}(\vec{y},t) := -\frac{\alpha^{3/2}}{(2\pi)^{3/2}} \sum_{\lambda=\pm} \int (\vec{v}(t)\cdot\vec{\varepsilon}(\vec{k},\lambda)^{*})\vec{\varepsilon}(\vec{k},\lambda)\Lambda(|k|)e^{-i\vec{k}\cdot(\vec{y}-\alpha\vec{x}(t))}d^{3}k + h.c. \tag{II.12}$$

with $\vec{v}(t) = e^{iHt}\vec{v}e^{-iHt} = e^{iHt}(-i\vec{\nabla}_{\vec{x}} - \alpha^{\frac{3}{2}}\vec{A}(\alpha\vec{x}))e^{-iHt}$ and $\vec{x}(t) = e^{iHt}\vec{x}e^{-iHt}$. Equation (II.11) is meaningful as an equation between densely defined operator-valued distributions.

By Cook's argument, the existence of the limits

$$\lim_{t\to\pm\infty} \vec{A}[\vec{f}_t, t]\psi, \tag{II.13}$$

for $\psi \in \mathcal{H}_{\Sigma}$, follows from the existence of the integral

$$\begin{aligned}
&\int_0^{\pm\infty} \frac{\partial}{\partial t}\vec{A}[\vec{f}_t, t]\psi dt = \\
&= \int_0^{\pm\infty} i\int \frac{\partial}{\partial t}\Big(\vec{A}(\vec{y},t)\cdot\frac{\partial\vec{f}_t(\vec{y})}{\partial t} - \frac{\partial\vec{A}(\vec{y},t)}{\partial t}\cdot\vec{f}_t(\vec{y})\Big)d^{3}y\psi dt \qquad \text{(II.14)}\\
&= \int_0^{\pm\infty} i\int \Big[\Big(\vec{\nabla}_{\vec{y}}\cdot\vec{\nabla}_{\vec{y}}\vec{A}(\vec{y},t) - \frac{\partial^{2}\vec{A}(\vec{y},t)}{\partial t^{2}}\Big)\cdot\vec{f}_t(\vec{y})\Big]d^{3}y\psi dt \qquad \text{(II.15)}
\end{aligned}$$

where, in passing from (II.14) to (II.15), we use the wave equation (II.1), and, taking into account the rapid spatial decay of $\vec{f}_t(\vec{y})$, we then integrate by parts twice in $\vec{y}$.

Introducing the notation

$$\vec{J}^{tr}[\vec{f}_t, t] := \int \vec{J}^{tr}(\vec{y},t)\cdot\vec{f}_t(\vec{y})dy, \tag{II.16}$$

and using the field equation (II.11), we may rewrite (II.14) as follows:

$$\int_0^{\pm\infty} \frac{\partial}{\partial_t}\vec{A}[\vec{f}_t, t]\psi dt = -i\int_0^{\pm\infty} \vec{J}^{tr}[\vec{f}_t, t]\psi dt. \tag{II.17}$$

The following lemma guarantees the convergence of the integral over time t on the right side of Eq. (II.17).

Lemma II.1. *Let ψ be a vector belonging to the subspace $\mathcal{H}_{\Sigma-\delta}$ defined in (I.18). For $\sum_{\lambda=\pm}\vec{\varepsilon}(\vec{k},\lambda)^{*}\hat{f}^{\lambda}(\vec{k}) =: \hat{\vec{f}}(\vec{k}) \in C_0^{\infty}(\mathbb{R}^3\backslash\{0\};\mathbb{C}^3)$ the following estimate holds:*

$$\|\vec{J}^{tr}[\vec{f}_t, t]\psi\| \le \frac{C_m}{1+|t|^{m}}, \tag{II.18}$$

for any $m \in \mathbb{N}$, where C_m is a finite constant (depending on m).

Proof.
We write the identity operator in electron position space as

$$\mathbf{1} = \chi(\langle\vec{x}\rangle - \beta|t|) + \chi^c(\langle\vec{x}\rangle - \beta|t|) \quad , \quad \langle\vec{x}\rangle := (\vec{x}\cdot\vec{x}+1)^{\frac{1}{2}} \tag{II.19}$$

for $0 < \beta < 1$, where the function $\chi(y)(= 1-\chi^c(y))$ is a non-negative $C^\infty(\mathbb{R})$-function equal to 1, for $y < -1$, and equal to 0, for $y > 1$. The operator $\vec{J}^{tr}[\vec{f}_t, t]$ is given by

$$\vec{J}^{tr}[\vec{f}_t, t] = \sum_{l=1}^{3} g_t^l(\vec{x}(t))v^l(t) \tag{II.20}$$

where the vector function $\vec{g}_t$ is as in Eq. (II.3). We use the partition of unity (II.19) to obtain the inequality

$$\|\sum_{l=1}^{3} g_t^l(\vec{x}(t))v^l(t)\psi\| \;\leq\; \sum_{l=1}^{3}\|g_t^l(\vec{x}(t))v^l(t)\chi(\langle\vec{x}(t)\rangle-\beta|t|)\psi\| \tag{II.21}$$

$$+\sum_{l=1}^{3}\|g_t^l(\vec{x}(t))v^l(t)\chi^c(\langle\vec{x}(t)\rangle-\beta|t|)\psi\|. \tag{II.22}$$

We treat each term in the two sums in Eqs. (II.21) and in (II.22) separately. To bound the terms in (II.21), the following norm inequality suffices:

$$\|g_t^l(\vec{x}(t))v^l(t)\chi(\langle\vec{x}(t)\rangle-\beta|t|)\psi\|$$

$$\leq \; \|g_t^l(\vec{x}(t))\frac{\partial\chi(\langle\vec{x}(t)\rangle-\beta|t|)}{\partial x^l(t)}\psi\| \tag{II.23}$$

$$+\|g_t^l(\vec{x}(t))\chi(\langle\vec{x}(t)\rangle-\beta|t|)\|\cdot\|v^l(t)\psi\|. \tag{II.24}$$

Similarly

$$\|g_t^l(\vec{x}(t))v^l\chi^c(\langle\vec{x}(t)\rangle-\beta|t|)\psi\| \tag{II.25}$$

$$\leq \; \|g_t^l(\vec{x}(t))\frac{\partial(\chi^c(\langle\vec{x}(t)\rangle-\beta|t|)\langle\vec{x}(t)\rangle^{-m})}{\partial x^l(t)}\|\cdot\|\langle\vec{x}(t)\rangle^m\psi\| \tag{II.26}$$

$$+\|g_t^l(\vec{x}(t))\chi^c(\langle\vec{x}(t)\rangle-\beta|t|)\langle\vec{x}(t)\rangle^{-m}\|\cdot\|v^l(t)\langle\vec{x}(t)\rangle^m\psi\|. \tag{II.27}$$

In order to prove (II.18), it is enough to notice that
i) the norms $\|v^l(t)\psi\|$ and $\|v^l(t)\langle\vec{x}(t)\rangle^m\psi\|$ are bounded, uniformly in time, because $\psi \in \mathcal{H}_{\Sigma-\delta}$; see, e.g., [9];
ii) the bound on the right side of Eq. (II.18) holds for $\sup_{|\vec{y}|<\beta|t|}|g_t^l(\vec{y})|$; see, e.g., [12]. □

III Reduction formulae for S-matrix elements

In this section we rigorously derive *reduction formulae* for the S-matrix elements corresponding to Rayleigh scattering. We study scattering processes, where the incoming state and the outgoing state describe a finite number of incoming and outgoing photons, respectively, and a hydrogen atom in its groundstate. Thus, we consider amplitudes of the form

$$\Big(\prod_{i=1}^{m'} \vec{A}^{out}[\vec{f_i}]\phi_{gs}, \prod_{j=1}^{m} \vec{A}^{in}[\vec{h}_j]\phi_{gs}\Big), \tag{III.1}$$

where $\{\vec{f_i}\}, \{\vec{h}_j\}$ are vector test functions as in (II.3). In order to be able to apply the results of the previous section, we must impose the following condition on the supports of the test functions $\{\vec{f_i}\}, \{\vec{h}_j\}$:

$$\begin{aligned} \chi(H \geq \Sigma - \delta) \prod_{i=1}^{m'} \vec{A}^{out}[\vec{f_i}]\phi_{gs} &= 0 \\ \chi(H \geq \Sigma - \delta) \prod_{j=1}^{m} \vec{A}^{in}[\vec{h}_j]\phi_{gs} &= 0 \end{aligned} \tag{III.2}$$

for an arbitrary $\delta > 0$.
Let

$$\omega_i' := \sup\{|\vec{k}| \,|\, \vec{k} \in \mathrm{supp}\hat{\vec{f_i}}(\vec{k})\} \tag{III.3}$$

$$\omega_j := \sup\{|\vec{k}| \,|\, \vec{k} \in \mathrm{supp}\hat{\vec{h}}_j(\vec{k})\}. \tag{III.4}$$

Then (III.3) and (II.10) imply that

$$E_{gs} + \sum_{i=1}^{m'} \omega_i' \leq \Sigma - \delta \tag{III.5}$$

and

$$E_{gs} + \sum_{j=1}^{m} \omega_j \leq \Sigma - \delta. \tag{III.6}$$

Assumption (III.2) implies that the states

$$\psi_{m'}^{out} := \prod_{i=1}^{m'} \vec{A}^{out}[\vec{f_i}]\phi_{gs} \tag{III.7}$$

and

$$\psi_m^{in} := \prod_{j=1}^{m} \vec{A}^{in}[\vec{h}_j]\phi_{gs} \tag{III.8}$$

exhibit exponential decay in the distance between the electron and the proton. Hence by Lemma II.1, one further asymptotic creation operator can be applied to $\psi_{m'}^{out}$,ψ_m^{in}, respectively.

In the presence of an arbitrarily small infrared cutoff in the interaction term of the Hamiltonian, asymptotic completeness of Rayleigh scattering has been proven in [8]; the first result about asymptotic completeness, for not solvable models in this context, has been provided in [6], where it is proven for massive scalar bosons. This implies that states $\psi_{m'}^{out}$ and ψ_m^{in}, as in Eqs. (III.7), (III.8), respectively, satisfying (III.2), with $\delta = 0$, span the space $\mathcal{H}_\Sigma$. It is expected, but not proven, that this result remains true when the infrared cutoff is removed.

The *reduction formulae* enable us to express the matrix elements in Eq. (III.1) in terms of (integrals of) time-ordered products of interpolating fields. These formulae will serve as a starting point to derive an infrared-convergent algorithm to explicitly calculate the scattering amplitudes, up to a remainder term of arbitrarily high order in α.

We first explain the reduction procedure for a matrix element describing a process with only one incoming photon in a wave function $\vec{h}$ and one outgoing photon in a wave function $\vec{f}$, i.e., for

$$\langle \vec{A}^{out}[-\overline{\vec{f}}]\vec{A}^{in}[\vec{h}]\rangle_{\phi_{gs}}, \tag{III.9}$$

where $\langle\cdot\rangle_{\phi_{gs}}$ denotes the expectation value with respect to the groundstate ϕ_{gs}.

