Inclusion of radiation damping in the close-coupling equations for electron-atom scattering

F. Robicheaux, T. W. Gorczyca, and M. S. Pindzola
Department of Physics, Auburn University, Auburn, Alabama 36849

N. R. Badnell
Department of Physics and Applied Physics, University of Strathclyde, Glasgow G4 0NG, United Kingdom
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The close-coupling approximation for electron-atom scattering is extended to include the effect of one-photon radiation damping at a level nonperturbative in the wave function. The complex potential is derived and introduced directly into the set of integro-differential equations used to calculate the S matrix. The formulation is ideal for inelastic scattering and photoionization with radiation damping and can be used to calculate photorecombination cross sections. The numerical solution of the resulting differential equation is accomplished through a combination of R-matrix, perturbation theory, and analytic techniques. Some of the implications of this method are discussed. The connections to previous theoretical approaches are discussed.

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I. INTRODUCTION

The effect of radiation damping on atomic dynamics has both a practical and a theoretical interest for atomic, plasma, and astrophysical [1] situations. The most difficult situation to describe theoretically occurs when a scattering electron is temporarily captured into a resonance state; the competition between autoionization and radiative decay as well as possible interference between indistinguishable paths should be accurately described. Most of the calculations that include radiation damping are based on the independent processes isolated resonance approximation and second-order perturbation theory [2]. In these calculations, all interference effects (interference or interaction between resonances, interference between resonances and continua, etc.) are ignored, which means radiation damping of autoionizing states contributes additional width to resonances and causes a rechanneling of flux from electron scattering channels to photon emission channels. Methods that sum probabilities work fairly well for total photorecombination cross sections but can have radical failures for photoionization, electron impact excitation, or partial dielectronic recombination cross sections even for highly charged systems. Photorecombination is the capture of an electron by an atom or an ion with the simultaneous emission of a photon. The more sophisticated theories of radiation damping [3–6] have not been utilized extensively because of the difficulty in constructing general computer programs based on these methods. Methods that are based on the application of detailed balance to photoionization cross sections [7] will only be accurate for near-neutral systems because radiation damping effects are much smaller than electrostatic effects.

The general status of radiation damping in atoms has prompted us to develop an approach that includes nonperturbative, radiative damping effects in the wave function in a form that could be computationally efficient [8]. A basic step of the method is the identification of the nonlocal radiation damping potential (to lowest order in the coupling to the radiation field) without reference to any representation of the wave function. The effect of the different types of final decay states can be examined in detail and different styles of computational tools can be exploited as necessary. We have modified existing R-matrix programs to include the effect of all types of radiation damping on the atomic dynamics. Test runs on multielectron systems have required roughly the same amount of computer time with radiation damping as the unmodified codes take with no damping. The modifications should allow the trivial inclusion of radiation damping into calculated atomic parameters.

In this paper, we focus on the derivation of the radiation damping potential and the general implications of this potential for the atomic part of the wave functions. As with all previous methods for treating the effect of radiation damping on the wave function [3–6], we use the pole approximation to obtain finite results for the radiation damping potential (i.e., only the effects of real one-photon emission are included while virtual photon emission and absorption are ignored). This potential describes one-photon damping but does not include quantum optics or Lamb shift terms. This approximation becomes increasingly problematic at higher residual charge due to the rapid increase of the Lamb shift and other virtual photon effects. The effects of radiation damping on the wave function are included in three different ways: (i) the change in the Hamiltonian due to type-I transitions (i.e., radiative decay of the core state) is included analytically by changing the core energy from $E_c \rightarrow E_c - i\Gamma_c/2$, where Γ_c is the total radiative decay rate; (ii) the change in the wave function due to type-IIS transitions (see Sec. VI) is included through a numerical procedure (the R-matrix method); and (iii) the type-

IIL transitions (see Sec. VI) are included perturbatively in unphysical wave functions (unphysical wave functions are solutions of the Schrödinger or Dirac equation that do not have the correct boundary conditions at $r \to 0$ or $r \to \infty$); the physical wave functions are constructed from a linear superposition of the unphysical solutions [9] and include nonperturbative effects.

The main goal of this paper is to describe the implications of the current method and the numerical methods that are needed to calculate the solutions of the atomic Hamiltonian with the radiation damping potential. In future papers, we will explore the effects of radiation damping on specific atomic systems, especially those related to electron scattering experiments.

We have endeavored to keep the description of the physics of this paper self-contained. We feel that there are several aspects of this work that deserve attention. The derivation of the radiation damping potential without reference to any particular representation is the base upon which the rest of the paper is constructed; opportunistic exploitation of different representations allows the compact description of many different types of radiation damping. We have derived a simple approximate expression for the photorecombination probability near one resonance embedded in one electron continuum with many possible final states for radiative capture; our simple expression is a very good approximation to more exact and complicated expressions derived by others. We have found that the effect of radiative decay of a core state on a Rydberg electron should be incorporated by replacing the core state energy E_c in the close-coupling equation for the Rydberg electron with $E_c - i\Gamma_c/2$, where Γ_c is the total radiative decay rate; this replacement contradicts the accepted method for describing radiative decay of core states. We have shown how the radiation damping potential can be incorporated into the close-coupling equations by using a variation of the usual R-matrix method; this variation preserves the rapid calculation of scattering parameters and thus allows the inclusion of radiation damping with relatively little effort. We have examined the effect of radiation damping utilizing multichannel quantum defect theory (MQDT), which clearly shows the connection between radiative and dielectronic recombination; this examination showed that radiation damping can be nonperturbatively included into the physical wave function if it is perturbatively included in the unphysical wave function.

II. RADIATION DAMPING POTENTIAL

Several authors [3–6] have obtained equations that describe the effect of an optical potential for one-photon radiation damping, although it has not often been used in close-coupling equations or methods to date. Reference [10] is an exception for an isolated resonance embedded in one continuum. The derivation of the optical potential for radiation damping has often been linked with a specific method for obtaining the atomic wave function (e.g., the projection operator formalism [11] applied to atomic resonances). In this section, we give a derivation of this potential to introduce notation that will be used throughout the rest of the paper. The derivation below is not truly rigorous because we will set to zero the interactions that cause the Lamb shift; the only effect that will be retained is the damping due to photon emission. This is the pole approximation applied to radiation damping. In Sec. V B, we will rederive the results of this section using the projection operator formalism of Feshbach [11] as applied to radiation damping without reference to the type of atomic wave functions in the P space; the results from Sec. V B will be used in Sec. V C. Atomic units will be used throughout this paper.

The wave functions $|\Psi^{\pm}_{Ej}\rangle$ will be the solutions of the Hamiltonian equation [Eq. (2) below] for an atom or an ion coupled to the radiation field; the + superscript represents the situation that as $t \to -\infty$ there is an electron coming towards the target ion in channel j and as $t \to \infty$ there are amplitudes for the electron to have elastically or inelastically scattered from the target or a photon was emitted. The − superscript represents the situation that as $t \to \infty$ the electron leaves the target only in channel j with no emitted photons and for $t \to -\infty$ there is a linear superposition of incoming waves in the photon and electron channels. Most of the practical calculations of electron scattering from atoms or ions separate the time dependence of the wave function from the spatial and spin dependence. Following this tradition, we write the wave function

$$|\Psi^{\pm}_{Ej}\rangle = e^{-iEt}\left[|\psi^{\pm}_{Ej}\rangle + \sum_{n,\mathbf{k},\hat{\boldsymbol{\epsilon}}} B^{\pm}_{n,\mathbf{k}\hat{\boldsymbol{\epsilon}},j}(E)|\psi_n\rangle a^{\dagger}_{\mathbf{k}\hat{\boldsymbol{\epsilon}}}\right]|\mathcal{V}\rangle, \tag{1}$$

where E is a real energy, $|\psi^{\pm}_{Ej}\rangle$ is an unknown atomic scattering wave function, the $|\psi_n\rangle$ are known atomic bound-state wave functions, $a^{\dagger}_{\mathbf{k}\hat{\boldsymbol{\epsilon}}}$ is the raising operator for a photon of wave vector $\mathbf{k}$ and polarization $\hat{\boldsymbol{\epsilon}}$, $|\mathcal{V}\rangle$ is the radiation field vacuum, and $B^{\pm}_{n\mathbf{k}\hat{\boldsymbol{\epsilon}},j}(E)$ are c-number coefficients. The wave function can be written in this form because the $|\psi^{\pm}_{Ej}\rangle$ are scattering-type functions and the radiation field decouples from the electron at large distances; if the $|\psi_E\rangle$ were bound-state functions the energy E would need to be complex if there were a lower state coupled to $|\psi_E\rangle$ through the radiation field.

The $|\Psi^{\pm}_{Ej}\rangle$ is a solution of

$$i\partial|\Psi^{\pm}_{Ej}\rangle/\partial t = (H_A + H_R + H_I)|\Psi^{\pm}_{Ej}\rangle, \tag{2}$$

where H_A is the atomic Hamiltonian, $H_R = \sum_{\mathbf{k},\hat{\boldsymbol{\epsilon}}} \omega_{\mathbf{k}} a^{\dagger}_{\mathbf{k}\hat{\boldsymbol{\epsilon}}} a_{\mathbf{k}\hat{\boldsymbol{\epsilon}}}$ is the Hamiltonian for the radiation field, and $H_I = -\sum_{\mathbf{k},\hat{\boldsymbol{\epsilon}}} \sqrt{2\pi/V\omega_{\mathbf{k}}}(\hat{\boldsymbol{\epsilon}} \cdot \mathbf{P} a_{\mathbf{k}\hat{\boldsymbol{\epsilon}}} + \hat{\boldsymbol{\epsilon}}^* \cdot \mathbf{P} a^{\dagger}_{\mathbf{k}\hat{\boldsymbol{\epsilon}}})$ is the part of the Hamiltonian that couples the electronic motion to the radiation field. The electron momentum operator is $\mathbf{P}$. We quantize the radiation field in a cube of volume V and take the limit $V \to \infty$ in all physical

parameters.

