QED effects in scattering processes involving atomic bound states: Radiative recombination

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The standard perturbative expansion of the S matrix cannot generally be used in the treatment of atomic scattering processes, involving atomic bound states, due to the special type of singularity that can appear here. It is demonstrated in the present paper that as a consequence of the optical theorem for free particles the effective Hamiltonian is closely related to the total cross section, a relation that is valid also when bound states are present. This implies that methods designed for structure calculations also can be used in dynamical processes. We have found that the covariant-evolution-operator technique that we have developed for structure calculations is here particularly useful. This is a consequence of the fact that the regular part of this operator (the Green's operator), running over all times, is essentially equal to the effective Hamiltonian and therefore directly related to the scattering cross section. In this paper the procedure is demonstrated for the case of radiative recombination.

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I. INTRODUCTION

There is presently an increasing interest in studying the effects of quantum electrodynamics (QED) on various dynamical processes. At GSI in Darmstadt high-energy collisions, involving highly charged ions, have been intensively studied, particularly the process known as *radiative electron capture*, where a loosely bound electron is being captured by a projectile ion under the emission of a photon [1,2]. A closely related process is *radiative recombination*, where an electron in the continuum is being captured by the target ion also under the emission of a photon.

The standard procedure for treating scattering processes for free particles is the scattering or S matrix. If bound-electron states are involved, however, a certain type of singularity appears in the perturbation expansion, which cannot be handled by the standard S-matrix formulation. These singularities appear when an intermediate bound state is degenerate or quasidegenerate with the initial state, referred to as intermediate model-space states. Several procedures have been developed for dealing with this problem in structure calculations. One procedure is the S matrix in combination with the Sucher energy formula, which contains counterterms to eliminate the singularities [3,4]. Another procedure is the two-times Green's function, developed by Shabaev and co-workers in St Petersburg [5]. A third method is the covariant-evolution-operator (CEO) method, developed by the Gothenburg group [6,7]. The evolution operator can be singular, and eliminating the singularities leads to what is referred to as the *Green's operator*, $\mathcal{G}$, due to its analogy with the Green's function.

The last procedure differs from the previous two in a fundamental way, mainly because it can also yield information about the wave function and not only about energy corrections. This implies that the QED perturbations can be included directly into the expansion of the wave operator. This is of great importance primarily for structure calculations in that QED and many-body perturbations (electron correlation) can be combined in a systematic way.

From the optical theorem for free particles [8] it follows that the diagonal element of the S matrix is proportional to the total scattering cross section. In the present paper it is shown that the total cross section is also proportional to the imaginary part of the effective Hamiltonian—a relation that is valid also when bound states are present. A corresponding relation holds for the transition rate between bound states, which is known to be proportional to the imaginary part of the energy and used, for instance, by Barbiery and Sucher as well as by Sapirstein *et al.* [9,10]. This is the reason why methods originally designed for structure problems (which involve the real part of the effective Hamiltonian) can be used also for dynamical problems. Recently, Shabaev *et al.* have studied the QED corrections to the radiative recombination process, involving a bare nucleus, by applying the two-times Green's function [11,12].

It is the main purpose of the present paper to demonstrate that also the CEO method we have developed is well suited for treating dynamical processes, when bound states are involved. It is shown that the Green's operator, when running over all times, is closely related to the imaginary part of the effective Hamiltonian and can be regarded as a generalization of the S matrix, where all singularities of the perturbative expansion due to intermediate model-space states are eliminated. As a consequence, using the Green's operator leads to a particularly simple and straightforward procedure for this kind of problem. This is demonstrated in detail in the present paper for the process of radiative recombination. The procedure is clearly available also for other dynamical problems, such as the transition rate between bound atomic states, and calculations of this kind are under way.

II. SCATTERING PROCESSES

Our treatment of the scattering process will be based upon the effective Hamiltonian and its relation to the scattering cross section. We shall first derive this relation from the optical theorem for free particles, a relation that holds also when

bound states are present. This procedure will be applied to the case of radiative recombination.

A. Optical theorem

The scattering process for free particles is normally described by means of the S matrix. An important tool in that study is the *optical theorem* (see, for instance, Peskin and Schröder [8, p. 230]), which can be shown as follows. We introduce

$$S = 1 + iT; \quad S^\dagger = 1 - iT^\dagger. \tag{1}$$

Since S is unitary, we have

$$1 = SS^\dagger = 1 + i(T - T^\dagger) + T^\dagger T, \tag{2}$$

or

$$-i(T - T^\dagger) = T^\dagger T. \tag{3}$$

We consider a diagonal element of this equation and insert a complete set of intermediate states on the right-hand side:

$$\begin{aligned} -i\langle p|T - T^\dagger|p\rangle &= \sum_q \langle p|T^\dagger|q\rangle\langle q|T|p\rangle \\ &= \sum_q \langle q|T|p\rangle^*\langle q|T|p\rangle, \end{aligned} \tag{4}$$

which gives

$$2\,\mathrm{Im}\langle p|T|p\rangle = \sum_q \langle q|T|p\rangle^*\langle q|T|p\rangle = \sum_q |\langle q|T|p\rangle|^2. \tag{5}$$

The scattering amplitude τ is related to the S matrix by

$$\langle q|T|p\rangle = 2\pi\delta(E_p - E_q)\,\tau(p \to q), \tag{6}$$

leading to

$$\boxed{2\,\mathrm{Im}\langle p|T|p\rangle = \sum_q |2\pi\delta(E_p - E_q)\tau(p \to q)|^2.} \tag{7}$$

Here, the left-hand side is twice the imaginary part of the forward-scattering amplitude, and the right-hand side is essentially the total cross section. This is the optical theorem for free particles.

