

## Unified description of radiative and dielectronic recombination, including the coupling between autoionization and radiation continua

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Although dielectronic and radiative recombination are usually treated as distinct noninterfering processes, Alber, Cooper, and Rau [Phys. Rev. A **30**, 2845 (1984)] have recently presented a scattering- or  $S$ -matrix analysis which provides a unified description of these processes. This description employs a diagonalization of the atom plus radiation field Hamiltonian using a limited basis set consisting of one discrete autoionizing state, a single-electron continuum, and a single-photon continuum. In the present work we extend Møller scattering operator and resolvent operator techniques, which have previously been used to discuss the decay of prepared systems, in order to provide an  $S$ -matrix analysis of the electron-ion photorecombination process near an isolated autoionizing resonance. We explicitly allow for degenerate magnetic sublevels of the atomic system and for multiple angular momentum contributions in the partial-wave expansion of the electron-continuum eigenstate. After the introduction of the pole approximation, in which only the  $\delta$ -function term is retained in the evaluation of the various self-energies that occur in the diagonalization of the Hamiltonian for the combined many-electron radiation-field system, we obtain the total electron-ion photorecombination cross section as the sum of the radiative and dielectronic recombination contributions together with the conventionally ignored interference term. The radiative and dielectronic recombination cross sections reduce to the familiar forms when the continuum-continuum coupling effects are neglected. Alternatively, the combined cross section for the entire electron-ion photorecombination process may be represented by a modified Fano line profile, which is shifted and broadened as a result of the coupling between the autoionization and radiation continua. Recombination processes that involve more than a single state of the initial ion, of the autoionizing resonance, or of the final system can be treated by appropriately augmenting the unperturbed basis set. It is anticipated that the effects of the interference between radiative and dielectronic recombination and of the continuum-continuum coupling will be most important for individual transitions involving low-lying autoionizing levels and will probably be negligible for the total dielectronic recombination rates due to the highly excited levels.

### I. INTRODUCTION

In the ordinary nonresonant radiative recombination process<sup>1</sup>

$$X^{+(Z)}(i) + e^{-}(\mathbf{p}) \rightarrow X^{+(Z-1)}(f) + \hbar\mathbf{k}, \quad (1)$$

an electron with momentum  $\mathbf{p}$  is captured by an ion with residual charge  $Z$  that is initially in the quantum eigenstate  $|i\rangle$ , and a photon is emitted simultaneously with momentum  $\hbar\mathbf{k}$ . The final state  $|f\rangle$  of the recombined ion, which is the result of this direct recombination process, is most probably low-lying bound state. The direct radiative recombination process is precisely the inverse of the ordinary nonresonant photoionization process from the state  $|f\rangle$ .

In a low-density high-temperature plasma, such as a so-

lar flare or a tokamak discharge, multiply charged atomic ions tend to recombine predominantly by the two-step dielectronic recombination process. Dielectronic recombination was first described by Bates and Massey<sup>2</sup> in 1943 in connection with low-temperature phenomena. The importance of dielectronic recombination in high-temperature plasma was not fully recognized until 1964 when Burgess<sup>3</sup> first pointed out that very large recombination rates can be derived by taking into account the relatively high probabilities for recombination into the highly excited levels  $|f\rangle$ , which form a Rydberg series converging to the level  $|i\rangle$  of the initial ion.

The initial step in the two-step resonant dielectronic recombination process is the radiationless capture of a plasma electron

$$X^{+(Z)}(i) + e^{-}(\mathbf{p}) \rightarrow X^{+(Z-1)}(a), \quad (2)$$

to form a doubly excited autoionizing state  $|a\rangle$ . The accompaniment of the radiationless capture process by the excitation of the recombining ion is necessary for total energy conservation. Recombination is accomplished if, instead of autoionizing by means of the inverse of the capture process (2), the doubly excited state  $|a\rangle$  undergoes a radiatively stabilizing transition to a bound final state  $|f\rangle$ ,

$$X^{+(Z-1)}(a) \rightarrow X^{+(Z-1)}(f) + \hbar\mathbf{k}. \quad (3)$$

This radiative stabilization occurs predominantly through the deexcitation of the recombining ion core when the incident electron is captured into a high Rydberg level. Such inner-electron stabilizations usually play the dominant role in the dielectronic recombination process.

Recently there has been intense activity in colliding beam investigations<sup>4,5</sup> of electron-ion photorecombination, which have led to spectacular experimental confirmations of the theoretically predicted<sup>6-8</sup> electric-field-induced dielectronic recombination process. There has also been a general recognition of the importance of dielectronic recombination, both in the determination of the ionization-recombination equilibrium charge-state distributions<sup>9,10</sup> of multiply charged ions in high-temperature plasmas, and in the production of the x-ray line emission spectra.<sup>11,12</sup> These developments have provided motivation for the formulation of a more fundamental quantum-mechanical description than the traditional picture of radiative and dielectronic recombination. While simplified calculations that are based on the conventional theory may ultimately be proven to be adequate for estimating the total recombination rates that occur in the determination of the ionization-recombination balance, a precise treatment, which is based on a fundamental quantum-mechanical foundation, is expected to be essential for the reliable theoretical prediction of emission spectra due to the individual radiatively stabilizing transitions of Eq. (3). These radiative transitions can produce prominent satellites in the vicinity of the resonance lines that are associated with deexcitations of the recombining ion. Resolvable dielectronic satellites can be utilized for spectroscopic determinations of basic plasma properties,<sup>13,14</sup> such as temperatures, densities, and states of ionization. Unresolvable satellites may provide substantial contributions to the observed intensities of the resonance lines.

In order to develop a fundamental quantum-mechanical description, it is necessary to abandon the artificial distinction between the nonresonant radiative and the resonant dielectronic recombination mechanisms. A unified description is natural because both recombination mechanisms obviously involve identical initial and final states of the combined electron-ion plus radiation-field system. It was first pointed out by Shore<sup>15</sup> that a unified treatment can be accomplished by fully utilizing the methods of multichannel collision theory<sup>16</sup> and quantum electrodynamics.<sup>17</sup> The total cross section describing the combined electron-ion photorecombination process that is obtained for an isolated resonance can thereby be expressed as the sum

$$\begin{aligned} \sigma(i, \mathbf{p} \rightarrow f, \mathbf{k}) = & \sigma_{\text{RR}}(i, \mathbf{p} \rightarrow f, \mathbf{k}) + \sigma_{\text{DR}}(i, \mathbf{p} \rightarrow f, \mathbf{k}) \\ & + \sigma_{\text{int}}(i, \mathbf{p} \rightarrow f, \mathbf{k}), \end{aligned} \quad (4)$$

of the radiative recombination (denoted by RR) and dielectronic recombination (denoted by DR) cross sections plus the usually ignored interference term (denoted by int).

In a rigorous quantum-mechanical description of the combined electron-ion photorecombination process, one should treat in a consistent manner the interactions responsible for autoionization and spontaneous radiative decay. Spontaneous radiative decay is well known to be the result of the interaction between the atomic electrons and the quantized radiation field, while autoionization is usually described in terms of the effective (configuration-space) interaction between the atomic electrons. In the lowest nonvanishing order of quantum electrodynamical perturbation theory,<sup>17</sup> this effective interaction is mediated by the virtual emission and reabsorption of a photon. Armstrong, Theodosiou, and Wall<sup>18</sup> presented a description of autoionization and radiative decay for a system initially in the doubly excited state in which both interactions were treated on an equal footing and in a consistent manner. They were able to derive approximate expressions for the modified autoionization and radiative transition probabilities from the autoionizing state in the presence of the electromagnetic coupling between the electron and photon continua. These transition probabilities have the same familiar branching-ratio form as the conventional unperturbed probabilities, but they are expressed in terms of effective autoionization and radiative decay rates that incorporate the continuum-continuum coupling. The approximate expressions obtained by Armstrong, Theodosiou, and Wall<sup>18</sup> were subsequently rederived by Haan and Cooper,<sup>19</sup> using multichannel scattering theory techniques, and were shown to have a wider region of validity than was originally recognized. This theory of autoionization and spontaneous radiative decay in the presence of the electromagnetic coupling between the final-state continua has been recently extended by Jacobs<sup>20</sup> to explicitly take into account the angular momentum degeneracy of the atomic levels and the multiplicity of angular momentum components in the partial-wave expansion for the electron-continuum state.

In order to predict the dielectronic recombination cross section and satellite line intensity, the analysis of autoionization and radiative decay must be combined with a description of the electron-ion collision mechanism that is responsible for the excitation of the intermediate autoionizing resonance state. The dielectronic recombination cross section [ $\sigma_{\text{DR}}$ —see Eq. (4)] can be expressed in the familiar Breit-Wigner form<sup>21,22</sup> (as the product of the radiationless electron-capture cross section and the probability for the radiatively stabilizing transition) by considering a system which is initially prepared in the doubly excited state (in contrast to a free electron and an ion) and by making the isolated-resonance approximation. The isolated-resonance approximation has been recently applied<sup>23</sup> in a investigation of the effects of the continuum-continuum coupling on dielectronic satellite line intensities. The continuum-continuum coupling effects were in-

corporated by the introduction of effective autoionization and radiative transition rates, which were defined in terms of the unperturbed rates and the Fano line-profile parameter.<sup>24</sup> The objective of the present investigation is to provide a unified  $S$ -matrix description, by means of which the continuum-continuum coupling effects can be consistently included in all three terms of Eq. (4).

An  $S$ -matrix description of the combined electron-ion photorecombination process has been presented by Davies and Seaton,<sup>25</sup> and their approach has been adopted by Bell and Seaton<sup>26</sup> and by Alber, Cooper, and Rau<sup>27</sup> to develop unified treatments of radiative and dielectronic recombination. These treatments rely on the preliminary determination of a structured electron continuum, which describes the combined resonant and nonresonant electron-ion collision process in the absence of the atom-field interaction. The electron-ion scattering and photorecombination cross sections that are obtained utilizing this structured electron-continuum eigenstate exhibit the characteristic Fano line shape<sup>28</sup> in the vicinity of the autoionizing resonance. The combined resonant plus nonresonant electron continuum together with the unperturbed photon continuum are subsequently employed in these treatments as a basis set for the exact diagonalization of the complete Hamiltonian that includes the atom-field interaction. The  $S$  matrix obtained from this exact sequential diagonalization then leads to the prediction of a modified Fano line shape, which incorporates the continuum-continuum coupling, as has been emphasized by Alber, Cooper, and Rau.<sup>27</sup>

In the present investigation the interactions responsible for autoionization and spontaneous radiative emission are treated on an equal footing by employing a simultaneous diagonalization procedure. Rather than introducing a perturbation expansion, we exploit the exact diagonalization of the Hamiltonian for the interacting atom-field system that can be accomplished by restricting the unperturbed basis set to include only a single discrete autoionizing state and the nonresonant electron- and photon-continuum states corresponding to the first-order autoionization and radiative decay processes. This exact diagonalization is achieved by utilizing the multichannel scattering-operator techniques that were exploited by Haan and Cooper<sup>19</sup> and subsequently extended by Jacobs<sup>20</sup> to derive exact closed-form expressions for the probabilities of autoionization and radiative emission in the presence of the continuum-continuum coupling. Instead of using the initial condition that the atomic system is prepared in the autoionizing state, we now present an  $S$ -matrix description of the electron-ion photorecombination process. The introduction of vertex functions and a modified autoionizing-state propagator enables the  $S$  matrix to be expressed in the familiar form as the sum of a resonant and a nonresonant transition amplitude.

The  $S$ -matrix formulation in terms of vertex functions and a modified propagator has been developed with the ultimate objective of providing a framework that would be suitable for the precise nonperturbative incorporation of radiative corrections, i.e., corrections to the lowest-order  $S$  matrix that would result from the application of relativistic quantum electrodynamical perturbation theory<sup>17</sup> to all

orders. These higher-order corrections could be represented by Feynman diagrams that would involve the virtual emissions and reabsorptions of photons. In the present investigation this nonperturbative analysis is accomplished by means of the exact diagonalization of the complete atom-field Hamiltonian within the subspace of a severely restricted basis set of unperturbed eigenstates. In addition, the total electron-ion photorecombination cross section is explicitly evaluated by introducing the pole approximation<sup>19</sup> in which only the  $\delta$ -function term is retained in the evaluation of the self-energy operators that arise from the exact simultaneous diagonalization. (The validity of the pole approximation will be discussed in Sec. III A.) In order to provide a fully consistent treatment of the higher-order corrections, it may be necessary in a future investigation not only to reconsider these two approximations but also to confront the well-known obstacles that have prevented the formulation of a rigorous and practical description of relativistic many-electron atomic systems.

The difficulties associated with the description of a relativistic many-electron atom are encountered in the partition of the lowest-order electron-electron interaction which is responsible for autoionization. We have chosen to include this interaction as a perturbation on an equal footing with the atom-field interaction. The relativistic electron-electron interaction may be represented to lowest order in the Møller form,<sup>29</sup> which corresponds to the virtual exchange of a single photon.<sup>17</sup> However, the inclusion of a substantial portion of the electron-electron interaction in the unperturbed Hamiltonian has been found to be essential for a practical description of a many-electron system. This modification of our treatment of the electron-electron interaction can be made in a precise manner by introducing the Feshbach projection operators<sup>30,31</sup>  $P$  and  $Q$ , which project onto the subspaces spanned by the open and closed electron-continuum channels, respectively. A more balanced definition would also involve the analogous photon-continuum channel projection operators, but this extension will not be needed for the description of the photorecombination process of interest. Unfortunately, the inclusion of some virtual photon-exchange effects in the unperturbed Hamiltonian not only appears unappealing from the viewpoint of quantum field theory but also, as has been demonstrated by Sucher,<sup>32</sup> has the disadvantage of providing a suitable unperturbed basis for the rigorous and systematic incorporation of radiative corrections only with the introduction of positive-energy projection operators, which immensely complicate the treatment of the unperturbed problem.