We solve for the scattering part of the wave function $|\psi^{\pm}_{Ej}\rangle$ by substituting the form of the total wave function from Eq. (1) into Eq. (2). We project onto Eq. (2) with $\langle\mathcal{V}|a_{\mathbf{k}\hat{\boldsymbol{\epsilon}}}\langle\psi_n|$ to obtain

$$B^{\pm}_{n\mathbf{k}\hat{\boldsymbol{\epsilon}},j}(E) = -\sqrt{2\pi/V\omega_k}\langle\psi_n|\hat{\boldsymbol{\epsilon}}^*\cdot\mathbf{P}|\psi^{\pm}_{Ej}\rangle/(E-E_n-\omega_k\pm i\delta), \tag{3}$$

where $(E_n - H_A)|\psi_n\rangle = 0$ and we will take the limit $\delta \to 0^+$ in any integrals. Finally, we project onto Eq. (2) with $\langle\mathcal{V}|$ to obtain the differential equation for which $|\psi^{\pm}_{Ej}\rangle$ is a solution:

$$(E-H_A)|\psi^{\pm}_{Ej}\rangle = \sum_{n\mathbf{k},\hat{\boldsymbol{\epsilon}}}\hat{\boldsymbol{\epsilon}}\cdot\mathbf{P}|\psi_n\rangle(-\sqrt{2\pi/V\omega_k})B^{\pm}_{n\mathbf{k}\hat{\boldsymbol{\epsilon}},j}(E). \tag{4}$$

In this form it appears the $|\psi^{\pm}_{Ej}\rangle$ are the solutions of inhomogeneous differential equations. However, the $B^{\pm}$ depend on the $|\psi^{\pm}_{Ej}\rangle$, which somewhat complicates matters. By substituting the expression for $B^{\pm}_{n\mathbf{k}\hat{\boldsymbol{\epsilon}},j}(E)$ from Eq. (3) into Eq. (4), we obtain an equation for $|\psi^{\pm}_{Ej}\rangle$ that has the form

$$(E-H_A)|\psi^{\pm}_{Ej}\rangle = \sum_{n,\mathbf{k},\hat{\boldsymbol{\epsilon}}}\hat{\boldsymbol{\epsilon}}\cdot\mathbf{P}|\psi_n\rangle\langle\psi_n|\hat{\boldsymbol{\epsilon}}^*\cdot\mathbf{P}|\psi^{\pm}_{Ej}\rangle \times\frac{2\pi}{V\omega_k}\Big/(E-E_n-\omega_k\pm i\delta), \tag{5}$$

where the right-hand side of Eq. (5) suggests an optical potential. The modes of the radiation field can be summed over exactly to lowest order in V by converting the sum to an integral

$$\sum_{\mathbf{k},\hat{\boldsymbol{\epsilon}}} = \int d^2\hat{k}\int d\omega\sum_{\hat{\boldsymbol{\epsilon}}}V\omega^2/(2\pi c)^3, \tag{6}$$

with c being the speed of light. We sum over the polarizations and integrate over emission angles to obtain

$$(E-H_A)|\psi^{\pm}_{Ej}\rangle = \sum_n\mathbf{P}|\psi_n\rangle\cdot\langle\psi_n|\mathbf{P}|\psi^{\pm}_{Ej}\rangle \times\int_0^{\infty}d\omega\frac{2\omega}{3\pi c^3}\Big/(E-E_n-\omega\pm i\delta). \tag{7}$$

The real part of the integral diverges. This term gives the shift in the energy position due to the interaction with the radiation field (when it is handled properly using renormalization theory); for electron scattering it gives a change in phase shift. This is analogous to the Lamb shift for bound states and is typically a small correction (except at very high charge) when it is correctly included in the equations of motion. The proper treatment of the Lamb shift term is beyond the scope of this paper so we set it to zero. The residue from the pole of the integral can be easily obtained to give

$$(E-H_A)|\psi^{\pm}_{Ej}\rangle = \mp\frac{2i}{3c^3}\sum_n(E-E_n)\mathbf{P}|\psi_n\rangle\cdot\langle\psi_n|\mathbf{P}|\psi^{\pm}_{Ej}\rangle. \tag{8}$$

Equation (8) is extremely important because it gives the differential equation for $|\psi^{\pm}_{Ej}\rangle$ and clearly shows that $|\psi^{+}_{Ej}\rangle$ is the solution of a differential equation different from the $|\psi^{-}_{Ej}\rangle$ wave function. This equation is also important because it does not presuppose any representation for the scattering function. The right-hand side of this equation can be written in terms of the nonlocal optical potential

$$V_R = -\frac{2i}{3c^3}\sum_n(E-E_n)\mathbf{P}|\psi_n\rangle\cdot\langle\psi_n|\mathbf{P}, \tag{9}$$

which we will call the radiation damping potential. This radiation damping potential is spherically symmetric and it is anti-Hermitian. This potential can be derived using a projection operator formalism [11] as applied to the second quantized radiation field; this derivation is given in Sec. V B.

There have been several methods that have been proposed for including radiation damping in electron-ion interactions [3–6]. Although it is sometimes difficult to see the connection between all of the different methods, every method can be expressed as an attempt at solving Eq. (8) because all of the methods derive from the same approximations utilized in this section. The nonobvious connections with other methods are discussed in Sec. V C.

III. PROPERTIES OF THE WAVE FUNCTION

In this section, we derive some of the properties of the wave function. Some of the questions about the scattering form of the wave function are addressed.

A. Normalization

The normalization properties of the scattering functions are examined in detail because the normalization of the wave functions and the photoionization cross sections are intimately related. This is a nontrivial question arising from the non-Hermitian nature of $H_A + V_R$.

We will begin by focusing on the normalization of the $|\psi^{\pm}_{Ej}\rangle$ atomic scattering functions. If the Hamiltonian is Hermitian the most important scattering functions are the $|\psi^{\pm}_{Ej}\rangle$ functions that have the asymptotic form (as $r\to\infty$) [12]

$$|\psi^{-}_{Ej}\rangle = \mathcal{A}\sum_{j'}|\Phi_{j'}\rangle[f^{+}_{\epsilon j'}(r)\delta_{j'j} - f^{-}_{\epsilon j'}(r)S^{\dagger}_{j'j}]/i\sqrt{2}, \tag{10}$$

$$|\psi^{+}_{Ej}\rangle = \mathcal{A}\sum_{j'}|\Phi_{j'}\rangle[f^{-}_{\epsilon j'}(r)\delta_{j'j} - f^{+}_{\epsilon j'}(r)S_{j'j}]i/\sqrt{2}, \tag{11}$$

where $\mathcal{A}$ is the antisymmetrization operator, $S_{j'j}$ is the S matrix connecting channels j' and j, $|\Phi_{j'}\rangle$ are the channel functions that include the target state as well as any angular momentum of the outer electron, and the $f^{\pm}_{\epsilon j'}(r)$ are the radial functions that are the solutions of the asymptotic Schrödinger or Dirac equation. All of the channels in Eqs. (10) and (11) are open. If the asymptotic potential is $-Z/r$, then these are Coulomb functions at energy $\epsilon_{j'} = E - E_{\mathrm{core},j'}$ with the properties [9]

$$f^{\pm}_{\epsilon j'}(r) \rightarrow \sqrt{1/\pi k_{j'}}\; r^{\pm Zi/k_{j'}} e^{\pm i(k_{j'}r+\eta_{j'})}, \tag{12}$$

where $k_{j'} = \sqrt{2\epsilon_{j'}}$ and $\eta_{j'}$ is the long-range Coulomb phase shift for channel j' and charge Z. In terms of Seaton's s and c functions $f^{\pm}(r) = c(r) \pm is(r)$ and in terms of the f and g functions (see Fano and Rau) $f^{\pm}(r) = [-g(r) \pm if(r)]/\sqrt{2}$. The $(f^{+})^{*} = f^{-}$ at real energies. Since the $f^{\pm}_{\epsilon j}$ are solutions of the same differential equation, the Wronskian of these two functions is independent of position and can therefore be evaluated at $r \rightarrow \infty$:

$$W(f^{+}_{\epsilon j}, f^{-}_{\epsilon j}) = -2i/\pi. \tag{13}$$

This Wronskian will be used in conjuction with Green's theorem to find integrals involving the solutions of the Schrödinger equation with the form of Eqs. (10) and (11).

When the Hamiltonian is Hermitian, the S matrix is unitary, which gives $\sum_{j''} S_{j''j} S^{*}_{j''j'} = \delta_{jj'}$. Using the unitarity of the S matrix and the properties of the $f^{\pm}$ one can show

$$|\psi^{-}_{Ej}\rangle = \sum_{j'} |\psi^{+}_{Ej'}\rangle S^{*}_{j'j} = |\psi^{+}_{Ej}\rangle^{*}, \tag{14}$$

where in the last equality the complex conjugation is only for the radial part of the wave function. Finally, the $|\psi^{\pm}_{Ej}\rangle$ are normalized per unit energy when they are the solution of a Hermitian Hamiltonian

$$\langle \psi^{\pm}_{Ej} | \psi^{\pm}_{E'j'} \rangle = \delta(E - E')\delta_{jj'} \; . \tag{15}$$

To obtain this result, one can use Green's theorem applied to a finite volume and then take the limit as the volume becomes infinite to obtain the δ function of energy.

When the Hamiltonian is not Hermitian, none of these relationships hold. First, if $|\psi^{+}_{Ej}\rangle$ is a solution of the Hamiltonian $H = H_A + V_R$ with an S matrix $S_{j'j}$, the $|\psi^{-}_{Ej}\rangle$ given by Eq. (10) is *not* a solution of the Hamiltonian; it is a solution of $(E - H^{\dagger})|\psi^{-}_{Ej}\rangle = 0$. This is fortunate because in Eq. (8), the $|\psi^{-}_{Ej}\rangle$ are defined as the solutions of $(E - H^{\dagger})|\psi^{-}_{Ej}\rangle = 0$ since the Hermitian conjugate of H_A equals H_A and the Hermitian conjugate of V_R equals $-V_R$. The one relationship between the $|\psi^{\pm}_{Ej}\rangle$ functions that still holds is

$$|\psi^{-}_{Ej}\rangle = |\psi^{+}_{Ej}\rangle^{*}, \tag{16}$$

where the complex conjugation is for the radial parts of the functions, the $|\psi^{+}_{Ej}\rangle$ are eigenstates of H, and the $|\psi^{-}_{Ej}\rangle$ are eigenstates of $H^{\dagger}$.

The $|\psi^{\pm}_{Ej}\rangle$ are not normalized per unit energy when the Hamiltonian is not Hermitian; the overlap integrals can be obtained by applying Green's theorem to the overlap over a finite volume and then taking the limit that the volume becomes infinite. These normalization integrals are

$$\langle \psi^{+}_{Ej} | \psi^{+}_{E'j'} \rangle = \frac{1}{2} \left(\delta_{jj'} + \sum_{j''} S^{*}_{j''j} S_{j''j'} \right) \delta(E - E'), \tag{17}$$

$$\langle \psi^{-}_{Ej} | \psi^{-}_{E'j'} \rangle = \frac{1}{2} \left(\delta_{jj'} + \sum_{j''} (S^{\dagger})^{*}_{j''j} (S^{\dagger})_{j''j'} \right) \delta(E - E'). \tag{18}$$

When the S matrix is unitary (i.e., the Hamiltonian is Hermitian), these results reduce to those given in Eq. (15).