The forward-scattering amplitude becomes imaginary when an intermediate state goes on-shell, and Cutkosky [13], [8, p. 236] has given the following rules for applying the optical theorem to a Feynman diagram:

(1) Cut through all diagrams in all possible ways such that the cut propagators can simultaneously be put on shell.

(2) For each cut, replace $1/(p^2 - m^2 + i\eta)$ by $-2\pi i\delta(p^2 - m^2)$ in each propagator and then perform the loop integrals.

(3) Sum the imaginary contributions for all possible cuts.

When bound states are involved, singularities may appear in the perturbative expansion of the S matrix, due to vanishing energy denominators, and the form (7) of the optical theorem is no longer valid. It is shown in the Appendix [Eq. (A33)] that the diagonal element of the forward-scattering amplitude is closely related to the *effective Hamiltonian*

$$PTP = -2\pi\delta(E_{\mathrm{in}} - E_{\mathrm{out}})W, \tag{8}$$

where W is the *effective interaction* $W = H_{\mathrm{eff}} - PH_0P$ and H_{eff} is the effective Hamiltonian. P is the projection operator for the model space, degenerate with the initial state. The optical theorem (7) can then be expressed as

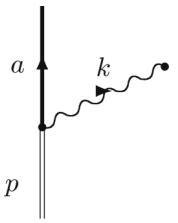

FIG. 1. Lowest-order process in radiative recombination. The solid line represents an electron in a bound state and a thin double line a "quasifree" electron in the continuum, moving in the nuclear potential.

$$\boxed{2\,\mathrm{Im}\langle p| - H_{\mathrm{eff}}|p\rangle = \sum_q 2\pi\delta(E_p - E_q)|\tau(p \to q)|^2,} \tag{9}$$

since the model Hamiltonian H_0 has no imaginary part. This is valid also when bound states are present, but the effective Hamiltonian then has to be evaluated in a different way.

In order to evaluate $2\,\mathrm{Im}(-H_{\mathrm{eff}})$ in the bound-state case, we can essentially use the same Cutkosky rules as before:

(1) Make one cut in all diagrams of the effective Hamiltonian in all possible ways so that the cut state can be degenerate with the initial and final states.

(2) For each cut, replace the singularity $1/(D + i\eta)$ by $-\pi i\delta(D)$.

(3) Sum all imaginary contributions.

There may in this case also be remaining degeneracies, due to the intermediate model-space states, which can be treated in the same way as in structure calculations [6,7].

III. RADIATIVE RECOMBINATION

We shall now apply the CEO and Green's-operator procedure to the process of radiative recombination.[1] In this process we assume that the incoming electron is captured by a naked nucleus (see Fig. 1), which is the process studied experimentally at GSI and theoretically by Shabaev *et al.* [11].

A. Lowest order

In lowest order the forward-scattering amplitude is represented by the Feynman diagram to the left in Fig. 2. The Green's operator is in this case identical to the S matrix and given by means of the Feynman rules for the S matrix ([14], Chap. 7 and [7], Appendix)

$$\begin{aligned} \langle p|S|p\rangle &= \langle p|\mathcal{G}(\infty, -\infty)|p\rangle \\ &= 2\pi\delta(E_{\mathrm{in}} - E_{\mathrm{out}})\langle p|iAi\Gamma iA|p\rangle, \end{aligned} \tag{10}$$

[1]For details concerning the covariant-evolution operator and the Green's operator we refer to the Appendix and to Ref. [7].

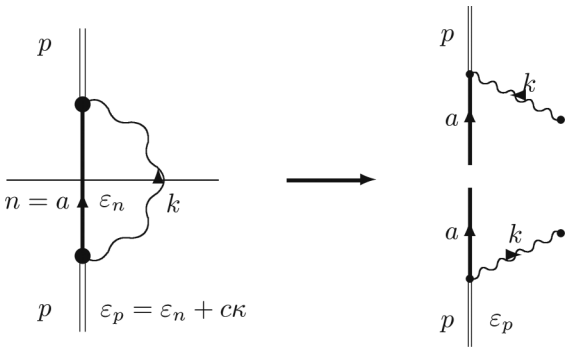

FIG. 2. Applying the optical theorem in lowest order. Left: forward-scattering amplitude. Right: after the cut.

where the photon-field operators are assumed to be contracted. A stands for the photon interaction $A = ec\alpha^{\mu}A_{\mu}$ and

$$\Gamma = \Gamma(\varepsilon_p) = \frac{|n+k\rangle\langle n+k|}{\varepsilon_p - \varepsilon_n - c\kappa + i\eta} \tag{11}$$

is the resolvent. The k vector is $k = (c\kappa, -\mathbf{k})$. A summation or integration over intermediate states is assumed.

Using the relation in the Appendix [Eq. (A32)],

$$PiG(\infty, -\infty)P = 2\pi\delta(E_{\text{in}} - E_{\text{out}})W, \tag{12}$$

we then get

$$\begin{aligned}\langle p| - W|p\rangle &= -\langle p|A\Gamma A|p\rangle \\ &= -\langle p|A\frac{|n+k\rangle\langle n+k|}{\varepsilon_p - \varepsilon_n - c\kappa + i\eta}A|p\rangle.\end{aligned} \tag{13}$$

This has a singularity, when $\varepsilon_p = \varepsilon_n + c\kappa$,

$$W \to \langle p|A\Gamma_P A|p\rangle \tag{14}$$

with $\Gamma_P = P\Gamma$, which lies in a *continuum*, since the photon energy is not fixed. Therefore, the integral leads to a principal integral and half a pole contribution $\mathcal{P} - \pi i\delta(\varepsilon_p - \varepsilon_n - c\kappa)$. Then

$$2\text{Im}\langle p| - H_{\text{eff}}|p\rangle = 2\pi\delta(\varepsilon_p - \varepsilon_a - c\kappa)\langle p|A|q\rangle\langle q|A|p\rangle, \tag{15}$$

since H_0 does not have any imaginary part. $|q\rangle$ stands here for the intermediate *degenerate* state $|a,k\rangle$, where k represents the photon. The renormalization of the self-energy leads to a counter mass term, which, however, does not contribute to the imaginary part.