For high- $Z$  few-electron systems, a treatment that fully utilizes the methods of relativistic quantum field theory would appear to be appropriate and could be successful. Such a treatment would have the attractive features that all radiative corrections could be incorporated in a systematic and consistent manner and that renormalization counter terms could be included in an unambiguous fashion. An approach that might be worthy of consideration would be an extension to the collision process of the full QED approach that has been recently applied by Mohr<sup>33</sup> in a precise evaluation of radiative corrections to

the energy eigenvalues of two-electron ions. In this full QED approach, perturbation theory is applied as an expansion in terms of a basis of noninteracting Dirac electrons and positrons that are bound by the static nuclear Coulombic potential, as in the Furry bound-state interaction picture<sup>34</sup> of quantum electrodynamics. Both the electron-electron interactions and radiative corrections then arise consistently as perturbations produced by the interaction of the bound electrons with the quantized radiation field. These perturbations are expected to decrease as the nuclear charge  $Z$  is increased. The adoption of such an approach to the description of the electron-ion photorecombination process would involve substantial modifications to the present analysis, in order to utilize a basis set consisting of both single-electron and single-positron states, and may ultimately have practical application only to very-few-electron systems.

The remainder of this paper has been arranged as follows: In Sec. II the  $S$ -matrix approach is developed to provide a unified description of radiative and dielectronic recombination. The one-discrete-autoionizing-level and two-continua approximation<sup>18,19</sup> is utilized in its extended form<sup>20</sup> to allow for the degenerate magnetic substates of the atomic eigenstates and for a multiplicity of angular momentum contributions in the partial-wave expansion for the electron-continuum state. Assuming that this severely restricted basis set of unperturbed eigenstates provides an adequate representation, the Møller scattering-operator method<sup>16</sup> is employed to perform an exact simultaneous diagonalization of the complete Hamiltonian for the interacting many-electron atom and quantized radiation-field system. The  $S$  matrix is thereby obtained in the familiar form, as the sum of a resonant and a non-resonant transition amplitude, with the introduction of vertex corrections and autoionizing-state propagator modifications. Exact closed-form expressions are presented for the vertex functions and for the modified propagator.

In Sec. III the vertex functions and the modified autoionizing-resonance propagator are evaluated in the pole approximation. The cross sections corresponding to radiative and dielectronic recombination, together with the contribution that involves the interference between the nonresonant and the resonant transition amplitudes, are thereby expressed in terms of the familiar unperturbed autoionization and radiative decay rates and the non-resonant photoionization cross sections. Through the introduction of effective decay rates, which incorporate the continuum-continuum coupling, the dielectronic recombination cross section  $\sigma_{DR}$  [Eq. (4)] is expressed in the same well-known Breit-Wigner form<sup>21,22</sup> as the cross section in the absence of the continuum-continuum coupling. The conclusions of the present investigation are presented in Sec. IV, together with a discussion of future extensions to incorporate multi-continuum-channel recombination, the effects of overlapping autoionizing resonances, renormalization, and the effects of collisional dephasing processes and plasma electric microfields.

## II. THE $S$ -MATRIX DESCRIPTION

Bell and Seaton<sup>26</sup> have pointed out that the scattering operator provides a unified description of four distinguish-

able elementary processes. By considering different elements of the scattering operator, we can treat electron-ion photorecombination, electron-ion scattering, photoionization, and photon-ion scattering. These binary collision processes may be schematically represented by the scattering diagrams shown in Fig. 1, which includes the relevant Fock-space  $S$ -matrix elements. The double lines represent bound states of the many-electron atomic system. The electron-spin projection and photon-polarization quantum numbers  $m_s$  and  $\lambda$  have been explicitly designated, whereas the total electronic angular-momentum-projection quantum numbers  $M_i$  and  $M_f$  are understood to be included in the detailed specifications of the states  $|i\rangle$  and  $|f\rangle$ , which refer, respectively, to the initial recombining ion and the final recombined atomic system in the photorecombination process. We emphasize that the contracted diagrams in Fig. 1 represent the complete  $S$ -matrix elements and not only the lowest-order nonvanishing perturbation theory contributions.

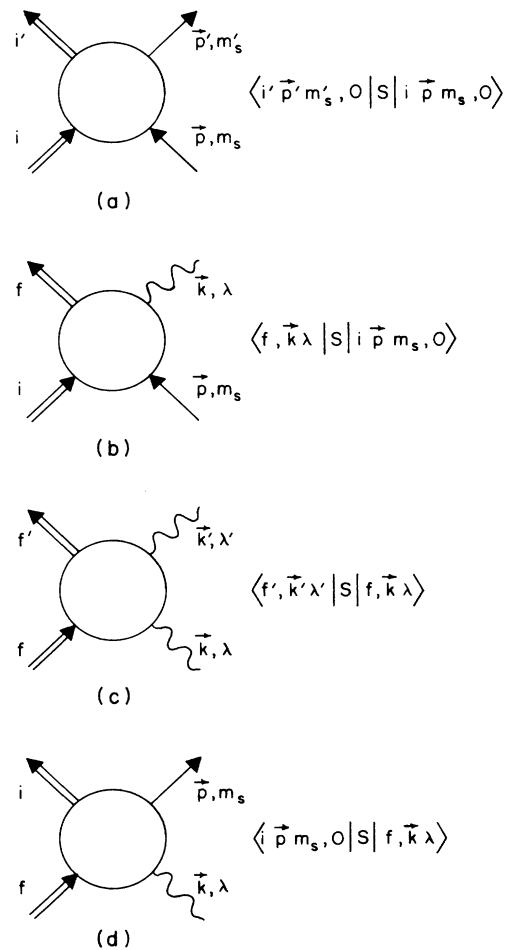


FIG. 1. Diagrams representing electron-ion scattering (a), electron-ion photorecombination (b), photon-ion scattering (c), and photoionization (d), together with the corresponding Fock-space  $S$ -matrix elements. Double lines represent many-electron bound states.

### A. Connection with the resolvent operator

Let us assume that we have obtained the eigenstates of the unperturbed Hamiltonian

$$H^0 = H_A + H_F, \quad (5)$$

which consists of the unperturbed Hamiltonian  $H_A$  for the relativistic many-electron atomic system and of the Hamiltonian  $H_F$  for the free radiation field. We select a restricted basis set of these unperturbed eigenstates that includes only the direct-product states  $|a,0\rangle$ ,  $|ipm_s,0\rangle$ , and  $|f,k\lambda\rangle$ . These states represent, respectively, the autoionizing state, the nonresonant electron-ion scattering continuum supporting a single electron of momentum  $\mathbf{p}$  (which is allowed to vary) and spin  $m_s = \pm \frac{1}{2}$ , and the photon-emission continuum supporting a photon of wave number  $\mathbf{k}$  (which is also allowed to vary) and polarization  $\lambda = 1, 2$ . The two continua are the two asymptotic decay channels of the autoionizing state. Note that the photon Fock-space basis is restricted to include only the occupation number state vectors  $|n_k\rangle$  with  $n_k = 0$  and  $n_k = 1$  photons in the quantized-radiation field. The atomic states  $|i\rangle$ ,  $|a\rangle$ , and  $|f\rangle$  are assumed to be eigenstates with total electronic-angular-momentum quantum numbers  $J_i$ ,  $J_a$ , and  $J_f$  and may each consist of degenerate magnetic substates specified by the projection quantum number  $M_i$ ,  $M_a$ , and  $M_f$ , respectively. The use of the one-discrete-level and two-continua basis set of unperturbed eigenstates clearly restricts the scope of our present treatment to elastic electron and photon scattering processes, to single-continuum-channel recombination and photoionization processes, and to isolated-resonance phenomena.

The interacting relativistic many-electron atom and quantized radiation-field system can be described in terms of the complete Hamiltonian operator

$$H = H_A + H_F + H_{AF} = H^0 + V, \quad (6)$$

which consists of the unperturbed Hamiltonians  $H_A$  and  $H_F$  for the atomic system and free radiation field combined with the atom-field interaction  $H_{AF}$ . To provide a precise description of the autoionization process, we now introduce the Feshbach projection operators<sup>30,31</sup>  $P$  and  $Q$ . The operator  $P$  projects onto the subspace of the open electron-continuum channel eigenstate  $|ipm_s,0\rangle$ , while the operator  $Q$  projects onto the subspace of the closed-channel autoionizing state  $|a,0\rangle$ . A third projection operator  $R$  could be introduced which projects onto the subspace of the photon-continuum channel eigenstate  $|f,k\lambda\rangle$ , but the explicit indication of this operator will not be necessary in the present investigation. The explicit representations of the projection operators  $P$  and  $Q$ , in terms of our restricted basis set, are given by the relations

$$P = \sum_{M_i} \sum_{m_s} \int d^3p |ipm_s,0\rangle \langle ipm_s,0|, \quad (7a)$$

$$Q = \sum_{M_a} |a,0\rangle \langle a,0|. \quad (7b)$$

The perturbation operator  $V$  can now be taken to be the sum of the atom-field interaction  $H_{AF}$  and the projected interaction  $PH_AQ + QH_AP$ , which is the precise form of the interaction that is responsible for autoionization. For a consistent partition of the Hamiltonian  $H$ , the unperturbed Hamiltonian  $H^0$  must now be taken as the sum of  $H_F$  and the projected atomic Hamiltonian  $PH_AP + QH_AQ$ . The electron-continuum state  $|ipm_s,0\rangle$  is rigorously an eigenstate of  $PH_AP$ , while the autoionizing state  $|a,0\rangle$  is precisely an eigenstate of  $QH_AQ$ .

In order to derive expressions for the scattering operator, it is advantageous to introduce the transition operator  $T$ . The matrix elements of the operators  $S$  and  $T$  for the electron-ion scattering and photorecombination processes are connected by the relationships

$$\begin{aligned} \langle i'p'm'_s,0 | S | ipm_s,0 \rangle &= \delta^3(\mathbf{p}' - \mathbf{p}) \delta(i', i) \delta(m'_s, m_s) \\ &\quad - 2\pi i \delta(E'_p - E_p) \lim_{\epsilon \rightarrow 0} \langle i'p'm'_s,0 | T(E_p + i\epsilon) | ipm_s,0 \rangle, \end{aligned} \quad (8a)$$

$$\begin{aligned} \langle f, k\lambda | S | ipm_s,0 \rangle &= -2\pi i \delta(E_k - E_p) \lim_{\epsilon \rightarrow 0} \langle f, k\lambda | T(E_k + i\epsilon) | ipm_s,0 \rangle, \end{aligned} \quad (8b)$$

where the total continuum energy eigenvalues are defined by

$$E_p = E_i + \epsilon_p, \quad (9a)$$

$$E_k = E_f + \hbar\omega_k. \quad (9b)$$

We now exploit the relationship<sup>16</sup>

$$G(z)V = G_0(z)T(z), \quad (10)$$

where  $G(z) = (z - H)^{-1}$  is the resolvent, or Green's operator, and where  $G_0(z)$  represents  $(z - H^0)^{-1}$ . Thus the  $T$  matrix is found to satisfy the relation

$$T(z) = (z - H^0)G(z)V, \quad (11)$$

which can be shown to be in agreement with the reduction formula that is employed in quantum field theory. With the introduction of our restricted basis set of unperturbed eigenstates and the use of the non-Hermitian properties  $T^\dagger(z) = T(z^*)$  and  $G^\dagger(z) = G(z^*)$ , the required matrix elements of  $T$  can be evaluated by means of the expansions

$$\begin{aligned} \langle f, k\lambda | T(z) | ipm_s,0 \rangle &= \sum_{M_a} \langle f, k\lambda | V | a,0 \rangle \langle a,0 | G(z)(z - H^0) | ipm_s,0 \rangle \\ &\quad + \sum_{M'_i} \sum_{m'_s} \int d^3p' \langle f, k\lambda | V | i'p'm'_s,0 \rangle \langle i'p'm'_s,0 | G(z)(z - H^0) | ipm_s,0 \rangle \\ &\quad + \sum_{M'_f} \sum_{\lambda'} \sum_{\mathbf{k}'} \langle f, k\lambda | V | f', \mathbf{k}'\lambda' \rangle \langle f', \mathbf{k}'\lambda' | G(z)(z - H^0) | ipm_s,0 \rangle, \end{aligned} \quad (12)$$

$$\begin{aligned}
\langle i'p'm'_s,0 | T(z) | ipm_s,0 \rangle &= + \sum_{M_a} \langle i'p'm'_s,0 | V | a,0 \rangle \langle a,0 | G(z)(z-H^0) | ipm_s,0 \rangle \\
&+ \sum_{M_i'' m_s''} \int d^3p'' \langle i'p'm'_s,0 | V | i''p''m_s'',0 \rangle \langle i''p''m_s'',0 | G(z)(z-H^0) | ipm_s,0 \rangle \\
&+ \sum_{M_f} \sum_{\lambda} \sum_{\mathbf{k}} \langle i'p'm'_s,0 | V | f,\mathbf{k}\lambda \rangle \langle f,\mathbf{k}\lambda | G(z)(z-H^0) | ipm_s,0 \rangle .
\end{aligned} \tag{13}$$

It should be noted that the severely restricted basis set of unperturbed eigenstates includes primed atomic eigenstates, such as  $|i'\rangle$  and  $|f'\rangle$ , which within our basis can differ from the corresponding unprimed eigenstates only with respect to the magnetic quantum numbers  $M_i$  and  $M_f$ . These expansions for the matrix elements of  $T$  are simplified substantially by taking advantage of the fact that the perturbation matrix elements satisfy the conditions

$$\langle ipm_s,0 | V | i'p'm'_s,0 \rangle = 0 , \tag{14}$$

$$\langle f,\mathbf{k}\lambda | V | f',\mathbf{k}'\lambda' \rangle = 0 . \tag{15}$$

Analogous expansions can be derived for the matrix elements of  $T$  that are required for photon-ion scattering and photoionization. We note that the  $S$ -matrix elements describing recombination and photoionization are related on account of charge-conjugation and time-reversal invariance.<sup>17</sup>

In the remaining sections of this paper we will find the necessary matrix elements of  $G(z)$ , and then we will construct the desired matrix elements of  $T(z)$  using Eqs. (12) and (13). We wish to close this section, however, with a short discussion of the relationship between the operator  $T$  and the Møller operator  $\Omega_+$ .