Exploiting Eq. (II.17), we find that

$$\begin{aligned}
&\langle \vec{A}^{out}[-\overline{\vec{f}}]\vec{A}^{in}[\vec{h}]\rangle_{\phi_{gs}} = && \text{(III.10)}\\
&= \langle \vec{A}^{out}[-\overline{\vec{f}}]\vec{A}^{out}[\vec{h}]\rangle_{\phi_{gs}} + \langle \vec{A}^{out}[-\overline{\vec{f}}](\vec{A}^{in}[\vec{h}] - \vec{A}^{out}[\vec{h}])\rangle_{\phi_{gs}} && \text{(III.11)}\\
&= (f,h) + i\int_{-\infty}^{+\infty} \langle \vec{A}^{out}[-\overline{\vec{f}}]\vec{J}^{tr}[\vec{h}_s, s]\rangle_{\phi_{gs}} ds && \text{(III.12)}\\
&\quad -i\int_{-\infty}^{+\infty} \langle \vec{J}^{tr}[\vec{h}_s, s]\vec{A}^{in}[-\overline{\vec{f}}]\rangle_{\phi_{gs}} ds,
\end{aligned}$$

where the third term in (III.12) can be added for free, because it actually vanishes. This is seen by noticing that the groundstate is a vacuum for the asymptotic annihilation operators; see, e.g., [8]. Now, using again Eq. (II.17), we get

$$
\begin{aligned}
&\langle \vec{A}^{out}[-\bar{\vec{f}}]\vec{A}^{in}[\vec{h}]\rangle_{\phi_{gs}} = && \text{(III.13)}\\
&= \quad (f,h) - \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int\int \overline{f_t(\vec{z})}\langle \mathcal{T}(\vec{J}^{tr}(\vec{z},t)\vec{J}^{tr}(\vec{y},s))\rangle_{\phi_{gs}}\vec{h}_s(\vec{y})d^3yd^3zdsdt\\
&\qquad +i\int_{-\infty}^{+\infty}\langle[\vec{A}[-\bar{\vec{f}}_s,s],\vec{J}^{tr}[\vec{h}_s,s]]\rangle_{\phi_{gs}}ds && \text{(III.14)}
\end{aligned}
$$

where $\mathcal{T}$ is the time ordered product. A scalar product between vector quantities depending on the same position variables is understood, here and in the following.
The equal time commutator in Eq. (III.14) corresponds to

$$
-\int\int \overline{f_s(\vec{z})}[\frac{\partial\vec{A}(\vec{z},s)}{\partial s},\vec{J}^{tr}(\vec{y},s)]\vec{h}_s(\vec{y})d^3yd^3z \qquad \text{(III.15)}
$$

that is, in general, a non vanishing function of the electron position.
In order to get a more symmetrical expression that can be easily generalized to scattering amplitudes with an arbitrary finite number of photons, starting from the expression in Eq. (III.12) we follow the standard *reduction formulae* procedure. Due to the results achieved in the previous sections, we can control the mathematical quantities that will be derived.
First we choose a smooth real function, ξ, of the time variable s with the following properties:

$$
\xi(s)=1, \qquad \text{for} \qquad -\alpha^{-\epsilon}+\frac{R}{2}\leq s\leq \alpha^{-\epsilon}-\frac{R}{2}, \qquad \text{(III.16)}
$$

$$
\xi(s)=0, \qquad \text{for} \qquad s\leq -\alpha^{-\epsilon}-\frac{R}{2} \quad \text{and} \quad s\geq \alpha^{-\epsilon}+\frac{R}{2}, \qquad \text{(III.17)}
$$

where $0<\epsilon<<1$ and $R>0$ is an α-independent number.
Remark
This is a crucial step for the expansion in α we are going to carry out. Because of the fast convergence proved in Lemma II.1, we can choose a "short" time scale, $\alpha^{-\epsilon}$, as a time cutoff, provided the cutoff-function ξ is smooth, uniformly in α.

It follows from Lemma II.1, Inequality (II.18), that

$$
i\int_{-\infty}^{+\infty}\langle \vec{A}^{out}[-\bar{\vec{f}}]\vec{J}^{tr}[\vec{h}_s,s]\rangle_{\phi_{gs}}ds \qquad \text{(III.18)}
$$

can be approximated by

$$
i\int_{-\infty}^{+\infty}\langle \vec{A}^{out}[-\bar{\vec{f}}]\vec{J}^{tr}(\vec{h}_s,s)\rangle_{\phi_{gs}}\xi(s)ds, \qquad \text{(III.19)}
$$

up to an error term of order $o(\alpha^N)$, for any $N \in \mathbb{N}$. After some integrations by parts, we end up with

$$-i\int_{-\infty}^{+\infty}\int\langle\vec{A}^{out}[-\overline{\vec{f}}]\vec{A}(\vec{y},s)\rangle_{\phi_{gs}}\Box(\vec{h}_s(\vec{y})\xi(s))d^3yds. \tag{III.20}$$

Similarly

$$-i\int_{-\infty}^{+\infty}\langle\vec{J}^{tr}[\vec{h}_s,s]\vec{A}^{in}[-\overline{\vec{f}}]\rangle_{\phi_{gs}}ds \tag{III.21}$$

is approximated by

$$i\int_{-\infty}^{+\infty}\langle\vec{A}(\vec{y},s)\vec{A}^{in}[-\overline{\vec{f}}]\rangle_{\phi_{gs}}\Box(\vec{h}_s(\vec{y})\xi(s))ds, \tag{III.22}$$

up to an error term of order $o(\alpha^N)$. We propose to express the sum of the two quantities (III.18) and (III.21) as the integral of a time-ordered product of the fields. For general S-matrix elements, we will basically apply the two operations i) and ii) explained below.
i) The sum of the two terms (III.18) and (III.21) is given by

$$-lim_{t\to+\infty}i^2\int_{-\infty}^{+\infty}\int\int\langle(\vec{A}_{\widehat{\theta}_{t,s}}(\vec{z},t)\cdot\overleftrightarrow{\partial}\overline{\vec{f}_t(\vec{z})})\vec{A}(\vec{y},s)\rangle_{\phi_{gs}}\times \tag{III.23}$$

$$\times\Box(\vec{h}_s(\vec{y})\xi(s))d^3zd^3yds$$

$$+\quad lim_{t\to-\infty}i^2\int_{-\infty}^{+\infty}\int\langle\vec{A}(\vec{y},s)(\vec{A}_{\widehat{\theta}_{s,t}}(\vec{z},t)\cdot\overleftrightarrow{\partial}\overline{\vec{f}_t(\vec{z})})\rangle_{\phi_{gs}}\times \tag{III.24}$$

$$\times\Box(\vec{h}_s(\vec{y})\xi(s))d^3zd^3yds$$

where

$$\vec{A}_{\widehat{\theta}_{t,s}}(\vec{z},t):=\vec{A}(\vec{z},t)\widehat{\theta}(t-s) \tag{III.25}$$

$$\vec{A}_{\widehat{\theta}_{t,s}}(\vec{z},t)\cdot\overleftrightarrow{\partial_t}\overline{\vec{f}_t(\vec{z})}:=\vec{A}_{\widehat{\theta}_{t,s}}(\vec{z},t)\cdot\frac{\partial\overline{\vec{f}_t(\vec{z})}}{\partial t}-\frac{\partial\vec{A}_{\widehat{\theta}_{t,s}}(\vec{z},t)}{\partial t}\cdot\overline{\vec{f}_t(\vec{z})} \tag{III.26}$$

and $\widehat{\theta}_{t,s}=\widehat{\theta}(t-s)$ is a non-negative, α-independent, C^∞ approximation of the Heaviside step function. We apply the fundamental theorem of calculus to (III.23), (III.24). From the derivative with respect to t of the expression

$$\vec{A}_{\widehat{\theta}_{t,s}}(\vec{z},t)\cdot\overleftrightarrow{\partial}\overline{\vec{f}_t(\vec{z})}, \tag{III.27}$$

with $|t|$ large enough, we get a current, $\vec{J}^{tr}[\overline{\vec{f}_t},t]$ applied to the groundstate; (an integration by parts in the $\vec{z}-$coordinates is involved here). Thanks to Estimate (II.18) in Lemma II.1, we can choose the function $\xi(t)$ in order

to cutoff the t-integration. This introduces an error of order $o(\alpha^N)$, for an arbitrarily large N.
ii) Since the groundstate vector ϕ_{gs} is in the domain of the fields $\vec{A}_{\widehat{\theta}_{t,s}}(\vec{z},t)$ and $\partial_t\vec{A}_{\widehat{\theta}_{t,s}}(\vec{z},t)$ when smeared out in space, we can rewrite the difference of the two limits (III.23) and (III.24) as

$$\begin{aligned}-i^2\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int\int & ds d^3z d^3y \xi(t)\times \\ \times\frac{\partial}{\partial t}\big\{ & \langle\vec{A}_{\widehat{\theta}_{t,s}}(\vec{z},t)\cdot\overleftrightarrow{\partial_t}\,\overline{\vec{f}_t(\vec{z})}\vec{A}(\vec{y},s)\rangle_{\phi_{gs}}\Box(\vec{h}_s(\vec{y})\xi(s)) \\ & +\langle\vec{A}(\vec{y},s)\vec{A}_{\widehat{\theta}_{s,t}}(\vec{z},t)\cdot\overleftrightarrow{\partial_t}\,\overline{\vec{f}_t(\vec{z})}\rangle_{\phi_{gs}}\Box(\vec{h}_s(\vec{y})\xi(s))\big\}\end{aligned} \tag{III.28}$$

up to an error term of arbitrarily high order in α. After an integration by parts, we finally conclude that if $(f,h)=0$ the expression in Eq. (III.9) is given by

$$i^2\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int\int\Box(\overline{\vec{f}_t(\vec{z})}\xi(t))\langle\mathcal{T}^{\widehat{\theta}}(\vec{A}(\vec{z},t)\vec{A}(\vec{y},s))\rangle_{\phi_{gs}}\Box(\vec{h}_s(\vec{y})\xi(s))d^3yd^3zdsdt, \tag{III.29}$$

up to an error of order $o(\alpha^N)$, for any $N\in\mathbb{N}$, where $\mathcal{T}^{\widehat{\theta}}$ denotes the smooth time-ordered product obtained when replacing the Heaviside function by the smooth function $\widehat{\theta}$.

In order to generalize this result to an arbitrary, finite number of asymptotic photons, we have to control the norm of vectors of the form

$$\begin{aligned}\int_{-\infty}^{+\infty}\cdot\cdot\int_{-\infty}^{+\infty}\int\cdot\cdot\int\ & \mathcal{T}^{\widehat{\theta}}(\vec{A}(\vec{y}_1,s_1)\cdots\vec{A}(\vec{y}_n,s_n))\phi_{gs}\times \\ & \times\prod_{i=1}^{n}\Box(\vec{h}_{i,s_i}(\vec{y}_i)\xi(s_i))\prod_{i=1}^{n}ds_id^3y_i.\end{aligned} \tag{III.30}$$

Some operator domain problems might, in principle, arise, because the vector potential (smeared in space) is an unbounded operator. However, because of the time integrations, and because the groundstate belongs to $D(H^m)$, for any $m\in\mathbb{N}$, the vector in Eq. (III.30) turns out to be well defined, and its norm is bounded uniformly in α.

