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Projection-operator approach to the unified treatment of radiative and dielectronic recombination

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A formalism that is based on projection operators is employed to obtain a general recipe for constructing matrix elements of the transition or T operator for electron-ion photorecombination processes in model systems featuring a limited number of discrete states and continua. The projection-operator formalism allows for a natural separation of the total transition operator into a direct, or radiative recombination, contribution and a resonance, or dielectronic recombination contribution. Implementation of the general recipe is discussed, and expressions for matrix elements of needed propagators in the combined Hilbert space of electron and photon continua are derived for model systems in which one makes the pole approximation on the photon continua, but not on the electron continua. The simplifications that occur when the pole approximation is made on all continua are presented. Finally, the recipe is employed to describe photorecombination for two model systems that feature an isolated autoionizing state. One model includes an arbitrary number of possible final-state photon continua, and the second model includes an arbitrary number of possible final-state electron continua. For the former model, it is shown how the various terms entering into the expression for the recombination transition amplitude can be obtained from a perturbation series and interpreted in terms of Feynman-like diagrams.

I. INTRODUCTION

Collisions between electrons and many-electron ions can be accompanied by free-bound spontaneous radiative emission processes. These processes can play an important role in the determination of the ionization-recombination balance of multiply charged ions in both colliding electron-ion beam experiments[1-3] and in high-temperature laboratory and astrophysical plasmas.[4-6] Radiative emission processes resulting from electron-ion collisions are responsible for the appearance of prominent spectral features in the far-ultraviolet and x-ray region, which are frequently employed for the investigation of fundamental atomic collisional and radiative interactions and for the spectroscopic determination of basic plasma properties,[7,8] such as temperatures, densities, and charge-state distributions. The free-bound radiation emission process is conventionally described as involving either direct (nonresonant) radiative recombination, which is the inverse of the ordinary photoionization process, or two-step (resonant) dielectronic recombination,[4] which consists of a radiationless electron capture (accompanied by excitation of the initial ion, to form a doubly excited autoionizing state) followed by a spontaneous radiatively stabilizing transition to a bound final state.

It has been pointed out in several scattering-theory investigations[9-11] that the treatment of radiative and dielectronic recombination as two distinct, noninterfering processes is not strictly permissible within the framework of a rigorous quantum-mechanical theory. In particular, the transition probability for the formation of a given bound final state of the recombined ion, accompanied by the spontaneous emission of a photon, must be expressed as the square of the sum of the nonresonant and the resonant transition amplitudes associated with the direct radiative recombination and the dielectronic recombination processes, respectively. The total cross section for the entire electron-ion photorecombination process is thereby expressed as the sum of the radiative and dielectronic recombination cross sections together with an additional contribution, which represents the interference between the transition amplitudes for radiative and dielectronic recombination. Moreover, it has been demonstrated in recent theoretical treatments[12-14] of the decay of unstable states that the exact diagonalization of the complete Hamiltonian for the interacting many-electron and radiation-field system results in the appearance of an additional interference phenomenon, which can be interpreted as an interference between the unperturbed autoionization and spontaneous radiative decay modes.

In a previous investigation,[11] we have presented a unified description of radiative and dielectronic recombination which includes the electromagnetic coupling between the autoionization and the radiative-decay continua. This description has provided a generalization of an earlier scattering or S-matrix analysis by Alber, Cooper, and Rau[9] to explicitly take into account degenerate magnetic sublevels of the atomic system and multiple angular momentum contributions in the partial-wave expansion for the electron-continuum eigenstate. The central result of this unified description is an exact expression for the transition matrix for the entire electron-ion photorecombination process. This exact expression is

naturally obtained as the sum of a nonresonant transition or radiative recombination amplitude, which is represented by a vertex operator, and a resonant transition or dielectronic recombination amplitude, which involves both the vertex operator and the projection of the resolvent operator onto the subspace of the autoionizing states. After the introduction of a limited basis set, consisting of a single discrete autoionizing state, a single-electron continuum, and a single-photon continuum, together with the pole approximation,[13,14] in which the various self-energy quantities are approximated by including only the δ-function terms, explicit expressions for the various contributions to the total electron-ion photorecombination cross section are obtained in terms of the familiar unperturbed matrix elements of the electron-electron and radiation-field interactions. In particular, the modified dielectronic recombination cross section is expressed in the familiar Breit-Wigner form by means of the introduction of effective autoionization and radiative decay rates,[12–14] which incorporate the interference between the autoionization and radiative decay continua. Alternatively, the combined cross section for the entire electron-ion photorecombination process may be represented in terms of a modified Fano line-profile function, which is shifted and broadened as a result of the electromagnetic coupling between the autoionization and radiative-decay continua.

For application to recombination processes involving multiple electron continua and/or multiple photon continua, it is advantageous to develop the S-matrix description by taking advantage of the projection-operator techniques originally introduced for nuclear reaction theory by Feshbach,[15,16] and also utilized in studies of the decay of virtual or prepared states[17–19] and in studies of multiphoton ionization processes in atomic systems.[20] Projection-operator techniques have also recently been applied[21] to the scattering-theory analysis of laser-induced autoionization phenomena involving several spontaneous radiative decay continua. It is convenient to introduce a natural extension of the usual Feshbach projection-operator formalism, which involves the electron-continuum projection operator P and the resonance state projection operator Q, to include the photon-continuum projection operator R.[22–24] Our objective shall be to provide an explicit procedure for obtaining the required projected transition amplitudes in terms of the unperturbed interaction matrix elements that are routinely evaluated in the course of standard multiconfiguration atomic structure and scattering calculations.

In the present work we use projection-operator techniques to investigate in detail the transition operator T that describes the electron-ion photorecombination process. We present an expression for T which separates naturally into two terms, one of which describes the direct radiative recombination process in the absence of autoionizing resonances, and the other which incorporates all effects of the autoionizing resonances. The projection-operator formalism allows us to present a general recipe for constructing matrix elements of the T operator for electron-ion photorecombination processes for particular model systems of interest featuring a limited number of discrete states and continua.

In Sec. II of this paper we present the projection-operator formalism in detail, and we derive a general expression for the T operator. In Sec. III we apply the projection-operator formalism to electron-ion photorecombination processes, and we present the general recipe mentioned above. The formalism involves certain continuum-continuum propagators whose matrix elements must be determined in order to construct the required matrix elements of T, and Sec. IV is devoted to finding explicit forms for these propagators in various levels of approximation. In Sec. V we apply the general recipe to two model systems. Finally, in Sec. VI we summarize some of the results of this study and discuss possible extensions of the present work.