$T(z)$  is defined by

$$T(z) \equiv V + VG(z)V , \tag{16}$$

and therefore

$$T(E_p + i\epsilon) | ipm_s,0 \rangle = V\Omega_+ | ipm_s,0 \rangle \equiv V | ipm_s,0+ \rangle , \tag{17}$$

where we have introduced the plus sign to denote the outgoing-wave boundary condition and have used the well-known relation

$$\Omega_+ | ipm_s,0 \rangle = [1 + G(E_p + i\epsilon)V] | ipm_s,0 \rangle . \tag{18}$$

Projecting Eq. (17) onto some final state such as  $|f,\mathbf{k}\lambda\rangle$  and using Eq. (8b) gives

$$\begin{aligned}
\langle f,\mathbf{k}\lambda | S | ipm_s,0 \rangle \\
= -2\pi i \delta(E_k - E_p) \langle f,\mathbf{k}\lambda | V | ipm_s,0+ \rangle .
\end{aligned} \tag{19}$$

Thus the scattering matrix for recombination is directly proportional to the matrix element of the interaction  $V$  between the unperturbed final state of interest and the diagonalized initial continuum state. An analogous relationship can be derived involving the unperturbed initial state

and the diagonalized final state by utilizing the Møller operator  $\Omega_-$  that corresponds to the incoming-wave boundary condition.

To cite the simplest case for illustration, suppose we neglect magnetic degeneracies and other complications and simply write  $|i\epsilon_p\rangle$  for  $|ipm_s,0\rangle$  and  $|f\omega_k\rangle$  for  $|f,\mathbf{k}\lambda\rangle$ . Our system then becomes equivalent to that studied by Alber, Cooper, and Rau.<sup>27</sup> Because of the separability of the coupling involving photon emission<sup>19</sup> [see, for example, Eqs. (26) and (27) of this work] we can write

$$\langle f\omega_k | V | i\epsilon_p+ \rangle = g^*(\omega_k) \langle f | V_d | i\epsilon_p+ \rangle , \tag{20}$$

where  $V_d$  represents essentially the electric dipole coupling and  $g$  is defined by Eq. (25) below. Finally  $|\langle f | V_d | i\epsilon_p+ \rangle|^2$  when considered as a function of  $\epsilon_p$  gives the modified Fano profile which we discuss further in Sec. III E and, as noted by Alber, Cooper, and Rau,<sup>27</sup> also gives the dependence of the recombination probability on the energy of the incident electron.

## B. The matrix elements of the Green's operator

The definition of the Green's operator  $G(z)$  can be written in the form

$$(z - H^0)G(z) = 1 + VG(z) , \tag{21}$$

where  $V$  represents the sum of the atom-field interaction  $H_{AF}$  and the projected electron-electron interaction  $QH_A P + PH_A Q$ . A set of coupled equations for the various matrix elements of  $G(z)$  is obtained simply by forming the matrix elements of both sides of Eq. (21) between the unperturbed eigenstates that have been included in our basis set. Some of the off-diagonal elements of  $G(z)$  can be related by taking advantage of the non-Hermitian property. Since the matrix elements  $\langle a,0 | G(z) | a,0 \rangle$ ,  $\langle ipm_s,0 | G(z) | a,0 \rangle$ , and  $\langle f,\mathbf{k}\lambda | G(z) | a,0 \rangle$  have already been obtained in previously reported investigations<sup>19,20</sup> of the autoionization and radiative decay amplitudes for systems initially in the state  $|a,0\rangle$ , only three additional independent matrix elements of  $G(z)$  will be required for the present  $S$ -matrix description. These additional matrix elements of  $G(z)$  may be denoted by  $\langle i'p'm'_s,0 | G(z) | ipm_s,0 \rangle$ ,  $\langle f,\mathbf{k}\lambda | G(z) | ipm_s,0 \rangle$ , and  $\langle f',\mathbf{k}'\lambda' | G(z) | f,\mathbf{k}\lambda \rangle$ . The last of these matrix elements is required only for the evaluation of the  $S$ -matrix element describing the photon-ion scattering process, which we will not pursue further in the present investigation.

The equation for  $\langle i'p'm'_s,0 | (z - H^0)G(z) | ipm_s,0 \rangle$  can be expanded in terms of our restricted basis set of unperturbed eigenstates to give the relationship

$$(z - E_p') \langle i' \mathbf{p}' m_s', 0 | G(z) | i \mathbf{p} m_s, 0 \rangle = \delta(M_i', M_i) \delta(m_s', m_s) \delta^3(\mathbf{p}' - \mathbf{p}) + \sum_{M_a} \langle i' \mathbf{p}' m_s', 0 | V | a, 0 \rangle \langle a, 0 | G(z) | i \mathbf{p} m_s, 0 \rangle + \sum_{M_f} \sum_{\lambda} \sum_{\mathbf{k}} \langle i' \mathbf{p}' m_s', 0 | V | f, \mathbf{k} \lambda \rangle \langle f, \mathbf{k} \lambda | G(z) | i \mathbf{p} m_s, 0 \rangle. \quad (22)$$

Analogous relationships are obtained for  $\langle f', \mathbf{k}' \lambda' | (z - H^0) G(z) | f, \mathbf{k} \lambda \rangle$  and for  $\langle f, \mathbf{k} \lambda | (z - H^0) G(z) | i \mathbf{p} m_s, 0 \rangle$ .

In order to proceed further, it will be necessary to introduce the explicit expressions for the various matrix elements of the interaction operator  $V$ . These expressions have been derived<sup>20</sup> by means of the introduction of a partial-wave expansion<sup>35</sup> for the unperturbed electron-continuum eigenstate and by the application of the Wigner-Eckart theorem.<sup>36</sup> In our present analysis, we retain only the electric dipole contribution that arises from the multipole expansion of the radiation field operator. The inclusion of higher-order multipole contributions in a future extension of this investigation may be necessary for an accurate description of high-Z atomic systems.

The interaction matrix element that is responsible for autoionization can be represented, in terms of the Wigner 3- $j$  symbols,<sup>36</sup> by means of the partial-wave expansion

$$\begin{aligned} \langle a, 0 | V | i \mathbf{p} m_s, 0 \rangle &= \langle a, 0 | QH_{AP} | i \mathbf{p} m_s, 0 \rangle \\ &= \sum_{l, m} \exp[i(l\pi/2 - \sigma_l)] Y_{lm}^*(\hat{\mathbf{p}}) \\ &\quad \times \sum_{K, N} (-1)^{s - J_i - N + K - l - M_a} [(2K + 1)]^{1/2} \begin{Bmatrix} J_i & s & K \\ M_i & m_s & -N \end{Bmatrix} \begin{Bmatrix} l & K & J_a \\ m & N & -M_a \end{Bmatrix} \\ &\quad \times \langle \gamma_a J_a || QH_{AP} || \gamma_i J_i, Kpl; J_a \rangle, \end{aligned} \quad (23)$$

where the double vertical bars denote the reduced matrix element of the projected interaction operator  $QH_{AP}$  that results from the application of the Wigner-Eckart theorem.<sup>36</sup> The symbols  $\gamma_a$  and  $\gamma_i$  denote the sets of additional quantum numbers and  $\sigma_l$  is the Coulomb phase shift. We emphasize that the unperturbed electron-continuum eigenstate  $|i \mathbf{p} m_s, 0\rangle$  that is introduced by this partial-wave expansion describes the electron-ion scattering in the absence of both the projected electron-electron interaction and the electromagnetic interaction  $H_{AF}$ . In the terminology of the Feshbach projection-operator formalism,<sup>30,31</sup> these states correspond to the nonresonant electron-ion scattering states that are eigenstates of the projected unperturbed atomic Hamiltonian  $PH_{AP}$ , which is defined within the subspace of the open electron-continuum channel  $|i \mathbf{p} m_s, 0\rangle$ .

The interaction matrix element that describes the spontaneous radiative decay process is given in the electric dipole approximation by

$$\begin{aligned} \langle a, 0 | V | f, \mathbf{k} \lambda \rangle &= \langle a, 0 | H_{AF} | f, \mathbf{k} \lambda \rangle \\ &= \sum_{\mu} g_{\mu}(\mathbf{k}, \lambda) (-1)^{J_a - M_a} \begin{Bmatrix} J_a & 1 & J_f \\ -M_a & \mu & M_f \end{Bmatrix} \\ &\quad \times \langle \gamma_a J_a || \mathbf{D} || \gamma_f J_f \rangle, \end{aligned} \quad (24)$$

where  $\mathbf{D}$  denotes the many-electron atomic dipole-moment operator that has the dimension of length and may be represented in its relativistic form. The quantity  $g_{\mu}(\mathbf{k}, \lambda)$  is defined by

$$g_{\mu}(\mathbf{k}, \lambda) = -i \left[ \frac{2\pi e^2 \hbar \omega_k}{V_F} \right]^{1/2} (\hat{\mathbf{e}}_{\mathbf{k}\lambda})_{\mu}^*, \quad (25)$$

where  $\mu$  designates the irreducible spherical tensor components of the unit photon-polarization vector  $\hat{\mathbf{e}}_{\mathbf{k}\lambda}$  and  $V_F$  denotes the volume within which the radiation field has been quantized.

The interaction matrix element that couples the unperturbed electron and photon continua may be expressed in the separable form

$$\begin{aligned} \langle i \mathbf{p} m_s, 0 | V | f, \mathbf{k} \lambda \rangle &= \langle i \mathbf{p} m_s, 0 | H_{AF} | f, \mathbf{k} \lambda \rangle \\ &= \sum_{\mu} f_{\mu}^*(M_i \mathbf{p} m_s, M_f) g_{\mu}(\mathbf{k}, \lambda). \end{aligned} \quad (26)$$

The quantity  $f_{\mu}^*(M_i \mathbf{p} m_s, M_f)$  is defined in the electric dipole approximation by the relation

$$f_{\mu}^*(M_i \mathbf{p} m_s, M_f) = \langle i \mathbf{p} m_s | \mathbf{D}_{\mu} | f \rangle, \quad (27)$$

and may be represented in this approximation by means of the partial-wave expansion

$$\begin{aligned} f_{\mu}^*(M_i \mathbf{p} m_s, M_f) &= \sum_{l, m} \exp[-i(l\pi/2 - \sigma_l)] Y_{lm}(\hat{\mathbf{p}}) \sum_{K, N, J, M} (-1)^{s - J_i - N + K - l - 2M + J} [(2K + 1)(2J + 1)]^{1/2} \\ &\quad \times \begin{Bmatrix} J_i & s & K \\ M_i & m_s & -N \end{Bmatrix} \begin{Bmatrix} l & K & J \\ m & N & -M \end{Bmatrix} \begin{Bmatrix} J & 1 & J_f \\ -M & \mu & M_f \end{Bmatrix} \\ &\quad \times \langle \gamma_i J_i, Kpl; J || \mathbf{D} || \gamma_f J_f \rangle. \end{aligned} \quad (28)$$

The notation in our subsequent analysis can be simplified substantially by the introduction of vector and tensor self-energies that are natural extensions of the definitions originally presented by Haan and Cooper.<sup>19</sup> These extended definitions, which include the magnetic quantum numbers, are as follows:<sup>20</sup>

$$\begin{aligned} \sigma_{\mu}^{fa}(M_f M_a, z) &= \sum_{M_i} \sum_{m_s} \int d^3p \frac{f_{\mu}(M_i \mathbf{p} m_s, M_f)}{(z - E_p)} \langle i \mathbf{p} m_s, 0 | V | a, 0 \rangle, \end{aligned} \quad (29)$$

$$\begin{aligned} \sigma_{\mu\nu}^{ff}(M_f M_f', z) &= \sum_{M_i} \sum_{m_s} \int d^3p \frac{f_{\mu}(M_i \mathbf{p} m_s, M_f)}{(z - E_p)} f_{\nu}^*(M_i \mathbf{p} m_s, M_f'), \end{aligned} \quad (30)$$

$$\sigma_{\mu}^{ga}(M_f M_a, z) = \sum_{\lambda} \sum_{\mathbf{k}} \frac{g_{\mu}(\mathbf{k}, \lambda)}{(z - E_k)} \langle f, \mathbf{k} \lambda | V | a, 0 \rangle, \quad (31)$$

$$\sigma_{\mu\nu}^{gg}(z) = \sum_{\lambda} \sum_{\mathbf{k}} \frac{g_{\mu}(\mathbf{k}, \lambda) g_{\nu}^*(\mathbf{k}, \lambda)}{(z - E_k)}. \quad (32)$$

The transposed elements are defined by relationships such

as the following:

$$\begin{aligned} \sigma_{\mu}^{af}(M_a M_f, z) &= \sum_{M_i} \sum_{m_s} \int d^3p \frac{\langle a, 0 | V | i \mathbf{p} m_s, 0 \rangle}{(z - E_p)} \\ &\quad \times f_{\mu}^*(M_i \mathbf{p} m_s, M_f) \\ &= [\sigma_{\mu}^{fa}(M_f M_a, z^*)]^*. \end{aligned} \quad (33)$$

The results obtained for the various matrix elements of  $G(z)$  can be simplified substantially by exploiting the special properties of the tensor self-energies  $\sigma_{\mu\nu}^{ff}(z)$  and  $\sigma_{\mu\nu}^{gg}(z)$ . The tensor self-energy  $\sigma_{\mu\nu}^{gg}(z)$  is found to have the diagonal form

$$\sigma_{\mu\nu}^{gg}(z) = \Sigma^{gg}(z) \delta_{\mu\nu}. \quad (34)$$

After converting the discrete summation over  $\mathbf{k}$  into an integral over the continuous photon-energy variable  $\hbar\omega_k$ , the scalar self-energy  $\Sigma^{gg}(z)$  can be expressed as

$$\Sigma^{gg}(z) = \frac{2e^2 \hbar}{3\pi c^3} \int_0^{\infty} \frac{d\omega_k \omega_k^3}{(z - E_k)}. \quad (35)$$