We have now found an expression that is proportional to the lowest-order scattering cross section. Next we shall consider higher-order contributions.

B. Self-energy insertion on the bound state

We begin the study of higher-order effects by considering the case when there is a self-energy insertion in the bound state. The forward-scattering amplitude is represented by the Feynman diagram in Figs. 3 and 4 (left), and we shall evaluate the effective Hamiltonian (12). The evolution operator, which is singular, is given by

$$\langle p|U|p\rangle = 2\pi\delta(E_{\text{in}} - E_{\text{out}})\,\langle p|iAi\Gamma(-i)\Sigma i\Gamma i A|p\rangle, \tag{16}$$

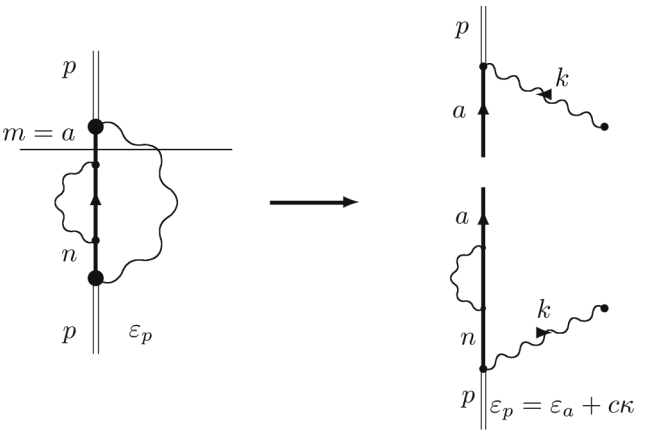

FIG. 3. Self-energy on the bound state—cut at upper state.

where Σ stands for self-energy insertion,

$$\Sigma = \Sigma(\varepsilon_a) = \Sigma(\varepsilon_p - c\kappa). \tag{17}$$

The corresponding part of $\langle p| - H_{\text{eff}}|p\rangle$ is

$$\langle p| - H_{\text{eff}}|p\rangle : \; -\langle p|A\Gamma\,\Sigma\Gamma A|p\rangle. \tag{18}$$

This has a regular part

$$-\langle p|A\Gamma_Q\,\Sigma\Gamma_Q A|p\rangle, \tag{19}$$

where the model-space states are eliminated by the reduced resolvent (A14b). This does not contribute to the scattering cross section, since only the imaginary part of the forward-scattering amplitude does.

The imaginary part of the forward-scattering amplitude is given by the singularities. One singularity can be treated as in first order, leading to

$$\begin{aligned}&-\langle p|A\Gamma_P\Sigma\Gamma A|p\rangle \\ &\quad = -\mathcal{P} + i\pi\delta(\varepsilon_p - \varepsilon_a - c\kappa)\langle p|A|q\rangle\langle q|\Sigma\Gamma A|p\rangle,\end{aligned} \tag{20}$$

$$\begin{aligned}&-\langle p|A\Gamma\Sigma\Gamma_P A|p\rangle \\ &\quad = -\mathcal{P} + i\pi\delta(\varepsilon_p - \varepsilon_a - c\kappa)\langle p|A\Gamma\Sigma|q\rangle\langle q|A|p\rangle,\end{aligned} \tag{21}$$

where $\Gamma_P = P\Gamma$. The photon energy is now *fixed*, and the other singularity lies in a *discrete* environment, and

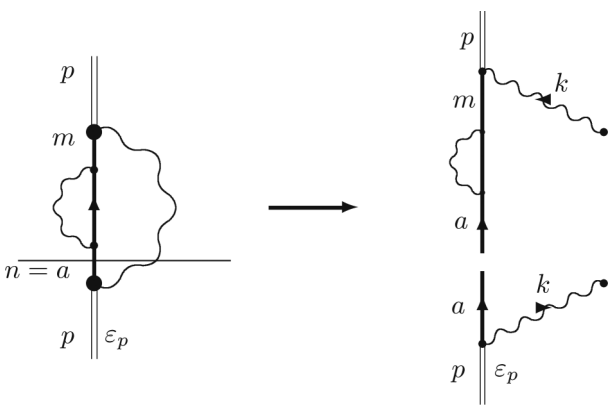

FIG. 4. Self-energy on the bound state—cut at lower state.

therefore leads to a model-space contribution (MSC) (see Appendix),

$$-\langle p|A\Gamma_P\Sigma\Gamma A|p\rangle \to i\pi\delta(\varepsilon_p-\varepsilon_a-c\kappa) \times\langle p|\left(\frac{\delta}{\delta\mathcal{E}}[A|q'\rangle\langle q'|\Sigma(\mathcal{E}-c\kappa)]_{\mathcal{E}=\varepsilon_p}\right) \times|q\rangle\langle q|A|p\rangle, \tag{22}$$

$$-\langle p|A\Gamma\Sigma\Gamma_P A|p\rangle \to i\pi\delta(\varepsilon_p-\varepsilon_a-c\kappa) \times\langle p|\left(\frac{\delta A}{\delta\mathcal{E}}\right)_{\mathcal{E}=\varepsilon_p}|q'\rangle\langle q'|\Sigma|q\rangle\langle q|A|p\rangle, \tag{23}$$

where $q=(n,k)$ and $q'=(m,k)$. The total imaginary part of the effective Hamiltonian (12) then becomes

$$\begin{aligned}2\mathrm{Im}\langle p|-H_{\mathrm{eff}}|p\rangle &= 2\pi\delta(\varepsilon_p-\varepsilon_a-c\kappa)\\ &\times\langle p|\Big(A|q\rangle\langle q|\Sigma\Gamma_Q A+A\Gamma_Q\Sigma|q\rangle\langle q|A\\ &+\frac{\delta}{\delta\mathcal{E}}(A|q\rangle\langle q|\Sigma)_{\mathcal{E}=\varepsilon_p}|q\rangle\langle q|A\\ &+\left(\frac{\delta A}{\delta\mathcal{E}}\right)_{\mathcal{E}=\varepsilon_p}|q\rangle\langle q|\Sigma|q\rangle\langle q|A\Big)|p\rangle.\end{aligned} \tag{24}$$

This is the corresponding contribution to the cross section in the case with a self-energy insertion on the bound-state line.