II. PROJECTION-OPERATOR FORMALISM

In this section we present in detail a projection-operator formalism that will be applied in subsequent sections. The formalism of this section is essentially application independent, although the context of the development and the subsequent application relate to describing electron-ion photorecombination processes. Variations of the formalism of this section have been used previously by other investigators in a variety of contexts. A discussion of the use of projection operators for describing the decay of unstable states has been presented by Goldberger and Watson[17] and by Mower.[18,19] Applications to scattering problems have been presented by Feschbach[15,16] and Rodberg,[25] while treatments of photoabsorption processes have been given by Shore[26] and others.[20]

We suppose that the Hamiltonian H for the many-electron atom and radiation-field system of interest has been decomposed as $H=H^0+V$, and we assume that the eigenstates of H^0 are known. We define two orthogonal projection operators, C and Q, which commute with H^0. Then of course $C^2=C$, $Q^2=Q$, $CQ=QC=0$, $H^0C=CH^0$, and $H^0Q=QH^0$. The interaction V couples the various eigenstates of H^0, so that in general CVC, CVQ, QVC, and QVQ are nonzero. We assume that V does not couple states which are in the spaces onto which C and Q project with states outside those combined spaces: $(C+Q)V=V(C+Q)=V$. (Thus, if the initial state is in the $C+Q$ space, then the $C+Q$ space is complete for describing the development of the system, and states outside the $C+Q$ space can be ignored. Within this $C+Q$ space, we can then write $C+Q=1$, where 1 is the identity operator, and $H^0=CH^0C+QH^0Q$.)

When we apply the projection-operator formalism to electron-ion photorecombination processes, we will suppose that the eigenstates of H^0 include electron continua (consisting of target positive ion and unbound electron), photon continua (which are product states of an emitted photon and bound discrete atomic states of the target plus electron), and discrete (doubly excited) states. C will be the operator that projects onto the set of all continuum eigenstates of H^0 (both electron and photon), and Q will be the operator which projects onto the set of all discrete (doubly excited) eigenstates of H^0. The potential

V will be taken to be the sum of the interactions responsible for autoionization processes and radiative transitions, and will couple the discrete states to the electron continua (autoionization coupling) and to the photon continua (spontaneous radiative decay coupling). V will also couple various continua together. The continuum projection operator C will subsequently be written as the sum of two projection operators, $C=P+R$, where P projects onto the subspace of electron continua, and R projects onto the subspace of photon continua. The operators P and Q will then be the usual Feshbach projection operators,[15,16] and R will be the projection operator introduced by Gau and Hahn,[22] and used by LaGattuta.[23,24]

The Green's operator is defined as $G(z)=(z-H^0-V)^{-1}$. Many studies involving Green's operators are based on the Lippmann-Schwinger equation $G(z)=G^0(z)+G^0(z)VG(z)$, where $G^0(z)=(z-H^0)^{-1}$ represents the Green's operator in the absence of the interaction V. In this work we will proceed from the different, but equivalent expression

$$(z-H^0)G(z)=1+VG(z)\ . \tag{2.1}$$

Acting on (2.1) with Q from both the left and right, and recalling that Q commutes with H^0, gives

$$(z-H^0)QG(z)Q=Q+QVCG(Z)Q+QVQG(Z)Q. \tag{2.2}$$

Acting on (2.1) from the left with C and from the right with Q, and defining

$$\Phi(z)=C[C(z-H^0-V)C]^{-1}\ , \tag{2.3}$$

one easily obtains, since both C and Q commute with H^0,

$$CG(z)Q=[C\Phi(z)C]V[QG(z)Q]\ . \tag{2.4}$$

Next defining

$$\Lambda(z)=V+VC\Phi(z)CV \tag{2.5}$$

and substituting (2.4) into (2.2), one obtains

$$QG(z)Q=Q\{Q[z-H^0-\Lambda(z)]Q\}^{-1}\ . \tag{2.6}$$

Two other useful equations which can be derived from (2.1) using similar straightforward methods are

$$QG(z)C=QG(z)Q[VC\Phi(z)C] \tag{2.7}$$

and

$$CG(z)C=C\Phi(z)C[1+VQG(z)C]\ . \tag{2.8}$$

Equations (2.3)–(2.8) are useful in a variety of problems involving photoionization, photodetachment, or photorecombination processes. The operator $\Lambda(z)$ has been frequently referred to as a "level shift operator" or "vertex operator," and in the contexts of photoionization and the decay of virtual states it has often been denoted by $R(z)$.[17–21] In the photoionization studies, the symbol P has often been used to denote the projector onto the discrete states, and the symbol Q is used for the projector onto the continuum states.

$\Lambda(z)$ is also closely related to optical potentials, which are frequently introduced in multichannel scattering theory.[27] In particular, $Q\Lambda(z)Q=QVQ+QVC\Phi(z)CVQ$ represents an optical potential in the Q subspace, which in the present work corresponds to the discrete state subspace. The above formalism is quite similar to the original Feshbach projection-operator formalism,[15,16] although in many discussions[28] and applications of the Feshbach formalism one constructs an optical potential in the subspace of the continua rather than in the subspace of the discrete states. These discussions accordingly do not use the continuum space propagator $\Phi(z)$, as defined in Eq. (2.3), but use a Q-space propagator $Q[Q(z-H^0-V)Q]^{-1}$. We note, however, that the original Feshbach papers contain expressions involving the continuum space propagator that we have called $\Phi(z)$ as well as expressions involving the Q space propagator $Q[Q(z-H^0-V)Q]^{-1}$.

To describe the photorecombination process we shall use the transition operator T; if H^0 denotes the unperturbed Hamiltonian and V the interaction, then[29]

$$T(z)=V+VG(z)V \tag{2.9a}$$

$$=V+V(C+Q)G(z)(C+Q)V\ . \tag{2.9b}$$

The transition operator T is related to the scattering operator S and provides a complete description of the electron-ion photorecombination process. The recombination cross section can be evaluated in terms of the matrix elements of T between the asymptotic continuum states. The complex variable z is used to specify the appropriate scattering boundary conditions on the asymptotic continuum states. For an incident electron with energy E, one takes $z=E+i0$, i.e., $T(z)=\lim_{\varepsilon\downarrow 0}T(E+i\varepsilon)$.

In this work our primary interest lies in describing electron-ion photorecombination processes for systems in which the initial states, consisting of incident electron and bound target ion, have energies close to the energies of autoionizing resonances. In order to concentrate on the effects of the interactions responsible for autoionization and spontaneous radiative decay, some of the interactions between the incident electron and the positive ion target are assumed to have been assimilated into the "unperturbed Hamiltonian" H^0. This assimilation poses no formal difficulties. In the Appendix we briefly show how the formalism of multichannel scattering theory[29] can be applied to the situation of interest, and how the assimilation of some of the interaction into H^0 can be carried out, with Eq. (2.9) as a resulting equation describing the effects of the interactions of interest.