Lemma III.1. *Let the function* ξ *be smooth and of compact support and such that* $sup_{s\in\mathbb{R}}|\frac{d^m\xi(s)}{ds^m}|$ *is* $\alpha-$*independent, for any* $m\in\mathbb{N}$. *Let* $\{\vec{h}_l(\vec{y}_l,s_l)|l=1,..,n\}$ *be smooth solutions of the free wave equation with properties as in Eq. (II.3). Then the following operator is bounded in the operator norm,* *uniformly in α:*

$$\begin{aligned}\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty}\int\cdots\int\ \mathcal{T}^{\widehat{\theta}}(\vec{X}(\vec{y}_1,s_1)\cdots\vec{X}(\vec{y}_n,s_n))\times\\ \times\prod_{l=1}^{n}\Box(\vec{h}_{l,s_l}(\vec{y}_l)\xi(s_l))\prod_{l=1}^{n}ds_l d^3y_l\frac{1}{(H+i)^n}\end{aligned}\tag{III.31}$$

where $\vec{X}(\vec{y},s)$ is either $\vec{A}(\vec{y},s)$ or $\dot{\vec{A}}(\vec{y},s)$ and

$$\begin{aligned}&\mathcal{T}^{\widehat{\theta}}(\vec{X}(\vec{y}_1,s_1)\cdots\vec{X}(\vec{y}_n,s_n)):=\\ =\ &\sum_{p\in\mathcal{P}}\vec{X}(\vec{y}_{p(1)},s_{p(1)})\cdots\vec{X}(\vec{y}_{p(n)},s_{p(n)})\times\\ &\qquad\times\widehat{\theta}(s_{p(1)}-s_{p(2)})\cdots\widehat{\theta}(s_{p(n-1)}-s_{p(n)}),\end{aligned}\tag{III.32}$$

and $\mathcal{P}$ being the group of permutations of n elements.

Proof. The proof is by induction in n.
Given the permutation $(p(1),\cdots,p(j))$, we assume that, for $1\leq j\leq n-1$, the following statements are true:

- H1) The operator

  $$\begin{aligned}\int_{-\infty}^{+\infty}\cdot\cdot\int_{-\infty}^{+\infty}\int\cdot\cdot\int\ \vec{X}(\vec{y}_{p(1)},s_{p(1)})\cdots\vec{X}(\vec{y}_{p(j)},s_{p(j)})\times\\ \times\prod_{l=1}^{j-1}\widehat{\theta}(s_{p(l)}-s_{p(l+1)})\prod_{l=1}^{j}\Box(\vec{h}_{p(l),s_{p(l)}}(\vec{y}_{p(l)})\xi(s_{p(l)}))\prod_{l=1}^{j}ds_{p(l)}d^3y_{p(l)}\frac{1}{(H+i)^j}\end{aligned}\tag{III.33}$$

  is bounded uniformly in α;

- H2) For $u\in\mathbb{R}$, and for functions ζ, $\vec{g}$ belonging to the families $\{\frac{d^k\xi(s_l)}{ds_l^k}|l=1,..,n\,;\,k=1,2,3,\cdots\}$ and $\{\frac{d^k\vec{h}_l(\vec{y}_l,s_l)}{ds_l^k}|l=1,..,n\,;\,k=1,2,3,\cdots\}$, respectively, the operator

  $$\int_{-\infty}^{+\infty}\int(H+i)^{j-1}\vec{X}(\vec{y},s))\widehat{\theta}(u-s)\vec{g}_s(\vec{y})\zeta(s))d^3yds\frac{1}{(H+i)^j}\tag{III.34}$$

  is bounded, uniformly in u and in α.

We first prove that H2) holds when j is replaced by $j+1$. For this purpose we consider the scalar product

$$(\psi,\int_{-\infty}^{+\infty}\int(H+i)^j\vec{X}(\vec{y},s))\widehat{\theta}(u-s)\vec{g}_s(\vec{y})\zeta(s))d^3yds\frac{1}{(H+i)^{j+1}}\phi)\tag{III.35}$$

where $\psi \in \mathcal{D}(H^m)$, for any $m \in \mathbb{N}$, and ϕ is an arbitrary vector. The expression in Eq. (III.35) can be written as (recall $\widehat{\theta}_{u,s} = \widehat{\theta}(t-s)$)

$$\int_{-\infty}^{+\infty}\int(\psi,(H+i)^{j-1}\vec{X}(\vec{y},s))\widehat{\theta}_{u,s}\vec{g}_s(\vec{y})\zeta(s))d^3yds\frac{1}{(H+i)^j}\phi) \tag{III.36}$$

$$- \quad i\int_{-\infty}^{+\infty}\int(\psi,(H+i)^{j-1}\frac{\partial\vec{X}(\vec{y},s)}{\partial s}\widehat{\theta}_{u,s}\vec{g}_s(\vec{y})\zeta(s))d^3yds\frac{1}{(H+i)^{j+1}}\phi) \tag{III.37}$$

Integrating by parts in the time variable s, the expression in Eq. (III.37) is seen to be given by

$$i\int_{-\infty}^{+\infty}\int(\psi,(H+i)^{j-1}\vec{X}(\vec{y},s)\frac{\partial}{\partial s}\Big(\widehat{\theta}_{u,s}\vec{g}_s(\vec{y})\zeta(s))\Big)\frac{1}{(H+i)^{j+1}}\phi)d^3yds. \tag{III.38}$$

By the induction hypothesis H2), we conclude that the absolute value of the scalar product (III.37) is bounded by

$$C\|\psi\|\|\phi\|, \tag{III.39}$$

where C is a positive constant independent of ψ and ϕ. Due to Riesz' lemma, the operator in (III.35) is bounded. Because of our assumptions on $\widehat{\theta}_{u-s}, \vec{g}_s(\vec{y}), \zeta(s)$, the constant C can be chosen to be independent of α and u.

Turning to H1), we first introduce a shorthand notation: Expression (III.33) is abbreviated by $\mathcal{X}(p(1),\cdot\cdot,p(j))$, and the expression in Eq. (III.34) by $\mathcal{A}_u(\vec{g},\zeta)$. Because of property H2), for $j+1$, and assuming H1) holds for j, the following inequality

$$\begin{aligned} &\|\mathcal{X}(p(1),\cdot\cdot,p(j+1))\| \\ \leq\ & 2\|\mathcal{X}(p(1),\cdot\cdot,p(j))\|\mathrm{sup}_{s_{p(j)}}\|\mathcal{A}_{s_{p(j)}}(\frac{d\vec{h}_{p(j+1)}(\vec{y}_{p(j+1)},s_{p(j+1)})}{ds_{p(j+1)}},\frac{d\xi(s_{p(j+1)})}{ds_{p(j+1)}})\| \\ & +\|\mathcal{X}(p(1),\cdot\cdot,p(j))\|\mathrm{sup}_{s_{p(j)}}\|\mathcal{A}_{s_{p(j)}}(\vec{h}_{p(j+1)},\frac{d^2\xi(s_{p(j+1)})}{ds^2_{p(j+1)}})\| \end{aligned} \tag{III.40}$$

implies that H1) holds for $j+1$, too. Since H1) and H2) are obviously true for $j=1$, they hold for any $j \leq n$. Lemma III.1 follows from H1) and H2). □

In our derivation of *reduction formulae* we neglect forward scattering, i.e., we assume that $(f_i, h_j) = 0$, for arbitrary i, j. The general case can easily be derived from the result below, at the price of more complicated expressions.

Proposition III.2. *Under the assumptions in Eq. (III.2) and of Lemma III.1 on* $\{\vec{h}_j\}$, $\{\vec{f}_p\}$ *and* ξ, *and if* $(f_p, h_j) = 0$, *for all* p *and* j, *the S-matrix element*

$$\Big(\prod_{p=1}^{m'} \vec{A}^{out}[\vec{f}_p]\phi_{gs}, \prod_{j=1}^{m} \vec{A}^{in}[\vec{h}_j]\phi_{gs}\Big) \tag{III.41}$$

is given by

$$i^{m+m'} \int_{-\infty}^{+\infty} \cdot\cdot \int_{-\infty}^{+\infty} \int \cdot\cdot \int \langle \mathcal{T}^{\widehat{\theta}}(\prod_{p=1}^{m'} \vec{A}(\vec{z}_p, t_p) \prod_{j=1}^{m} \vec{A}(\vec{y}_j, s_j)\rangle_{\phi_{gs}} \times \tag{III.42}$$

$$\times \prod_{p=1}^{m'} \Box(\overline{\vec{f}_{p,t_p}}(\vec{z}_p)\xi(t_p)) \prod_{j=1}^{m} \Box(\vec{h}_{j,s_j}(\vec{y}_j)\xi(s_j)) \prod_{p=1}^{m'} dt_p d^3 z_p \prod_{j=1}^{m} ds_j d^3 y_j,$$

up to an error term of arbitrarily high order in α.

Proof. The proof is by induction. If there are only one incoming and one outgoing photon, we have proven this result at the beginning of the section. Notice that, using the same arguments, we can eliminate one incoming and one outgoing photon from the asymptotic states in the scalar product (III.41). The inductive assumption is that $l + l' = n - 1 (< m + m')$ photons can be eliminated yielding the expression

$$\int \Big(\prod_{p=1}^{m'-l'} \vec{A}^{out}[\vec{f}_p]\phi_{gs}, \mathcal{T}^{\widehat{\theta}}(\prod_{p=1}^{l'} \vec{A}(\vec{z}_p, t_p) \prod_{j=1}^{l} \vec{A}(\vec{y}_j, s_j)) \prod_{j=1}^{m-l} \vec{A}^{in}[\vec{h}_j]\phi_{gs}\Big) \times \tag{III.43}$$

$$\times \prod_{p=1}^{l'} \Box(\overline{\vec{f}_{p,t_p}}(\vec{z}_i)\xi(t_p)) \prod_{j=1}^{l} \Box(\vec{h}_{j,s_j}(\vec{y}_j)\xi(s_j)) \prod_{p=1}^{l'} dt_p d^3 z_p \prod_{j=1}^{l} ds_j d^3 y_j,$$

up to an error term of arbitrarily high order in α. To prove (III.41) for $l + l' + 1 = n$, another photon, for example an outgoing photon, must be eliminated from the outgoing state in Expression (III.41), with $l + l' = n - 1$. This can be accomplished by repeating operations i) and ii) at the beginning of this section, with the following modifications:

a) The counterpart of the expectation value in (III.23) is given by:

$$\Big(\psi^{out}_{m'-l'-1}, T^{\widehat{\theta}}(\vec{A}(\vec{z}_1, t_1) \cdot\cdot \vec{A}(\vec{z}_{l'+1}, t_{l'+1}) \cdot \overleftrightarrow{\partial}\,\overline{\vec{f}_{l'+1,t_{l'+1}}(\vec{z}_{l'+1})} \cdot\cdot \vec{A}(\vec{y}_l, s_l))\psi^{in}_{m-l}\Big) \tag{III.44}$$

where

$$\psi^{out}_{m'-l'-1} := \prod_{p=1}^{m'-l'-1} \vec{A}^{out}[\vec{f}_p]\phi_{gs} \tag{III.45}$$

$$\psi^{in}_{m-l} := \prod_{j=1}^{m-l} \vec{A}^{in}[\vec{h}_j]\phi_{gs}; \tag{III.46}$$

b) As before, using Lemma III.1, we may cutoff the integration over $t_{l'+1}$ by introducing the smooth function of compact support (see (III.16),(III.17)), $\xi(t_{l'+1})$, up to an error of, at most, order $o(\alpha^N)$. We then integrate by parts, which is legitimate because of Lemma III.1, applied to the product of $l + l' = n - 1$ fields. □