The terms with the derivative of the photon interaction $ec\alpha^\nu A_\nu$ correspond to the correction of the photon energy due to the modification of the bound-state electron energy, caused by first-order QED corrections, separately added by Shabaev *et al.* [11, Eq. (34)].

C. Vertex correction

Next we consider the contribution to the scattering amplitude, when there is a vertex correction as illustrated in Figs. 5 and 6 (left). The contribution to the forward-scattering

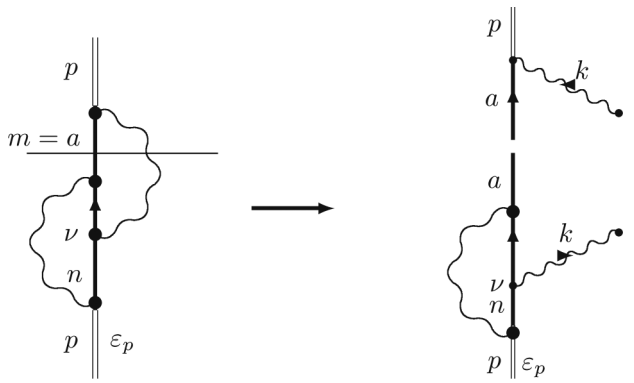

FIG. 5. Scattering with a vertex correction—cut at the upper state.

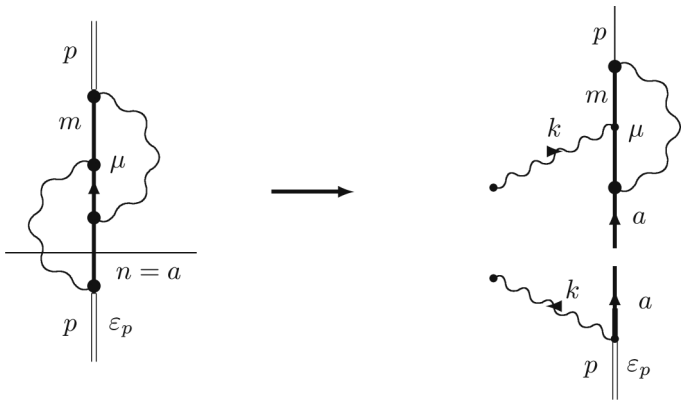

FIG. 6. Scattering with a vertex correction—cut at the lower state.

amplitude is[2]

$$\begin{aligned}&2\pi\delta(E_{\mathrm{in}}-E_{\mathrm{out}})\,\langle p|-iAi\Gamma i\Lambda|p\rangle \quad \text{or}\\ &\times 2\pi\delta(E_{\mathrm{in}}-E_{\mathrm{out}})\,\langle p|-i\Lambda i\Gamma iA|p\rangle\end{aligned} \tag{25}$$

with contractions between the field operators. Λ stands for the vertex-correction interaction $\Lambda=ec\Lambda^\mu A_\mu$. The corresponding part of the effective interaction becomes

$$\langle p|-W|p\rangle=\langle p|\Lambda\Gamma A|p\rangle \quad \text{or} \quad \langle p|A\Gamma\Lambda|p\rangle. \tag{26}$$

One singularity can be eliminated as before, leading to

$$\langle p|\Lambda\Gamma_P A|p\rangle = \mathcal{P}\,-i\pi\delta(\varepsilon_p-\varepsilon_a-c\kappa)\langle p|\Lambda|q\rangle\langle q|A|p\rangle, \tag{27}$$

$$\langle p|A\Gamma_P\Lambda|p\rangle = \mathcal{P}\,-i\pi\delta(\varepsilon_p-\varepsilon_a-c\kappa)\langle p|A|q\rangle\langle q|\Lambda|p\rangle. \tag{28}$$

There are no MSCs in this case. This leads to

$$\begin{aligned}2\,\mathrm{Im}\langle p|-H_{\mathrm{eff}}|p\rangle &= -2\pi\delta(\varepsilon_p-\varepsilon_a-c\kappa)\\ &\times[\langle p|\Lambda|q\rangle\langle q|A|p\rangle+\langle p|A|q\rangle\langle q|\Lambda|p\rangle].\end{aligned} \tag{29}$$

Our result differs in the relative sign from that of Shabaev *et al.*, which might be due to different sign conventions.[2]

D. Self-energy insertion on the free-electron state

When there is a self-energy insertion in the (quasi)free electron state, the forward-scattering amplitude is represented by the Feynman diagram in Fig. 7 (left), corresponding to the evolution operator

$$\langle p|U|p\rangle=2\pi\delta(E_{\mathrm{in}}-E_{\mathrm{out}})\,\langle p|iAi\Gamma iAi\Gamma(-i)\Sigma|p\rangle, \tag{30}$$

where $q=(n,k)$. This leads to

$$\langle p|-W|p\rangle=-\langle p|A\Gamma A\Gamma\Sigma|p\rangle. \tag{31}$$

[2]Sign conventions (see, for instance, Ref. [7]): $\Sigma(\varepsilon_a)=i\int\frac{dz}{2\pi}S_{\mathrm{F}}(\varepsilon_a-z;\boldsymbol{x}_2,\boldsymbol{x}_1)\,I(z;\boldsymbol{x}_2,\boldsymbol{x}_1)$. $\Lambda^\mu(\varepsilon_a,\varepsilon_a)=-i\alpha^\mu\int\frac{dz}{2\pi}S_{\mathrm{F}}(\varepsilon_a-z;\boldsymbol{x}_2,\boldsymbol{x}_3)\,S_{\mathrm{F}}(\varepsilon_a-z;\boldsymbol{x}_3,\boldsymbol{x}_1)\,I(z;\boldsymbol{x}_2,\boldsymbol{x}_1)$. $I(z;\boldsymbol{x}_1,\boldsymbol{x}_2)=e^2c^2\alpha_1^\mu\alpha_2^\nu D_{\mathrm{F}\mu\nu}(z;\boldsymbol{x}_1,\boldsymbol{x}_2)$.