To show the origin of the nonunitarity of the S matrix we examine the properties of

$$\langle \psi^{+}_{Ej} | (H_A + V_R) \psi^{+}_{Ej'} \rangle - \langle (H_A + V_R) \psi^{+}_{Ej} | \psi^{+}_{Ej'} \rangle = 0. \tag{19}$$

Since the V_R is anti-Hermitian, Eq. (19) is identical to

$$\langle \psi^{+}_{Ej} | H_A \psi^{+}_{Ej'} \rangle - \langle H_A \psi^{+}_{Ej} | \psi^{+}_{Ej'} \rangle = -2 \langle \psi^{+}_{Ej} | V_R | \psi^{+}_{Ej'} \rangle. \tag{20}$$

The H_A contains Hermitian potential terms and kinetic energy operators; the contribution from the potential cancels out in Eq. (20). The contribution from the kinetic energy terms goes to a constant at finite distance because the two wave functions are at the same energy; by using Green's theorem, the contribution from the kinetic energy can be expressed as a surface integral as long as the surface is large enough to completely contain the effects from the core electrons:

$$\langle \psi^{+}_{Ej} | H_A \psi^{+}_{Ej'} \rangle - \langle H_A \psi^{+}_{Ej} | \psi^{+}_{Ej'} \rangle = -\frac{1}{4} \sum_{j''} W(f^{+}_{j''} \delta_{j''j} - f^{-}_{j''} S^{*}_{j''j}, f^{-}_{j''} \delta_{j''j'} - f^{+}_{j''} S_{j''j'}). \tag{21}$$

If we use Eq. (13) for the Wronskian of each term in Eq. (21) and substitute this expression into Eq. (20), we find

$$\delta_{jj'} - \sum_{j''} S^{*}_{j''j} S_{j''j'} = 4\pi i \langle \psi^{+}_{Ej} | V_R | \psi^{+}_{Ej'} \rangle. \tag{22}$$

The radiation damping potential V_R is $-i$ times a positive definite operator, which means $1 - S^{\dagger}S$ is a positive definite matrix as it must be (electron flux is lost due

to radiation damping). We can substitute Eq. (22) into (17) to obtain

$$\langle\psi^+_{Ej}|\psi^+_{E'j'}\rangle = (\delta_{jj'} - 2\pi i\langle\psi^+_{Ej}|V_R|\psi^+_{E'j'}\rangle)\delta(E-E'). \tag{23}$$

This equation clearly shows the effect of radiation damping on the normalization of the atomic scattering function. The $|\psi^+_{Ej}\rangle$ in Eq. (22) is the solution of Eq. (8). Radiation damping can be calculated at the perturbative level [7] by utilizing Eq. (22) with the $|\psi^+_{Ej}\rangle$ being the solution of $(E-H_A)|\psi^+_{Ej}\rangle = 0$.

Now we turn to the difficult question of finding the normalization of the total wave function $|\Psi^\pm_{Ej}\rangle$ that includes both zero- and one-photon terms. To reduce notational difficulties we will find the normalization for the "+" solution only. We use the expression for the total wave function from Eq. (1) to obtain

$$\langle\Psi^+_{Ej}|\Psi^+_{E'j'}\rangle = \langle\psi^+_{Ej}|\psi^+_{E'j'}\rangle + \sum_{n,\mathbf{k},\hat{\boldsymbol{\epsilon}}} B^{+*}_{n\mathbf{k}\hat{\boldsymbol{\epsilon}},j}(E)B^+_{n\mathbf{k}\hat{\boldsymbol{\epsilon}},j'}(E'). \tag{24}$$

We have already derived an expression for $\langle\psi^+_{Ej}|\psi^+_{E'j'}\rangle$ so it is only necessary to find an expression for the second term of this equation. We substitute the form of B from Eq. (3) to obtain

$$\sum_{n,\mathbf{k},\hat{\boldsymbol{\epsilon}}} B^{+*}_{n\mathbf{k}\hat{\boldsymbol{\epsilon}},j}(E)B^+_{n\mathbf{k}\hat{\boldsymbol{\epsilon}},j'}(E')$$

$$= \lim_{\delta,\delta'\to 0^+}\sum_{n,\mathbf{k},\hat{\boldsymbol{\epsilon}}}\frac{2\pi}{V\omega_k}\langle\psi^+_{Ej}|\hat{\boldsymbol{\epsilon}}\cdot\mathbf{P}|\psi_n\rangle\langle\psi_n|\hat{\boldsymbol{\epsilon}}^*\cdot\mathbf{P}|\psi^+_{Ej}\rangle \times[(E-E_n-\omega_k-i\delta)(E'-E_n-\omega_k+i\delta')]^{-1}. \tag{25}$$

Using Eq. (6), the sum over $\mathbf{k}$ and $\hat{\boldsymbol{\epsilon}}$ can be converted to an integral to give

$$\sum_{n,\mathbf{k},\hat{\boldsymbol{\epsilon}}} B^{+*}_{n\mathbf{k}\hat{\boldsymbol{\epsilon}},j}(E)B^+_{n\mathbf{k}\hat{\boldsymbol{\epsilon}},j'}(E')$$

$$= \lim_{\delta,\delta'\to 0^+}\sum_n\frac{4(E-E_n)i}{3c^3} \times\langle\psi^+_{Ej}|\mathbf{P}|\psi_n\rangle\cdot\langle\psi_n|\mathbf{P}|\psi^+_{E'j'}\rangle/(E'-E+i\delta+i\delta') = 2\pi i\langle\psi^+_{Ej}|V_R|\psi^+_{E'j'}\rangle\delta(E-E'). \tag{26}$$

Substituting the overlap of the atomic scattering function from Eqs. (23) and (26) for the overlap of the B coefficients into Eq. (24), we obtain

$$\langle\Psi^+_{Ej}|\Psi^+_{E'j'}\rangle = \delta_{jj'}\delta(E-E'). \tag{27}$$

A similar treatment would show the $|\Psi^-_{Ej}\rangle$ to be normalized per unit energy. This treatment demonstrates that the full wave function is energy normalized as it must be to be useful in atomic scattering calculations. Equation (27) allows us to use the results from usual scattering theory, except we use the wave function $|\Psi^\pm_{Ej}\rangle$ instead of the $|\psi^\pm_{Ej}\rangle$, although we will be able to express all of the physical parameters of interest in terms of the functions $|\psi^\pm_{Ej}\rangle$.

B. Photon emission probability

In the scattering formulation of radiation damping the total probability for photon emission can be obtained from the S matrix of the electron scattering wave function Eq. (11). The S-matrix element $S_{jj'}$ is the amplitude for the electron to scatter from channel j to channel j' without emitting a photon. The probability for the electron to scatter from channel j to any channel j' is $\sum_{j'}|S_{jj'}|^2$ and is equal to 1 if the Hamiltonian is Hermitian. Radiation damping reduces this probability because there is a nonzero probability for emitting a photon. The probability for approaching the nucleus in channel j and emitting a photon is

$$P_j(E) = 1 - \sum_{j'}|S_{jj'}|^2 = 4\pi i\langle\psi^+_{Ej}|V_R|\psi^+_{Ej}\rangle. \tag{28}$$

This probability can be written as the sum of the partial probabilities P_{jn}, which are the probabilities for an electron to approach the nucleus in channel j, emit a photon in any direction and polarization, and be captured in state n. The P_{jn} are given by

$$P_{jn}(E) = \frac{8\pi(E-E_n)}{3c^3}\langle\psi^+_{Ej}|\mathbf{P}|\psi_n\rangle\cdot\langle\psi_n|\mathbf{P}|\psi^+_{Ej}\rangle. \tag{29}$$

These probabilities can be related to the total photoionization cross section through simple factors. The total probability for photon emission is $P_j = \sum_n P_{jn}$. The P_{jn} can be expressed as reduced matrix elements and geometrical factors that depend on the type of angular momentum coupling that is appropriate for the scattering problem. In LS coupling the expression is

$$P_{jn}(E) = \frac{8\pi(E-E_n)}{3c^3(2L+1)}|\langle\psi^+_{Ej}||\nabla||\psi_n\rangle|^2, \tag{30}$$

where L is the total angular momentum of channel j. A final probability that may be of interest is the probability for the electron to approach the core in the $\hat{\mathbf{z}}$ direction with the target in state c' and emit a photon in direction $\hat{k}$ with polarization $\hat{\boldsymbol{\epsilon}}$ and captured in state $|\psi_n\rangle$. This probability is

$$\frac{d^2P^{\hat{\boldsymbol{\epsilon}}}_{c'n}}{d^2\hat{k}}(E) = \frac{(E-E_n)}{c^3}|\langle\psi^+_{Ec'\hat{z}}|\hat{\boldsymbol{\epsilon}}\cdot\mathbf{P}|\psi_n\rangle|^2, \tag{31}$$

where the $|\psi^+_{Ec'\hat{z}}\rangle$ is the superposition of states $|\psi^+_{Ej}\rangle$ that gives an incoming wave in the $\hat{\mathbf{z}}$ direction on the target in state c'. This probability can be rewritten in terms of standard angular factors and reduced matrix elements in exactly the same fashion as differential photoionization cross sections.

IV. PHYSICAL PARAMETERS

Radiation damping changes some of the standard properties of wave functions. Therefore, we would like to completely specify how to obtain physical parameters from wave functions that have included the effects of radiation damping.

A. Elastic and inelastic scattering cross sections

The elastic and the inelastic scattering cross sections are obtained by comparing the rate of scattering into certain directions and/or channels to the incident flux of electrons [12]. This idea does not change when there is radiation damping present; photon emission is simply another channel. The application of these ideas involves the $|\Psi^+_{Ei}\rangle$ wave functions of Eq. (1); the probability for scattering from channel i to channel j and not emit a photon is simply $|S_{ij}|^2$ (whether or not radiation damping is included) since the electron flux toward the nucleus in channel i is 1 and the flux away from the atom in channel j is $|S_{ij}|^2$. The formulas for elastic and inelastic cross sections with radiation damping are identical to those with no radiation damping as long as the S matrix is used (or the T matrix is obtained from the S matrix). Radiation damping changes the S matrix but does not change the formulas used to calculate the scattering cross sections.