Multiplying out the right-hand term in Eq. (2.9b) and using Eqs. (2.4), (2.7), and (2.8) gives, after some rearranging,

$$T(z)=\Lambda(z)+\Lambda(z)QG(z)Q\Lambda(z)\ . \tag{2.10}$$

Equation (2.10) is an operator equation which, when applied to electron-ion photorecombination problems, generalizes previous work in providing a unified description of radiative and dielectronic recombination.[30] Equation (2.10) has previously been presented by Rodberg[25] and by Feschbach[16] in the context of resonances in the scattering of nucleons by nuclei, and by Shore[26] in the context of photoabsorption resonances. All of these investigators

have indicated that the first term in the sum, which we have called $\Lambda(z)$, describes scattering in the absence of the set of states Q, and that the resonance effects arising because of the states Q are entirely included in the second term.

III. APPLICATION TO ELECTRON-ION PHOTORECOMBINATION PROCESSES

In discussing photorecombination processes it is convenient to write the continuum projection operator C as the sum of projection operators for electron and photon continua: $C=P+R$, where $PH^0=H^0P$, $RH^0=H^0R$, and of course $PR=RP=0$. Then the photorecombination process, in which the system evolves from an electron continuum state (in the subspace onto which P projects) into a photon continuum state (in the subspace onto which R projects), is described by

$$RT(z)P=R\Lambda(z)P+R\Lambda(z)QG(z)Q\Lambda(z)P\ . \tag{3.1}$$

Equation (3.1) provides a natural separation of the total transition operator for electron-ion photorecombination into a direct, or radiative recombination, contribution and a resonance, or dielectronic recombination, contribution. The first term in the sum, $R\Lambda(z)P$, represents the transition amplitude that would be obtained for $RT(z)P$ if there were no autoionizing states present in the system, and this nonresonant term can be said to represent direct, or free-bound, radiative recombination. All effects of the autoionizing states are included in the second, or resonance, term, $R\Lambda(z)QG(z)Q\Lambda(z)P$, in which $QG(z)Q$ can be thought of as representing a propagator through the subspace of autoionizing states. The resonance term differs from the conventional transition amplitude for dielectronic recombination, however, because effects of the couplings between the electron and photon continua have been included; it has been demonstrated that this coupling can affect the matrix elements of $R\Lambda(z)Q$, $QG(z)Q$, and $Q\Lambda(z)P$.[8] A different division into radiative and dielectronic recombination contributions, which is based on a separation of the incident electron-continuum wave function, has been adopted by LaGattuta.[23,24]

In order to treat the electron-ion photorecombination process, we will assume that V does not mix photon continua with other photon continua, i.e., that $RVR=0$. We will also assume that the interaction of electron continua with other electron continua, which would be described by PVP, has been included in the unperturbed Hamiltonian H^0, as discussed in the Appendix. After application of this condition we have $PVP=0$, and we take V to be the sum of the interactions leading to autoionization and to spontaneous radiative decay. We emphasize that the eigenstates of H^0 are not plane-wave states, but are the scattering eigenstates in the absence of autoionization and spontaneous radiative decay.

A. Derivation of general recipe for calculating matrix elements of T operator

Evaluation of matrix elements of (3.1) will require knowledge about the matrix elements of $\Lambda(z)$, and hence of $\Phi(z)$. For the case $PVP=RVR=0$, it follows immediately from its definition, Eq. (2.3), that in the space C

$$(z-H^0)\Phi(z)=1+PVR\Phi(z)+RVP\Phi(z)\ . \tag{3.2}$$

If one acts on both the left- and right-hand sides of (3.2) with P, one finds

$$(z-PH^0P)P\Phi(z)P=P+PVR\Phi(z)P\ . \tag{3.3}$$

Acting on the left of (3.2) with R and on the right with P gives

$$(z-RH^0R)R\Phi(z)P=RVP\Phi(z)P\ . \tag{3.4}$$

Combined, Eqs. (3.3) and (3.4) give

$$P\Phi(z)P=P[Pz-PH^0P-PVRG^0(z)RVP]^{-1}P \tag{3.5a}$$

and

$$R\Phi(z)P=RG^0(z)RVP\Phi(z)P\ , \tag{3.5b}$$

where

$$G^0(z)=(z-H^0)^{-1}\ , \tag{3.6a}$$

$$RG^0(z)R=R[R(z-H^0)R]^{-1}\ . \tag{3.6b}$$

Similarly one can write

$$R\Phi(z)R=R[Rz-RH^0R-RVPG^0(z)PVR]^{-1}R\ , \tag{3.7a}$$

$$P\Phi(z)R=PG^0(z)PVR\Phi(z)R\ , \tag{3.7b}$$

where

$$PG^0(z)P=P[P(z-H^0)P]^{-1}\ . \tag{3.7c}$$

We are now able to write a general recipe for constructing matrix elements of the T operator for electron-ion photorecombination processes for particular model systems of interest featuring a limited number of discrete states and continua.

(1) Evaluate matrix elements of $P\Phi(z)P$, $R\Phi(z)R$, $R\Phi(z)P$ and $P\Phi(z)R$ using Eqs. (3.5) and (3.7). [Note that $R\Phi(z)P$ and $P\Phi(z)R$ can be constructed from $P\Phi(z)P$ and $R\Phi(z)R$, respectively.]

(2) Find matrix elements of $R\Lambda(z)P$, $R\Lambda(z)Q$, $Q\Lambda(z)P$, and $Q\Lambda(z)Q$ using Eq. (2.5).

(3) Invert the matrix corresponding to the operator $Q[z-H^0-Q\Lambda(z)Q]Q$ in the Q space to obtain the Q-space projection of the resolvent. (If there are N_d discrete states being considered in the problem, then this will be an $N_d\times N_d$ matrix.)

(4) Evaluate matrix elements of $RT(z)P$ using Eq. (3.1).