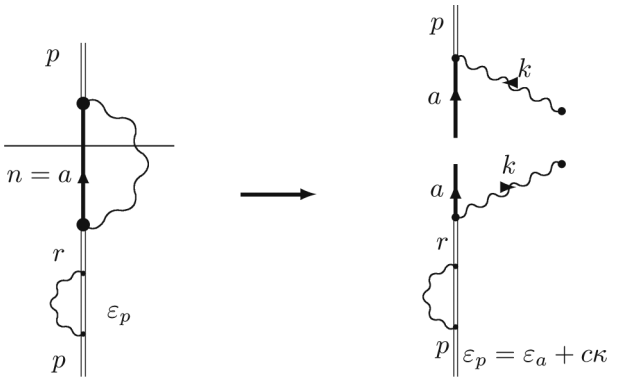

FIG. 7. Scattering with a self-energy correction on the free electron.

A cut at the leftmost singularity leads to

$$-\langle p|A\Gamma_P A\Gamma\Sigma|p\rangle = -\not{P} + i\pi\delta(\varepsilon_p - \varepsilon_a - c\kappa) \times\langle p|A|q\rangle\langle q|A\Gamma\Sigma|p\rangle \tag{32}$$

and

$$\langle p|2\,\mathrm{Im}(-H_{\mathrm{eff}})|p\rangle = 2\pi\delta(\varepsilon_p - \varepsilon_a - c\kappa) \times \langle p|A|q\rangle\langle q|A\Gamma\Sigma|p\rangle. \tag{33}$$

A cut at the singularity of the intermediate electron propagator would not contribute to this process.

There can also be a singularity inside the lower self-energy, which corresponds to the inverted diagram with a self-energy perturbation on the outgoing line. This yields the total contribution

$$\begin{aligned}&\langle p|2\,\mathrm{Im}(-H_{\mathrm{eff}})|p\rangle \\ &= 2\pi\delta(\varepsilon_p - c\kappa - \varepsilon_a) \\ &\quad\times\langle p|A|q\rangle\langle q|A\Gamma\Sigma + \Sigma\Gamma A|q\rangle\langle q|A|p\rangle \\ &= 2\pi\delta(\varepsilon_p - c\kappa - \varepsilon_a)\langle p|A|q\rangle\langle q|\left(A\frac{|r\rangle\langle r|}{\varepsilon_p - \varepsilon_n + i\eta}\Sigma\right. \\ &\quad\left.+\Sigma\frac{|r\rangle\langle r|}{\varepsilon_p - \varepsilon_n + i\eta}A\right)|q\rangle\langle q|A|p\rangle.\end{aligned} \tag{34}$$

Since the states r here form a continuum, the singularity leads to a principal integral and half a pole, of which only the latter contributes to the imaginary part. There is no MSC here.

IV. SCATTERING AMPLITUDE

By summing all contributions of $2\,\mathrm{Im}\langle p| - H_{\mathrm{eff}}|p\rangle$ for this particular process, we have according to (9),

$$2\,\mathrm{Im}\langle p| - H_{\mathrm{eff}}|p\rangle = 2\pi\delta(E_p - E_q)|\tau(p\to q)|^2. \tag{35}$$

All contributions above are of the form

$$2\,\mathrm{Im}\langle p| - H_{\mathrm{eff}}|p\rangle = 2\pi\delta(E_p - E_q)\langle p|\cdots|p\rangle, \tag{36}$$

which leads to the relation

$$\langle p|\cdots|p\rangle = |\tau(p\to q)|^2. \tag{37}$$

In the present case we do not have an explicit expression for the scattering amplitude as in the free case (6). Instead, if we want to have an expression for the amplitude, this has to be extracted from the cross section (37).

From the expressions derived above we have

$$\begin{aligned}|\tau(p\to q)|^2 = \langle p|A|q\rangle\langle q|\Bigg(&A + \Sigma\Gamma_Q A + \left(\frac{\delta\Sigma}{\delta\mathcal{E}}\right)_{\mathcal{E}=\varepsilon_p} \\ &\times|q\rangle\langle q|A - \Lambda + A\frac{|n+k\rangle\langle n+k|}{\varepsilon_p - \varepsilon_n + i\eta}\Sigma\Bigg)|p\rangle \\ &+\langle p|\Bigg(A\Gamma_Q\Sigma + 2\left(\frac{\delta A}{\delta\mathcal{E}}\right)_{\mathcal{E}=\varepsilon_p}|q\rangle\langle q|\Sigma - \Lambda \\ &+\Sigma\frac{|n+k\rangle\langle n+k|}{\varepsilon_p - \varepsilon_n + i\eta}A\Bigg)|q\rangle\langle q|A|p\rangle,\end{aligned} \tag{38}$$

which is of the form

$$|\tau(p\to q)|^2 = \langle p|A|q\rangle\langle q|A + X|p\rangle + \langle p|Y|q\rangle\langle q|A|p\rangle. \tag{39}$$