B. Photoionization cross section

The photoionization cross section is obtained by comparing the rate of electron ejection in a certain direction and/or channel to the incident photon flux [13]. The usual method is to use a representation of the wave function in terms of the solution with incoming wave boundary conditions, i.e., the $|\Psi^-_{Ej}\rangle$. In this representation, there are outgoing waves only in channel j. The dipole matrix elements between these states and the initial state give the amplitude for ionization into channel j. The reduced dipole matrix elements can be obtained from

$$\begin{aligned} d^-_{Ej} &= \langle \Psi^-_{Ej} || D || \Psi_g \rangle \\ &= \langle \psi^-_{Ej} || D || \psi_g \rangle, \end{aligned} \tag{32}$$

where $|\Psi_g\rangle = |\psi_g\rangle|\mathcal{V}\rangle$ and the $(H_A - V_R - E)|\psi^-_{Ej}\rangle = 0$ [with asymptotic form given by Eq. (10)]. We have used the equivalence of Eq. (16) to obtain photoionization cross sections in terms of the $|\psi^+_{Ej}\rangle$,

$$d^-_{Ej} = \langle \psi^+_{Ej} || D || \psi_g \rangle^*. \tag{33}$$

The dipole matrix element give by Eq. (32) or (33) is used in the usual cross section formulas to obtain the differential, partial, or total photoionization cross sections. The formulas for the photoionization cross section do not change, but the radiation damping changes the d^-_{Ej} and can therefore change the cross section.

The photoionization cross section can be written in many different forms that are equivalent when no damping is present (e.g., using standing-wave solutions of the Schrödinger equation). Some of these forms do not give correct results when radiation damping is present.

C. Photorecombination cross section

The photorecombination cross section can be obtained from the $|\Psi^+_{Ej}\rangle$ wave functions in a very simple manner. The cross section is obtained by comparing the rate for emitting photons compared to the incoming electron flux. In the scattering formulation of radiation damping, the photorecombination cross section is a simple extension of the usual inelastic scattering cross section. From Sec. III B, we can obtain the probability for emitting photons during one electronic collision. The cross section for photon emission when the target ion is in state c' is

$$\sigma_{c'}(E) = \frac{\pi}{k^2_{c'}} \sum_j g_j P_j(E), \tag{34}$$

where $k^2_{c'} = 2(E - E_{c'})$ is the squared wave number of the incoming electron, g_j is a statistical factor, and P_j is from Eq. (28). The sum is over all channels j for which the target state of channel j is the state c'. The factor g_j is

$$g_j = (2J_j + 1)/2(2J_{c'} + 1), \tag{35}$$

where $J_{c'}$ is the total angular momentum of the core and J_j is the total angular momentum of channel j when jj coupling is used and

$$g_j = (2L_j + 1)(2S_j + 1)/2(2L_{c'} + 1)(2S'_c + 1), \tag{36}$$

where $L_{c'}$ ($S_{c'}$) is the total orbital angular momentum (spin) of the core and L_j (S_j) is the total orbital angular momentum (spin) of channel j when LS coupling is used.

The partial and the differential photorecombination cross sections can be obtained in a similar manner by using the partial and differential photorecombination probabilities from Sec. III B.

V. CONNECTIONS TO OTHER METHODS

In this section, we sketch the connection of the present formulation to other theoretical methods.

A. Fano profile with damping

We would like to examine the effect of radiation damping when there is one resonance embedded in one continuum. We will use the formalism that was utilized by Fano [14] to describe scattering near an isolated resonance. In this treatment we will only account for the main effect of the resonance on the wave function and obtain the probability for recombination from Eq. (22).

We construct the wave function using a representation

of states that are solutions of the Hamiltonian when the coupling of the resonance to the continuum and all photodecay channels are neglected. Let $|f_r\rangle$ be the resonance state and $|f_E\rangle$ be the real, energy normalized continuum function. We will find the solution

$$(H-E)|\psi_E^+\rangle = 0, \tag{37}$$

where $H = H_A + V_R$ and $|\psi_E^+\rangle$ has the form

$$|\psi_E^+\rangle = a(E)|f_r\rangle + \int dE'|f_{E'}\rangle b_{E'E}. \tag{38}$$

We need to know the matrix elements of the Hamiltonian in this representation

$$\langle f_r|H|f_r\rangle = E_r - i\Gamma_R/2, \tag{39}$$

$$\langle f_E|H|f_r\rangle = V_E, \tag{40}$$

$$\langle f_{E'}|H|f_E\rangle = E\delta(E-E'), \tag{41}$$

where we have neglected the small amount of radiative recombination in the last relationship. E_r is the energy of the resonance and Γ_R is the *full radiative* width of the resonance, which may have contributions from many final states. Projecting on the left-hand side of Eq. (37) with $\langle f_r|$ gives

$$(E_r - i\Gamma_R/2 - E)a(E) + \int dE' V_{E'}^* b_{E'E} = 0 \tag{42}$$

and projecting on the left-hand side with $\langle f_{E'}|$ gives

$$V_{E'}a(E) + (E'-E)b_{E'E} = 0. \tag{43}$$

The formal relationship between $b_{E'E}$ and $a(E)$ in Eq. (43) can be recast in the form

$$b_{E'E} = \left[\frac{\mathrm{P}}{E-E'} + Z(E)\delta(E-E')\right] V_{E'}a(E), \tag{44}$$

where P indicates the principal part of any integration with this term. Substituting this expression for $b_{E'E}$ into Eq. (42) shows that

$$Z(E) = (E - \bar{E}_r + i\Gamma_R/2)/|V_E|^2, \tag{45}$$

where

$$\bar{E}_r = E_r + \mathrm{P}\int dE'|V_{E'}|^2/(E-E') \tag{46}$$

is a slowly varying function of energy.

To find the wave function we substitute this value for Z into $b_{E'E}$ and $b_{E'E}$ into Eq. (38) to obtain

$$|\psi_E^+\rangle = a(E)\Big[|f_r\rangle + |f_E\rangle V_E Z(E) + \mathrm{P}\int dE'|f_{E'}\rangle\langle f_{E'}|H|f_r\rangle/(E-E')\Big]. \tag{47}$$

Note that the integral term is simply $G_0V|f_r\rangle$, where G_0 is the standing-wave Green's function for the unstructured continuum. For distances larger than the interaction range of H, this Green's function term can be obtained from the solution that oscillates 90° out of phase from $|f_E\rangle$ (we denote this function $|g_E\rangle$),

$$|\psi_E^+\rangle = a(E)V_E Z(E)[|f_E\rangle + \pi|g_E\rangle/Z(E)] \quad r > r_0. \tag{48}$$

To find an expression for $a(E)$, we use the asymptotic form of $|\psi_E^+\rangle$ and the expressions for $|f_E\rangle$ and $|g_E\rangle$. This procedure gives

$$a(E) = V_E^*/(E - \bar{E}_r + i\Gamma_R/2 + i\Gamma_A/2), \tag{49}$$

where we have substituted in the autoionizing width $\Gamma_A = 2\pi|V_E|^2$.

We now turn to an exploration of the squared dipole matrix element, which is important for both photoionization cross sections and the probability for photorecombination. For this exploration, we will be careful of contributions from interference terms because we only have one dipole matrix element. Following Fano, we write the reduced dipole matrix elements as

$$D_r = \langle f_r||D||\psi_g\rangle + \mathrm{P}\int dE' V_{E'}^* D_{E'}/(E-E') \tag{50}$$

and

$$D_E = \langle f_E||D||\psi_g\rangle. \tag{51}$$

The matrix coupling the ground state to the final state is

$$\langle\psi_E^+||D||\psi_g\rangle^* = [D_r^*V_E^* + D_E^*(E-\bar{E}_r + i\Gamma_R/2)]/[E - \bar{E}_r + i(\Gamma_A+\Gamma_R)/2]. \tag{52}$$

If we choose the normalization of $|f_r\rangle$ and $|f_E\rangle$ appropriately, the elements V, D_r, and D_E will be real and thus

$$\begin{aligned}|\langle\psi_E^+||D||\psi_g\rangle|^2 &= \{[VD_r + (E-\bar{E}_r)D_E]^2 \\ &\quad + D_E^2\Gamma_R^2/4\}/[(E-\bar{E}_r)^2 \\ &\quad + (\Gamma_R+\Gamma_A)^2/4] \\ &= D_E^2[(q_R+\varepsilon)^2+\mu^2]/(\varepsilon^2+1),\end{aligned} \tag{53}$$

where $q_R = 2D_rV/[D_E(\Gamma_R+\Gamma_A)]$, $\varepsilon = 2(E-\bar{E}_r)/(\Gamma_A+\Gamma_R)$, and $\mu = \Gamma_R/(\Gamma_R+\Gamma_A)$. Note that the usual Fano profile obtains when $\Gamma_R \to 0$. Also, as the radiative rate increases, $q_R \to 0$ and $\mu \to 1$, which gives $|\langle\psi_E^+||D||\psi_E^+\rangle|^2 = D_E^2$ (i.e., as the radiative rate increases all of the effects of the resonance disappear from the photoionization cross section). This formula shows the q for a resonance changes in the presence of radiation damping $q_r = q\Gamma_A/(\Gamma_R+\Gamma_A)$ (i.e., the asymmetry parameter with damping equals the asymmetry parameter with no damping times the branching ratio for autoionization). The parameter μ is equal to the branching ratio for photorecombination and is zero when there is no radiation damping. Note that without damping the photoionization cross section goes to zero at $\varepsilon = -q$ due to the in-

terference between direct and resonant ionization paths. With radiation damping, $\mu \neq 0$ and the ionization cross section does not go exactly to zero. It is well known that damping destroys coherence and interference effects and therefore it should not be surprising that such a term is present. The form of Eq. (53) agrees with Eq. (5.12) of Ref. [6] when high-order effects from radiative decay are neglected in their formula; but the form of Eq. (53) does not agree with the form of Eq. (5a) of Ref. [15] because they are describing a different physical situation. Equation (53) can be derived with the formalism of Ref. [3] by using two final radiative states. One state is weakly radiatively coupled to the resonance and has an interference type dipole matrix element and the second state is strongly coupled to the resonance but not coupled to the continuum.