B. Comparison with related work

Before proceeding further, comparison with two recent works of LaGattuta[23,24] is warranted. He has considered the same topic as the present work, and although many aspects of his approach are different, his results are equivalent. However, the implementation of his results may be different from ours because the operator inverses have been written in different forms. To make the comparison more explicit, we note that our projected Φ

operators $P\Phi(z)P$ and $R\Phi(z)R$ [Eqs. (3.5a) and (3.7a)], which can be thought of as modified propagators within the P and R subspaces, correspond, respectively, to his g_P and g_R of Eqs. (15) and (18) of his paper II.[24]

LaGattuta uses the identity

$$(A-B)^{-1}=[A(1-A^{-1}B)]^{-1}=(1-A^{-1}B)^{-1}A^{-1} . \tag{3.8}$$

This identity allows one to write alternative forms for several quantities, and we write them below for reference. Equation (3.8) applied to our Eqs. (3.5a) and (3.7a) gives

$$P\Phi(z)P=P[P-PG^0(z)PVRG^0(z)RVP]^{-1}PG^0(z)P \tag{3.9}$$

and

$$R\Phi(z)R=R[R-RG^0(z)RVPG^0(z)PVR]^{-1}RG^0(z)R . \tag{3.10}$$

It follows that one can write

$$\begin{aligned} C\Phi(z)C&=(P+R)\Phi(z)(P+R)\\ &=[1+RG^0(z)RVP]P\Phi(z)P\\ &\quad+[1+PG^0(z)PVR]R\Phi(z)R \end{aligned} \tag{3.11}$$

and

$$\begin{aligned} Q\Lambda(z)Q&=QVQ+QV[1+RG^0(z)RVP]P\Phi(z)PVQ\\ &\quad+QV[1+PG^0(z)PVR]R\Phi(z)RVQ . \end{aligned} \tag{3.12}$$

Using Eq. (3.11), together with the equivalences of our PG^0P and RG^0R with the quantities g_P and g_R defined by LaGattuta[24] [see our Eqs. (3.6) and (3.7c)], it can be shown that the diagonal matrix elements of our Q-space projection of the resolvent operator QGQ are equivalent to those matrix elements which can be obtained from Eq. (24) of his paper II.[24] When more than a single Q-space state is included in the basis set, the Q-space projection of the resolvent operator can only be obtained by employing the full matrix inversion referred to in item number three of our general recipe. An alternative representation of this matrix inversion is the general relation given by Eq. (20) of LaGattuta's paper II.[24]

In paper I (Ref. 23) LaGattuta considered the case in which the direct coupling between different continua was neglected, i.e., $RVP=PVR=PVP=RVR=0$. For this case Eq. (3.2) immediately gives

$$\Phi(z)=C(z-H^0)^{-1}=CG^0(z) . \tag{3.13}$$

Then (2.5) gives

$$\Lambda(z)=V+VPG^0(z)PV+VRG^0(z)RV , \tag{3.14}$$

and (2.6) gives

$$\begin{aligned} QG(z)Q=Q[&Q(z-H^0)Q-QVQ-QVPG^0(z)PVQ\\ &-QVRG^0(z)RVQ]^{-1}Q . \end{aligned} \tag{3.15}$$

His Eq. (17) can then be obtained by taking the modulus squared of the appropriate matrix elements of Eq. (3.1) and using Eqs. (3.8), (3.14), and (3.15) (with $QVQ=0$). For this special case of no direct coupling between continua, Eq. (3.1) becomes

$$RT(z)P=0+RVQG(z)QVP . \tag{3.16}$$

The first term in the sum is zero because there is no direct radiative recombination, and the second term represents conventional dielectronic recombination [with $QG(z)Q$ given by Eq. (3.15)].

IV. FINDING EXPLICIT FORMS FOR THE PROJECTIONS $P\Phi(z)P$ AND $R\Phi(z)R$

The usefulness of the above formalism depends to a great extent on being able to perform the necessary operator inversions in finding $P\Phi(z)P$ and $R\Phi(z)R$.

The inversions can in principle be accomplished for particular model systems of interest featuring a limited number of discrete states and continua if one takes into account the separability of the coupling between the electron and photon continua.[31] In this section we consider these inversions in a general context, and we first obtain expressions for the inversions for the case where the pole approximation is made on the photon continua but not on the electron continua (we will define what we mean by the "pole approximation" below). We then present expressions obtained by introducing the pole approximation for both the electron and photon continua.

We will assume that the continuum eigenstates of H^0 have a δ-function normalization with respect to energy. Accordingly, we will write the electron continuum eigenstates as $|\alpha E\rangle$, where α denotes the relevant quantum numbers of the state and E denotes its total energy, and we will write the photon continuum eigenstates as $|f\omega\rangle$, where f denotes relevant quantum numbers and ω denotes the total energy (the use of a separate symbol ω for the energy of photon continuum states is unnecessary, but it is useful as a reminder that one is dealing with a photon continuum rather than electron continuum). We will assume $\langle\alpha E|\alpha' E'\rangle=\delta_{\alpha\alpha'}\delta(E-E')$, $\langle f\omega|f'\omega'\rangle=\delta_{ff'}\delta(\omega-\omega')$, and of course $\langle\alpha E|f\omega\rangle=0$. For these states the projection operators can be written

$$\begin{aligned} P&=\sum_\alpha\int dE|\alpha E\rangle\langle\alpha E| ,\\ R&=\sum_f\int d\omega|f\omega\rangle\langle f\omega| . \end{aligned} \tag{4.1}$$

(Throughout this work all integrals are definite integrals over all continuum energies.)

A. Explicit form for the projection $P\Phi(z)P$ in the pole approximation for the photon continua alone

Our starting point for finding matrix elements of $P\Phi(z)P$ is Eq. (3.5a), which may be rewritten as

$$(z-PH^0P)P\Phi(z)P=P+[PVRG^0(z)RVP]P\Phi(z)P . \tag{4.2a}$$

Taking matrix elements of Eq. (4.2a) gives

$$(z-E)\langle\alpha E|\Phi(z)|\alpha' E'\rangle=\delta_{\alpha\alpha'}\delta(E-E')+\sum_{\alpha''}\int dE''\langle\alpha E|VRG^0(z)RV|\alpha'' E''\rangle\langle\alpha'' E''|\Phi(z)|\alpha' E'\rangle \ . \tag{4.2b}$$

The matrix element $\langle\alpha E|VRG^0(z)RV|\alpha'' E''\rangle$ appearing in (4.2b) can be expanded in terms of the photon continuum states in the form

$$\langle\alpha E|VRG^0(z)RV|\alpha'' E''\rangle=\sum_{f'}\int d\omega'\frac{\langle\alpha E|V|f'\omega'\rangle\langle f'\omega'|V|\alpha'' E''\rangle}{z-\omega'} \ . \tag{4.3}$$

We will eventually be interested in $z=z_p\equiv\omega_p+i0$ for some energy ω_p. It is well known that one can write

$$\frac{1}{\omega_p+i0-\omega'}=P\left[\frac{1}{\omega_p-\omega'}\right]-i\pi\delta(\omega_p-\omega') \ , \tag{4.4}$$

where P represents the principal part. If we neglect the principal part of the integral over the photon continuum appearing in (4.3) (in this work we will refer to the neglect of the principal part as the "pole approximation"), we obtain

$$\langle\alpha E|VRG^0(z_p)RV|\alpha'' E''\rangle=-i\pi\sum_{f'}\langle\alpha E|V|f'\omega_p\rangle\langle f'\omega_p|V|\alpha'' E''\rangle \ . \tag{4.5}$$