IV Asymptotic expansion of the scattering amplitudes

The expression in Eq. (III.42) derived in the previous Section must be evaluated in terms of explicit convergent integrals, up to an error term that, as we will prove, can be chosen to be of arbitrarily high order in the finestructure constant α.
The *reduction formulae* derived in the previous Section are not a particularly convenient starting point to develop an algorithm for calculating S-matrix elements. However, with a slight modification that depends on the desired order, $o(\alpha^N)$, $N = 1, 2, 3, ..$, of accuracy of the algorithm, we can, in essence, repeat the reduction procedure in Proposition III.2. This procedure gives rise to time-ordered products. Our modified version of the reduction procedure does not rely on Lemma III.1, and, more importantly, it will yield an expression that can be expanded up to error terms of $o(\alpha^N)$, by making use of the Duhamel expansion of the propagators and the infrared-finite algorithm developed in [2] for the calculation of the groundstate and the groundstate energy.

IV.1 A modified reduction procedure

Let $o(\alpha^N)$ be the desired order of the error term in the calculation of the scattering amplitude (III.41). Since the leading order is $\alpha^{\frac{3}{2}(m+m')}$, we may assume that $N > \frac{3}{2}(m + m')$. The $N-$dependent, modified reduction procedure differs from the usual one in the following way: Before eliminating a photon from one of the asymptotic states, e.g. from the incoming state

$$\psi_m^{in} = \prod_{j=1}^{m} \vec{A}^{in}[\vec{h}_j]\phi_{gs}, \tag{IV.1}$$

we apply the operator $(H+i)^n$, $n=[N-\frac{3}{2}(m+m')+1]$ (where $[\cdot]$ is the integer part) to obtain

$$\begin{aligned} &\sum_{p=1}^{n}\binom{n}{p}(E_{gs}+i)^{n-p}\sum_{l_1=1}^{m}\sum_{l_2=1}^{m}\cdots\sum_{l_p=1}^{m}\prod_{j=1}^{m}\vec{A}^{in}[\vec{h}_j^{(l_1,l_2,\cdot\cdot,l_p)}]\phi_{gs} \qquad \text{(IV.2)}\\ +\quad &(E_{gs}+i)^n\prod_{j=1}^{m}\vec{A}^{in}[\vec{h}_j]\phi_{gs}\end{aligned}$$

where

$$\vec{h}_j^{(l_1,l_2,\cdot\cdot,l_p)}(\vec{y}):=\sum_{\lambda=\pm}\int\vec{\varepsilon}(\vec{k},\lambda)^*|k|^{(\sum_{q=1}^{p}\delta_{l_q,j})}\hat{h}_j^{\lambda}(\vec{k})e^{+i\vec{k}\cdot\vec{y}}\frac{d^3k}{(2\pi)^{3/2}\sqrt{2|k|}} \qquad \text{(IV.3)}$$

where $\delta_{l_q,j}$ is Kronecker's symbol. The original vector can be written as

$$\begin{aligned}\phi_m^{in} &=\\ &= (H+i)^{-n}\sum_{p=1}^{n}\binom{n}{p}(E_{gs}+i)^{n-p}\sum_{l_1=1}^{m}\cdot\cdot\sum_{l_p=1}^{m}\prod_{j=1}^{m}\vec{A}^{in}[\vec{h}_j^{(l_1,l_2,\cdot\cdot,l_p)}]\phi_{gs} \qquad \text{(IV.4)}\\ &\quad +(H+i)^{-n}(E_{gs}+i)^n\prod_{j=1}^{m}\vec{A}^{in}[\vec{h}_j]\phi_{gs}. \qquad \text{(IV.5)}\end{aligned}$$

We now eliminate the m-th photon from the state in Eq. (IV.2), using the procedure already employed in Proposition III.2. The same manipulations must be repeated for each photon. The final expression consists of finitely many terms similar to the expression in Eq. (III.42) except that

1) the test functions are the ones obtained in Eqs. (IV.2),(IV.3); and

2) the time-ordered product is given by

$$\begin{aligned}&\mathcal{T}_N^{\widehat{\theta}}\Big(\prod_{l=1}^{m'}\vec{A}(\vec{z}_l,t_l)\prod_{j=1}^{m}\vec{A}(\vec{y}_i,s_i)\Big):= \qquad \text{(IV.6)}\\ &=\mathcal{T}^{\widehat{\theta}}\Big(\prod_{l=1}^{m'}\{\vec{A}(\vec{z}_l,t_l)\frac{1}{(H+i)^n}\}\prod_{j=1}^{m}\{\frac{1}{(H+i)^n}\vec{A}(\vec{y}_j,s_j)\}\Big) \qquad \text{(IV.7)}\end{aligned}$$

The operation $\mathcal{T}_N^{\widehat{\theta}}$ in (IV.6) can be expanded in α. In fact, a factor of $\frac{1}{(H+i)}$ can be put next to each field operator $\vec{A}(\vec{z}_l,0)$, and a factor of $\frac{1}{(H+i)^{n-1}}$ remains next to each propagator $e^{-iH(t_l-t_{l+1})}$. Then we use the Duhamel expansion

$$\frac{1}{(H+i)^{n-1}}e^{iHt} = \tag{IV.8}$$

$$\begin{aligned}
= \ & \frac{1}{(H+i)^{n-1}}e^{iH_0t} + \frac{i}{(H+i)^{n-1}}\int_0^t e^{iH_0\tau_1}\frac{1}{(H+i)}H_I e^{-iH_0\tau_1}d\tau_1 e^{iH_0t} \\
& \cdots\cdots\cdots\cdots\cdots\cdots\cdots \\
& +\frac{i^{n-1}}{(H+i)}\int_0^t\Big(\prod_{l=1}^{n-2}\int_0^{\tau_l}\Big)\prod_{j=1}^{n-1}\Big(e^{iH_0\tau_{n-j}}\frac{1}{(H+i)}H_I e^{-iH_0\tau_{n-j}}\Big)\times \\
& \qquad\qquad \times d\tau_{n-1}\cdots d\tau_1 e^{iH_0t}
\end{aligned}$$

$$\begin{aligned}
& +i^n\int_0^t\Big(\prod_{l=1}^{n-1}\int_0^{\tau_l}\Big)e^{iH\tau_n}\frac{1}{(H+i)}H_I e^{-iH_0\tau_n}\times \\
& \quad \times\prod_{j=1}^{n-1}\Big(e^{iH_0\tau_{n-j}}\frac{1}{(H+i)}H_I e^{-iH_0\tau_{n-j}}\Big)d\tau_n\cdots d\tau_1 e^{iH_0t},
\end{aligned} \tag{IV.9}$$

where H_0 has been defined in Eq. (I.17), and $H_I := H - H_0$. We then apply the Neumann series expansion of the resolvent

$$\frac{1}{(H+i)} = \sum_{j=0}^{n-1}\Big[\frac{1}{(H_0+i)}\Big(-H_I\frac{1}{(H_0+i)}\Big)^j\Big] \tag{IV.10}$$

$$+\frac{1}{(H_0+i)}\Big(-H_I\frac{1}{(H+i)}\Big)^n, \tag{IV.11}$$

and we exploit the α-independence on the norm bounds of the operators

$$\alpha^{-\frac{3}{2}}\frac{1}{(H_0+i)^{\frac{1}{2}}}H_I\frac{1}{(H_0+i)^{\frac{1}{2}}}, \quad \alpha^{-\frac{3}{2}}\frac{1}{(H+i)^{\frac{1}{2}}}H_I\frac{1}{(H_0+i)^{\frac{1}{2}}} \tag{IV.12}$$

$$\int\vec{A}(\vec{z}_l,0)\overline{\vec{f}_l(\vec{z}_l,0)}d^3z_l\frac{1}{(H_0+i)^{\frac{1}{2}}}, \quad \int\vec{A}(\vec{z}_l,0)\overline{\vec{f}_l(\vec{z}_l,0)}d^3z_l\frac{1}{(H+i)^{\frac{1}{2}}}. \tag{IV.13}$$

Using the fact that the time-integrations extend over intervals of length proportional to $\alpha^{-\epsilon}$, we conclude that the remainder term (IV.9) in the Duhamel expansion is bounded by $const\cdot\alpha^{n(\frac{3}{2}-\epsilon)}$. Therefore the operator (IV.6) can be approximated, up to an error term of $o(\alpha^N)$, by finitely many expressions only involving the propagator and the resolvent of the Hamiltonian H_0, besides the groundstate ϕ_{gs} and the groundstate energy E_{gs}. These latter quantities can be calculated using the algorithm developed in [2] and outlined in next section. We can therefore state the main result of the paper:

Theorem IV.1. *For $\alpha \leq \bar{\alpha}$, with $\bar{\alpha} \equiv \bar{\alpha}_N$ small enough, the S-matrix elements $S_\alpha^{m',m}(\{\vec{f}_i\},\{\vec{h}_j\})$, where $(f_i, h_j) = 0$, have expansions of the form*

$$S_\alpha^{m',m}(\{\vec{f}_i\},\{\vec{h}_j\})^{conn} = \sum_{\ell=6}^{2N} S_l^{m',m}(\{\vec{f}_i\},\{\vec{h}_j\};\alpha)\alpha^{\frac{\ell}{2}} \; + \; o(\alpha^N) \qquad \text{(IV.14)}$$

with

$$\lim_{\alpha\to 0} \alpha^\delta |S_l^{m',m}(\{\vec{f}_i\},\{\vec{h}_j\};\alpha) = 0 \qquad , \quad \textit{for arbitrary} \quad \delta > 0, \qquad \text{(IV.15)}$$

for $N = 3, 4, 5, \ldots$. The coefficients $S_l^{m',m}(\{\vec{f}_i\},\{\vec{h}_j\};\alpha)$ are computable in terms of finitely many convergent integrals, for arbitrary $l < \infty$ (with $l \geq 6$).

IV.2 Expansion of the groundstate and the groundstate energy

The final and technically most subtle step in the calculation of the S-matrix elements concerns the calculation of the groundstate and the groundstate energy. Because of infrared divergences, which invalidate a straightforward Taylor expansion, an iterative construction must be employed to remove an infrared cutoff in photon momentum space and to devise a convergent algorithm. Such a construction has been developed in [2] on the basis of results in [10] and [1]. In the following, we describe the results of [2] without providing proofs; but see [1], [2] and [10]. The main ideas underlying the construction of the groundstate will be discussed, and the strategy of the re-expansion will be outlined.