A simple formula obtains when there is no direct excitation to the continuum $D_E = 0$. For this case

$$|\langle\psi_E^+||D||\psi_g\rangle|^2 = \frac{D_r^2\Gamma_A/2\pi}{(E-\bar{E}_r)^2+(\Gamma_R+\Gamma_A)^2/4}, \quad (54)$$

which is a Lorentzian of width $\Gamma_A + \Gamma_R$ as expected. Often the experimental resolution is insufficient to resolve this line and the important parameter is this function convolved with the experimental resolution, giving

$$\int dE W(E-E')|\langle\psi_E^+||D||\psi_g\rangle|^2 \simeq W(\bar{E}_r - E')D_r^2\Gamma_A/(\Gamma_R+\Gamma_A). \quad (55)$$

The radiation damping has reduced the height of the experimentally observed peak by the factor $\Gamma_A/(\Gamma_R+\Gamma_A)$, which is the branching ratio for autoionization.

We can also utilize Eq. (22) to obtain the total probability for photorecombination

$$R(E) = 4\pi i\langle\psi_E^+|V_R|\psi_E^+\rangle = \frac{\Gamma_R\Gamma_A}{(E-\bar{E}_r)^2+(\Gamma_A+\Gamma_R)^2/4} + T_E + \bar{T}_E, \quad (56)$$

where $T_E = 4\pi i\langle f_E|V_R|f_E\rangle$ is the radiative recombination probability in the absence of the resonance and $\bar{T}_E$ contains cross terms between the resonance and the continuum photorecombination amplitudes and it contains effects of the resonance on the continuum. For most systems where the treatment of this section is applicable, the contributions from $\bar{T}_E$ have relatively small integrated contributions to the photorecombination probability. In general, $\bar{T}_E$ does not make a large contribution due to the large number of final states that contribute to the photorecombination probability, which effectively averages over the q and removes the simple interference profile. Finally, for most applications, the experimental scattering energy has an energy distribution $W(E)$, so it is necessary to obtain a convolved probability

$$\langle R\rangle(E') = \int dE R(E)W(E-E') \simeq \frac{2\pi\Gamma_A\Gamma_R}{\Gamma_A+\Gamma_R}W(E_r-E') + T_{E'}, \quad (57)$$

which is a good approximation when the width of the convolution function W is much larger than $\Gamma_A+\Gamma_R$ and much smaller than the energy variation in T_E.

B. Connection to projection-operator methods

The radiation damping potential of Eq. (9) may also be derived using the projection operator technique introduced by Feshbach [11]. The electron continuum projection operator is given by P, the resonance state projection operator is given by Q, and following Gau and Hahn [4] the photon continuum projection operator is given by R. In keeping with a nonperturbative close-coupling theory that includes a structured continuum, we subsume Q space into P space. The coupled time-independent Schrödinger equation is given by

$$PH_APP\psi_P + PDR\psi_R = E\psi_P \quad (58)$$

and

$$RH_AR\psi_R + RDP\psi_P = E\psi_R\ , \quad (59)$$

where $\psi = \psi_P + \psi_R$, H_A is the Hamiltonian for the isolated atom, and D is the electron-photon interaction. Substituting Eq. (59) into Eq. (58) one obtains

$$[PH_AP + PDR(E-RH_AR)^{-1}RDP - E]\psi_P = 0\ , \quad (60)$$

which reduces in the pole approximation to

$$(PH_AP - i\pi PDR|\psi_n\rangle\langle\psi_n|RDP - E)\psi_P = 0\ , \quad (61)$$

for a single bound state $|\psi_n\rangle$. The generalization of the second term in Eq. (61) to include multiple bound states can be identified with the radiation damping potential of Eq. (9).

C. Connection to time-dependent methods

The radiation damping theory of Weisskopf and Wigner [16] for transitions between bound states was extended by Davies and Seaton [3] to cover transitions from the continuum. In keeping with a nonperturbative close-coupling theory, Davies and Seaton also assumed a structured continuum. The resulting time-dependent matrix equations for the probability amplitudes were solved by application of Laplace transforms. The connection between the complex potential method for radiation damping and the time-dependent approach is found in the original work of Feshbach [11]. The formal solution of Eq. (61) is given by

$$\psi_P = \psi_0^+ + A(E-PH_AP)^{-1}PDR|\psi_n\rangle\ , \quad (62)$$

where

$$(PH_AP - E)\psi_0^+ = 0 \quad (63)$$

and

$$A = -i\pi\langle\psi_n|RDP|\psi_P\rangle \ . \tag{64}$$

Substituting Eq. (62) into Eq. (64), the resulting linear equation for A can be solved to yield

$$A = -i\pi(1+Z)^{-1}\langle\psi_n|RDP|\psi_0^+\rangle \ , \tag{65}$$

where

$$Z = i\pi\langle\psi_n|RDP(E-PH_AP)^{-1}PDR|\psi_n\rangle \ . \tag{66}$$

The multichannel generalization of Eq. (66) can be identified with the Z matrix introduced by Davies and Seaton [3].

From the asymptotic behavior of Eq. (62), the transition matrix is given by

$$T = T_0 + A\langle\psi_0^-|PDR|\psi_n\rangle \ , \tag{67}$$

where T_0 is the transition matrix describing the asymptotic behavior of ψ_0^+. For the simple case of elastic scattering of spinless systems

$$\psi_0^{\pm} = e^{\pm i\delta}\psi_E \ , \tag{68}$$

where

$$\psi_E \rightarrow \sqrt{\frac{2}{\pi k}}\sin(kr+\delta) \ . \tag{69}$$

The resulting scattering matrix is given by

$$S_0 = e^{2i\delta} \ . \tag{70}$$

Using the relationship

$$S = 1 - 2\pi i T \tag{71}$$

and substituting Eq. (67) for T yields the scattering matrix including radiation damping

$$S = S_0(1 - 2\pi^2\mathcal{H}(1+Z)^{-1}\mathcal{H}^{\dagger}) \ , \tag{72}$$

where

$$\mathcal{H} = \langle\psi_E|PDR|\psi_n\rangle \ . \tag{73}$$

The multichannel genralizations of Eqs. (72) and (73) may be identified with the $\mathcal{H}$ and S matrices of Davies and Seaton.

D. MQDT formulation of photorecombination

The scattering formulation of radiation damping has many interesting features. In this section, we explore some of the properties and discuss some of the features of this treatment when it is used in conjunction with MQDT [9]. The final result obtained by applying MQDT is identical to that obtained when solving for the wave function using other methods. However, additional insight may be obtained by dissecting the dynamics with this tool. In this section, we will focus on the case where the outer electron experiences a long-range potential of $-Z/r$.

The basic idea in MQDT is that the wave function when an electron leaves the core region can be represented as a superposition of regular and irregular functions

$$|\psi_j\rangle = \sum_{j'}|\Phi_{j'}\rangle(f_{j'}\delta_{j'j} - g_{j'}\mathcal{K}_{j'j}) \tag{74}$$

or incoming and outgoing functions

$$|\psi_j^-\rangle = \sum_{j'}|\Phi_{j'}\rangle[f_{j'}^-\delta_{j'j} - f_{j'}^+(\mathcal{S}^{\dagger})_{j'j}]/i\sqrt{2}, \tag{75}$$

$$|\psi_j^+\rangle = \sum_{j'}|\Phi_{j'}\rangle(f_{j'}^+\delta_{j'j} - f_{j'}^-\mathcal{S}_{j'j})i/\sqrt{2}. \tag{76}$$

The important conceptual difference between Eqs. (74)–(76) and Eqs. (10) and (11) is that the summation over channels in Eqs. (10) and (11) is only over open channels and S is the physical S matrix while the summation in Eqs. (74)–(76) is over both open and closed channels. The wave functions in Eqs. (74)–(76) are not physical because the radial functions in the closed channels diverge as $r \rightarrow \infty$. Because we have not applied the correct boundary condition at $r \rightarrow \infty$, the unphysical $\mathcal{K}$ and $\mathcal{S}$ matrices in Eqs. (74)–(76) do not have a strong energy dependence near thresholds. The physical K and S matrices can be obtained by superposing the unphysical wave functions to eliminate the divergence in the closed channels. This superposition can be formally accomplished analytically (because the asymptotic forms of the Coulomb functions are known) to obtain

$$K_{oo} = \mathcal{K}_{oo} - \mathcal{K}_{oc}(\mathcal{K}_{cc} + \tan\beta_c)^{-1}\mathcal{K}_{co} \tag{77}$$

and

$$\begin{aligned} S_{oo} &= \mathcal{S}_{oo} - \mathcal{S}_{oc}(\mathcal{S}_{cc} + \exp 2i\beta_c)^{-1}\mathcal{S}_{co} \\ &= (1+iK_{oo})/(1-iK_{oo}), \end{aligned} \tag{78}$$

where $\beta_c = \pi(\nu_c - \ell_c)$ with ν_c the effective quantum number $\nu_c = Z/\sqrt{2(E_c - E)}$ and the unphysical $\mathcal{K}$ matrix has been partitioned into blocks according to whether the channel is open or closed

$$\mathcal{K} = \begin{pmatrix} \mathcal{K}_{oo} & \mathcal{K}_{oc} \\ \mathcal{K}_{co} & \mathcal{K}_{cc} \end{pmatrix}; \tag{79}$$

a similar partition holds for the $\mathcal{S}$ matrix. When there is radiation damping present the $\mathcal{K}$ matrix is complex symmetric.

For most dynamical situations, the radiation damping gives a perturbative change to the *unphysical* $\mathcal{K}$ matrix. This is because all channels are treated as if they were open and the only type of damping present has the same form as radiative recombination. "Radiative recombination" in closed channels becomes dielectronic recombination when the unphysical wave functions are superposed to obtain the physical functions. One exception is the

type-I transitions where the core electrons emit the photon; a method for including this type of transition is described in Sec. VI B. The other exception is when the unphysical $\mathcal{K}$ matrix itself has a pole; this effect is accounted for nonperturbatively using the R-matrix method as described in Sec. VI A.