The partial-wave expansion Eq. (28) can be employed to reduce the tensor self-energy  $\sigma_{\mu\nu}^{ff}(z)$  to the form

$$\sigma_{\mu\nu}^{ff}(M_f M_f', z) = \sum_{J, M} \begin{bmatrix} J & 1 & J_f \\ -M & \mu & M_f \end{bmatrix} \begin{bmatrix} J & 1 & J_f \\ -M & \nu & M_f' \end{bmatrix} (2J+1) \Sigma^{ff}(z), \quad (36)$$

where the scalar self-energy  $\Sigma^{ff}(z)$  is defined by the integral

$$\Sigma^{ff}(z) = \frac{1}{(2J+1)} \int_0^{\infty} \frac{p^2 dp}{(z - E_p)} \sum_K \sum_I |\langle \gamma_i J_i, K p l; J || \mathbf{D} || \gamma_f J_f \rangle|^2. \quad (37)$$

An equation that involves only matrix elements of  $G(z)$  having the forms  $\langle f, \mathbf{k} \lambda | G(z) | i \mathbf{p} m_s, 0 \rangle$  and  $\langle a, 0 | G(z) | i \mathbf{p} m_s, 0 \rangle$  can be deduced by eliminating matrix elements of the type  $\langle i' \mathbf{p}' m_s', 0 | G(z) | i \mathbf{p} m_s, 0 \rangle$  from the set of coupled equations consisting of Eq. (22) together with the analogous relationship for  $\langle f, \mathbf{k} \lambda | (z - H^0) G(z) | i \mathbf{p} m_s, 0 \rangle$ . In order to extract the desired solution for the matrix elements  $\langle f, \mathbf{k} \lambda | G(z) | i \mathbf{p} m_s, 0 \rangle$ , it is first necessary to multiply both sides of this equation by the factor

$$\begin{bmatrix} J_a & 1 & J_f \\ -M_a & \mu & M_f \end{bmatrix} g_{\mu}(\mathbf{k}, \lambda),$$

for some fixed value of the index  $\mu$ , and then to perform the summations over  $M_f$ ,  $\mu$ ,  $\lambda$ , and  $\mathbf{k}$ . This procedure is evidently analogous to that employed previously in connection with Eq. (19) of the derivation of the autoionization and radiative decay probabilities.<sup>20</sup>

The properties of the tensor self-energies expressed by Eqs. (34) and (36) allow the extraction of an exact closed-form expression for the matrix elements  $\langle f, \mathbf{k} \lambda | G(z) | i \mathbf{p} m_s, 0 \rangle$ , which can be presented in the form

$$\begin{aligned} \langle f, \mathbf{k} \lambda | G(z) | i \mathbf{p} m_s, 0 \rangle &= \frac{\langle f, \mathbf{k} \lambda | V | i \mathbf{p} m_s, 0 \rangle}{(z - E_k)(z - E_p) \Psi(z)} + \sum_{M_a} \left[ \langle f, \mathbf{k} \lambda | V | a, 0 \rangle + \sum_{\mu} \frac{g_{\mu}^*(\mathbf{k}, \lambda)}{\Psi(z)} [\sigma_{\mu}^{fa}(M_f M_a, z) \right. \\ &\quad \left. + \Sigma^{ff}(z) \sigma_{\mu}^{ga}(M_f M_a, z)] \right] \frac{\langle a, 0 | G(z) | i \mathbf{p} m_s, 0 \rangle}{(z - E_k)}, \end{aligned} \quad (38)$$

where

$$\Psi(z) = 1 - \Sigma^{gg}(z) \Sigma^{ff}(z). \quad (39)$$

The corresponding solution obtained for the matrix elements  $\langle i' \mathbf{p}' m_s', 0 | G(z) | i \mathbf{p} m_s, 0 \rangle$  can be expressed as



$$\begin{aligned}
& \langle i' \mathbf{p}' m'_s, 0 | G(z) | i \mathbf{p} m_s, 0 \rangle \\
&= \frac{\delta(M'_i, M_i) \delta(m'_s, m_s) \delta^3(\mathbf{p}' - \mathbf{p})}{(z - E'_p)} + \sum_{M_f} \sum_{\mu} \frac{f_{\mu}^*(M'_i \mathbf{p}' m'_s, M_f) \Sigma^{gg}(z) f_{\mu}(M_i \mathbf{p} m_s, M_f)}{(z - E'_p)(z - E_p) \Psi(z)} \\
&+ \sum_{M_a} \left[ \langle i' \mathbf{p}' m'_s, 0 | V | a, 0 \rangle \right. \\
&\quad \left. + \sum_{M_f} \sum_{\mu} \frac{f_{\mu}^*(M'_i \mathbf{p}' m'_s, M_f)}{\Psi(z)} [\sigma_{\mu}^{ga}(M_f M_a, z) + \Sigma^{gg}(z) \sigma_{\mu}^{fa}(M_f M_a, z)] \right] \frac{\langle a, 0 | G(z) | i \mathbf{p} m_s, 0 \rangle}{(z - E'_p)}. \quad (40)
\end{aligned}$$

An analogous exact closed-form expression can be obtained for the matrix elements  $\langle f', \mathbf{k}' \lambda' | G(z) | f, \mathbf{k} \lambda \rangle$ , which are required only for the photon-ion scattering matrix element.

In order to complete the determination of the matrix elements given by Eqs. (38) and (40), it is necessary to utilize our previously derived result for  $\langle a, 0 | G(z) | i \mathbf{p} m_s, 0 \rangle$ , which may be presented in the form<sup>19,20</sup>

$$\begin{aligned}
& \langle i \mathbf{p} m_s, 0 | G(z) | a, 0 \rangle \\
&= \left[ \langle i \mathbf{p} m_s, 0 | V | a, 0 \rangle + \sum_{\mu} \sum_{M_f} \frac{f_{\mu}^*(M_i \mathbf{p} m_s, M_f)}{\Psi(z)} [\sigma_{\mu}^{ga}(M_f M_a, z) + \Sigma^{gg}(z) \sigma_{\mu}^{fa}(M_f M_a, z)] \right] \frac{\langle a, 0 | G(z) | a, 0 \rangle}{(z - E_p)}. \quad (41)
\end{aligned}$$

The modified propagator for the autoionizing state is given by<sup>19,20</sup>

$$\begin{aligned}
& [\langle a, 0 | G(z) | a, 0 \rangle]^{-1} = z - E_a - \Sigma^{aa}(z) - \sum_{\mu} \sum_{M_f} \frac{\sigma_{\mu}^{af}(M_a M_f, z)}{\Psi(z)} [\sigma_{\mu}^{ga}(M_f M_a, z) + \Sigma^{gg}(z) \sigma_{\mu}^{fa}(M_f M_a, z)] \\
&\quad - \sum_{\mu} \sum_{M_f} \frac{\sigma_{\mu}^{ag}(M_a M_f, z)}{\Psi(z)} [\sigma_{\mu}^{fa}(M_f M_a, z) + \Sigma^{ff}(z) \sigma_{\mu}^{ga}(M_f M_a, z)], \quad (42)
\end{aligned}$$

where

$$\Sigma^{aa}(z) = \sum_{M_i} \sum_{m_s} \int d^3 p \frac{|\langle a, 0 | V | i \mathbf{p} m_s, 0 \rangle|^2}{(z - E_p)} + \sum_{M_f} \sum_{\lambda} \sum_{\mathbf{k}} \frac{|\langle a, 0 | V | f, \mathbf{k} \lambda \rangle|^2}{(z - E_k)}. \quad (43)$$

### C. The transition operator for electron-ion scattering and photorecombination

The matrix elements of the transition operator  $T$  that describe the electron-ion scattering and photorecombination processes may now be expressed, by means of Eqs. (12) and (13) together with our results for the matrix elements of  $G$ , as sums of a resonant and a nonresonant transition amplitude in the familiar forms<sup>15</sup>

$$\begin{aligned}
\langle i' \mathbf{p}' m'_s, 0 | T | i \mathbf{p} m_s, 0 \rangle &= \lim_{\epsilon \rightarrow 0} \left[ \langle i' \mathbf{p}' m'_s, 0 | \tilde{V}(E_p + i\epsilon) | i \mathbf{p} m_s, 0 \rangle \right. \\
&\quad \left. + \sum_{M_a} \langle i' \mathbf{p}' m'_s, 0 | \tilde{V}(E_p + i\epsilon) | a, 0 \rangle \langle a, 0 | G(E_p + i\epsilon) | a, 0 \rangle \langle a, 0 | \tilde{V}(E_p + i\epsilon) | i \mathbf{p} m_s, 0 \rangle \right], \quad (44)
\end{aligned}$$

$$\begin{aligned}
\langle f, \mathbf{k} \lambda | T | i \mathbf{p} m_s, 0 \rangle &= \lim_{\epsilon \rightarrow 0} \left[ \langle f, \mathbf{k} \lambda | \tilde{V}(E_k + i\epsilon) | i \mathbf{p} m_s, 0 \rangle \right. \\
&\quad \left. + \sum_{M_a} \langle f, \mathbf{k} \lambda | \tilde{V}(E_k + i\epsilon) | a, 0 \rangle \langle a, 0 | G(E_k + i\epsilon) | a, 0 \rangle \langle a, 0 | \tilde{V}(E_k + i\epsilon) | i \mathbf{p} m_s, 0 \rangle \right]. \quad (45)
\end{aligned}$$

The matrix elements of the vertex operator  $\tilde{V}(z)$  that correspond to the nonresonant transition amplitudes are obtained in the forms

$$\langle i' \mathbf{p}' m'_s, 0 | \tilde{V}(z) | i \mathbf{p} m_s, 0 \rangle = \sum_{M_f} \sum_{\mu} \frac{f_{\mu}^*(M'_i \mathbf{p}' m'_s, M_f) \Sigma^{gg}(z) f_{\mu}(M_i \mathbf{p} m_s, M_f)}{\Psi(z)}, \quad (46)$$

$$\langle f, \mathbf{k} \lambda | \tilde{V}(z) | i \mathbf{p} m_s, 0 \rangle = \langle f, \mathbf{k} \lambda | V | i \mathbf{p} m_s, 0 \rangle + \sum_{M'_f} \sum_{\mu} \sum_{\nu} \frac{g_{\mu}^*(\mathbf{k}, \lambda) \sigma_{\mu\nu}^{ff}(M'_f M'_f, z) \Sigma^{gg}(z) f_{\nu}(M_i \mathbf{p} m_s, M'_f)}{\Psi(z)}, \quad (47)$$

which incorporate our nonperturbative results for the vertex modifications. Note the absence from the right-hand side of Eq. (46) of the lowest-order contribution  $\langle i'p'm'_s, 0 | V | ipm_s, 0 \rangle$ , which has been assumed to vanish, as indicated by Eq. (14). The vanishing of this contribution is in accord with our initial assumption that the nonresonant electron-ion scattering process, in the absence of the electromagnetic interaction  $H_{AF}$ , is completely described by the unperturbed electron-continuum states  $|ipm_s\rangle$ .

The matrix elements of the vertex operator  $\tilde{V}(z)$  that are required for the evaluation of the autoionizing-resonance contributions to the transition amplitudes can also be expressed as sums of unmodified and modified interaction matrix elements as follows:

$$\langle ipm_s, 0 | \tilde{V}(z) | a, 0 \rangle = \langle ipm_s, 0 | V | a, 0 \rangle + \sum_{M_f} \sum_{\mu} \frac{f_{\mu}^*(M_i p m_s, M_f)}{\Psi(z)} [\sigma_{\mu}^{ga}(M_f M_a, z) + \Sigma^{gg}(z) \sigma_{\mu}^{fa}(M_f M_a, z)], \quad (48)$$

$$\begin{aligned} \langle f, \mathbf{k}\lambda | \tilde{V}(z) | a, 0 \rangle &= \langle f, \mathbf{k}\lambda | V | a, 0 \rangle + \sum_{\mu} g_{\mu}^*(\mathbf{k}, \lambda) \sigma_{\mu}^{fa}(M_f M_a, z) \\ &+ \sum_{\mu} \sum_{\nu} \sum_{M'_f} \frac{g_{\mu}^*(\mathbf{k}, \lambda) \sigma_{\mu\nu}^{ff}(M_f M'_f, z)}{\Psi(z)} [\sigma_{\nu}^{ga}(M'_f M_a, z) + \Sigma^{gg}(z) \sigma_{\nu}^{fa}(M'_f M_a, z)]. \end{aligned} \quad (49)$$

If only the matrix elements of the unmodified interaction operator  $V$  are retained in the vertex functions defined by Eqs. (47), (48), and (49), and the corresponding approximation is introduced into the autoionizing-resonance propagator given by Eqs. (42) and (43), we recover the familiar expression for the lowest-order combined transition amplitude describing radiative and dielectronic recombination.<sup>15</sup>

The resonant and nonresonant transition amplitudes, which appear in Eqs. (44) and (45), may be represented schematically by the Feynman-type diagrams shown in Figs. 2 and 3, for electron-ion scattering and photorecombination, respectively. In the diagrams associated with

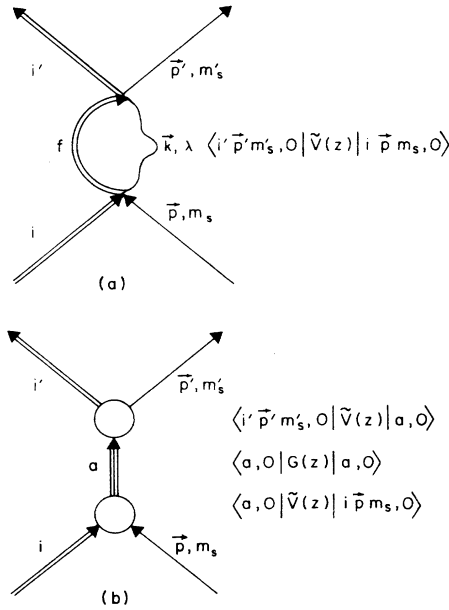


FIG. 2. Diagrams representing the lowest-order contribution (a) to the nonresonant transition amplitude and the entire resonant transition amplitude (b) for electron-ion scattering. The open circles represent the indicated matrix elements of the vertex operator  $\tilde{V}(z)$ , while the triple lines represent the indicated matrix element of the modified propagator  $G(z)$ .

the autoionizing-resonance contributions, the open circles represent the vertex functions while the triple lines designate the modified propagator. These modifications incorporate radiative corrections to all orders in quantum electrodynamical perturbation theory, but within the limitations of our restricted basis set of unperturbed eigenstates. The nonresonant transition amplitudes are represented by Feynman-type diagrams that indicate the lowest-order photorecombination amplitude [Fig. 3(a)]

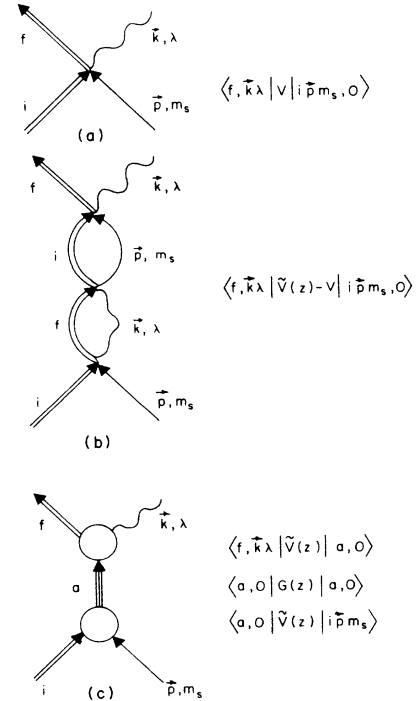


FIG. 3. Diagrams representing the unperturbed contribution (a) and the lowest-order radiative correction (b) to the nonresonant transition amplitude together with the entire resonant transition amplitude (c) for electron-ion photorecombination. The open circles represent the indicated matrix elements of the vertex operator  $\tilde{V}(z)$ , while the triple lines represent the indicated matrix element of the modified propagator  $G(z)$ .

and the leading radiative corrections [Figs. 2(a) and 3(b)], which correspond to the replacement of  $\Psi(z)$  by unity in Eqs. (46) and (47). The higher-order radiative corrections, which involve more than one virtual photon emission and reabsorption, are generated by the remaining terms in the expansion of  $1/\Psi(z)$  in powers of the product  $\Sigma^{gg}(z)\Sigma^{ff}(z)$ .