IV.2.1 Notation

In the following of this Section, we simplify our notation by setting

$$k \;:=\; (\vec{k}, \lambda)\,, \quad \omega(k) \;\equiv\; |k| \;:=\; |\vec{k}|\,, \quad \text{and} \quad \int f(k)\, dk \;:=\; \sum_{\lambda=\pm} \int f(\vec{k}, \lambda)\, d^3k\,,$$

for any integrable functions $f(\cdot, \lambda)$,$\lambda = \pm$. Given an operator-valued function $F : \mathbb{R}^3 \times \mathbb{Z}_2 \to \mathcal{B}(\mathcal{H}_{el})$, we write

$$a^*(F) \;\; := \;\; \int F(k) \otimes a^*(k) dk \qquad \text{(IV.16)}$$

$$a(F) \;\; := \;\; \int F(k)^* \otimes a(k) dk. \qquad \text{(IV.17)}$$

This allows us to write the velocity operator $\vec{v}$ (rescaled by 2) as

$$\vec{v} \;:=\; -i\vec{\nabla}_x \;+\; a^*(\vec{G}) \;+\; a(\vec{G})\,, \qquad \text{(IV.18)}$$

where $\vec{G} : \mathbb{R}^3 \times \mathbb{Z}_2 \to \mathcal{B}(\mathcal{H}_{el})^3$ are the multiplication operators defined by

$$\vec{G}(k) \;:=\; \frac{\alpha^{3/2}}{(2\pi)^{3/2}} \, \frac{\Lambda(k)}{\sqrt{2\,|k|}} \, e^{-i\alpha\vec{k}\cdot\vec{x}} \, \vec{\varepsilon}(k) \, . \tag{IV.19}$$

In terms of the velocity operator, the Hamiltonian assumes the simple form

$$H \;=\; \vec{v}^{\,2} \,-\, V(x) \,+\, \check{H}. \tag{IV.20}$$

We define a decreasing sequence, $(\sigma_n)_{n=0}^{\infty}$, of energy scales by setting

$$\sigma_n \;:=\; \kappa\,\alpha^n \, . \tag{IV.21}$$

Note, in passing, that, for all $n \in \mathbb{N}_0$, we have that $\sigma_{n+1} \leq \kappa\alpha < 1$. To cut the interaction Hamiltonian into slices corresponding to ever lower energy scales, we make use of the operators

$$\vec{G}_n(k) \;:=\; \mathbf{1}\Big(\sigma_n \leq |k|\Big)\, \vec{G}(k) \, , \quad \text{and} \quad \vec{G}_n^m(k) \;:=\; \mathbf{1}\Big(\sigma_n \leq |k| < \sigma_m\Big)\, \vec{G}(k) \, , \tag{IV.22}$$

for all $k \in \mathbb{R}^3 \times \mathbb{Z}_2$ and $m, n \in \mathbb{N}_0$, with $m < n$. Note that $\vec{G} = \sum_{n=0}^{\infty} \vec{G}_{n+1}^n$ and that $\vec{G}_n$ is the coupling function of the interaction Hamiltonian cutoff in the infrared region, $|k| \leq \sigma_n$. We factorize Fock space $\mathcal{F} = \mathcal{F}(\mathfrak{h})$ into tensor products by introducing suitable subspaces corresponding to the one-photon Hilbert space corresponding to different energy scales:

$$\mathfrak{h}_n \;:=\; L^2\Big[\mathcal{K}_n\Big] \quad \text{and} \quad \mathfrak{h}_n^m \;:=\; L^2\Big[\mathcal{K}_n^m\Big] \, , \tag{IV.23}$$

where,

$$\text{for } 0 \leq n \leq \infty, \quad \mathcal{K}_n \;:=\; \Big\{(\vec{k}, \tau) \in \mathbb{R}^3 \times \mathbb{Z}_2 \;\Big|\; \sigma_n \leq \omega(\vec{k})\Big\} \, , \tag{IV.24}$$

$$\text{for } 0 \leq m < n \leq \infty, \quad \mathcal{K}_n^m \;:=\; \Big\{(\vec{k}, \tau) \in \mathbb{R}^3 \times \mathbb{Z}_2 \;\Big|\; \sigma_n \leq \omega(\vec{k}) < \sigma_m\Big\} . \tag{IV.25}$$

Note that $\mathcal{K}_n^0 \subset \mathcal{K}_n$ is a proper subset. For integers $1 \leq m < n < \ell \leq \infty$, we have the disjoint decomposition $\mathcal{K}_\ell = \mathcal{K}_m \cup \mathcal{K}_n^m \cup \mathcal{K}_\ell^n$, and hence the direct sum

$$\mathfrak{h}_\ell \;\cong\; \mathfrak{h}_m \oplus \mathfrak{h}_n^m \oplus \mathfrak{h}_\ell^n \, , \tag{IV.26}$$

which gives rise to the isomorphism

$$\mathcal{F}_\ell \;\cong\; \mathcal{F}_m \otimes \mathcal{F}_n^m \otimes \mathcal{F}_\ell^n \, , \tag{IV.27}$$

with $\mathcal{F}_n := \mathcal{F}(\mathfrak{h}_n)$ and $\mathcal{F}_n^m := \mathcal{F}(\mathfrak{h}_n^m)$. In particular, for any $n \in \mathbb{N}$,

$$\mathcal{F} \;=\; \mathcal{F}_\infty \;\cong\; \mathcal{F}_n \otimes \mathcal{F}_{n+1}^n \otimes \mathcal{F}_\infty^{n+1} \, . \tag{IV.28}$$

We set

$$\mathcal{H}_n \;:=\; \mathcal{H}_{el} \otimes \mathcal{F}_n \quad \text{and} \quad \mathcal{H}_n^m \;:=\; \mathcal{H}_{el} \otimes \mathcal{F}_n^m . \tag{IV.29}$$

For energy-scale indices $m, n \in \mathbb{N}_0$, with $m < n$, we define the velocity operator $\vec{v}_n$, the field-energy operators $\check{H}_n$, $\check{H}_n^m$, and the Hamiltonian H_n by

$$\begin{aligned} \vec{v}_n \;&:=\; -i\vec{\nabla}_x \,+\, a^*(\vec{G}_n) \,+\, a(\vec{G}_n)\,, && \text{(IV.30)} \\ \check{H}_n \;&:=\; \int \mathbf{1}(\sigma_n \leq |k|)\, \omega(k)\, a^*(k)a(k)\, dk\,, && \text{(IV.31)} \\ \check{H}_n^m \;&:=\; \int \mathbf{1}(\sigma_n \leq |k| < \sigma_m)\, \omega(k)\, a^*(k)a(k)\, dk\,, && \text{(IV.32)} \\ H_n \;&:=\; \vec{v}_n^{\,2} \,-\, V(x) \,+\, \check{H}_n\,, && \text{(IV.33)} \end{aligned}$$

as operators on $\mathcal{H}_n$ and $\mathcal{H}_n^m$, respectively. We introduce the groundstate energy at scale n and groundstate energy differences

$$E_n \;:=\; \inf \sigma(H_n) \quad \text{and} \quad E_n^m \;:=\; E_m - E_n\,. \tag{IV.34}$$

To compare Hamiltonians, H_n and H_{n+1}, at successive energy scales, it is convenient to define positive operators H_n^+ and $\widetilde{H}_n^+$ on $\mathcal{H}_n$ and $\mathcal{H}_{n+1}$, respectively, by

$$\begin{aligned} H_n^+ \;&:=\; H_n \,-\, E_n\,, && \text{(IV.35)} \\ \widetilde{H}_n^+ \;&:=\; H_n^+ \otimes \mathbf{1}_{n+1}^n \,+\, \mathbf{1}_n \otimes \check{H}_{n+1}^n\,, && \text{(IV.36)} \end{aligned}$$

where we denote the identity operator on $\mathcal{H}_n$ and on $\mathcal{F}_n^m$ by $\mathbf{1}_n$ and $\mathbf{1}_n^m$, respectively. We identify $\vec{v}_n$ with $\vec{v}_n \otimes \mathbf{1}_{n+1}^n$ acting on $\mathcal{H}_{n+1}$. Note that, for $n \in \mathbb{N}_0$,

$$\vec{v}_{n+1} \;=\; \vec{v}_n \,+\, a^*(\vec{G}_{n+1}^n) \,+\, a(\vec{G}_{n+1}^n)\,. \tag{IV.37}$$

Similarly, given $\psi_n \in \mathcal{H}_n$, we define a vector

$$\tilde{\psi}_n \;:=\; \psi_n \otimes \Omega_{n+1}^n \;\in\; \mathcal{H}_{n+1}\,, \tag{IV.38}$$

where Ω_n and Ω_n^m denote the vacuum vectors in $\mathcal{F}_n$ and $\mathcal{F}_n^m$, respectively. With these notations, we have that

$$H_{n+1}^+ = \widetilde{H}_n^+ \,+\, W_{n+1}^n \,+\, E_{n+1}^n\,, \tag{IV.39}$$

where

$$\begin{aligned} W_{n+1}^n \;&:=\; (\vec{v}_{n+1})^2 \,-\, (\vec{v}_n)^2 && \text{(IV.40)} \\ &=\; 2\,a^*(\vec{G}_{n+1}^n)\cdot\vec{v}_n \,+\, 2\,\vec{v}_n\cdot a(\vec{G}_{n+1}^n) \,+\, \Big(a^*(\vec{G}_{n+1}^n) + a(\vec{G}_{n+1}^n)\Big)^2 \\ &=\; 2\,a^*(\vec{G}_{n+1}^n)\cdot\vec{v}_n \,+\, 2\,\vec{v}_n\cdot a(\vec{G}_{n+1}^n) \,+\, a^*(\vec{G}_{n+1}^n)\cdot a^*(\vec{G}_{n+1}^n) \\ &\quad\;+\, a(\vec{G}_{n+1}^n)\cdot a(\vec{G}_{n+1}^n) \,+\, 2\,a^*(\vec{G}_{n+1}^n)\cdot a(\vec{G}_{n+1}^n) \,+\, \Big\|\vec{G}_{n+1}^n\Big\|^2\,, \end{aligned}$$

with $\left\|\vec{G}^n_{n+1}\right\|^2 := \int |\vec{G}^n_{n+1}(k)|^2\, dk$. In Eq. (IV.39), we make use of the Coulomb gauge condition $\vec{\nabla} \cdot \vec{A}(x) = 0$, which implies that

$$a^*(\vec{G}^n_{n+1}) \cdot \vec{v}_n \;=\; \vec{v}_n \cdot a^*(\vec{G}^n_{n+1}) \quad \text{and} \quad a(\vec{G}^n_{n+1}) \cdot \vec{v}_n \;=\; \vec{v}_n \cdot a(\vec{G}^n_{n+1})\,. \tag{IV.41}$$

IV.2.2 Preliminary results and outline of strategy

Here we describe some results derived in [1], concerning the construction of the groundstate of H, that will be used again and again in the re-expansion procedure. A key ingredient used in our construction of the groundstate of H is the simple identity

$$2\,\vec{v} \;=\; i\,[H\,,\,\vec{x}], \tag{IV.42}$$

which implies that the interaction term in H, which is *marginal* in the *infrared* region (in the sense of power counting), is actually *infrared-irrelevant* on the subspace of all those states where the electron is bound to the nucleus.