We would like to examine in detail the formulas that apply when there are two coupled channels with one channel being closed. To make the derivation simpler, we utilize shifted Coulomb functions

$$F_i = f_i \cos \pi\mu_i - g_i \sin \pi\mu_i, \tag{80}$$

$$G_i = f_i \sin \pi\mu_i + g_i \cos \pi\mu_i, \tag{81}$$

where the μ_i have been chosen so the real diagonal elements of the $\mathcal{K}$ matrix have been set to zero; the asymptotic form of the wave function is

$$|\psi_j\rangle = \sum_{j'} |\Phi_{j'}\rangle (F_{j'}\delta_{j'j} - G_{j'}\mathcal{K}_{j'j}), \tag{82}$$

with $\mathrm{Re}(\mathcal{K}_{jj}) = 0$. We will take channel 1 as open and 2 as closed. In order to simplify the treatment still further we ignore the radiation damping from the open channel $\mathrm{Im}(\mathcal{K}_{11}) = \mathrm{Im}(\mathcal{K}_{12}) = 0$. The physical K matrix is

$$K_{11} = -\mathcal{K}_{12}^2/[\tan(\beta_2 + \pi\mu_2) + i\kappa_{22}], \tag{83}$$

where $\kappa_{22} = \mathrm{Im}(\mathcal{K}_{22})$. We wish to examine the physical S matrix near the resonance $\beta_2 + \pi\mu_2 = n\pi$. If we expand $\tan(\beta_2 + \pi\mu_2)$ into terms linear in the energy difference from the resonance [i.e., $\tan(\beta_2 + \pi\mu_2) \simeq (E - E_r)d\beta_2/dE = (E - E_r)\pi\nu^3/Z^2$] we obtain the following expression for the physical S matrix:

$$S_{11} \simeq \left[(E - E_r)\frac{\pi\nu^3}{Z^2} + i\kappa_{22} - i\mathcal{K}_{12}^2\right] \Big/ \left[(E - E_r)\frac{\pi\nu^3}{Z^2} + i\kappa_{22} + i\mathcal{K}_{12}^2\right]. \tag{84}$$

The photoemission probability is given by

$$1 - |S_{11}|^2 = 4(\kappa_{22}Z^2/\pi\nu^3)(\mathcal{K}_{12}^2 Z^2/\pi\nu^3)/[(E - E_r)^2 + (\kappa_{22}Z^2/\pi\nu^3 + \mathcal{K}_{12}^2 Z^2/\pi\nu^3)^2]. \tag{85}$$

Now we note that using Fermi's golden rule $\kappa_{22}Z^2/\pi\nu^3$ is the radiative half-width of the state n and $\mathcal{K}_{12}^2 Z^2/\pi\nu^3$ is the autoionization half-width of the state n; this identification is obtained by converting the energy normalization of channel 2 to normalization per unit volume. (Note that the radiative width is proportional to κ_{22} while the autoionization width is proportional to $\mathcal{K}_{12}^2$. This indicates that the imaginary part of the $\mathcal{K}$ matrix can be much smaller than the real part of the $\mathcal{K}$ matrix and still have a dominant effect when the channels are closed.) This identification gives

$$1 - |S_{11}|^2 = \Gamma_R\Gamma_A/[(E - E_r)^2 + (\Gamma_R + \Gamma_A)^2/4], \tag{86}$$

which should be compared to the first term of Eq. (56). We use this derivation to emphasize that although the radiation damping potential only has a perturbative effect on the *unphysical* $\mathcal{K}$ matrix (and $\mathcal{S}$ matrix) and wave function, the damping has a nonperturbative effect on the *physical* S matrix and wave function. Note that if we used the radiation damping potential as a perturbation on the physical wave function and S matrix we would obtain

$$1 - |S_{11}|^2 = \Gamma_R\Gamma_A/[(E - E_r)^2 + \Gamma_A^2/4], \tag{87}$$

which will give horrible results when $\Gamma_R > \Gamma_A$.

In Sec. VI C, we describe a method for perturbatively including the radiation damping potential. We emphasize here that for the case in Sec. VI C, the damping is given as a perturbation on the unphysical $\mathcal{K}$ matrix and wave function, not as a perturbation on the physical wave function. By including the perturbation in the unphysical K matrix and wave functions, the dominant nonperturbative effects on the physical parameters are accounted for.

VI. NUMERICAL DESCRIPTION OF RADIATION DAMPING

In this section, we focus on the types of analytic and computational methods that are needed for practical implementation of radiation damping in atomic scattering problems. These methods have already proven accurate for recombination in Li-like Ar, He-like O, and H-like Fe [8].

We explore the implications for the calculation of the scattering wave function when radiation damping is present. By exploring the general aspects of specific situations, we can identify useful approximations that should hold for all practical applications. A specific purpose of this section is to identify approximations that include the nonperturbative effects due to radiation damping.

In radiation damping, type-I transitions are identified with the radiative decay of core states (i.e., the inverse of isolated core excitations). An example of this decay is $1s\epsilon\ell \leftrightarrow 2pn\ell' \rightarrow 1sn'\ell' + \hbar\omega$ in electron scattering from hydrogenlike ions. Type-II transitions involve the radiative decay of the "outer electron." An example of this in electron scattering from Li-like ions is $1s^2 2s\epsilon\ell \leftrightarrow 1s^2 2pn\ell' \rightarrow 1s^2 2pn''\ell'' + \hbar\omega$, where the $n''\ell''$electron is bound with respect to the $1s^2 2s$ threshold. For the purpose of R-matrix calculations we distinguish type-II transitions into two subgroups: type IIS and type IIL. In the type-IIS transitions, the final state is small and fits inside the R-matrix volume (e.g., $n'' = 2$ and maybe $n'' = 3$ in the Li-like example above). In the type-IIL transitions, the final state is large and does not fit inside the R-matrix volume.

A. Radiation damping in the R-matrix method

Multielectron atomic wave functions can be obtained only by approximate or numerical methods. The R-matrix method has proven to be a very useful tool for obtaining electronic scattering functions. In this section, we derive formulas for the variational estimate [17–19]

of the R matrix when the Hamiltonian is not Hermitian. The Wigner-Eisenbud R matrix [20,21] can be obtained from the variational R matrix by restricting all of the basis functions to have zero derivative on the R-matrix boundary. More importantly, we rewrite the expression for the R matrix in a form that can be efficiently solved on a computer.

There are special solutions of the Schrödinger equation at energy E that have a constant logarithmic derivative over a closed surface [17]. These special solutions, which we will write as $\psi_{E\beta}$, are defined by $(E-H)\psi_{E\beta}=0$ and $(\partial\psi_{E\beta}/\partial n + b_\beta\psi_{E\beta})|_{\text{surface}}=0$, where $\partial\psi_{E\beta}/\partial n$ is the normal derivative at the surface. To find a variational estimate for b_β, we need a trial wave function $\psi^t_{E\beta}=\psi_{E\beta}+\delta_{E\beta}$, where $\delta_{E\beta}$ is a small function compared to $\psi_{E\beta}$. Using the properties of $\psi_{E\beta}$ it is possible to show that

$$b_\beta\int dS\psi^t_{E\beta}\psi^t_{E\beta}=2\int dV\psi^t_{E\beta}(E-H)\psi^t_{E\beta} - \int dS\psi^t_{E\beta}\partial\psi^t_{E\beta}/\partial n+O(\delta^2_{E\beta}) \quad (88)$$

where $\int dV$ means integration over the volume contained inside the surface and $\int dS$ means integration over the surface. To show this relationship, substitute $\psi^t_{E\beta}=\psi_{E\beta}+\delta_{E\beta}$ into Eq. (88) and discard all terms that contain $\delta^2_{E\beta}$. An important point to note is that $(\psi^t_{E\beta})^*$ does not appear in the variational expression and that $H^\dagger$ is not used in any step of the derivation. This means that Eq. (88) is a variational estimate of $b_\beta(E)$ even when H is not Hermitian. Equation (88) is the usual starting point for the variational estimates of the R matrix, but now the Hamiltonian is not restricted to be Hermitian. The usual method for using Eq. (88) is to expand the trial function in a basis set with linear coefficients $\psi^t_{E\beta}=\sum_a y_a C_{a\beta}(E)$. The variational R-matrix equations do not restrict the logarithmic derivative of the y_a basis functions at the surface; however, in the Wigner-Eisenbud treatment, the y_a must have zero derivative at the boundary. The value of the basis functions at the surface is given by $y_a|_{\text{surface}}=\sum_j|\Phi_j\rangle y_{ja}$. The y_{ja} are important parameters in the R-matrix equations, as will be seen below.

Taking the derivative of Eq. (88) with respect to the $C_{a\beta}$ results in a generalized eigenvalue matrix equation for the $C_{a\beta}$ and the eigenvalues $b_\beta(E)$. The $b_\beta(E)$ are the eigenvalues of the inverse of the R matrix. The $\psi_{E\beta}$ (and the generalized eigenvalue equations) are somewhat difficult to work with compared to other solutions. Except for normalization, the R matrix completely describes the behavior of the wave function since it is the inverse of the logarithmic derivative matrix. We will utilize solutions of the Schrödinger equation that have the form [18,19]

$$\psi_{Ej}|_{\text{surface}}=\sum_{j'}|\Phi_{j'}\rangle R_{j'j}(E),$$
$$\partial\psi_{Ej}/\partial n|_{\text{surface}}=|\Phi_j\rangle. \quad (89)$$

The ψ_{Ej} can be constructed from the basis functions y_a, $\psi_{Ej}=\sum_a y_a C_{aj}(E)$. The variational estimate of the R matrix is

$$R_{jj'}(E)=-\frac{1}{2}\sum_{a,a'}y_{ja}y_{j'a'}[(E-\tilde{H})^{-1}]_{aa'}, \quad (90)$$

where the $\tilde{H}$ matrix is complex symmetric and given by

$$\tilde{H}_{aa'}=\langle y_a|H|y_{a'}\rangle+\frac{1}{2}\int dS y_a\partial y_{a'}/\partial n\ . \quad (91)$$

The coefficients of the expansion of the trial function ψ^t_{Ej} are important for calculation of photoionization and partial photorecombination cross sections and are given by

$$C_{aj}(E)=-\frac{1}{2}\sum_{a'}y_{ja'}[(E-\tilde{H})^{-1}]_{a'a}. \quad (92)$$

To this point, all of the equations in this section are the same as those used in standard atomic calculations. However, the Hamiltonian is complex symmetric and therefore not Hermitian. The resulting R matrix is also complex symmetric. The only new term in $\tilde{H}$ arises from the radiation damping potential so we will focus on this term. It is only necessary to find the matrix elements of the radiation damping potential $\langle y_a|V_R|y_{a'}\rangle$ in order to include this potential in the R-matrix equations. The radiation damping potential is a spherically symmetric operator so it only connects functions with the same J and M_J. In LS coupling, this potential conserves L, M_L, S, and M_S as well. In order to derive the factors in the matrix elements of the radiation damping potential we expand the symbol denoting the basis function $y_a=|aLSM_LM_S\rangle$ and the photon decay state $|\psi_n\rangle=|nL^nS^nM^n_LM^n_S\rangle$. With these symbols, the matrix elements of the radiation damping potential are

$$\langle y_a|V_R|y_{a'}\rangle$$
$$=-\frac{2i}{3c^3}\sum_n(E-E_n) \times\sum_{q,M^n_L,M^n_S}(-1)^q\langle aLSM_LM_S|P_q|nL^nS^nM^n_LM^n_S\rangle \times\langle nL^nS^nM^n_LM^n_S|P_{-q}|a'LSM_LM_S\rangle. \quad (93)$$

The P_q do not operate on the spins, therefore the spin part of the matrix element reduces to $\delta_{M_SM^n_S}\delta_{SS^n}$. This matrix element can be expressed as reduced matrix elements and simple factors by using the Wigner-Eckart theorem

$$\langle y_a|V_R|y_{a'}\rangle=-\frac{2i}{3c^3(2L+1)} \times\sum_n(E-E_n)\delta_{SS^n}\langle aLS||\nabla||nL^nS^n\rangle \times\langle a'LS||\nabla||nL^nS^n\rangle, \quad (94)$$

where we have used sum rules for 3-j symbols and the definition of the momentum operator for the last step. The matrix elements for jj-coupled calculations can be

obtained from a similar derivation.