The vertex functions that are represented by the open circles in Figs. 2 and 3 may be depicted in greater detail by means of the Feynman-type diagrams shown in Figs. 4 and 5 for external electron and photon lines, respectively. The unmodified interaction matrix elements that occur as the leading terms in the expressions Eqs. (48) and (49) for the vertex functions are represented by the diagrams labeled (a) in Figs. 4 and 5. The diagrams labeled (b) and (c) exhibit the lowest-order radiative corrections that are generated by the vertex correction operator  $\tilde{V}(z) - V$ . In Sec. III the pole approximation will be employed in an approximate evaluation of the vertex and propagator

modifications, which results in expressions for the modified electron-ion photorecombination cross sections involving the familiar unperturbed atomic transition probabilities. It would be necessary to employ the renormalization program of modern relativistic quantum field theory<sup>37</sup> in order to properly treat the various divergent quantities that would be encountered in a precise evaluation of these corrections.

The diagrams that are labeled (a) in Figs. 3–5 represent the elementary interactions that serve as the fundamental structures in the diagrammatic perturbation theory expansion of the transition amplitudes describing the electron-ion scattering and photorecombination processes. It is desirable to present the relationships between these elementary interactions and the basic interaction of quantum electrodynamics, which is represented by a vertex formed by two electron lines and a single photon line. For concreteness, we present these relationships by adopting for

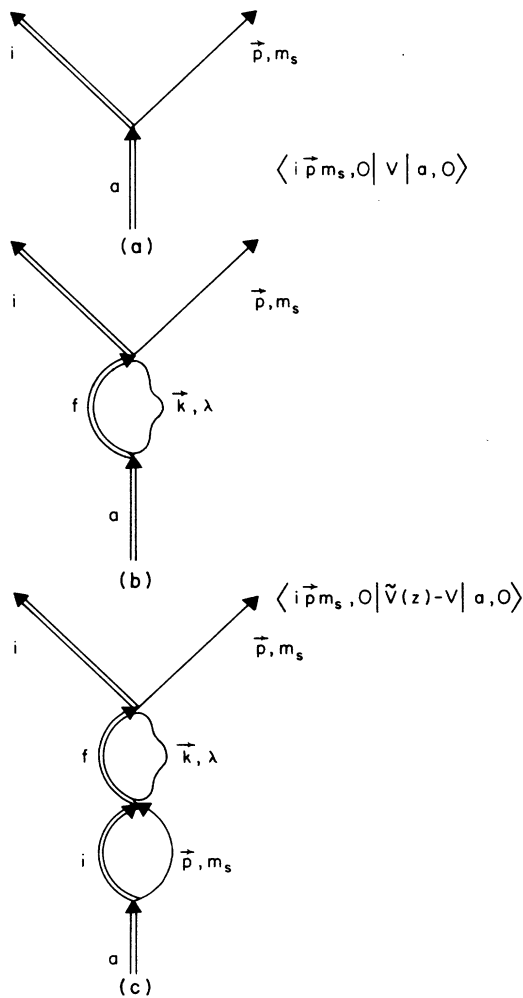


FIG. 4. Vertex diagrams containing an external electron line. The indicated matrix element of the unmodified interaction operator  $V$  is represented by (a), while the lowest-order radiative corrections that are generated by the vertex correction operator  $\tilde{V}(z) - V$  are represented by (b) and (c).

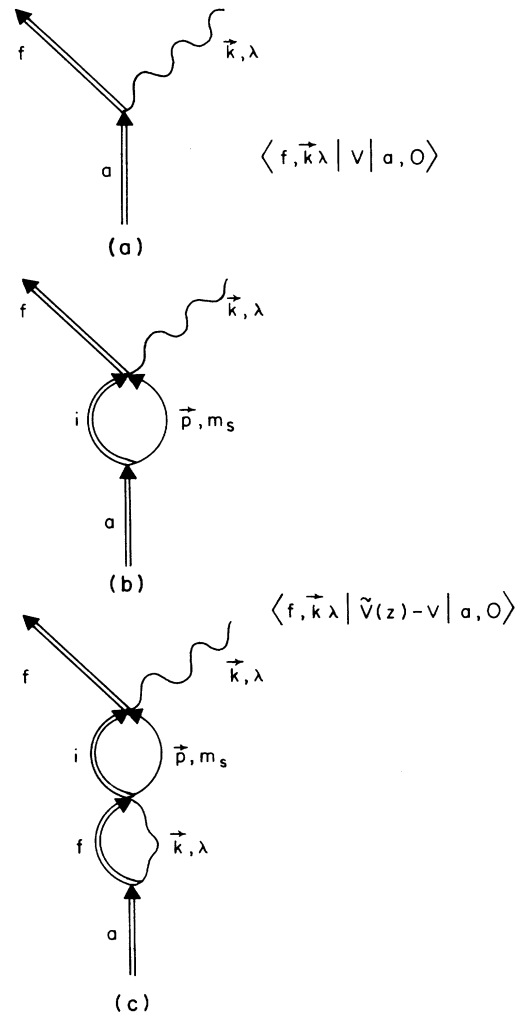


FIG. 5. Vertex diagrams containing an external photon line. The indicated matrix element of the unmodified interaction operator  $V$  is represented by (a), while the lowest-order radiative corrections that are generated by the vertex correction operator  $\tilde{V}(z) - V$  are represented by (b) and (c).

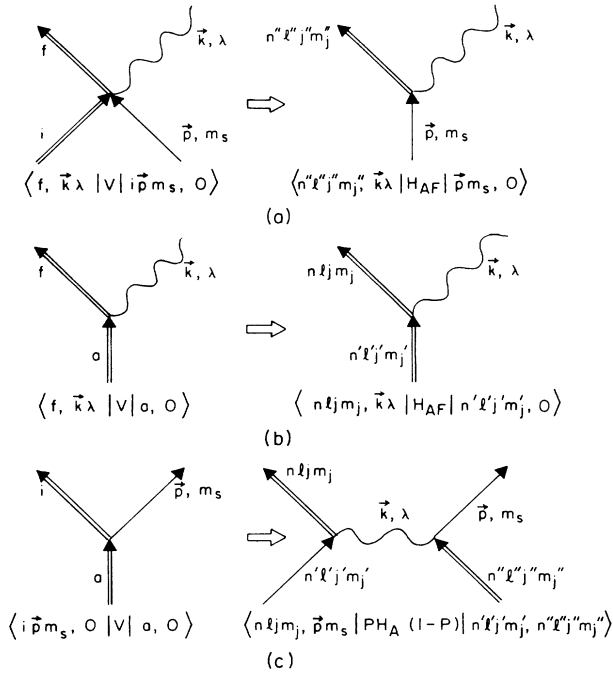


FIG. 6. Relationships between the elementary interactions that are represented by the unmodified vertices in Figs. 2–5 and the basic interaction diagram of quantum electrodynamics, which is a vertex formed by two electron lines and a singlet photon line. The atomic eigenstates are specified by  $|i\rangle = |nljm_j\rangle$ ,  $|a\rangle = |n'l'j'm'_j, n''l''j''m''_j\rangle$ , and  $|f\rangle = |nljm_j, n''l''j''m''_j\rangle$ . The vertex diagrams (a) and (b) represent the indicated basic interaction matrix elements, while diagram (c) designates the indicated matrix element of the single-photon-exchange approximation to the electron-electron interaction.

the atomic basis states the simplified uncoupled-electron specifications

$$|i\rangle = |nljm_j\rangle, \\ |a\rangle = |n'l'j'm'_j, n''l''j''m''_j\rangle,$$

and

$$|f\rangle = |nljm_j, n''l''j''m''_j\rangle.$$

These uncoupled representations are most suitable for the treatment of processes involving the high-Rydberg autoionizing states with  $n'' \gg n' > n$ , for which the dominant stabilizing radiative decay channel involves the

inner-electron transition  $n'l'j'm'_j \rightarrow nljm_j$ .

The pairs of diagrams that are labeled (a) and (b) in Fig. 6 illustrate the connections between the elementary photon emission processes and the basic single-electron transition resulting from the relativistic atomic-electron–radiation-field interaction

$$H_{AF} = -e \left[ \frac{2\pi\hbar}{\omega_k} \right]^{1/2} \underline{\alpha} \cdot \hat{\epsilon}_{\vec{k}\lambda}^* e^{-ik \cdot \mathbf{r}}, \quad (50)$$

where  $\underline{\alpha}$  denotes the Dirac matrix. The single-photon exchange approximation for the relativistic interaction between the atomic electrons is illustrated by the pair of diagrams labeled (c). The configuration-space interaction operator that corresponds to this approximation for the relativistic electron-electron interaction can be expressed in the Møller form<sup>29</sup>

$$V(r_{12}) = (1 - \underline{\alpha}_1 \cdot \underline{\alpha}_2) \frac{\exp(ikr_{12})}{r_{12}}, \quad (51)$$

where  $k$  represents the momentum of the virtual photon. It can be seen that the diagram labeled (c) is in fact a combination of the two basic diagrams labeled (a) and (b). This provides a physical understanding for the widely used approximation<sup>3,10</sup> in which the autoionization rates are expressed in terms of the radiative decay rate for the inner-electron transition.

### III. THE ELECTRON-ION PHOTORECOMBINATION CROSS SECTIONS

A very general description of electron-ion photorecombination can be presented in terms of a final-state density matrix, which can be defined in terms of the individual transition matrix elements and an initial-state density matrix representing the polarization states of the incident electron and the initial state. An analogous description has been presented in connection with the atomic photoionization process.<sup>35</sup> In the present investigation we treat only the recombination processes in which the magnetic sublevels of the incident electron and the initial ion are equally populated and the magnetic quantum numbers and polarizations of the final-state products are not measured. In addition, the differential cross sections will be integrated over the final electron and photon directions to obtain the total cross sections.

The total cross sections for electron-ion scattering and photorecombination are defined, in terms of the respective matrix elements of the transition operator  $T$ , by the expressions

$$\sigma(i, \epsilon_p \rightarrow i, \epsilon'_p) = \left[ \frac{2\pi}{\hbar} \right] \left[ \frac{m_e}{p} \right] \frac{1}{(2J_i + 1)(2s + 1)} \sum_{M_i} \sum_{m_s} \sum_{M'_i} \sum_{m'_s} \int d\Omega_p \rho(\epsilon'_p) |\langle i', \mathbf{p}', m'_s, 0 | T | i, \mathbf{p}, m_s, 0 \rangle|^2, \quad (52)$$

$$\sigma(i, \epsilon_p \rightarrow f, \omega_k) = \left[ \frac{2\pi}{\hbar} \right] \left[ \frac{m_e}{p} \right] \frac{1}{(2J_i + 1)(2s + 1)} \sum_{M_i} \sum_{m_s} \sum_{M_f} \sum_{\lambda} \int d\Omega_k \rho(\hbar\omega_k) |\langle f, \mathbf{k}, \lambda | T | i, \mathbf{p}, m_s, 0 \rangle|^2, \quad (53)$$

where the nonrelativistic expression for the incident electron flux has now been introduced. The densities of final electron and photon states per unit energy and solid angle intervals are denoted by  $\rho(\varepsilon_p')$  and  $\rho(\hbar\omega_k)$ , respectively. The cross section for electron-ion scattering that would be predicted with the results obtained from our severely restricted basis set could describe only the uninteresting elastic scattering process, which will not be considered further in the present investigation.

When Eq. (45) is substituted into Eq. (53), three contributions to  $\sigma(i, \varepsilon_p \rightarrow f, \omega_k)$  are obtained which arise from the modulus squared of the nonresonant transition amplitude, from the modulus squared of the resonant transition amplitude, and from the interference terms involving the nonresonant and resonant transition amplitudes. We will denote these contributions by  $\tilde{\sigma}_{RR}(i, \varepsilon_p \rightarrow f, \omega_k)$ ,  $\tilde{\sigma}_{DR}(i, \varepsilon_p \rightarrow f, \omega_k)$ , and  $\tilde{\sigma}_{int}(i, \varepsilon_p \rightarrow f, \omega_k)$ , respectively. We will treat them separately in Secs. III B, III C, and III D and we will combine them in Sec. III E. First, however, we will introduce the pole approximation.