Next dividing Eq. (4.2b) by z_p-E, multiplying by $\langle f\omega_p|V|\alpha E\rangle$, summing over α, and integrating over E gives

$$\sum_{\alpha}\int dE\langle f\omega_p|V|\alpha E\rangle\langle\alpha E|\Phi(z_p)|\alpha' E'\rangle$$
$$=\sum_{\alpha}\int dE\frac{\langle f\omega_p|V|\alpha E\rangle}{z_p-E}\left[\delta_{\alpha\alpha'}\delta(E-E')-i\pi\sum_{f'}\langle\alpha E|V|f'\omega_p\rangle\sum_{\alpha''}\int dE''\langle f'\omega_p|V|\alpha'' E''\rangle\langle\alpha'' E''|\Phi(z_p)|\alpha' E'\rangle\right] . \tag{4.6}$$

Denoting the left-hand side of Eq. (4.6) by $\tilde{I}_{f\alpha'}(z_p,E')$, Eq. (4.6) becomes

$$\tilde{I}_{f\alpha'}(z_p,E')=\frac{\langle f\omega_p|V|\alpha' E'\rangle}{z_p-E'}+\sum_{f'}\tilde{\sigma}_{ff'}(z_p)\tilde{I}_{f'\alpha'}(z_p,E') \tag{4.7}$$

where

$$\tilde{\sigma}_{ff'}(z)\equiv-i\pi\sum_{\alpha}\int dE\frac{\langle f\omega_p|V|\alpha E\rangle\langle\alpha E|V|f'\omega_p\rangle}{z-E} \ . \tag{4.8}$$

If there are M photon continua in the problem, then $\tilde{\sigma}(z_p)$ is simply an $M\times M$ matrix, and if there are N electron continua, then $\tilde{I}(z_p,E')$ is an $M\times N$ (electron energy dependent) matrix. We have placed the tildes over σ and I to serve as explicit reminders that they are finite-dimensional matrices corresponding to the limited numbers of electron and photon continua explicitly included. Equation (4.7) can be solved to give

$$\tilde{I}_{f\alpha'}(z_p,E')=\sum_{f'}\{[\tilde{1}-\tilde{\sigma}(z_p)]^{-1}\}_{ff'}\frac{\langle f'\omega_p|V|\alpha' E'\rangle}{z_p-E'} \ , \tag{4.9}$$

where $\tilde{1}$ denotes the $M\times M$ identity matrix. Finally, substituting Eq. (4.9) into Eq. (4.2b) and making the pole approximation on the photon continua gives the result

$$\langle\alpha E|\Phi(z_p)|\alpha' E'\rangle=\frac{\delta_{\alpha\alpha'}\delta(E-E')}{z_p-E}-i\pi\sum_{f}\frac{\langle\alpha E|V|f\omega_p\rangle}{z_p-E}\tilde{I}_{f\alpha'}(z_p,E') \ . \tag{4.10}$$

This provides the required matrix elements of the projection $P\Phi(z)P$.

B. Explicit form for the projection $R\Phi(z)R$ in the pole approximation for the photon continua alone

An expression analogous to (4.10) can be derived for the matrix elements of $R\Phi(z)R$. For notational convenience, we first define

$$K(z)\equiv RVPG^0(z)PVR \ . \tag{4.11}$$

Equation (3.7a) then gives

$$(z-\omega)\langle f\omega|\Phi(z)|f'\omega'\rangle=\delta_{ff'}\delta(\omega-\omega')+\sum_{f''}\int d\omega''\langle f\omega|K(z)|f''\omega''\rangle\langle f''\omega''|\Phi(z)|f'\omega'\rangle \ . \tag{4.12}$$

Multiplying both sides of (4.12) by $\langle f'''\omega'''|K(z)|f\omega\rangle$, dividing by $z-\omega$, summing over f, and integrating over ω gives

$$\int d\omega \sum_f \langle f'''\omega'''|K(z)|f\omega\rangle\langle f\omega|\Phi(z)|f'\omega'\rangle$$

$$= \int d\omega \sum_f \frac{\langle f'''\omega'''|K(z)|f\omega\rangle}{z-\omega}\delta_{ff'}\delta(\omega-\omega')$$

$$+ \int d\omega \sum_f \frac{\langle f'''\omega'''|K(z)|f\omega\rangle}{z-\omega}\int d\omega'' \sum_{f''} \langle f\omega|K(z)|f''\omega''\rangle\langle f''\omega''|\Phi(z)|f'\omega'\rangle \ . \quad (4.13)$$

Next let us examine the matrix elements of $K(z)$,

$$\langle f\omega|K(z)|f''\omega''\rangle = \sum_\alpha \int dE \frac{\langle f\omega|V|\alpha E\rangle\langle \alpha E|V|f''\omega''\rangle}{z-E} \ . \quad (4.14)$$

$K(z)$ represents an indirect coupling between pairs of photon continua by way of the electron continua. It depends on photon continuum energies through the continuum-continuum matrix elements $\langle f\omega|V|\alpha E\rangle$ and $\langle \alpha E|V|f''\omega''\rangle$, which are weakly dependent on the photon energy, and hence ω, in the electric-dipole approximation. If we neglect this dependence on ω of the continuum-continuum matrix elements of V, and replace them with their values at $\omega=\omega_p$, we can write

$$\langle f\omega|K(z)|f''\omega''\rangle = \langle f\omega_p|K(z)|f''\omega_p\rangle = \frac{i}{\pi}\tilde{\sigma}_{ff''}(z) \ . \quad (4.15)$$

(Recall that ω denotes the total energy of the product state $|f\omega\rangle$, and thus is the sum of the photon energy and the energy of atomic state $|f\rangle$. Thus setting $\omega=\omega_p$ in the matrix elements of V fixes the photon energies at different energy values for different atomic states $|f\rangle$.)