This leads to the approximate amplitude

$$\tau(p\to q) \approx \langle q|A + \tfrac{1}{2}(X + Y^\dagger)|p\rangle, \tag{40}$$

and

$$\begin{aligned}\tau(p\to q) \approx \langle q|\Bigg(&A + \Sigma\Gamma_Q A + \Sigma|q\rangle\langle q|\left(\frac{\delta A}{\delta\mathcal{E}}\right)_{\mathcal{E}=\varepsilon_p} \\ &+\frac{1}{2}\left(\frac{\delta\Sigma}{\delta\mathcal{E}}\right)_{\mathcal{E}=\varepsilon_p}|q\rangle\langle q|A - \Lambda \\ &+A\frac{|n+k\rangle\langle n+k|}{\varepsilon_p - \varepsilon_n + i\eta}\Sigma\Bigg)|p\rangle.\end{aligned} \tag{41}$$

This agrees with the result of Shabaev *et al.* [11] (apart from sign difference for the vertex part, which might be due to different sign conventions).

The self-energies and vertex corrections that are not affected by the cuts have to be properly renormalized. For the effects affected by the cut the renormalization does not contribute to the imaginary part.

It can be noted that the derivative of the self-energy appears only once in the cross section, which explains the factor of $1/2$ in the amplitude. The derivative of the photon energy, on the other hand, appears twice and hence appears with the factor of unity in the amplitude.

The effect of the vacuum polarization is not included here but can be evaluated in very much the same way, and in doing so, here we also find agreement with the result of Shabaev *et al.*

A new numerical evaluation of the QED effects treated here are presently under way and will be published separately [15].

V. SUMMARY AND CONCLUSIONS

We have here demonstrated that the procedure of the covariant-evolution operator and Green's operator, originally developed for structure calculations, can also be readily applied in dynamical processes involving bound particles. This is here demonstrated particularly for the process of radiative recombination, but the procedure should be applicable also to other dynamical processes. Due to the presence of bound

states in the process, the standard perturbative expansion of the S matrix is not applicable. The results we obtain are in excellent agreement with those obtained by Shabaev *et al.*, using the two-times Green's function, also originally developed for structure calculations. Our procedure is based upon the effective Hamiltonian, which according to the optical theorem is closely related to the scattering cross section.

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APPENDIX: THE COVARIANT-EVOLUTION OPERATOR AND THE GREEN'S OPERATOR

1. S matrix

We shall first consider the S matrix, which relates the final and initial states in a dynamical process

$$\Phi(t=+\infty) = S\,\Phi(t=-\infty) \tag{A1}$$

and is related to the standard evolution operator by

$$S = U(\infty,-\infty). \tag{A2}$$

The S matrix can be expanded as ([14, Eq. 6.23] and [7, Eq. (4.3)])

$$S = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{-i}{c}\right)^n \int dx_1^4 \cdots \int dx_n^4\; T \times [\mathcal{H}(x_1)\cdots\mathcal{H}(x_n)]\, e^{-\gamma(|t_1|+|t_2|\cdots|t_n|)}, \tag{A3}$$

integrated over all space and time. Here, γ is an adiabatic-damping parameter and

$$\mathcal{H}(x) = -\hat{\psi}^\dagger(x) ec\alpha^\mu A_\mu(x)\hat{\psi}(x) \tag{A4}$$

represents the interaction between the electron (charge $-e$) and the electromagnetic field

$$A_\mu(x) = \frac{1}{\sqrt{2\kappa c(2\pi)^3}} \sum_r \epsilon_{\mu r}[a_{kr}e^{-ikx} + a_{kr}^\dagger e^{ikx}], \tag{A5}$$

$k = (c\kappa, -\boldsymbol{k})$ being the covariant k vector, $a_{kr}^\dagger, a_{kr}$ the creation and annihilation operators, and $\epsilon_{\mu r}$ the components of the polarization vector, r representing the polarization direction. $\hat{\psi}(x), \hat{\psi}^\dagger(x)$ represent the electron-field operators.

The energy can be calculated by means of the Sucher formula [4]

$$S = \sum_n S^{(n)}, \tag{A6}$$

$$\Delta E = \lim_{\gamma\to 0} \frac{i\gamma}{2} \frac{\sum n\langle\Phi|S^{(n)}|\Phi\rangle}{\langle\Phi|S|\Phi\rangle}. \tag{A7}$$

This formula eliminates the singularity of the S matrix that appears when there is an intermediate model-space state.

2. Covariant-evolution operator and the Green's operator[3]

The S matrix is relativistically covariant in the sense that all internal integrations run over all times. This is not the case for the standard evolution operator for finite initial and final times. This can be modified, though, in such way that it becomes covariant in this sense for all times, leading to what we refer to as the CEO. In the single-particle case it can be defined

$$U(t,t_0) = \iint d^3\boldsymbol{x}\, d^3\boldsymbol{x}_0\, \hat{\psi}^\dagger(x) \times \langle 0_{\rm H}|T[\hat{\psi}_{\rm H}(x)\hat{\psi}_{\rm H}^\dagger(x_0)]|0_{\rm H}\rangle\, \hat{\psi}(x_0), \tag{A8}$$

using the *Heisenberg representation* and T being the *Wick time-ordering* operator. The vacuum expectation value appearing here is the same as in the definition of the Green's function.