Proposition IV.2. *Assume Hypothesis 1. Then there exist constants* $0 < C' \leq C$, $C \geq 4$ *such that, for all* $\alpha < \frac{1}{2C}$, E_n *is an eigenvalue of multiplicity one. Moreover*

$$\inf\Big[\sigma(H^+_n) \setminus \{0\}\Big] \;=:\; \mathrm{gap}_n \;\geq\; [1 - \frac{3}{4}C\alpha]\,\sigma_n\,, \tag{IV.43}$$

$$\inf\Big[\sigma(\widetilde{H}^+_n) \setminus \{0\}\Big] \;=:\; \widetilde{\mathrm{gap}}_n \;=\; \sigma_{n+1}\,, \tag{IV.44}$$

and

$$\sup_{z\in\Gamma_{n+1}} \Big\| \Big(\frac{1}{\widetilde{H}^+_n - z}\Big)^{1/2} \Big(-W^n_{n+1}\Big) \Big(\frac{1}{\widetilde{H}^+_n - z}\Big)^{1/2} \Big\| \;\leq\; C\,\alpha\,, \tag{IV.45}$$

where $\Gamma_{n+1} := \{\frac{1}{4}\sigma_{n+1}e^{i\vartheta} \in \mathbb{C} | \vartheta \in [0, 2\pi)\}$. *The spectral projections* $\widetilde{P}_n := |\widetilde{\phi}_n\rangle\langle\widetilde{\phi}_n\|$ *and* $P_{n+1} := |\phi_{n+1}\rangle\langle\phi_{n+1}|$, *where* $\widetilde{\phi}_n$ *and* ϕ_{n+1} *are groundstates of* $\widetilde{H}_n$ *and* H_{n+1}, *respectively, correspond to*

$$\widetilde{P}_n \;=\; \frac{-1}{2\pi i}\int_{\Gamma_{n+1}} \frac{dz_{n+1}}{\widetilde{H}^+_n - z_{n+1}}\,, \tag{IV.46}$$

and

$$P_{n+1} \;=\; \frac{-1}{2\pi i}\int_{\Gamma_{n+1}} \frac{dz_{n+1}}{H_{n+1} - E_{n+1} - z_{n+1}}\,, \tag{IV.47}$$

respectively, with $\Gamma_n := \{\frac{1}{4}\sigma_n e^{i\vartheta} \in \mathbb{C} | \vartheta \in [0, 2\pi)\}$. *Their difference has a norm convergent series expansion*

$$P_{n+1} - \widetilde{P}_n \;=\; \frac{-1}{2\pi i}\sum_{\nu=1}^{\infty}\int_{\Gamma_{n+1}} (-1)^\nu\, Y^{(\nu)}_{n+1}(z_{n+1})\, dz_{n+1}\,, \tag{IV.48}$$

where

$$Y_{n+1}^{(\nu)}(z) := \frac{1}{\widetilde{H}_n^+ - z}\Big(W_{n+1}^n \frac{1}{\widetilde{H}_n^+ - z}\Big)^\nu , \tag{IV.49}$$

and

$$\|P_{n+1} - \widetilde{P}_n\| \ \leq \ C' \alpha^{(n+2)/2} . \tag{IV.50}$$

The eigenvalue $E_\infty \equiv E_{gs}$ is non degenerate.

If we are interested in deriving an explicit expression for ϕ_{gs} up to a remainder term of order $o(\alpha^N)$, we may as well consider the vector ϕ_{2N-1}, because

$$\|\phi_{2N-1} - \phi_{gs}\| \leq o(\alpha^N). \tag{IV.51}$$

The bound (IV.51) follows from Proposition IV.2. Up to normalization, the vector ϕ_{2N-1} is given by the product $P_{2N-1}P_{2N-2}\cdots P_1$ of the projections $\{P_{2N-1}, ..., P_1\}$ applied to the groundstate, ϕ_0, of the bare Hamiltonian H_0^+, i.e.

$$\phi_{2N-1} \propto P_{2N-1}\cdot\cdot\cdot P_1\phi_0. \tag{IV.52}$$

For a more precise version of Formula (IV.52) see [2]. From Proposition IV.2, more precisely from estimate (IV.45), we infer that the expansion (IV.48) can be truncated at a finite order in such a way that the remainder term is $o(\alpha^N)$. Thus, the vector

$$P_{2N-1}^T\cdot\cdot\cdot P_1^T\phi_0 \quad , \tag{IV.53}$$

where

$$(P_m)^T := -\frac{1}{2\pi i}\sum_{j=0}^{N}\int_{\Gamma_m} dz_m \frac{1}{\widetilde{H}_{m-1}^+ - z_m}\Big[(-W_m^{m-1})\frac{1}{\widetilde{H}_{m-1}^+ - z_m}\Big]^j, \tag{IV.54}$$

is an approximate expression for ϕ_{gs}, up to a remainder term $o(\alpha^N)$ and up to a normalization factor. The truncation in the definition of P_m^T only depends on N.

From now on, we focus our attention on the analysis of the finitely many resolvents appearing on the right side of (IV.54), for $m = 2N-1$.

Our derivation of explicit finite expressions for the vector (IV.53) relies on three operations to be iterated a finite number of times:

i) The photon creation- and annihilation operators are Wick-ordered, shell by shell;

ii) the identity operator, $\mathbf{1}_n$, in the space $\mathcal{H}_n$ is decomposed into the sum $P_n + P_n^\perp$;

iii) two slightly different, truncated Neumann expansions, which we call $\mathcal{A}$ and $\mathcal{B}$, are used to re-expand the contributions associated with $P_n^{\perp}$ coming from operation ii).

Re-expansion procedure
As a first step, we expand the resolvents

$$\frac{1}{\widetilde{H}^{+}_{2N-2} - z_{2N-1}} \tag{IV.55}$$

appearing in the truncated projection P^{T}_{2N-1} in Expression (IV.53) until only resolvents of the Hamiltonian H^{+}_{2N-3} are left. We then put the expressions obtained in a form that enables us to iterate the operation, until only resolvents of the bare Hamiltonian H_0^{+} are left.
This can be accomplished if we take into account that the operator in Eq. (IV.55) is applied to a vector containing only a finite, N-dependent, but α-independent, number of photons with momenta in the shell $\mathcal{K}^{2N-2}_{2N-1}$, thanks to the truncation in P^{T}_{2N-1}. After Wick-ordering of the photon operators in the shell $\mathcal{K}^{2N-2}_{2N-1}$, the original resolvent (IV.55) is replaced by a finite, N-dependent number of resolvents of the form

$$\frac{1}{H^{+}_{2N-2} - z_{2N-1} + \sum_j |k_j|} \tag{IV.56}$$

applied to a vector in $\mathcal{H}_{2N-2}$, where the sum, $\sum_j |k_j|$, of energies $|k_j|$, $\{k_j : \sigma_{2N-1} \leq |k_j| \leq \sigma_{2N-2}\}$ is finite and depends only on N. The key idea underlying the re-expansion of ϕ_{gs} is to split the operator (IV.56) into two pieces,

$$\frac{1}{H^{+}_{2N-2} - z_{2N-1} + \sum_j |k_j|} P_{2N-2} \quad \text{and} \quad \frac{1}{H^{+}_{2N-2} - z_{2N-1} + \sum_j |k_j|} P^{\perp}_{2N-2}. \tag{IV.57}$$

The first one is proportional to the projection P_{2N-2}, the factor of proportionality being an explicit number. Up to a remainder term of order $o(\alpha^N)$, P_{2N-2} can be expanded by using Eq. (IV.48) and then truncated as in Eq. (IV.54). The second term in (IV.57) is analyzed by using the Neumann expansion below, which we call of type $\mathcal{A}$:

$$\begin{aligned} & P^{\perp}_{2N-2} \frac{1}{\widetilde{H}^{+}_{2N-3} - z_{2N-1} + \sum_j |k_j|} P^{\perp}_{2N-2} \\ + \;& P^{\perp}_{2N-2} \frac{1}{\widetilde{H}^{+}_{2N-3} - z_{2N-1} + \sum_j |k_j|} P^{\perp}_{2N-2} + P^{\perp}_{2N-2} \frac{1}{\widetilde{H}^{+}_{2N-3} - z_{2N-1} + \sum_j |k_j|} P^{\perp}_{2N-2} \times \\ & \times \sum_{j=1}^{\infty} \Big[\Big(- W^{2N-3}_{2N-2} - (E^{2N-3}_{2N-2}) \Big) \frac{1}{\widetilde{H}^{+}_{2N-3} - z_{2N-1} + \sum_j |k_j|} P^{\perp}_{2N-2} \Big]^{j}. \end{aligned} \tag{IV.58}$$

This expansion converges, because the absolute value of the energy shift E^{2N-3}_{2N-2} is very small, namely of order $\mathcal{O}(\alpha^{2N})$; and
the expression

$$\frac{1}{\widetilde{H}^{+}_{2N-3} - z_{2N-1} + \sum_j |k_j|} P^{\perp}_{2N-2} \tag{IV.59}$$

is bounded in norm by σ^{-1}_{2N-2}, because of the orthogonal projection $P^{\perp}_{2N-2}$. The expansion in Eq. (IV.58) yields additional powers of α. It can therefore be truncated at some $N-$dependent order. Finally, $P^{\perp}_{2N-2} = \mathbf{1}_{2N-2} - P_{2N-2}$ has to be expanded and truncated similarly to P_{2N-2}. As a result of the previous operations (decomposition (IV.57), and Neumann expansion $\mathcal{A}$), the resolvent (IV.56) is represented by a polynomial in the following operators:

- the resolvents

$$\frac{1}{\widetilde{H}^{+}_{2N-3} - z_{2N-1} + \sum_j |k_j|} \quad , \quad \frac{1}{\widetilde{H}^{+}_{2N-3} - z_{2N-2}}; \tag{IV.60}$$

- the slice interaction W^{2N-3}_{2N-2};
- and the energy shift E^{2N-3}_{2N-2}.