We now can solve Eq. (4.13). Defining the left-hand side of Eq. (4.13) to be $\tilde{\xi}_{f'''f'}(z,\omega')$ [$\tilde{\xi}$ is independent of ω''' because of the approximation made in Eq. (4.15)], we obtain, after once again neglecting the principal value integral over the photon continuum

$$\tilde{\xi}_{f'''f'}(z_p,\omega') = \tilde{\sigma}_{f'''f'}(z_p)\delta(\omega'-\omega_p) + \sum_f \tilde{\sigma}_{f'''f}\tilde{\xi}_{ff'}(z_p,\omega') \ . \quad (4.16)$$

Thus

$$\tilde{\xi}_{f'''f'}(z_p,\omega') = \sum_f \{[\tilde{1}-\tilde{\sigma}(z_p)]^{-1}\}_{f'''f}\tilde{\sigma}_{ff'}(z_p)\delta(\omega'-\omega_p) \ . \quad (4.17)$$

Finally Eq. (4.12) gives

$$\langle f\omega|\Phi(z_p)|f'\omega'\rangle = \frac{\delta_{ff'}\delta(\omega-\omega')}{z_p-\omega} + \frac{1}{z_p-\omega}\sum_{f''}\{[\tilde{1}-\tilde{\sigma}(z_p)]^{-1}\}_{ff''}\tilde{\sigma}_{f''f'}(z_p)\delta(\omega'-\omega_p) \ , \quad (4.18a)$$

which becomes, if we write

$$\frac{1}{z_p-\omega} = -i\pi\delta(\omega_p-\omega) \ ,$$

$$\langle f\omega|\Phi(z_p)|f'\omega'\rangle = -i\pi\delta(\omega-\omega_p)\delta(\omega'-\omega_p)\left[\delta_{ff'}+\sum_{f''}\{[\tilde{1}-\tilde{\sigma}(z_p)]^{-1}\}_{ff''}\tilde{\sigma}_{f''f'}(z_p)\right] \ . \quad (4.18b)$$

This provides the required matrix elements of the projection $R\Phi(z)R$. On first inspection of Eq. (4.18b), one might be tempted to write the matrix product as

$$[\tilde{1}-\tilde{\sigma}(z)]^{-1}\tilde{\sigma}(z) = [\tilde{1}-\tilde{\sigma}(z)]^{-1}\{[\tilde{\sigma}(z)]^{-1}\}^{-1}$$

$$= \{[\tilde{\sigma}(z)]^{-1}[\tilde{1}-\tilde{\sigma}(z)]\}^{-1}$$

$$= \{[\tilde{\sigma}(z)]^{-1}-\tilde{1}\}^{-1} \ .$$

However, such a procedure is invalid if $\tilde{\sigma}(z)$ is not invertible.

C. Explicit forms for the projections $P\Phi(z)P$ and $R\Phi(z)R$ in the pole approximation for both electron and photon continua

We conclude this section by giving expressions for the matrix elements of $P\Phi(z_p)P$ and $R\Phi(z_p)R$ for the case in which the pole approximation is made on the electron continua as well as on the photon continua. We will write the electron continuum energy in the pole approximation as E_p to distinguish between photon and electron continua. Numerically $E_p=\omega_p=\mathrm{Re}(z_p)$. Then

$$\tilde{\sigma}_{f'f} = -\pi^2 \sum_\alpha \langle f'\omega_p|V|\alpha E_p\rangle\langle \alpha E_p|V|f\omega_p\rangle \quad (4.19)$$

and

$$\langle \alpha E|\Phi(E_p+i0)|\alpha' E'\rangle = -i\pi\delta(E-E_p)\delta(E'-E_p)\left[\delta_{\alpha\alpha'}-\pi^2\sum_f\sum_{f'}\langle \alpha E_p|V|f\omega_p\rangle[(\tilde{1}-\tilde{\sigma})^{-1}]_{ff'}\langle f'\omega_p|V|\alpha' E_p\rangle\right] . \tag{4.20}$$

$\langle f\omega|\Phi(\omega_p+i0)|f'\omega'\rangle$ retains the form (4.18b), but now with $\tilde{\sigma}$ given by Eq. (4.19). Since there must be symmetry between the two sets of continua, an alternative expression for $\langle f\omega|\Phi(\omega_p+i0)|f'\omega'\rangle$ can be obtained from Eqs. (4.19) and (4.20) by interchanging electron and photon continuum symbols in both equations

$$\langle f\omega|\Phi(\omega_p+i0)|f'\omega'\rangle = -i\pi\delta(\omega-\omega_p)\delta(\omega'-\omega_p)\left[\delta_{ff'}-\pi^2\sum_\alpha\sum_{\alpha'}\langle f\omega_p|V|\alpha E_p\rangle[(\tilde{1}-\tilde{\rho})^{-1}]_{\alpha\alpha'}\langle \alpha' E_p|V|f'\omega'\rangle\right] \tag{4.21a}$$

where

$$\tilde{\rho}_{\alpha\alpha'} \equiv -i\pi\sum_f\int d\omega\frac{\langle \alpha E_p|V|f\omega\rangle\langle f\omega|V|\alpha' E_p\rangle}{z-\omega} = -\pi^2\sum_f\langle \alpha E_p|V|f\omega_p\rangle\langle f\omega_p|V|\alpha' E_p\rangle . \tag{4.21b}$$

One can also write an expression for $\langle \alpha E|\Phi(E_p+i0)|\alpha' E'\rangle$ that is of the form (4.18b) by similarly interchanging electron and photon continuum symbols

$$\langle \alpha E|\Phi(E_p+i0)|\alpha' E'\rangle = -i\pi\delta(E-E_p)\delta(E'-E_p)\left[\delta_{\alpha\alpha'}+\sum_{\alpha''}[(\tilde{1}-\tilde{\rho})^{-1}]_{\alpha\alpha''}\tilde{\rho}_{\alpha''\alpha'}\right] . \tag{4.21c}$$

Thus for the case where one makes the pole approximation on the electron continua as well as the photon continua, explicit forms for $\langle \alpha E|\Phi(E_p+i0)|\alpha' E'\rangle$ and $\langle f\omega|\Phi(E_p+i0)|f'\omega'\rangle$ can be obtained from either of two sets of equations—Eqs. (4.20) and (4.18b) involving $(\tilde{1}-\tilde{\sigma})^{-1}$, or Eqs. (4.21a) and (4.21c) involving $(\tilde{1}-\tilde{\rho})^{-1}$. Which set is easier to use will depend on how many electron and photon continua are included in the problem.