In the *interaction representation* this leads to the perturbation expansion

$$U(t,t_0) = \sum_{n=0}^{\infty} \frac{1}{n!} \iint d^3\boldsymbol{x}\, d^3\boldsymbol{x}_0 \left(\frac{-i}{c}\right)^n \int d^4x_1 \cdots \int d^4x_n \times \hat{\psi}^\dagger(x)\, T[\hat{\psi}(x)\,\mathcal{H}(x_1)\cdots\mathcal{H}(x_n)\,\hat{\psi}^\dagger(x_0)] \times \hat{\psi}(x_0) e^{-\gamma(|t_1|+|t_2|\cdots)}, \tag{A9}$$

where γ is the adiabatic damping parameter. The operators are connected to form a one-body operator. In second order this becomes (leaving out the damping factor)

$$U^{(2)}(t,t_0) = \iint d^3\boldsymbol{x}\, d^3\boldsymbol{x}_0\, \hat{\psi}^\dagger(x) i S_{\rm F}(x,x_4)(-i)V(x_4,x_3) \times i S_{\rm F}(x_3,x_2)(-i)V(x_2,x_1) i S_{\rm F}(x_1,x_0)\hat{\psi}(x_0), \tag{A10}$$

where V is the perturbation. The factor of $1/2$ is eliminated, if we consider only one of the two permutations of the perturbations.

If we let $t_0 \to -\infty$, then

$$\int d^3\boldsymbol{x}_0 i S_{\rm F}(x_1,x_0)\hat{\psi}(x) \to \hat{\psi}(x_1), \tag{A11}$$

and this reduces to

$$U^{(2)}(t,-\infty) = \int d^3\boldsymbol{x}\, \hat{\psi}^\dagger(x) S_{\rm F}(x,x_4) \times V(x_4,x_3) S_{\rm F}(x_3,x_2) V(x_2,x_1)\hat{\psi}(x_1). \tag{A12}$$

This process is closely related to the Lehmann-Symanzik-Zimmermann reduction procedure ([16], Sec. 16.7 and [8], Sec. 7.2) where an electron propagator is removed from the vacuum expectation value (A8).

After Fourier transforming the operators, this can be expressed as

$$U^{(2)}(t,-\infty)P_{\mathcal{E}} = e^{-it(\mathcal{E}-H_0)}\Gamma(\mathcal{E})V(\mathcal{E})\Gamma(\mathcal{E})V(\mathcal{E})P_{\mathcal{E}}, \tag{A13}$$

[3] See further Refs. [6,7], Chap. 6.

where $P_{\mathcal{E}}$ is the projection operator for a part of the model space of energy $\mathcal{E}$ and

$$S_{\rm F}(\mathcal{E}) = \Gamma(\mathcal{E}) = \frac{1}{\mathcal{E} - H_0} \tag{A14a}$$

is the *resolvent operator*. Later we shall also need the *reduced resolvent operator*

$$\Gamma_Q(\mathcal{E}) = \frac{Q}{\mathcal{E} - H_0}, \tag{A14b}$$

where $Q = 1 - P$ is the projection operator for the space outside the model space. H_0 is the zeroth-order or model Hamiltonian that generates the zeroth-order or model functions.

A general single-particle evolution operator can be expressed as

$$U^{(n)}(t,-\infty)P_{\mathcal{E}} = e^{-it(\mathcal{E}-H_0)}\Gamma(\mathcal{E})V(\mathcal{E}) \times \Gamma(\mathcal{E})V(\mathcal{E})\Gamma(\mathcal{E})V(\mathcal{E})\cdots P_{\mathcal{E}}. \tag{A15}$$

This becomes (quasi)singular, when an intermediate or final state is (quasi)degenerate with the initial state. In order to remedy that we introduce the *Green's operator*, defined by the relation

$$U(t,-\infty)P = \mathcal{G}(t,-\infty)\circ PU(0,-\infty)P, \tag{A16}$$

where "$\circ$" indicates that the Green's operator acts on the *intermediate* model-space state. The Green's operator can be shown to be *regular*.

We apply the definition (A16) to the operator (A15) (with simplified notations):

$$U^{(n)}(\mathcal{E})P_{\mathcal{E}} = \mathcal{G}^{(n)}(\mathcal{E})P_{\mathcal{E}} + \mathcal{G}^{(n-1)}(\mathcal{E}')P_{\mathcal{E}'}U^{(1)}(\mathcal{E})P_{\mathcal{E}} + \mathcal{G}^{(n-2)}(\mathcal{E}')P_{\mathcal{E}'}U^{(2)}(\mathcal{E})P_{\mathcal{E}} + \cdots, \tag{A17}$$

noting that $U^{(0)}(0) = 1$. Solving for $\mathcal{G}^{(n)}$, we have

$$\mathcal{G}^{(n)}(\mathcal{E})P_{\mathcal{E}} = U^{(n)}(\mathcal{E})P_{\mathcal{E}} - \mathcal{G}^{(n-1)}(\mathcal{E}')P_{\mathcal{E}'}U^{(1)}(\mathcal{E})P_{\mathcal{E}} - \mathcal{G}^{(n-2)}(\mathcal{E}')P_{\mathcal{E}'}U^{(n-2)}(\mathcal{E})P_{\mathcal{E}} - \cdots. \tag{A18}$$

The negative terms are known as *counterterms* and have the effect of removing the (quasi)singularities.

Suppose the evolution operator is a combination of two lower-order evolution operators

$$U(\mathcal{E})P_{\mathcal{E}} = U_2(\mathcal{E})(P_{\mathcal{E}'} + Q)U_1(\mathcal{E}) \tag{A19}$$

with a possible intermediate model-space state of energy $\mathcal{E}'$, which could lead to a (quasi)singularity. We can express this as

$$U(\mathcal{E})P_{\mathcal{E}} = U_2(\mathcal{E})QU_1(\mathcal{E})P_{\mathcal{E}} + U_2(\mathcal{E})\Gamma_P(\mathcal{E}')W_1(\mathcal{E})P_{\mathcal{E}}, \tag{A20}$$

where

$$\Gamma_P(\mathcal{E}') = \frac{P_{\mathcal{E}'}}{\mathcal{E} - \mathcal{E}'}, \quad \Gamma(\mathcal{E}')W_1 = U_1. \tag{A21}$$