#### A. The pole approximation

The electron-ion photorecombination cross sections will now be evaluated by introducing into the definitions of the various self-energies the pole approximation

$$\lim_{\varepsilon \rightarrow 0} \frac{1}{E - E' \pm i\varepsilon} = \text{P} \left[ \frac{1}{E - E'} \right] \mp i\pi\delta(E - E') \\ \cong \mp i\pi\delta(E - E'), \quad (54)$$

in which the principal-value integral arising from the contribution denoted by P is to be ignored. The validity of the pole approximation has been investigated by Haan and Cooper,<sup>19</sup> and they have concluded that this approximation can be expected to be valid in a region in which the transition amplitude is a slowly and smoothly varying function of the continuous energy variable. However, they have pointed out that incorrect results can be obtained if the pole approximation is introduced prior to performing an integration over the entire energy range since it is not valid for the entire continuum. This difficulty can occur when the one-discrete-level and two-continua diagonalization is performed in a sequential manner, which often gives rise to a rapid energy variation. Here we avoid the problems by working with undiagonalized continuum states.

The self-energy  $\Sigma^{aa}(z)$ , which is defined by Eq. (43), reduces in the pole approximation to the familiar result

$$\Sigma^{aa}(z) = -\frac{i\hbar}{2} [\delta(z, E_i + \varepsilon_p) A_a(a \rightarrow i\varepsilon_p) \\ + \delta(z, E_f + \hbar\omega_k) A_r(a \rightarrow f)], \quad (55)$$

which is simply the sum of the usual autoionization and spontaneous radiative decay rates  $A_a(a \rightarrow i\varepsilon_p)$  and

$A_r(a \rightarrow f)$  in the absence of the continuum-continuum coupling. These unperturbed transition rates are expressed in terms of the appropriate reduced matrix elements by the relationships

$$A_a(a \rightarrow i\varepsilon_p) = \sum_{K,l} A_a(a \rightarrow i, K\varepsilon_p l) \\ = \frac{2\pi}{\hbar} \delta(\varepsilon_p, E_a - E_i) \\ \times \sum_{K,l} \frac{|\langle \gamma_a J_a \| QH_A P \| \gamma_i J_i, K\varepsilon_p l; J_a \rangle|^2}{(2J_a + 1)}, \quad (56)$$

$$A_r(a \rightarrow f) = \left[ \frac{4}{3} \right] \left[ \frac{e^2 \omega_k^3}{\hbar c^3} \right] \\ \times \delta(\hbar\omega_k, E_a - E_f) \frac{|\langle \gamma_a J_a \| \mathbf{D} \| \gamma_f J_f \rangle|^2}{(2J_a + 1)}. \quad (57)$$

Note that the electron-continuum states in Eq. (56) have now been normalized to a Dirac  $\delta$  function in the electron energy  $\varepsilon_p$ .

The scalar self-energies  $\Sigma^{ff}(z)$  and  $\Sigma^{gg}(z)$  are given in the pole approximation by the expressions

$$\Sigma^{ff}(z) = - \left[ \frac{i}{4\pi} \right] \left[ \frac{3}{\alpha \hbar \omega_k} \right] \left[ \frac{2J_f + 1}{2J_a + 1} \right] \\ \times \delta(z, E_i + \varepsilon_p) \sigma_p(f, \omega_k \rightarrow i, \varepsilon_p; J_a), \quad (58)$$

$$\Sigma^{gg}(z) = -i \left[ \frac{2}{3} \right] \left[ \frac{e^2}{c^3} \right] \omega_k^3 \delta(z, E_f + \hbar\omega_k), \quad (59)$$

where  $\alpha$  denotes the fine-structure constant. The continuum-continuum coupling parameter, which is defined by Eq. (39), is accordingly given in the pole approximation by the relationship

$$\Psi(z) = 1 + \left[ \frac{\alpha^2}{2\pi} \right] \left[ \frac{\hbar\omega_k}{2E_H} \right]^2 \left[ \frac{2J_f + 1}{2J_a + 1} \right] \left[ \frac{1}{a_0^2} \right] \\ \times \delta(z, E_i + \varepsilon_p) \delta(z, E_f + \hbar\omega_k) \sigma_p(f, \omega_k \rightarrow i, \varepsilon_p; J_a), \quad (60)$$

where  $E_H = e^2/2a_0$  and  $a_0 = \hbar^2/(e^2 m_e)$ . The quantity  $\sigma_p(f, \omega_k \rightarrow i, \varepsilon_p; J_a)$  denotes the unperturbed photoionization cross section corresponding to the partial-wave component of the electron-continuum state with total electronic angular momentum  $J_a$ . This unperturbed photoionization cross section is given by the relationship

$$\begin{aligned}\sigma_p(f, \omega_k \rightarrow i, \varepsilon_p; J_a) &= \sum_{K,l} \sigma_p(f, \omega_k \rightarrow i, K \varepsilon_p l; J_a) \\ &= \frac{4\pi^2 \alpha \hbar \omega_k}{3(2J_f + 1)} \sum_{K,l} |\langle \gamma_i J_i, K \varepsilon_p l; J_a \| \mathbf{D} \| \gamma_f J_f \rangle|^2.\end{aligned}\quad (61)$$

Note that by the introduction of the pole approximation we have avoided the problem of the divergent principal-value integral in the expression for  $\Sigma^{gg}(z)$ .

The tensor self-energies  $\sigma_{\mu\nu}^{ff}(M_f M_f', z)$  and  $\sigma_{\mu\nu}^{gg}(z)$  are obtained in the pole approximation simply by substituting the results for  $\Sigma^{ff}(z)$  and  $\Sigma^{gg}(z)$ , which are given by Eqs. (58) and (59), into the defining expressions Eqs. (30) and (32), respectively. The defining relations for the vector self-energies  $\sigma_{\mu}^{fa}(M_f M_a, z)$  and  $\sigma_{\mu}^{ga}(M_f M_a, z)$  can be reduced in the pole approximation to the forms

$$\begin{aligned}\sigma_{\mu}^{fa}(M_f M_a, z) &= \frac{-i\pi(-1)^{J_a - M_a}}{(2J_a + 1)^{1/2}} \begin{bmatrix} J_f & J_a & 1 \\ M_f & -M_a & \mu \end{bmatrix} \\ &\quad \times \delta(z, E_i + \varepsilon_p) \sum_{K,l} \langle \gamma_f J_f \| \mathbf{D} \| \gamma_i J_i, K \varepsilon_p l; J_a \rangle \langle \gamma_i J_i, K \varepsilon_p l; J_a \| PH_A Q \| \gamma_a J_a \rangle,\end{aligned}\quad (62)$$

$$\sigma_{\mu}^{ga}(M_f M_a, z) = (-1)^{J_a - M_a} \begin{bmatrix} J_f & J_a & 1 \\ M_f & -M_a & \mu \end{bmatrix} \Sigma^{gg}(z) \langle \gamma_f J_f \| \mathbf{D} \| \gamma_a J_a \rangle,\quad (63)$$

where  $\Sigma^{gg}(z)$  must be replaced by the result given in the pole approximation by Eq. (59).

The exact closed-form expression Eq. (42) for the modified autoionizing-state propagator simplifies in the pole approximation to the result

$$\begin{aligned}[\langle a, 0 | G(z) | a, 0 \rangle]^{-1} &= (z - E_a) + \delta(z, E_i + \varepsilon_p) \delta(z, E_f + \hbar\omega) \\ &\quad \times \left[ \frac{\hbar A_r(a \rightarrow f)}{\Psi(z) Q_f} + \frac{i\hbar}{2} A_a(a \rightarrow i\varepsilon_p) + \frac{i\hbar}{2\Psi(z)} A_r(a \rightarrow f) \left[ 1 - \frac{1}{Q_f^2} \right] \right],\end{aligned}\quad (64)$$

where  $Q_f$  is the multichannel Fano line profile parameter<sup>24</sup> defined by

$$\frac{1}{Q_f} = \frac{\pi \sum_{K,l} \langle \gamma_a J_a \| QH_A P \| \gamma_i J_i, K \varepsilon_p l; J_a \rangle \langle \gamma_i J_i, K \varepsilon_p l; J_a \| \mathbf{D} \| \gamma_f J_f \rangle}{(2J_a + 1)^{1/2} \langle \gamma_a J_a \| \mathbf{D} \| \gamma_f J_f \rangle}.\quad (65)$$

For the case in which only a single angular momentum term is retained in the partial-wave expansion for the electron-continuum state, Eqs. (56), (57), (60), and (61) can be used to reduce Eq. (65) to the simple result

$$\frac{1}{Q_f^2} = \frac{A_a(a \rightarrow i\varepsilon_p)}{A_r(a \rightarrow f)} [\Psi(z) - 1].\quad (66)$$

We note that this modified propagator has the familiar Lorentzian form

$$[\langle a, 0 | G(z) | a, 0 \rangle]^{-1} = (z - E_a) - \Delta(a) + \frac{i\Gamma(a)}{2},\quad (67)$$

where the shift  $\Delta(a)$  and width  $\Gamma(a)$  produced by the interaction  $V$  are given by

$$\Delta(a) = -\frac{\hbar A_r(a \rightarrow f)}{\Psi(z) Q_f},\quad (68)$$

$$\Gamma(a) = \hbar A_a(a \rightarrow i\varepsilon_p) + \frac{\hbar A_r(a \rightarrow f)}{\Psi(z)} \left[ 1 - \frac{1}{Q_f^2} \right].\quad (69)$$

We will denote by  $\tilde{A}(a)$  the total perturbed decay rate that is given by  $\Gamma(a)/\hbar$ .

## B. The modified radiative recombination cross section

The nonresonant transition amplitude in Eq. (45) determines the modified radiative recombination cross section according to the relation

$$\begin{aligned} \bar{\sigma}_{\text{RR}}(i, \varepsilon_p \rightarrow f, \omega_k) &= \left( \frac{2\pi}{\hbar} \right) \left( \frac{m_e}{p} \right) \frac{1}{(2J_i + 1)(2s + 1)} \\ &\times \sum_{M_i} \sum_{m_s} \sum_{M_f} \sum_{\lambda} \int d\Omega_k \rho(\hbar\omega_k) \left| \lim_{\varepsilon \rightarrow 0} \langle f, \mathbf{k}\lambda | \tilde{V}(E_k + i\varepsilon) | i\mathbf{p}m_s, 0 \rangle \right|^2, \end{aligned} \quad (70)$$

which differs from the usual radiative recombination cross section  $\sigma_{\text{RR}}(i, \varepsilon_p \rightarrow f, \omega_k)$  because of the appearance of the vertex operator  $\tilde{V}(z)$  in place of the interaction operator  $V$ . The vertex function, which is defined by Eq. (47), reduces in the pole approximation to the simple result

$$\begin{aligned} \langle f, \mathbf{k}\lambda | \tilde{V}(z) | i\mathbf{p}m_s, 0 \rangle &= \frac{1}{\Psi(z)} \sum_{\mu} g_{\mu}^*(\mathbf{k}, \lambda) f_{\mu}(M_i \mathbf{p}m_s, M_f) \\ &= \frac{1}{\Psi(z)} \langle f, \mathbf{k}\lambda | V | i\mathbf{p}m_s, 0 \rangle, \end{aligned} \quad (71)$$

where  $\Psi(z)$  is now given by Eq. (60). It can be seen that this result is the lowest-order dipole transition amplitude multiplied by a factor of  $\Psi(z)^{-1}$ . This factor incorporates to all orders the radiative corrections that are generated by the use of our limited basis set of unperturbed eigenstates in the diagonalization of the complete Hamiltonian  $H$ .

The final result for the modified radiative recombination cross section may be expressed in the form

$$\begin{aligned} \bar{\sigma}_{\text{RR}}(i, \varepsilon_p \rightarrow f, \omega_k) &= \frac{4\pi^2}{3} \left( \frac{\alpha^3}{a_0^3} \right) \left( \frac{\hbar\omega_k}{2E_H} \right)^3 \left( \frac{\hbar}{a_0 p} \right) \left( \frac{1}{2J_i + 1} \right) \frac{1}{\Psi(E_f + \hbar\omega_k)^2} \\ &\times \sum_K \sum_l \sum_J |\langle \gamma_f J_f || \mathbf{D} || \gamma_i J_i, Kpl; J \rangle|^2 \\ &= \frac{1}{\Psi(E_f + \hbar\omega_k)^2} \sigma_{\text{RR}}(i, \varepsilon_p \rightarrow f, \omega_k), \end{aligned} \quad (72)$$

where  $\Psi(E_f + \hbar\omega_k)$  is given by Eq. (60). The modified photoionization cross section  $\bar{\sigma}_p(f, \omega_k \rightarrow i, \varepsilon_p)$  corresponding to the inverse process can be obtained from the unperturbed partial-wave cross sections given by Eq. (61) simply by including the factor  $\Psi(E_k + \hbar\omega_k)^{-2}$  and performing the summation over the total electronic angular momentum  $J_a$ . Taking into account the connection between the alternative normalizations of the electron-continuum state per unit electron energy and per unit electron density, which may be expressed in the form

$$\frac{|\langle \gamma_f J_f || \mathbf{D} || \gamma_i J_i, K\varepsilon_p l; J \rangle|^2}{|\langle \gamma_f J_f || \mathbf{D} || \gamma_i J_i, Kpl; J \rangle|^2} = \left( \frac{p}{\hbar} \right) \left( \frac{1}{2E_H a_0^2} \right), \quad (73)$$

we can confirm that the modified radiative recombination and photoionization cross sections satisfy the well-known Kramers relationship<sup>38</sup>

$$\frac{\bar{\sigma}_{\text{RR}}(i, \varepsilon_p \rightarrow f, \omega_k)}{\bar{\sigma}_p(f, \omega_k \rightarrow i, \varepsilon_p)} = \left( \frac{\hbar\omega_k}{2E_H} \right)^2 \left( \frac{2E_H}{cp} \right)^2 \left( \frac{2J_f + 1}{2J_i + 1} \right). \quad (74)$$

### C. The modified dielectronic recombination cross section

The autoionizing-resonance contribution to the transition amplitude determines the modified dielectronic recombination cross section according to the relation

$$\begin{aligned} \bar{\sigma}_{\text{DR}}(i, \varepsilon_p \rightarrow f, \omega_k) &= \left( \frac{2\pi}{\hbar} \right) \left( \frac{m_e}{p} \right) \frac{1}{(2J_i + 1)(2s + 1)} \\ &\times \sum_{M_i} \sum_{m_s} \sum_{M_f} \sum_{\lambda} \int d\Omega_k \rho(\hbar\omega_k) \\ &\times \left| \lim_{\varepsilon \rightarrow 0} \sum_{M_a} \langle f, \mathbf{k}\lambda | \tilde{V}(E_k + i\varepsilon) | a, 0 \rangle \langle a, 0 | G(E_k + i\varepsilon) | a, 0 \rangle \right. \\ &\quad \left. \times \langle a, 0 | \tilde{V}(E_k + i\varepsilon) | i\mathbf{p}m_s, 0 \rangle \right|^2. \end{aligned} \quad (75)$$

The modified dielectronic recombination cross section may be expressed in the familiar Breit-Wigner form<sup>21,22</sup> by the introduction of effective autoionization and radiative decay rates that incorporate the continuum-continuum coupling.<sup>18-20</sup> These effective decay rates may be defined in the same forms as the usual expressions Eqs. (56) and (57) for the corresponding unperturbed decay rates, provided that in the reduced matrix elements the interaction operators are replaced by the effective operators that arise from the vertex operator  $\tilde{V}(z)$ .