Returning to the expression (IV.53), we then Wick-order the photon operators corresponding to photon momenta in the shell $\mathcal{K}^{2N-3}_{2N-2}$. This yields finitely many terms, and the resolvents in Eq. (IV.60) are replaced by resolvents of the form

$$\frac{1}{H^{+}_{2N-3} - z_{2N-1} + \sum_j |k_j| + \sum_i |q_i|} \quad , \quad \frac{1}{H^{+}_{2N-3} - z_{2N-2} + \sum_i |q_i|} \tag{IV.61}$$

where the photon momenta q_i all belong to the shell $\mathcal{K}^{2N-3}_{2N-2}$, and the number of terms in the sum $\sum_i |q_i|$ is bounded by an $N-$dependent number, thanks to the truncation in P^{T}_{2N-2}. As before, we decompose the resolvents into two pieces, using the projections P_{2N-3} and $P^{\perp}_{2N-3}$. This yields terms proportional to the projection P_{2N-3}, with an explicit factor of proportionality, and terms of the form

$$\frac{1}{H^{+}_{2N-3} - z_{2N-2} + \sum_i |q_i|} P^{\perp}_{2N-3} \quad , \quad \frac{1}{H^{+}_{2N-3} - z_{2N-1} + \sum_j |k_j| + \sum_i |q_i|} P^{\perp}_{2N-3}. \tag{IV.62}$$

The first term in Eq. (IV.62) is analyzed by using the Neumann expansion of type $\mathcal{A}$, see (IV.58), with $2N-2$ replaced by $2N-3$. The second term in

Eq. (IV.62) is treated by applying the following expansion, which we call of type $\mathcal{B}$:

$$
\begin{aligned}
& P^{\perp}_{2N-3} \frac{1}{\widetilde{H}^{+}_{2N-4} - z_{2N-2} + \sum_i |q_i|} P^{\perp}_{2N-3} && \text{(IV.63)} \\
+ \; & P^{\perp}_{2N-3} \frac{1}{\widetilde{H}^{+}_{2N-4} - z_{2N-2} + \sum_i |q_i|} P^{\perp}_{2N-3} \times \\
& \times \sum_{j=1}^{2N} \Big[\Big(- W^{2N-4}_{2N-3} - E^{2N-4}_{2N-3} \Big) \frac{1}{\widetilde{H}^{+}_{2N-4} - z_{2N-2} + \sum_i |q_i|} P^{\perp}_{2N-3} \\
& \qquad + \Big(z_{2N-2} - z_{2N-1} + \sum_j |k_j| \Big) \frac{1}{\widetilde{H}^{+}_{2N-4} - z_{2N-2} + \sum_i |q_i|} P^{\perp}_{2N-3} \Big]^{j} \\
+ \; & \frac{1}{H^{+}_{2N-3} - z_{2N-1} + \sum_i |q_i|} P^{\perp}_{2N-3} \times && \text{(IV.64)} \\
& \times \Big[\Big(- W^{2N-4}_{2N-3} - E^{2N-4}_{2N-3} \Big) \frac{1}{\widetilde{H}^{+}_{2N-4} - z_{2N-2} + \sum_i |q_i|} P^{\perp}_{2N-3} \\
& \qquad + \Big(z_{2N-2} - z_{2N-1} + \sum_j |k_j| \Big) \frac{1}{\widetilde{H}^{+}_{2N-4} - z_{2N-2} + \sum_i |q_i|} P^{\perp}_{2N-3} \Big]^{N+1}
\end{aligned}
$$

In this truncated expansion, the remainder term (IV.64) is proven to be of order $o(\alpha^N)$ with respect to the original expression in (IV.62). To see this, we use the bounds on the shift of the integration variable, $z_{2N-1} - z_{2N-2}$, and on the sum $\sum_j |k_j|$: Both quantities are of order σ_{2N-2}, the first one by definition of z_{2N-2} and z_{2N-1}, and the second one because of the fact that the number of terms in $\sum_j |k_j|$ is finite and α-independent.
The new features of our expansion of type $\mathcal{B}$, as compared to an expansion of type $\mathcal{A}$, are as follows:
The replacement of the integration variable z_{2N-1} by the variable z_{2N-2} is possible because of Estimate (IV.44) on the spectral gap: One then expands in the energies $|k_j|$, which are bounded by $const \cdot \sigma_{2N-2}$.
The norm of the remaining resolvents is bounded by $const \cdot \sigma^{-1}_{2N-3}$. Finally we truncate $P^{\perp}_{2N-3}$.
Hence, starting with a resolvent of the form given in Eq. (IV.56), and then performing the operations just described we end up with a polynomial in the following operators:
* Resolvents,

$$
\frac{1}{\widetilde{H}^{+}_{2N-4} - z_{2N-2} + \sum_i |q_i|} \quad , \frac{1}{\widetilde{H}^{+}_{2N-4} - z_{2N-3}} ; \qquad \text{(IV.65)}
$$

* slice interactions W^{2N-4}_{2N-3};

* energy shifts E^{2N-4}_{2N-3}, difference of integration variables, $z_{2N-1} - z_{2N-2}$, and energy sums, $\sum_j |k_j|$.
We proceed by Wick-ordering the photon creation- and annihilation operators in the shell $\mathcal{K}^{2N-4}_{2N-3}$ in every term obtained so far, starting from the vector in Eq. (IV.53), using (IV.54), for $m = 2N - 1$, and then expanding the resolvents as described above. Two types of resolvents result:

$$\frac{1}{H^{+}_{2N-4} - z_{2N-2} + \sum_i |q_i| + \sum_{i'} |q'_{i'}|} \quad , \frac{1}{H^{+}_{2N-4} - z_{2N-3} + \sum_{i'} |q'_{i'}|}; \tag{IV.66}$$

where the new sum, $\sum'_i |q'_{i'}|$, corresponds to photon momenta, $q'_{i'}$, in the shell $\mathcal{K}^{2N-4}_{2N-3}$, and the number of terms is bounded by an N-dependent, but α-independent integer.

After inserting the partition of unity, $\mathbf{1}_{2N-4} = P_{2N-4} + P^{\perp}_{2N-4}$, we arrive at the expressions in (IV.62), but with $2N-3$ replaced by $2N-4$. Thus , our re-expansion procedure, based on truncated Neumann expansions of type $\mathcal{A}$ and $\mathcal{B}$ and on Wick-ordering, can be iterated.
By applying the re-expansion procedure, scale by scale, to all the resolvents appearing in the truncated projections of Expression (IV.53), we eventually end up with an expansion of (IV.53) involving only "bare" resolvents, i.e., resolvents of the form

$$\frac{1}{H^{+}_{0} - z_{2} + \sum_i |q_i| + \sum_{i'} |q'_{i'}|} \quad , \frac{1}{H^{+}_{0} - z_{1} + \sum_{i'} |q'_{i'}|}, \tag{IV.67}$$

with momenta $\{q_i\}$, $\{q'_{i'}\}$ belonging to the shells $\mathcal{K}^1_2$ and $\mathcal{K}^0_1$, respectively.

The arguments described above represent the essential ingredients in the re-expansion procedure developed in [2], where the mathematical details are presented.

The main difficulty in the inductive proof of convergence of the re-expansion procedure is related to determining the energy shifts E^n_m more explicitly. In re-expanding ϕ_{2N-1}, all the energy shifts up to scale $2N - 1$ appear in our formulas. The energy shifts can be expressed in terms of the groundstate vectors on scales up to $2N - 2$. Explicit expressions for the energy shifts E^n_m are obtained from the re-expansions of $\{\phi_i | i = 1, ..., 2N-2\}$, up to remainder terms of $o(\alpha^N)$. The result of the re-expansion of the groundstate and the groundstate energy presented in [2] is:
For $\alpha \leq \bar{\alpha}$, with $\bar{\alpha} \equiv \bar{\alpha}_N$ small enough, the groundstate energy $E_{\mathrm{gs}} \equiv E_{\mathrm{gs}}(\alpha)$

and the groundstate $\phi_{\rm gs} \equiv \phi_{\rm gs}(\alpha^{\frac{1}{2}})$ *have expansions of the form*

$$E_{\rm gs}(\alpha) \;=\; E_0 + \sum_{\ell=3}^{N} \varepsilon_\ell\,(\alpha)\,\alpha^\ell \;+\; o(\alpha^N) \tag{IV.68}$$

$$\phi_{\rm gs}(\alpha^{\frac{1}{2}}) \;=\; \phi_0 + \sum_{\ell=3}^{2N} \varphi_\ell(\alpha)\,\alpha^{\ell/2} \;+\; o(\alpha^N) \tag{IV.69}$$

with

$$\lim_{\alpha\to 0} \alpha^\delta |\varepsilon_\ell\,(\alpha)| = 0 \qquad\qquad \forall \delta > 0, \tag{IV.70}$$

and

$$\lim_{\alpha\to 0} \alpha^\delta \|\varphi_\ell\,(\alpha)\| = 0 \qquad\qquad \forall \delta > 0, \tag{IV.71}$$

for arbitrary $N = 1, 2, 3, \dots$ *The coefficients* $\varepsilon_\ell(\alpha)$ *and* $\varphi_\ell(\alpha)$ *are computable in terms of finitely many convergent integrals, for any* $3 \leq \ell < \infty$.
Eqs. (IV.72),(IV.73) account for the possible appearance of powers of $\ln[1/\alpha]$ ("infrared logarithms"). We expect that infrared logarithms are not an artefact of our algorithm, but are an expression of infrared divergences in naive perturbation theory: The quantities $E_{\rm gs}(\alpha)$ and $\phi_{\rm gs}(\alpha^{\frac{1}{2}})$ are not analytic, nor even smooth, at $\alpha = 0$; rather, derivatives in $\alpha^{\frac{1}{2}}$ of sufficiently high order of these quantities diverge, as $\alpha \to 0$.

By combining the expansion of the modified *reduction formulae* developed in Section IV.1 with Expressions (IV.68) and (IV.69), Expansion (I.20) for the S-matrix elements of Rayleigh scattering is established.

V Bohr's frequency condition

In this last section, we explicitly compute the scattering amplitude in Eq. (III.9) to leading order in α.

In Section III, Eq. (III.13), we have derived that

$$i\langle \vec{A}^{out}[-\bar{\vec{f}}]\vec{A}^{in}[\vec{h}]\rangle_{\phi_{gs}} - i(f,h) =: (f, Th) \tag{V.1}$$

corresponds to

$$-i\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int\int \overline{f_t(\vec{z})}\langle \mathcal{T}(\vec{J}^{tr}(\vec{z},t)\vec{J}^{tr}(\vec{y},s))\rangle_{\phi_{gs}}\vec{h}_s(\vec{y})d^3y d^3z ds dt \tag{V.2}$$

$$-\int_{-\infty}^{+\infty}\langle[\vec{A}[-\bar{\vec{f}}_s, s], \vec{J}^{tr}[\vec{h}_s, s]]\rangle_{\phi_{gs}} ds \tag{V.3}$$

where we have used the standard definition for T, the T-matrix operator. The leading order term is of order α^3 and arises from the expression in Eq. (V.2).