V. APPLICATION TO MODEL SYSTEMS IN THE POLE APPROXIMATION

A. First application: one electron continuum, multiple photon continua

For a first detailed application of the general recipe, we consider a system featuring only a single electron continuum $|\alpha E\rangle$, but with an arbitrary number of photon continua. We will make the pole approximation on all the continua. Because we have only one electron continuum, $\tilde{\rho}$ is simply a scalar, and we define [see Eq. (4.21b)]

$$\psi \equiv 1-\tilde{\rho} = 1+\pi^2\sum_{f'}|\langle \alpha E_p|V|f'\omega_p\rangle|^2 . \tag{5.1}$$

Equation (4.21a) gives

$$\langle f\omega|\Phi(E_p+i0)|f'\omega'\rangle = -i\pi\delta(\omega-E_p)\delta(\omega'-E_p)\times\left[\delta_{ff'}-\frac{\pi^2\langle f\omega|V|\alpha E_p\rangle\langle \alpha E_p|V|f'\omega'\rangle}{\psi}\right] , \tag{5.2a}$$

and Eq. (4.21c) gives, after minor simplification,

$$\langle \alpha E|\Phi(E_p+i0)|\alpha E'\rangle = -\left[\frac{i\pi}{\psi}\right]\delta(E-E_p)\delta(E'-E_p) . \tag{5.2b}$$

From Eqs. (3.5b) and (3.7b) one obtains

$$\langle f\omega|\Phi(E_p+i0)|\alpha E\rangle = -\left[\frac{\pi^2}{\psi}\right]\delta(\omega-E_p)\delta(E-E_p)\langle f\omega|V|\alpha E\rangle \tag{5.2c}$$

and

$$\langle \alpha E|\Phi(E_p+i0)|f\omega\rangle = -\left[\frac{\pi^2}{\psi}\right]\delta(\omega-E_p)\delta(E-E_p)\langle \alpha E|V|f\omega\rangle . \tag{5.2d}$$

Before calculating the relevant matrix elements of the vertex operator Λ indicated in step (2) of our general recipe, we introduce the following notation. Discrete autoionizing states will be denoted by $|a\rangle$, with $\langle a|a'\rangle=\delta_{aa'}$ and $H^0|a\rangle=E_a|a\rangle$; $Q=\sum_a|a\rangle\langle a|$. We define

$$V_{fa}=\langle f\omega_p|V|a\rangle , \tag{5.3a}$$

$$V_{a\alpha}=\langle a|V|\alpha E_p\rangle , \tag{5.3b}$$

$$V_{f\alpha}=\langle f\omega_p|V|\alpha E_p\rangle , \tag{5.3c}$$

and we assume that all matrix elements are real. (Thus $V_{af}=V_{fa}$, etc.) The matrix elements V_{fa}, $V_{a\alpha}$, and $V_{f\alpha}$ represent, respectively, the lowest-order perturbation-theory contributions to the transition operators describing the processes of radiative decay from the autoionizing state, autoionization, and direct radiative recombination. We also will neglect the continuum-energy dependence of

all matrix elements of V. Then Eq. (2.5) gives

$$\langle f\omega|\Lambda(E_p+i0)|\alpha E\rangle=\frac{1}{\psi}V_{f\alpha}\ , \tag{5.4a}$$

$$\langle f\omega|\Lambda(E_p+i0)|a\rangle=V_{fa}-\frac{\pi^2}{\psi}V_{f\alpha}\sum_{f'}V_{\alpha f'}V_{f'a}-\frac{i\pi}{\psi}V_{f\alpha}V_{\alpha a}\ , \tag{5.4b}$$

$$\langle a|\Lambda(E_p+i0)|\alpha E\rangle=\frac{1}{\psi}\left[V_{a\alpha}-i\pi\sum_f V_{al}V_{f\alpha}\right]\ , \tag{5.4c}$$

$$\langle a|\Lambda(E_p+i0)|a\rangle=-\frac{2\pi^2}{\psi}V_{a\alpha}\sum_f V_{\alpha f}V_{fa}-\frac{i\pi}{\psi}\left[\psi\sum_f V_{af}^2+V_{a\alpha}^2-\pi^2\sum_f V_{af}V_{f\alpha}\sum_{f'}V_{\alpha f'}V_{f'a}\right]\ . \tag{5.4d}$$

In what follows we will treat the case of only one discrete autoionizing state $|a\rangle$; $\langle a|\Lambda(z)|a\rangle$ is then the only nonzero matrix element of $Q\Lambda(z)Q$, and the inverse of $Q[z-H^0-Q\Lambda(z)Q]Q$ is simply $Q/[z-E_a-\langle a|\Lambda(z)|a\rangle]$. In order to simplify notation further, we define

$$\Gamma=2\pi V_{a\alpha}^2\ , \tag{5.5a}$$

$$\gamma_f=2\pi V_{af}^2\ , \tag{5.5b}$$

$$q_f=\frac{V_{af}}{\pi V_{a\alpha}V_{\alpha f}}\ , \tag{5.5c}$$

where Γ and γ_f represent the lowest-order unperturbed autoionization and radiation decay rates (or widths), respectively, and g_f is the usual Fano line-profile parameter.[32] We emphasize that q_f is the pole-approximation result for the line-profile parameter corresponding to weak-field photoabsorption from the atomic state $|f\rangle$ to the asymptotic electron continuum $|\alpha E\rangle$ at continuum energies near the energy of the autoionizing state (or resonance) $|a\rangle$, and in the absence of spontaneous radiative decay. We will also assume that the signs of the continuum wavefunctions have been chosen so that the discrete state-continuum matrix elements of V (V_{af}, etc.) are positive. (Of course, the continuum-continuum matrix elements of V, $V_{f\alpha}$, can then be either positive or negative.) After substitution we obtain

$$\pi V_{\alpha f}=\frac{1}{q_f}\left[\frac{\gamma_f}{\Gamma}\right]^{1/2}\ , \tag{5.6a}$$

$$\psi=1+\sum_f\frac{\gamma_f}{\Gamma q_f^2}\ , \tag{5.6b}$$

$$\Lambda_{f\alpha}=\frac{1}{\pi\psi}\frac{1}{q_f}\left[\frac{\gamma_f}{\Gamma}\right]^{1/2}\ , \tag{5.7a}$$

$$\Lambda_{fa}=\left[\frac{\gamma_f}{2\pi}\right]^{1/2}\left[1-\frac{1}{\psi}\sum_{f'}\frac{\gamma_{f'}}{q_{f'}q_f\Gamma}-\frac{i}{\psi q_f}\right]\ , \tag{5.7b}$$

$$\Lambda_{a\alpha}=\frac{1}{\psi}\left[\frac{\Gamma}{2\pi}\right]^{1/2}\left[1-i\sum_f\frac{\gamma_f}{q_f\Gamma}\right]\ , \tag{5.7c}$$

and

$$\Lambda_{aa}=\frac{\Gamma}{2}(\Delta_a-i\eta)\ , \tag{5.7d}$$

where

$$\Delta_a=-\left[\frac{2}{\psi}\right]\sum_f\frac{\gamma_f}{\Gamma q_f}\ , \tag{5.7e}$$

$$\eta=\frac{1}{\psi}\left[1+\sum_f\frac{\gamma_f}{\Gamma}+\sum_{f,f'}\frac{\gamma_f\gamma_{f'}}{\Gamma^2 q_{f'}}\left[\frac{1}{q_{f'}}-\frac{1}{q_f}\right]\right] \tag{5.7f}$$

$$=\frac{1}{\psi}\left\{1+\psi\sum_f\frac{\gamma_f}{\Gamma}-\left[\sum_f\frac{1}{q_f}\left[\frac{\gamma_f}{\Gamma}\right]\right]^2\right\}\ . \tag{5.7g}$$

The quantity $(\Gamma/2)\Delta_a$ can be thought of as an energy shift of the discrete autoionizing state induced by the continuum-continuum couplings, and $\eta\Gamma$ as the total width or decay rate of the discrete autoionizing state. These expressions for Δ_a and η are generalizations of those presented earlier for systems featuring a single electron continuum and a single[13] or two[21,33] photon continua.