The matrix elements of the radiation damping potential cause problems in the usual formulation of the R-matrix equations. The number of basis functions in an R-matrix equation can be very large and thus the matrix inversion in Eq. (90) can be computationally very slow. The usual method for avoiding this bottleneck is to diagonalize the $\tilde{H}$ matrix. When the radiation damping potential is not present, the $\tilde{H}$ matrix does not depend on energy and is real symmetric; therefore, the eigenvalues and eigenvectors of $\tilde{H}$ greatly simplify Eq. (90). This is accomplished as

$$\sum_{a'} \tilde{H}_{aa'} U_{a'\alpha} = U_{a\alpha} E_\alpha \tag{95}$$

and the new basis functions are

$$y_\alpha = \sum_a y_a U_{a\alpha} \ . \tag{96}$$

The R matrix is

$$R_{jj'}(E) = -\frac{1}{2} \sum_\alpha y_{j\alpha} y_{j'\alpha} / (E - E_\alpha) \tag{97}$$

and the coefficients of the y_α needed to construct the ψ_{Ej} function are given by

$$C_{\alpha j} = -\frac{1}{2} y_{j\alpha} / (E - E_\alpha) \ . \tag{98}$$

The radiation damping potential is complex symmetric and energy dependent, which does not allow such a simple expression for the R matrix. However, it is important to note that the radiation damping potential is of very low rank compared to the rank of $\tilde{H}$. When the methods of Secs. VIB and VIC are utilized the rank of the radiation potential is usually between 0 and 5 (rank 0 means all of the radiation damping potential can be completely incorporated into the close-coupling equations using the methods of Secs. VIB and VIC). The low rank of V_R can be used to find an expression for the R matrix that is computationally efficient. For this purpose, we assume that the atomic part of the Hamiltonian has been diagonalized as if no radiation damping were present. The matrix $E - \tilde{H}$ has the form $A + XBW$, where $A_{\alpha\alpha'} = (E - E_\alpha)\delta_{\alpha\alpha'}$, $X_{\alpha n} = \langle \alpha || \nabla || n \rangle$, $W_{n\alpha} = X_{\alpha n}$, $B_{nn'} = \delta_{nn'} 2i(E - E_n)/3c^3(2L+1)$ in LS coupling, and $B_{nn'} = \delta_{nn'} 2i(E - E_n)/3c^3(2J+1)$ in jj coupling. Matrices of the form $A + XBW$ can be inverted as

$$(A + XBW)^{-1} = A^{-1} - A^{-1} X (B^{-1} + W A^{-1} X)^{-1} W A^{-1} . \tag{99}$$

Using the definitions for A, B, X, and W gives an important new matrix

$$\gamma_{nn'} \equiv (B^{-1} + W A^{-1} X)_{nn'} = \frac{3c^3(2L+1)}{2i(E - E_n)} \delta_{nn'} + \sum_\alpha \langle \alpha || \nabla || n \rangle \langle \alpha || \nabla || n' \rangle / (E - E_\alpha) \tag{100}$$

for LS coupling (change $L \to J$ for jj coupling). Note that the only inversion in Eq. (99) that is nontrivial is γ^{-1}, which only has dimension equal to the number of decay states (usually ≤ 5). The R matrix is equal to

$$R_{jj'}(E) = -\frac{1}{2} \left(\sum_\alpha y_{j\alpha} y_{j'\alpha} / (E - E_\alpha) \right) - \sum_{\alpha\alpha' nn'} y_{j\alpha} y_{j'\alpha'} (\gamma^{-1})_{nn'} \langle \alpha || \nabla || n \rangle \times \langle \alpha' || \nabla || n' \rangle / [(E - E_\alpha)(E - E_{\alpha'})] \ . \tag{101}$$

If there were no radiation damping present, the elements

$$d^0_{jn} = -\frac{1}{2} \sum_\alpha y_{j\alpha} \langle \alpha || \nabla || n \rangle / (E - E_\alpha) \tag{102}$$

would be the reduced dipole matrix elements connecting the state $|\psi_n\rangle$ to the state $|\psi_{Ej}\rangle$ defined by Eq. (89) and the R matrix with no radiation damping is given by

$$R^0_{jj'}(E) = -\frac{1}{2} \sum_\alpha y_{j\alpha} y_{j'\alpha} / (E - E_\alpha). \tag{103}$$

The R matrix with radiation damping can be given very simply in terms of the γ matrix and these parameters when no radiation damping is present

$$R_{jj'}(E) = R^0_{jj'}(E) + 2 \sum_{n,n'} d^0_{jn} d^0_{j'n'} (\gamma^{-1})_{nn'} \ . \tag{104}$$

This is the main result of this section, which shows that the R-matrix method can be quickly and efficiently adapted to include radiation damping. For photoionization calculations the $R^0_{jj'}$ and d^0_{jn} are already calculated in standard R-matrix programs; the only term of Eq. (104) that needs to be added to the standard code is the calculation of the complex matrix γ^{-1}. In general this is a very small matrix that does not add much time to the regular close-coupling calculations. The coefficients of the basis functions are

$$C_{\alpha j}(E) = -\frac{1}{2} \left[y_{j\alpha} + 2 \sum_{n,n'} d^0_{jn} (\gamma^{-1})_{nn'} \times \langle \alpha || \nabla || n' \rangle \right] \Big/ (E - E_\alpha). \tag{105}$$

We have demonstrated in this section how the R-matrix method can be adapted to include radiation damping in the close-coupling equations. The modifications to the usual programs are not extensive. However, there are two classes of radiative decay that would be impossible to include using this method. The first type is the decay of high Rydberg states by photon emission from the core (called type-I transitions, e.g., $2pn\ell \to 1sn'\ell + \hbar\omega$, which occurs in scattering from hydrogenlike ions). The second type comes from high Rydberg states decaying to bound Rydberg states, which we call type-IIL (e.g., $1s^2 2p11\ell \to 1s^2 2p7\ell + \hbar\omega$, which occurs in scattering from Li-like Ar). The reason these types of decays cannot be included in an R-matrix treatment is because the

potential needs to be contained inside the R-matrix volume; these Rydberg states would necessitate an excessively large volume, which defeats the purpose of the R-matrix method.

B. Radiative decay of core states

The type-I transitions are the most important source of radiative decay in the near neutral atoms and near the Rydberg series limit. This type of decay is characterized by the decay of the core state, which leaves the outer electron's orbital almost unchanged. The prototype example of this type of decay is $1s\epsilon\ell \leftrightarrow 2pn\ell' \rightarrow 1sn'\ell' + \hbar\omega$ in scattering of electrons from hydrogenlike ions. This type of interaction was treated by Bell and Seaton [22]; our results reduce to theirs for long-range Coulomb interactions.

We wish to derive the equation governing the electronic wave function in the outer region of a multichannel scattering problem. To keep the derivation simple, we explicitly derive the results for when the channels are not coupled; the change to the close-coupling equations are identical when there is coupling between the channels. We do not assume any form for the potential outside of the core region so this method is applicable to scattering from ions with [23] and without electric fields.

We will let the decay state $|n\rangle$ be represented by $|n\rangle = |\Phi_c\rangle F_{nc}(\mathbf{r})$ (the decay states also include continuum states that have total energy less than E) and the scattering function by $|\psi_E^+\rangle = |\Phi_{c'}\rangle F_{Ec'}^+(\mathbf{r})$. If we project Eq. (8) with $\langle\Phi_{c'}|$ we obtain the differential equation

$$
\begin{aligned}
&(E - H_{c'} - E_{c'})F_{Ec'}(\mathbf{r}) \\
&= -\frac{2i}{3c^3}\sum_{n,j}|\langle\Phi_{c'}|P_j|\Phi_c\rangle|^2(E - E_n)F_{nc}(\mathbf{r})\langle F_{nc}|F_{Ec'}\rangle \\
&= -\frac{2i}{3c^3}\sum_{n,j}|\langle\Phi_{c'}|P_j|\Phi_c\rangle|^2(E - H_c - E_c) \\
&\quad\times F_{nc}(\mathbf{r})\langle F_{nc}|F_{Ec'}\rangle, \qquad (106)
\end{aligned}
$$

where E_c is the energy of the core state and $H_c = \langle\Phi_c|H|\Phi_c\rangle$. We note that an approximate expression can be obtained for the right-hand side of Eq. (106) by using closure

$$
\sum_n F_{nc}(\mathbf{r})\langle F_{nc}|F_{Ec'}\rangle \simeq F_{Ec'}(\mathbf{r}). \qquad (107)
$$

This approximate expression is actually extremely good because the sum over n also includes an integration over continuum states to energy $E - E_c$, where the overlap in Eq. (107) is extremely small. The approximation in Eq. (107) is much smaller than most other numerical approximations in atomic calculations and can therefore be considered an equivalence. Substituting this expression into Eq. (106) gives

$$
\begin{aligned}
&(E - H_{c'} - E_{c'})F_{Ec'}(\mathbf{r}) \\
&= \left[-\frac{2i}{3c^3}\sum_{n,j}|\langle\Phi_{c'}|P_j|\Phi_c\rangle|^2(E_{c'} - E_c)\right] \\
&\quad\times(E - H_c - E_c)F_{Ec'}/(E_{c'} - E_c). \qquad (108)
\end{aligned}
$$

The term in square brackets is $-i/2$ times the radiative decay rate from core state $|\Phi_{c'}\rangle$ to state $|\Phi_c\rangle$. We obtain the following expression for the other terms on the right-hand side of Eq. (108):

$$
\begin{aligned}
&(E - H_c - E_c)F_{Ec'}/(E_{c'} - E_c) \\
&= \left(1 + O(\Gamma_{c'}/\omega) + \frac{V_c - V_{c'}}{E_c - E_{c'}}\right)F_{Ec'} \simeq F_{Ec'}. \qquad (109)
\end{aligned}
$$

This is an extremely accurate approximation since the difference in core energies is much larger than the change in potential and the radiative decay rate is much smaller than the frequency of the emitted photon. The derivation of the asymptotic differential equations when the channels are coupled involves the same approximations as Eq. (109); the only change is that the difference in potentials on the right-hand side of this equation becomes a difference in multichannel potentials times multichannel wave functions. When we include all possible decay paths for the core, the equation governing type-I transitions is

$$
(E - H_{c'} - E_{c'})F_{Ec'} = -i\frac{\Gamma_{c'}}{2}F_{Ec'}, \qquad (110)
$$

where $\Gamma_{c'}$ is the total photodecay rate of the core state $|\Phi_{c'}\rangle$. The close-coupling equation governing type-I transitions (i.e., photodecay of a core state) is obtained by replacing the core energy

$$
E_{c'} \rightarrow E_{c'} - i\Gamma_{c'}/2. \qquad (111)
$$

This substitution holds for coupled channels and is independent of the type of long-range field acting on the electron. This is the main result of this section.