In fact, due to one power of α multiplying the electron position operator, $\vec{x}$, in the transverse current, the term in Eq. (V.3) is of order α^4. In computing the leading term, we first rewrite the integrand in Expression (V.2) as

$$\begin{aligned} & e^{iE_{gs}(t-s)}\overline{\vec{f}_t(\vec{z})}\langle \vec{J}^{tr}(\vec{z},0)e^{-iH(t-s)}\vec{J}^{tr}(\vec{y},0)\rangle_{\phi_{gs}}\theta(t-s)\vec{h}_s(\vec{y}) && \text{(V.4)} \\ + \quad & e^{iE_{gs}(s-t)}\overline{\vec{f}_t(\vec{z})}\langle \vec{J}^{tr}(\vec{y},0)e^{-iH(s-t)}\vec{J}^{tr}(\vec{z},0)\rangle_{\phi_{gs}}\theta(s-t)\vec{h}_s(\vec{y}). && \text{(V.5)} \end{aligned}$$

Then we approximate $\vec{J}^{tr}(\vec{y},0)$ by

$$-\frac{\alpha^{3/2}}{(2\pi)^{3/2}}\sum_{\lambda=\pm}\int(\vec{p}\cdot\vec{\varepsilon}(\vec{k},\lambda)^*)\vec{\varepsilon}(\vec{k},\lambda)\Lambda(|k|)e^{-i\vec{k}\cdot\vec{y}}d^3k + h.c., \qquad \text{(V.6)}$$

where $\vec{p} := -i\nabla_{\vec{x}}$, and we approximate ϕ_{gs} by $\varphi_{el}\otimes\Omega$, φ_{el} being the ground state of the Coulomb system alone with corresponding Hamiltonian

$$H_{el} \ := -\Delta_{\vec{x}} - V(x). \qquad \text{(V.7)}$$

Finally, we replace the propagator $e^{-iH(t-s)}$ by $e^{-iH_0(t-s)}$, and we rewrite the identity operator between the two currents as a sum of projections onto eigenstates (and generalized eigenstates) of the Hamiltonian H_{el} tensor the vacuum state Ω. To compute the contribution of order α^3 to the transition amplitudes corresponding to an intermediate eigenstate ψ_n of the Hamiltonian H_{el}, we first analyze the contribution of the term in Eq. (V.4) to order α^3, by using the identity $\vec{p} = \frac{i}{2}[H_{el},\vec{x}]$:

$$\begin{aligned} -i\int_{-\infty}^{+\infty}ds\int_{-\infty}^{+\infty}dt\int\int(\Delta_n\mathcal{E})^2\sum_{\lambda,\lambda'}(\psi_0,\vec{x}\cdot\vec{\varepsilon}(\vec{k},\lambda)\psi_n)(\psi_n,\vec{x}\cdot\vec{\varepsilon}(\vec{q},\lambda')^*\psi_0)\ \times & \text{(V.8)} \\ \times e^{-i(\mathcal{E}_n-\mathcal{E}_0-|\vec{k}|)t}e^{-i(-\mathcal{E}_n+\mathcal{E}_0+|\vec{q}|)s}\theta(t-s)\frac{\overline{\hat{f}^{\lambda(\vec{k})}}}{\sqrt{|\vec{k}|}}\frac{\hat{h}^{\lambda'}(\vec{q})}{\sqrt{|\vec{q}|}}\frac{\Lambda(|k|)\Lambda(|q|)}{8}d^3kd^3q. & \end{aligned}$$

where $\Delta_n\mathcal{E} := \mathcal{E}_n - \mathcal{E}_0$ and $\mathcal{E}_n$ is the energy of the eigenstate ψ_n. Introducing the variable $u := t-s > 0$, the integral in Eq. (V.8) can be written as

$$\begin{aligned} i\int_{-\infty}^{+\infty}dt\int_{0}^{+\infty}du\int\int(\Delta_n\mathcal{E})^2\sum_{\lambda,\lambda'}(\psi_0,\vec{x}\cdot\vec{\varepsilon}(\vec{k},\lambda)\psi_n)(\psi_n,\vec{x}\cdot\vec{\varepsilon}(\vec{q},\lambda')^*\psi_0)\times & \text{(V.9)} \\ \times e^{i(|\vec{k}|-|\vec{q}|)t}e^{i(-\mathcal{E}_n+\mathcal{E}_0+|\vec{q}|)u}\frac{\overline{\hat{f}^{\lambda}(\vec{k})}}{\sqrt{|\vec{k}|}}\frac{\hat{h}^{\lambda'}(\vec{q})}{\sqrt{|\vec{q}|}}\frac{\Lambda(|k|)\Lambda(|q|)}{8}d^3kd^3q. & \end{aligned}$$

We insert regularizing factors $e^{-\epsilon|t|}$, $\epsilon > 0$, and $e^{-\mu|u|}$, $\mu > 0$, and then pass to the limits $\epsilon \to 0$ and $\mu \to 0$ of

$$\begin{aligned} & i\int_{-\infty}^{+\infty} dt \int_0^{+\infty} du \int\int (\Delta_n\mathcal{E})^2 \sum_{\lambda,\lambda'} (\psi_0, \vec{x}\cdot\vec{\varepsilon}(\vec{k},\lambda)\psi_n)(\psi_n,\vec{x}\cdot\vec{\varepsilon}(\vec{q},\lambda')^*\psi_0) \qquad \text{(V.10)} \\ & \times e^{i(|\vec{k}|-|\vec{q}|)t} e^{-\epsilon|t|} e^{i(-\mathcal{E}_n+\mathcal{E}_0+|\vec{q}|)u} e^{-\mu u} \frac{\overline{\hat{f}^\lambda(\vec{k})}}{\sqrt{|\vec{k}|}} \frac{\hat{h}^{\lambda'}(\vec{q})}{\sqrt{|\vec{q}|}} \frac{\Lambda(|k|)\Lambda(|q|)}{8} d^3k d^3q. \end{aligned}$$

An explicit calculation gives

$$\begin{aligned} & lim_{\epsilon\to 0} lim_{\mu\to 0} i\int d^3q \int d^3k (\Delta\mathcal{E}_n)^2 \sum_{\lambda,\lambda'} (\psi_0, \vec{x}\cdot\vec{\varepsilon}(\vec{k},\lambda)\psi_n)(\psi_n,\vec{x}\cdot\vec{\varepsilon}(\vec{q},\lambda')^*\psi_0)\times \qquad \text{(V.11)} \\ & \qquad \times \frac{2\epsilon}{(|\vec{k}|-|\vec{q}|)^2+\epsilon^2} \cdot \frac{i}{\mathcal{E}_0-\mathcal{E}_n+|\vec{q}|+i\mu} \frac{\overline{\hat{f}^\lambda(\vec{k})}}{\sqrt{|\vec{k}|}} \frac{\hat{h}^{\lambda'}(\vec{q})}{\sqrt{|\vec{q}|}} \frac{\Lambda(|k|)\Lambda(|q|)}{8} \\ & = \; i\int\int d^3q d^3k (\Delta_n\mathcal{E})^2 \sum_{\lambda,\lambda'} (\psi_0, \vec{x}\cdot\vec{\varepsilon}(\vec{k},\lambda)\psi_n)(\psi_n,\vec{x}\cdot\vec{\varepsilon}(\vec{q},\lambda')^*\psi_0) \times \qquad \text{(V.12)} \\ & \qquad \times 2\pi^2\delta(|\vec{k}|-|\vec{q}|)\delta(\mathcal{E}_0-\mathcal{E}_n+|\vec{q}|) \frac{\overline{\hat{f}^\lambda(\vec{k})}}{\sqrt{|\vec{k}|}} \frac{\hat{h}^{\lambda'}(\vec{q})}{\sqrt{|\vec{q}|}} \frac{\Lambda(|k|)\Lambda(|q|)}{8} \\ & \qquad -P\int d^3q \frac{1}{\mathcal{E}_0-\mathcal{E}_n+|\vec{q}|} \int d^3k (\Delta_n\mathcal{E})^2 \sum_{\lambda,\lambda'} (\psi_0, \vec{x}\cdot\vec{\varepsilon}(\vec{k},\lambda)\psi_n)(\psi_n,\vec{x}\cdot\vec{\varepsilon}(\vec{q},\lambda')^*\psi_0) \qquad \text{(V.13)} \\ & \qquad \times 2\pi\delta(|\vec{k}|-|\vec{q}|) \frac{\overline{\hat{f}^\lambda(\vec{k})}}{\sqrt{|\vec{k}|}} \frac{\hat{h}^{\lambda'}(\vec{q})}{\sqrt{|\vec{q}|}} \frac{\Lambda(|k|)\Lambda(|q|)}{8} \end{aligned}$$

where P stands for the principal part of $\frac{1}{\mathcal{E}_0-\mathcal{E}_n+|\vec{q}|}$. By similar calculations we see that contribution in Eq. (V.5) gives:

$$\begin{aligned} & i\int\int d^3q d^3k (\Delta_n\mathcal{E})^2 \sum_{\lambda,\lambda'} (\psi_0, \vec{x}\cdot\vec{\varepsilon}(\vec{k},\lambda)\psi_n)(\psi_n,\vec{x}\cdot\vec{\varepsilon}(\vec{q},\lambda')^*\psi_0) \times \qquad \text{(V.14)} \\ & \quad \times 2\pi^2\delta(|\vec{k}|-|\vec{q}|)\delta(-\mathcal{E}_0+\mathcal{E}_n+|\vec{q}|) \frac{\overline{\hat{f}^\lambda(\vec{k})}}{\sqrt{|\vec{k}|}} \frac{\hat{h}^{\lambda'}(\vec{q})}{\sqrt{|\vec{q}|}} \frac{\Lambda(|k|)\Lambda(|q|)}{8} \\ & \quad -\int d^3q \frac{1}{-\mathcal{E}_0+\mathcal{E}_n+|\vec{q}|} \int d^3k (\Delta_n\mathcal{E})^2 \sum_{\lambda,\lambda'} (\psi_0, \vec{x}\cdot\vec{\varepsilon}(\vec{k},\lambda)\psi_n)(\psi_n,\vec{x}\cdot\vec{\varepsilon}(\vec{q},\lambda')^*\psi_0) \qquad \text{(V.15)} \\ & \quad \times 2\pi\delta(|\vec{k}|-|\vec{q}|) \frac{\overline{\hat{f}^\lambda(\vec{k})}}{\sqrt{|\vec{k}|}} \frac{\hat{h}^{\lambda'}(\vec{q})}{\sqrt{|\vec{q}|}} \frac{\Lambda(|k|)\Lambda(|q|)}{8} \qquad \text{(V.16)} \end{aligned}$$

Now we observe that the real part of a (connected) scattering amplitude of the type calculated above, with $f = h$, is different from zero, in leading order, only if the photon wave function does not vanish for photon energies corresponding to a difference, $\mathcal{E}_n - \mathcal{E}_0$, of the energy $\mathcal{E}_n$ of an excited boundstate and the groundstate energy $\mathcal{E}_0$. In fact, it corresponds to Expression (V.12). Assuming the validity of the optical theorem, the total cross section for an incoming photon of wave function f is proportional to the imaginary part of (f, Tf). Therefore, in leading order, the total cross section for an incoming photon of wave function f vanishes if, for any n, $f(\vec{q}) = 0$ when $|\vec{q}| = \mathcal{E}_n - \mathcal{E}_0$. This is Bohr's frequency condition! Since we have assumed that the spectral support, with respect to H, of the initial (and the final) state is strictly below the ionization threshold Σ, transitions corresponding to intermediate states in the continuous spectrum do not contribute to the total cross section to leading order in α.

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