The vertex functions that occur in the expression Eq. (75) for the modified dielectronic recombination cross section may be represented in terms of the desired reduced matrix elements by means of the expansions

$$\begin{aligned} \langle i p m_s, 0 | \tilde{V}(z) | a, 0 \rangle &= \sum_{l,m} \exp[-i(l\pi/2 - \sigma_l)] Y_{lm}(\hat{p}) \\ &\times \sum_{K,N} (-1)^{s-J_i-N+K-l-M_a} (2K+1)^{1/2} \begin{Bmatrix} J_i & s & K \\ M_i & m_s & -N \end{Bmatrix} \begin{Bmatrix} l & K & J \\ m & N & -M_a \end{Bmatrix} \\ &\times \langle \gamma_i J_i, K p l; J_a | P \tilde{H}_A(z) Q | \gamma_a J_a \rangle, \end{aligned} \quad (76)$$

$$\langle f, \mathbf{k} \lambda | \tilde{V}(z) | a, 0 \rangle = \sum_{\mu} g_{\mu}^*(\mathbf{k}, \lambda) (-1)^{J_a - M_a} \begin{Bmatrix} J_a & 1 & J_f \\ -M_a & \mu & M_f \end{Bmatrix} \langle \gamma_f J_f | \tilde{\mathbf{D}}(z) | \gamma_a J_a \rangle, \quad (77)$$

which are identical in their forms to the corresponding expansions Eqs. (23) and (24) for the unmodified interactions.

The reduced matrix elements of the effective interaction operators  $P \tilde{H}_A(z) Q$  and  $\tilde{\mathbf{D}}(z)$  with  $z = E_k \pm i\epsilon$  may be related to the reduced matrix elements of the corresponding unmodified interaction operators by means of the pole approximation as follows:

$$\langle \gamma_i J_i, K p l; J_a | P \tilde{H}_A(z) Q | \gamma_a J_a \rangle = \frac{\langle \gamma_i J_i, K p l; J_a | P H_A Q | \gamma_a J_a \rangle}{\Psi(z)} \left[ \Psi(z) - \frac{A_r(a \rightarrow f)(\pm i + 1/Q_f)}{A_a(a \rightarrow i, K \epsilon_p l) Q_f(Kl)} \right], \quad (78)$$

$$\langle \gamma_f J_f | \tilde{\mathbf{D}}(z) | \gamma_a J_a \rangle = \frac{\langle \gamma_f J_f | \mathbf{D} | \gamma_a J_a \rangle}{\Psi(z)} \left[ 1 \mp \frac{i}{Q_f} \right], \quad (79)$$

where in Eq. (75)  $Q_f(Kl)$  denotes the individual contribution to the summation Eq. (65) associated with the partial wave  $K, l$ .

The modified dielectronic recombination cross section may be expressed in the familiar Breit-Wigner form<sup>21,22</sup>

$$\bar{\sigma}_{\text{DR}}(i, \epsilon_p \rightarrow f, \omega_k) = 2\pi^2 a_0^2 \left[ \frac{\hbar}{a_0 p} \right]^2 \left[ \frac{\hbar}{2E_H} \right] (2E_H) L_a(\hbar\omega_k) \frac{(2J_a + 1)}{2(2J_i + 1)} \frac{\tilde{A}_r(a \rightarrow f) \tilde{A}_a(a \rightarrow i, \epsilon_p)}{\tilde{A}(a)}. \quad (80)$$

The effective autoionization and radiative decay rates are related to the corresponding unperturbed rates in the pole approximation by means of the expressions<sup>20</sup>

$$\tilde{A}_a(a \rightarrow i, \epsilon_p) = \frac{A_a(a \rightarrow i, \epsilon_p)}{\Psi^2} \left[ \Psi^2 - \frac{2\Psi A_r(a \rightarrow f)}{Q_f^2 A_a(a \rightarrow i, \epsilon_p)} + (\Psi - 1) \left[ 1 + \frac{1}{Q_f^2} \right] \frac{A_r(a \rightarrow f)}{A_a(a \rightarrow i, \epsilon_p)} \right], \quad (81)$$

$$\tilde{A}_r(a \rightarrow f) = \frac{A_r(a \rightarrow f)}{\Psi^2} \left[ 1 + \frac{1}{Q_f^2} \right], \quad (82)$$

where  $\Psi$  represents  $\Psi(E_f + \hbar\omega_k)$ . The energy-normalized Lorentzian profile function obtained from Eq. (66) is given by

$$L_a(\hbar\omega_k) = \frac{\Gamma(a)}{2\pi} \frac{1}{[E_f - E_a + \hbar\omega_k - \Delta(a)]^2 + \Gamma(a)^2/4}, \quad (83)$$

and  $\Gamma(a) = \hbar \tilde{A}(a)$  represents the total width, which differs from the width obtained in the absence of the continuum-continuum coupling.<sup>19</sup>

For the case in which only a single angular momentum term is retained in the partial-wave expansion for the electron-continuum state, it follows from Eqs. (81) and (82) that the total perturbed decay rate  $\tilde{A}(a)$  is reduced from its unperturbed value  $A(a)$  according to the relation

$$\begin{aligned} \tilde{A}(a) &= \tilde{A}_a(a \rightarrow i \epsilon_p) + \tilde{A}_r(a \rightarrow f) \\ &= \frac{1}{\Psi} [A_a(a \rightarrow i \epsilon_p) + A_r(a \rightarrow f)] \\ &= \frac{1}{\Psi} A(a). \end{aligned} \quad (84)$$



#### D. The modified interference cross section

The cross section that arises from the interference between the resonant and nonresonant modified transition amplitudes in Eq. (45) can be expressed in the form

$$\begin{aligned} \bar{\sigma}_{\text{int}}(i, \varepsilon_p \rightarrow f, \omega_k) = & \left[ \frac{2\pi}{\hbar} \right] \left[ \frac{m_e}{p} \right] \frac{1}{(2J_i + 1)(2S + 1)} \\ & \times \sum_{M_i} \sum_{m_s} \sum_{M_f} \sum_{\lambda} \sum_{M_a} \int d\Omega_k \rho(\hbar\omega_k) \lim_{\varepsilon \rightarrow 0} [\langle f, \mathbf{k}\lambda | \tilde{V}(E_k + i\varepsilon) | i\mathbf{p}m_s, 0 \rangle \langle f, \mathbf{k}\lambda | \tilde{V}(E_k + i\varepsilon) | a, 0 \rangle^* \\ & \times \langle a, 0 | G(E_k + i\varepsilon) | a, 0 \rangle^* \langle a, 0 | \tilde{V}(E_k + i\varepsilon) | i\mathbf{p}m_s, 0 \rangle^* + \text{c.c.} ], \end{aligned} \quad (85)$$

where c.c. denotes the complex conjugate contribution. The complex conjugate of  $\langle f, \mathbf{k}\lambda | \tilde{V}(E_k + i\varepsilon) | a, 0 \rangle$  can be obtained by first substituting the relation Eq. (79) with  $z = E_k + i\varepsilon$  into the expansion Eq. (77) and then taking the complex conjugate. The complex conjugate of  $\langle a, 0 | \tilde{V}(E_k + i\varepsilon) | i\mathbf{p}m_s, 0 \rangle$  can be obtained by first utilizing the non-Hermitian property  $\tilde{V}^\dagger(z) = V(z^*)$ , which implies that  $\langle a, 0 | \tilde{V}(E_k + i\varepsilon) | i\mathbf{p}m_s, 0 \rangle^* = \langle i\mathbf{p}m_s, 0 | \tilde{V}(E_k - i\varepsilon) | a, 0 \rangle$ , and then substituting the relation Eq. (78) with  $z = E_k - i\varepsilon$  into the expansion Eq. (76).

In the pole approximation the modified interference cross section may thereby be reduced to the form

$$\begin{aligned} \bar{\sigma}_{\text{int}}(i, \varepsilon_p \rightarrow f, \omega_k) = & 2\pi^2 a_0^2 \left[ \frac{\hbar}{a_0 p} \right]^2 \left[ \frac{\hbar}{2E_H} \right] (2E_H) L_a(\hbar\omega_k) \frac{(2J_a + 1)}{2(2J_i + 1)} \frac{\tilde{A}_r(a \rightarrow f) \tilde{A}_a(a \rightarrow i, \varepsilon_p)}{\tilde{A}(a)} \frac{2}{\hbar \tilde{A}_a(a \rightarrow i, \varepsilon_p)} \left[ 1 + \frac{1}{Q_f^2} \right]^{-1} \frac{1}{\Psi} \\ & \times 2 \left[ \left[ \frac{2 - \Psi}{Q_f} \right] [E_f + \hbar\omega_k - E_a - \Delta(a)] - \left[ \frac{1}{Q_f^2} + \Psi - 1 \right] \frac{\Gamma(a)}{2} \right], \end{aligned} \quad (86)$$

where  $\Psi$  represents  $\Psi(E_f + \hbar\omega_k)$ .

The interference between the resonant and nonresonant modified transition amplitudes produces a departure from the standard Breit-Wigner form, which exhibits the usual Lorentzian energy dependence that is characteristic of the dielectronic recombination cross section. This departure from the Lorentzian line shape is manifest by the additional energy-dependent factor  $[E_f + \hbar\omega_k - E_a - \Delta(a)]$  in Eq. (86) and is completely analogous to the interference phenomena that was first theoretically described in the context of photoionization by Fano.<sup>28</sup> It should be emphasized that the modified interference cross section presented by Eq. (86) incorporates the additional shift and broadening that is produced by the coupling between the autoionization and radiation continua. The appearance of the interference contribution in the total electron-ion photorecombination cross section implies that the standard picture, in which radiative and dielectronic recombination are described as independent processes, is not strictly valid. The accuracy of the standard picture will obviously depend on the relative importance of the interference term.

#### E. The combined electron-ion photorecombination cross section

It is of interest to investigate the energy-dependence of the transition amplitude for the combined electron-ion photorecombination process without separating the nonresonant radiative and resonant dielectronic recombination contributions, since this separation has no fundamental foundation in our unified description. For simplicity we first treat only the case for which the tensor self-energy  $\sigma_{\mu\nu}^{ff}(M_f M_f', z)$  can be assumed to have the diagonal form  $\Sigma^{ff}(z) \delta_{\mu\nu}$ , and we omit all magnetic quantum number specifications. In other words, we now proceed according to the one-dimensional analysis presented by Haan and Cooper.<sup>19</sup> If the unperturbed electron- and photon-continuum state vectors are now denoted by  $|i\varepsilon_p\rangle$  and  $|f\omega_k\rangle$ , respectively, the total electron-ion photorecombination amplitude, which is obtained from Eqs. (42), (45), (48), (49), and (71), is given in the notationally simplified form

$$\begin{aligned} \langle f\omega_k | T | i\varepsilon_p \rangle = & \frac{1}{\Psi(z)} \langle f\omega_k | V | i\varepsilon_p \rangle \\ & + \left[ \langle f\omega_k | V | a \rangle + \frac{g^*(\omega_k)}{\Psi(z)} [\Sigma^{fa}(z) + \Sigma^{ff}(z) \Sigma^{ga}(z)] \right] \\ & \times \left[ (z - E_a) - \Sigma^{aa}(z) - \frac{1}{\Psi(z)} [\Sigma^{af}(z) \Sigma^{ga}(z) + \Sigma^{ag}(z) \Sigma^{fa}(z) \Sigma^{af}(z) \Sigma^{gg}(z) \Sigma^{fa}(z) + \Sigma^{ag}(z) \Sigma^{ff}(z) \Sigma^{ga}(z)] \right]^{-1} \\ & \times \left[ \langle a | V | i\varepsilon_p \rangle + \frac{f(\varepsilon_p)}{\Psi(z^*)^*} [\Sigma^{ag}(z^*)^* + \Sigma^{gg}(z^*)^* \Sigma^{af}(z^*)^*] \right], \end{aligned} \quad (87)$$

where all  $z$ -dependent quantities are to be evaluated at  $z = E_k + i\epsilon$ . In conformity with the notation of Haan and Cooper,<sup>19</sup> the vector self-energies without the magnetic quantum numbers are denoted by  $\Sigma^{fa}(z)$  and  $\Sigma^{ga}(z)$ , and the autoionizing state in the unperturbed basis set is designated simply by  $|a\rangle$ .