We would like to point out a complication that arises in applying this equation when calculating photoionization or photorecombination cross sections. In deriving this substitution we used closure, summing over bound states and integrating over continuum states. When $E < E_{c'}$ most of the overlap comes from bound states and when $E > E_{c'}$ most of the overlap comes from continuum states. This introduces complications in calculating photoionization and photorecombination cross sections since there are some cases when a photon is emitted but the electron can still escape the ion or the atom. The simplest way to account for this effect is to make the substitution $E_{c'} \rightarrow E_{c'} - i\Gamma_{c'}/2$ when $E < E_{c'}$ and not make the substitution when $E > E_{c'}$. This introduces errors when $|E - E_{c'}| < \Gamma_{c'}$. When $E < E_{c'}$, the approximation gives a photoionization (recombination) cross section that is too small (large) and when $E > E_{c'}$ this approximation gives a photoionization (recombination) cross section that is too large (small). When the calculated cross

section is convolved with a weight function, the errors from this approximation go to zero very rapidly as the width of the convolution function exceeds $\Gamma_{c'}$.

In the MQDT formulation discussed in Sec. V D, replacing $E_{c'}$ with $E_{c'} - i\Gamma_{c'}/2$ when $E < E_{c'}$ changes the asymptotic boundary conditions in the closed channels. This change entails replacing $\beta_{c'}(E) = Z\pi/\sqrt{2(E'_c - E)}$ with $\beta_{c'}(E) = Z\pi/\sqrt{2(E_{c'} - i\Gamma_{c'}/2 - E)}$; the branch of the square root needs to be chosed such that $\mathrm{Re}(\beta_{c'}) > 0$. When the energy is several widths below threshold

$$\beta_{c'}(E) \simeq Z\pi/\sqrt{2(E_{c'} - E)} + i\frac{\Gamma_{c'}}{2} Z\pi/[2(E_{c'} - E)]^{3/2}$$
$$= \pi\nu + i\frac{\Gamma_{c'}}{2}\pi\nu^3/Z^2. \quad (112)$$

When this form of $\beta_{c'}$ is substituted into Eq. (78) we find the physical S matrix to be

$$S_{oo} = \mathcal{S}_{oo} - \mathcal{S}_{oc}[\mathcal{S}_{cc} - G(\nu_c)e^{-2i\pi\nu_c}]^{-1}\mathcal{S}_{co}, \quad (113)$$

where $G(\nu_{c'}) = \exp(\pi\Gamma_{c'}\nu_{c'}^3/Z^2)$. This is the formula obtained by Bell and Seaton [22].

There are two possible methods for numerically implementing this type of radiation damping. The first method calculates the damping through the use of unphysical scattering functions Eqs. (74)–(76) without including *any* effect from the type-I radiation damping. When the closed channels are eliminated, use $\beta_c(E) = Z\pi/\sqrt{2(E_c - i\Gamma_c/2 - E}$ with the branch $\mathrm{Re}(\beta_c) > 0$ in the MQDT equations. This treatment is very similar in spirit to the usual use of MQDT in physics of complicated atoms (for example, see Ref. [17]). In the usual calculations the unphysical scattering parameters are obtained by matching the R-matrix solutions to the outer functions using the theoretical thresholds; however, in the MQDT part of the calculation the experimental thresholds are used. The second method includes the final decay state in the R-matrix part of the calculation and matches to outer solutions of the close-coupling equations with the complex core energies. (For high n it is a good approximation to neglect the type-I radiative decay in the R-matrix region and match to outer solutions of the close-coupling equations with the complex core energies.) If it is computationally feasible, the first method should be preferred.

C. Decay of Rydberg state to Rydberg state

The dominant mode of radiative decay depends on the charge on the ion and the principal quantum number of the Rydberg state. For near neutral atoms and near the series limit, type-I transitions dominate the decay. As the charge on the ion increases, type-II transitions become more important and can be more important than the type-I transitions. Type-II transitions to small final states (type IIS) can be included in R-matrix calculations described in Sec. VI A. Type-II transitions to large final states (type IIL) cannot be included in R-matrix calculations but can be included using a perturbative treatment for the unphysical $\mathcal{K}$ matrix or for the asymptotic wave function. We can obtain accurate results with *either* method because these types of transitions only become important when the ionic charge becomes large and thus the $\mathcal{K}$ matrix is small. As discussed in Sec. V D, treating the radiation damping potential as a perturbation on the $\mathcal{K}$ matrix of the unphysical wave function gives much more accurate results than treating the radiation damping potential as a perturbation on the physical wave function.

One way to obtain the $\mathcal{K}$ matrix including type-IIL transitions is to use a Born-type perturbation theory

$$\mathcal{K}_{jj'} = \mathcal{K}^0_{jj'} - \pi\langle\psi^0_j|V|\psi^0_{j'}\rangle, \quad (114)$$

where the $\mathcal{K}^0_{jj'}$ is the $\mathcal{K}$ matrix excluding type-IIL transitions, the potential V is the radiation damping potential for type-IIL transitions, and the $|\psi^0_j\rangle$ have the form

$$|\psi^0_j\rangle = \sum_{j'} |\Phi_{j'}\rangle(f_{j'}\delta_{j'j} - g_{j'}\mathcal{K}^0_{j'j}), \quad (115)$$

where the sum extends over both closed and open channels. The $|\psi^0_j\rangle$ diverge in the closed channels; however, the integrals in Eq. (114) are well defined because the potential V converges exponentially to zero with distance faster than the $|\psi^0_j\rangle$ diverge.

We do not evaluate Eq. (114) exactly because of the complications of evaluating that sort of multichannel matrix element. For most applications, the $|\psi^0_j\rangle$ and the $|\psi_n\rangle$ states in the potential V are multichannel wave functions. However, the channel couplings are usually very small and the change in quantum defect as the total $JLS\Pi$ of the wave function changes is also very small for highly charged ions. We can obtain a good approximation to the correction of the $\mathcal{K}$ matrix by using a configuration average type approach

$$-\pi\langle\psi^0_j|V|\psi^0_{j'}\rangle$$
$$\simeq \delta_{jj'}\frac{2\pi i}{3c^3(2\ell^j_o + 1)}$$
$$\times \sum_n \delta_{\ell^n_o \pm 1, \ell^j_o}(E - E_{c,j} - \varepsilon_n)|\langle F_n||\nabla||f_j\rangle|^2, \quad (116)$$

where ℓ^j_o (ℓ^n_o) is the orbital angular momentum of the outer electron in channel j (for state n), $\varepsilon_n = -Z^2/2(n-\mu)^2$ where μ is the quantum defect, f_j is the energy normalized continuum function, and F_n is the volume normalized radial function of the outer electron. This expression is for LS coupling; in jj coupling, ℓ_o would need to be replaced by the total angular momentum of the outer electron. Both F_n and f_j are calculated as distorted waves in a static Hartree potential. Essentially identical results are obtained when F_n and f_j are Coulomb waves for all space and $\mu = 0$. This approximation has been tested [8] in scattering from Ar^{15+} by increasing the size of the R-matrix volume and including more decay states in the R-matrix calculation and including less states through the approximation of Eq. (114). For this

ion, we obtained errors at the percent level when using Eqs. (114) and (116) for states $n \geq 3$ and including the $2s^2$, $2s2p$, and $2p^2$ decay states in the R-matrix calculation.

VII. DISCUSSION

The majority of this paper addresses the ramifications and positive aspects of describing radiation damping using an optical potential and the R-matrix method to describe radiation damping. In order to give a realistic assessment of the impact this method may have we would like to address some of the "liabilities" of using this method.

The power of using this method is that existing R-matrix programs can be modified in a relatively straightforward manner to incorporate radiation damping. These codes have been successful in describing very complicated atomic scattering processes. A possible drawback of the method is that it may be necessary to include a large number of decay states in the R-matrix equations. As the number of decay states increases the matrix inversion in Eq. (104) becomes increasingly time consuming. This may make the practical solution of the R-matrix equations too slow in some cases. Although this is a possibility, it does not seem likely that the number of decay channels will be large due to the approximate methods discussed in Secs. VI B and VI C.

Another difficulty of the method is an inherent problem in all R-matrix methods. The only large-scale practical method for obtaining convolved cross sections is to calculate the infinite resolution cross section on an energy mesh fine enough to trace out all of the relevant resonances. In practice, this may mean an extremely fine mesh and a huge number of mesh points. (This problem is not as acute for electron scattering cross sections as it is for photoionization and photorecombination cross sections.) This is not a problem in perturbative calculations since the energies, widths, and branching ratios for each resonance are calculated directly, which means convolved cross sections can be simply obtained by analytically integrating Lorentzians with the weight functions. We note that in certain circumstances, especially electron scattering and photoionization cross sections, this liability can be a strength since the R-matrix method easily allows all of the resonances and continua to interact with each other. Also, any interference phenomena are automatically included in the calculation.

In this paper we have described a method for including radiation damping in atomic scattering calculations. The successful application of this method has resulted from a combination of numerical, analytical, and perturbative techniques applied to the solutions of atomic Hamiltonians with the nonlocal radiation damping potential. In this paper we have not presented any applications of this method to any specific problems. However, the method has successfully described photorecombination cross sections in Ar^{15+} and model calculations on photoionization of Fe^{24+} [8]. We will report further applications of this method for electron impact excitation cross sections in later papers.

We have formulated the problem and the solution of radiation damping in a way that could be easily incorporated within standard atomic scattering programs without much effort. This should allow the routine inclusion of radiation damping effects into atomic scattering calculations.

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