Then there will be a counter term

$$-U_2(\mathcal{E}')\Gamma(\mathcal{E}')W_1(\mathcal{E})P_{\mathcal{E}}, \tag{A22}$$

where we note the energy parameter $\mathcal{E}'$ in U_2. This leads to a "*model-space contribution*"

$$\frac{\delta U_2}{\delta \mathcal{E}}P_{\mathcal{E}'}W_1P_{\mathcal{E}} \tag{A23}$$

and the Green's operator, corresponding to the evolution operator (A19),

$$\mathcal{G}(\mathcal{E}) = U_2(\mathcal{E})\Gamma_Q W_1(\mathcal{E})P_{\mathcal{E}} + \frac{\delta U_2}{\delta \mathcal{E}}P_{\mathcal{E}'}W_1P_{\mathcal{E}}. \tag{A24}$$

Here, the model-space contribution has eliminated the singularity due to the *intermediate* model-space state. In addition, there might be other singularities, which can be handled similarly.

The operator [7, Chap. 6]

$$\mathcal{R} = \left(i\frac{\partial \mathcal{G}(t,-\infty)}{\partial t}\right)_{t=0} \tag{A25}$$

is known as the *reaction operator* and closely related to the *effective interaction*

$$W = P\mathcal{R}P = P\left(i\frac{\partial \mathcal{G}(t,-\infty)}{\partial t}\right)_{t=0}P, \tag{A26}$$

and the *effective Hamiltonian*

$$H_{\rm eff} = W + PH_0P; \quad (H = H_0 + V). \tag{A27}$$

The Green's operator has the same time dependence as the evolution operator (A13), and applying the formula (A25) to a Green's operator then eliminates the denominator of the resolvent (A14a). Therefore, the Green's operator (A24) yields

$$W = PW_2(\mathcal{E})\Gamma_Q W_1(\mathcal{E})P_{\mathcal{E}} + P\frac{\delta W_2}{\delta \mathcal{E}}P_{\mathcal{E}'}W_1P_{\mathcal{E}}. \tag{A28}$$

This is the corresponding effective interaction, and the last term is the MSC.

The Green's operator at finite final times for a single-particle system can generally be written in the form

$$\begin{aligned}\mathcal{G}(t,-\infty) &= \int d^3\boldsymbol{x}\int d^4x_1\,\hat{\psi}^\dagger(x)S_{\rm F}(x,x_1)\mathcal{F}\hat{\psi}(x_1)\\ &= c_m^\dagger\langle m|\int\frac{d\omega}{2\pi}\,S_{\rm F}(\omega,\boldsymbol{x},\boldsymbol{x}_1)\mathcal{F}|n\rangle \times c_n e^{-it(\omega-\varepsilon_m)}e^{-it_1(\varepsilon_n-\omega)},\end{aligned} \tag{A29}$$

where $c_n, c_m^\dagger$ are electron creation and annihilation operators. We shall demonstrate below that the operator $\mathcal{F}$ is identical to the reaction operator $\mathcal{R}$ (A25).

Integration over t_1 and ω gives $\omega = \varepsilon_n$,

$$\begin{aligned}\mathcal{G}(t,-\infty) &= e^{-it(\varepsilon_n-\varepsilon_m)}c_m^\dagger\langle m|S_{\rm F}(\varepsilon_n)\mathcal{F}|n\rangle c_n\\ &= e^{-it(\varepsilon_n-H_0)}S_{\rm F}(\varepsilon_n)\mathcal{F}.\end{aligned}$$

If we operate on a space $P_{\mathcal{E}}$ with energy $\mathcal{E}$, then $\varepsilon_n = \mathcal{E}$,

$$\mathcal{G}(t,-\infty)P_{\mathcal{E}} = e^{-it(\mathcal{E}-H_0)}S_{\rm F}(\mathcal{E})\mathcal{F}P_{\mathcal{E}}.$$

If we here take the derivative with respect to t at $t = 0$, using (A14a), we find from the definition (A25) that the unknown operator $\mathcal{F}$ in (A29) is the reaction operator $\mathcal{R}$.

If we let $t \to \infty$, then

$$\begin{aligned}i\mathcal{G}(\infty,-\infty) &= \int d^4x\,\hat{\psi}^\dagger(x_1)\mathcal{R}\hat{\psi}(x_1)e^{-\gamma|t_1|}\\ &= \int dt_1\,c_m^\dagger\langle m|\mathcal{R}|n\rangle c_n e^{-it_1(\varepsilon_n-\varepsilon_m)}e^{-\gamma|t_1|}.\end{aligned} \tag{A30}$$

Integration over t_1 gives[4]

$$i\mathcal{G}(\infty,-\infty)P = 2\pi\,\Delta_\gamma(E_{\rm in}-E_{\rm out})\mathcal{R}P \rightarrow 2\pi\,\delta(E_{\rm in}-E_{\rm out})\mathcal{R}P \quad \text{(A31)}$$

[4]where the delta factor is given by

$$\Delta_\gamma(a) = \tfrac{1}{2\pi}\int_{-\infty}^{\infty} dt\, e^{-iat}e^{-\gamma|t|} = \tfrac{1}{\pi}\tfrac{\gamma}{a^2+\gamma^2} \rightarrow \delta(a) \quad \text{as} \quad \gamma\rightarrow 0.$$

and the effective interaction

$$\boxed{Pi\mathcal{G}(\infty,-\infty)P = 2\pi\,\delta(E_{\rm in}-E_{\rm out})W.} \quad \text{(A32)}$$

In the free-electron case there are no intermediate model-space states, and the Green's operator $\mathcal{G}(\infty,-\infty)$ is identical to the S matrix, which leads to the corresponding relation

$$PiSP = 2\pi\,\delta(E_{\rm in}-E_{\rm out})W. \quad \text{(A33)}$$

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