In order to combine the resonant and nonresonant transition amplitudes, we exploit the separable form of the dipole-interaction matrix elements. It is also advantageous to separate the electron- and photon-continuum contributions to the self-energy  $\Sigma^{aa}(z)$  by writing

$$\Sigma^{aa}(z) = \Sigma_{\text{elec}}^{aa}(z) + \Sigma_{\text{phot}}^{aa}(z). \quad (88)$$

The matrix elements of the electronic dipole-moment operator between the unperturbed atomic eigenstates are explicitly introduced by employing the relationships

$$\langle f\omega_k | V | i\epsilon_p \rangle = g^*(\omega_k) \langle f | \mathbf{D} | i\epsilon_p \rangle, \quad (89)$$

$$\langle f\omega_k | V | a \rangle = g^*(\omega_k) \langle f | \mathbf{D} | a \rangle, \quad (90)$$

$$f(\epsilon_p) = \langle f | \mathbf{D} | i\epsilon_p \rangle, \quad (91)$$

$$\Sigma^{ga}(z) = \Sigma^{gg}(z) \langle f | \mathbf{D} | a \rangle, \quad (92)$$

$$\Sigma_{\text{phot}}^{aa}(z) = \Sigma^{gg}(z) |\langle f | \mathbf{D} | a \rangle|^2. \quad (93)$$

The resonant and nonresonant contributions in Eq. (87) may now be combined to form the result

$$\langle f\omega_k | T | i\epsilon_p \rangle = g^*(\omega_k) \frac{\langle f | \mathbf{D} | i\epsilon_p \rangle [(z - E_a) - \Sigma_{\text{elec}}^{aa}(z)] + [\langle f | \mathbf{D} | a \rangle + \Sigma^{fa}(z)] \langle a | V | i\epsilon_p \rangle}{\Psi(z) [(z - E_a) - \Sigma_{\text{elec}}^{aa}(z)] - \Sigma^{gg}(z) [\langle f | \mathbf{D} | a \rangle + \Sigma^{fa}(z)] [\langle a | \mathbf{D} | f \rangle + \Sigma^{af}(z)]}. \quad (94)$$

The self-energies  $\Sigma_{\text{elec}}^{aa}(z)$ ,  $\Sigma^{fa}(z)$ , and  $\Sigma^{gg}(z)$  can be evaluated in the pole approximation to obtain the expressions

$$\Sigma_{\text{elec}}^{aa}(z) = -i\pi |\langle a | V | i\epsilon_p \rangle|^2, \quad (95)$$

$$\Sigma^{fa}(z) = -i\pi \langle f | \mathbf{D} | i\epsilon_p \rangle \langle i\epsilon_p | V | a \rangle, \quad (96)$$

$$\Sigma^{gg}(z) = -i\pi |g(\omega_k)|^2. \quad (97)$$

It is now convenient to introduce the parameters which are conventionally used in the Fano line shape theory,<sup>28</sup> i.e.,

$$\epsilon_f = \frac{(E_k - E_a)}{\Gamma_a/2} = \frac{(E_f - E_a + \hbar\omega_k)}{\Gamma_a/2}, \quad (98)$$

$$\frac{1}{Q_f} = \frac{\pi \langle f | \mathbf{D} | i\epsilon_p \rangle \langle i\epsilon_p | V | a \rangle}{\langle f | \mathbf{D} | a \rangle}, \quad (99)$$

$$\frac{\Gamma_a}{2} = \frac{\hbar A_a}{2} = \pi |\langle a | V | i\epsilon_p \rangle|^2. \quad (100)$$

(Note that we have now restricted our analysis to the case of a single electron-continuum partial-wave component.) In addition the continuum-continuum coupling parameter  $\Psi(z)$  can be expressed in the pole approximation by

$$\Psi(z) = 1 + \pi^2 |g(\omega_k)|^2 |\langle f | \mathbf{D} | i\epsilon_p \rangle|^2, \quad (101)$$

and the radiative decay rate  $A_r$  is given by

$$\frac{\hbar A_r}{2} = \pi |g(\omega_k)|^2 |\langle a | \mathbf{D} | f \rangle|^2. \quad (102)$$

The combined electron-ion photorecombination amplitude is finally obtained in the pole approximation in the parametrized form

$$\langle f\omega_k | T | i\epsilon_p \rangle = \frac{g^*(\omega_k) |\langle f | \mathbf{D} | i\epsilon_p \rangle|^2 (\epsilon_f + Q_f)}{\Psi \left[ \epsilon_f + \frac{2A_r}{\Psi Q_f A_a} \right] + i \left[ 1 + \frac{A_r}{A_a} \right]}, \quad (103)$$

and the total electron-ion photorecombination cross section is accordingly given in terms of the unperturbed radiative recombination cross section  $\sigma_{\text{RR}}(i, \epsilon_p \rightarrow f, \omega_k)$  by the result

$$\sigma(i, \epsilon_p \rightarrow f, \omega_k) = \frac{\sigma_{\text{RR}}(i, \epsilon_p \rightarrow f, \omega_k) (\epsilon_f + Q_f)^2}{\left[ \Psi^2 \left[ \epsilon_f + \frac{2A_r}{\Psi Q_f A_a} \right]^2 + \left[ 1 + \frac{A_r}{A_a} \right]^2 \right]}, \quad (104)$$

which is in agreement with Eq. (5a) in the paper of Alber, Cooper, and Rau.<sup>27</sup> In the limit of very large  $Q_f$ , Eq. (104) reduces to a Lorentzian profile function corresponding to the total unperturbed width  $\hbar(A_a + A_r)$  and therefore yields the conventional unperturbed dielectronic recombination cross section. In general, Eq. (104) represents a modified Fano profile characterized by a shift of the closed-channel resonance given by  $\hbar A_r / \Psi Q_f$  and by a reduced total width of  $\hbar(A_a + A_r) / \Psi$ , which are the result of the continuum-continuum coupling. This modified Fano profile has also been predicted for the process of laser-induced autoionization by Agarwal, Haan, and Cooper.<sup>39,40</sup>

For application to the general case of degenerate magnetic sublevels and multiple electron-continuum partial-wave components, Eqs. (72), (80), and (86) can be combined to form the total electron-ion photorecombination cross section

$$\begin{aligned}
\sigma(i, \varepsilon_p \rightarrow f, \omega_k) = & \left[ \Psi^2 \left[ \varepsilon_f + \frac{2A_r}{\Psi Q_f A_a} \right]^2 + \left[ \Psi \frac{\tilde{A}(a)}{A_a} \right]^2 \right]^{-1} \sigma_{\text{RR}}(i, \varepsilon_p \rightarrow f, \omega_k) \left[ \left[ \varepsilon_f + \frac{2A_r}{\Psi Q_f A_a} \right]^2 + \left[ \frac{\tilde{A}(a)}{A_a} \right]^2 \right] \\
& + \pi a_0^2 \left[ \frac{\hbar}{a_0 p} \right]^2 \frac{(2J_a + 1)}{2(2J_i + 1)} 4 \frac{A_r \tilde{A}_a}{A_a^2} \left[ 1 + \frac{1}{Q_f^2} \right] \\
& + \frac{8A_r}{\Psi A_a} \left[ \left[ \frac{2 - \Psi}{Q_f} \right] \left[ \varepsilon_f + \frac{2A_r}{\Psi Q_f A_a} \right] - \left[ \frac{1}{Q_f^2} + \Psi - 1 \right] \frac{\tilde{A}(a)}{A_a} \right]. \tag{105}
\end{aligned}$$

This general expression can be reduced to the special case represented by Eq. (104) by utilizing Eqs. (66), (81), (84), and the relationship

$$\sigma_{\text{RR}}(i, \varepsilon_p \rightarrow f, \omega_k) = \pi a_0^2 \left[ \frac{\hbar}{a_0 p} \right]^2 \frac{(2J_a + 1)}{2(2J_i + 1)} \frac{4A_r}{A_a Q_f^2}. \tag{106}$$

Consequently, the equivalence between the final result (105) of the present investigation and that of Alber, Cooper, and Rau<sup>27</sup> has been established, for the nondegenerate-level and single-partial-wave problem, by two different methods.

In the limit of very large values of  $Q_f$ , Eq. (105) can be reduced to the Lorentzian form

$$\begin{aligned}
\sigma(i, \varepsilon_p \rightarrow f, \omega_k) \xrightarrow[Q_f \rightarrow \infty]{} & 4\pi^2 a_0^2 \left[ \frac{\hbar}{a_0 p} \right]^2 \frac{(2J_a + 1)}{2(2J_i + 1)} \\
& \times \left[ \frac{A_r}{A_a} \right] \left[ \varepsilon_f^2 + \left[ 1 + \frac{A_r}{A_a} \right]^2 \right]^{-1}, \tag{107}
\end{aligned}$$

which is the conventional expression for the cross section describing dielectronic recombination in the absence of the coupling between the autoionization and radiation continua. The radiative recombination and interference contributions, together with the effects of the continuum-continuum coupling, must consequently become more important with decreasing values of  $Q_f$ . In the case of inner-electron radiatively stabilizing transitions, it can be deduced that  $Q_f$  increases as  $n^3$  where  $n$  denotes the principal quantum number of the outer electron. Moreover, it can be shown that  $Q_f$  scales in this case as  $Z$ , where  $Z$  represents the nuclear charge. From these properties it might be anticipated that the most important modifications to Eq. (107) will arise for transitions corresponding to the lowest possible values of  $n$  in low- and medium- $Z$  elements. Consequently, the modifications are expected to be most important for individual transitions involving low-lying autoionizing levels and to be negligible for total dielectronic recombination rates which are dominated by the contributions from highly excited levels. However, a more precise assessment of the importance of these modifications, together with the radiative corrections, can only be made after a more detailed analysis together with systematic numerical calculations for a variety of satellite transitions.

#### IV. CONCLUSIONS

In this investigation a unified description of radiative and dielectronic recombination has been presented that incorporates a nonperturbative treatment of the electromagnetic coupling between the autoionization and radiative decay continua. Particular attention has been given to the angular momentum degeneracy of the atomic levels and to the multiplicity of angular momentum components in the partial-wave expansion for the electron-continuum state. Through the introduction of vertex functions and of a modified propagator, the  $S$  matrix describing the combined electron-ion photorecombination process has been expressed as the sum of a resonant and a non-resonant transition amplitude. Within the limitations of our restricted basis set of unperturbed eigenstates, this formulation incorporates radiative corrections to all orders in quantum electrodynamical perturbation theory.

In a previous reported investigation<sup>20</sup> of radiative corrections to the intensities of dielectronic recombination satellite lines, the isolated-resonance approximation was employed to derive an expression that is found to be in agreement with the modified resonant contribution to the electron-ion photorecombination cross section obtained in our present unified description. This previous investigation is accordingly given a precise foundation by our unified expression, which would predict that the observed intensity of photoemission is determined completely by adding to the resonant contribution the conventionally neglected nonresonant and interference terms. By considering the case of a single electron-continuum partial-wave component, the unified expression for the modified electron-ion photorecombination cross section that has been derived in the present investigation is found to be in agreement with the corresponding result obtained by Alber, Cooper, and Rau.<sup>27</sup>

The full expression for the combined photorecombination cross section, given by Eq. (105), is quite complicated. However, it is clear that the interference and continuum-continuum coupling modifications are most important for small values of the Fano line profile parameter  $Q_f$ , which are most likely to occur for satellite lines with small principal quantum number. For these lines, detailed numerical calculations will be needed to assess the overall importance of the corrections considered here.

In order to correctly treat the multi-continuum-channel electron-ion photorecombination processes that are known to play an important role in determining the charge-state distributions and the photoemission spectra of high-temperature plasma, it will be necessary to enlarge the

basis set of unperturbed eigenstates to include several electron-continuum channels  $|ip_i m_s, 0\rangle$  and several photon-continuum channels  $|f, \mathbf{k}, \lambda\rangle$ . This extension of our unified description of radiative and dielectronic recombination is not expected to present any fundamental difficulties in view of the fact that the theory of autoionization and radiative decay into several final-state electron- and photon-continuum channels has already been developed<sup>18,20</sup> for an atomic system that has been initially prepared in the doubly excited state. Another situation in which an enlargement of our unperturbed basis set will be required arises in the case of overlapping resonances, i.e., autoionizing states whose widths exceed their energy-level separations. The autoionizing states that correspond to highly excited  $nl$  states of the outer electron must ultimately form a Rydberg series of overlapping resonances, because the width due to the dominant inner-electron radiative decay process is independent of  $n$  whereas the energy-level separations decreases as  $n^{-3}$ . The effects of overlapping resonances are expected to be significant for the resonance properties, such as level shifts and widths,

and for the dielectronic recombination cross sections associated with the high-Rydberg autoionizing levels.<sup>26</sup> Finally, the photon Fock-space basis can be extended to allow for many photons in the quantized-radiation-field modes for application to photoionization and stimulated recombination processes in the presence of intense laser radiative fields, such as has been treated by Agarwal, Haan, and Cooper.<sup>39,40</sup>

In a precise evaluation of the modified electron-ion photorecombination cross sections, the vertex and propagator modifications must be obtained without making the pole approximation. In order to properly treat the divergent self-energy quantities that would appear in this evaluation, it will be necessary to derive a renormalized expression for the transition operator. We anticipate that the renormalization procedure will involve the replacement of the modified propagator and the vertex correction operator by the corresponding renormalized operators. The renormalization must be consistent with the integral relationship between the vertex and propagator modifications, which can be expressed in the form

$$\begin{aligned}
 [ \langle a, 0 | G(z) | a, 0 \rangle ]^{-1} = & z - E_a - \sum_{M_i} \sum_{m_s} \int d^3 p \frac{\langle a, 0 | V | ip m_s, 0 \rangle \langle ip m_s, 0 | \tilde{V}(z) | a, 0 \rangle}{(z - E_p)} \\
 & - \sum_{M_f} \sum_{\lambda} \sum_{\mathbf{k}} \frac{\langle a, 0 | V | f, \mathbf{k}, \lambda \rangle \langle f, \mathbf{k}, \lambda | \tilde{V}(z) | a, 0 \rangle}{(z - E_k)}. \quad (108)
 \end{aligned}$$

Analogous relationships have been encountered in quantum electrodynamics.<sup>41</sup>

For application to electron-ion photorecombination in high-density plasmas, the analysis presented in this investigation should be extended to allow for the effects of both collisional dephasing processes and plasma electric microfields. Ballagh and Cooper<sup>42</sup> have recently presented a density-matrix description that takes into account the correlation effects that result when collision and spontaneous decay processes are of comparable duration. They demonstrated that the presence of this correlation phenomena invalidates the usual assumption that the total transition rates can be obtained as the sums of the rates that would be produced by the individual actions of the collision and spontaneous decay processes. It appears

desirable to develop a density-matrix description of the combined radiative and dielectronic recombination processes that would incorporate electron-ion collisional dephasing processes and plasma electric microfields.

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