It is now straightforward to obtain a final expression for the T matrix using Eq. (2.10). One finds

$$\langle f\omega T(E_p+i0)|\alpha E\rangle=\frac{1}{E_p-E_a-\Lambda_{aa}}[\langle f\omega|\Lambda|\alpha E\rangle(E_p-E_a-\Lambda_{aa})+\langle f\omega|\Lambda|a\rangle\langle a|\Lambda|\alpha E\rangle]\ , \tag{5.8}$$

which after simplification gives

$$\langle f\omega|T(E_p+i0)|\alpha E\rangle=\frac{1}{E_p-E_a-\Lambda_{aa}}\left[\frac{1}{\psi}\right]\left[(E_p-E_a)V_{f\alpha}+V_{fa}V_{a\alpha}-i\pi\sum_{f'}(V_{fa}V_{af'}V_{f'\alpha}-V_{f\alpha}V_{af'}^2)\right] \tag{5.9}$$

[where Λ_{aa} is given in Eq. (5.4d)], or

$$\langle f\omega|T(E_p+i0)|\alpha E\rangle=\left[\frac{1}{\pi\psi q_f}\right]\left[\frac{\gamma_f}{\Gamma}\right]^{1/2}\left[\frac{\epsilon+q_f+i\sum_{f'}(1-q_f/q_{f'})(\gamma_{f'}/\Gamma)}{\epsilon-\Delta_a+i\eta}\right]\ , \tag{5.10}$$

$$\epsilon=\frac{E_p-E_a}{(\Gamma/2)} \ . \tag{5.11}$$

Thus

$$|\langle f\omega|T(E_p+i0)|\alpha E\rangle|^2=\left[\frac{1}{\pi q_f}\right]^2\frac{\gamma_f}{\Gamma}\left[\frac{(\epsilon+q_f)^2+\left[\sum_{f'}(1-q_f/q_{f'})\gamma_{f'}/\Gamma\right]^2}{\psi^2[(\epsilon-\Delta_a)^2+\eta^2]}\right] . \tag{5.12}$$

For the case of only a single photon continuum, Eq. (5.12) agrees with the result of Alber *et al.*[9] The term in very large parentheses also agrees with the previously presented modified Fano profiles for the one-photon-continuum system[21,33] and for the two-photon-continuum system.[34] The modified profiles arise when one probes the system by photoionization from a bound atomic discrete state; the bound state corresponds to our atomic state $|f\rangle$. [The modulus squared of the matrix element of V coupling $|f\rangle$ with the diagonalized continuum is obtained by substituting $|\langle f|V|\alpha E\rangle|^2$ for $[1/(\pi q_f)]^2\gamma_f/\Gamma$ in Eq. (5.12).] The modification is due to spontaneous radiative decay.

Equation (5.12) describes photorecombination to the particular atomic state $|f\rangle$. An expression describing the total photorecombination process for the case of a single electron continuum and multiple photon continua can be obtained by summing over the final-state index f. The result can be shown to be equivalent to that presented by LaGattuta in Eq. (79) of Ref. 24.

B. Discussion of first application: Perturbation series expansion of Φ and Λ

The operator $\Phi(z)$ defined by Eq. (2.3) can be thought of as a propagator in the continuum space C which takes into account to all orders the couplings between continuum subspaces P and R. It can be expanded in an infinite series in powers of V which features the "unperturbed propagator" $G^0(z)=(z-H^0)^{-1}$

$$C\Phi C=CG^0C+CG^0VCG^0C+CG^0VCG^0VCG^0C+\cdots \tag{5.13}$$

(where we have suppressed the argument z) so that, for example,

$$P\Phi R=0+G_p^0V_{PR}G_R^0+0+G_P^0V_{PR}G_R^0V_{RP}G_P^0V_{PR}G_R^0+\cdots \tag{5.14}$$

where $G_P^0=PG^0P$, $V_{RP}=RVP$, etc. If one thinks of each power of V as representing a virtual transition, and of each G^0 as a "free propagator," then the first nonzero term on the right-hand side of Eq. (5.14) can be thought of as representing propagation in R space followed by a virtual transition to P space, and subsequent propagation in the P space. Higher-order nonzero terms can be thought of as representing multiple virtual transitions and propagations.

For the case of only a single electron continuum $|\alpha E\rangle$ and several photon continua $|f\omega\rangle$, one can write, in the pole approximation,

$$G_P^0=\int dE\frac{|\alpha E\rangle\langle\alpha E|}{z-E}=-i\pi|\alpha E_p\rangle\langle\alpha E_p| \ , \tag{5.15}$$

$$G_R^0=\sum_f\int d\omega\frac{|f\omega\rangle\langle f\omega|}{z-\omega}=-i\pi\sum_f|f\omega_p\rangle\langle f\omega_p| \ . \tag{5.16}$$

We note, however, that these relations are legitimate applications of the pole approximation only if it is understood that G_P^0 and G_R^0 are subsequently to be multiplied on the left and right by operators whose matrix elements are slowly varying functions of energy. Such is certainly the case in the present discussion of intermediate state propagators, since each one will be multiplied on the left and right by V.

Equation (5.15) and (5.16) give, for example,

$$G_P^0V_{PR}G_R^0=(-i\pi)^2\sum_f|\alpha E_p\rangle V_{\alpha f}\langle f\omega_p| \ , \tag{5.17}$$

$$\begin{aligned}G_P^0V_{PR}G_R^0V_{RP}G_P^0V_{PR}G_R^0&=(-i\pi)^4\sum_{f,f'}|\alpha E_p\rangle V_{\alpha f'}V_{f'\alpha}V_{\alpha f}\langle f\omega_p|\\&=\xi\cdot G_P^0V_{PR}G_R^0 \ ,\end{aligned} \tag{5.18}$$

where

$$\begin{aligned}\xi&\equiv(-i\pi)^2\sum_{f'}V_{\alpha f'}V_{f'\alpha}\\&=-\pi^2\sum_{f'}|V_{\alpha f'}|^2 \ .\end{aligned} \tag{5.19}$$

Higher-order terms in the sum (5.13) give higher powers of ξ, and

$$\begin{aligned}P\Phi R&=G_P^0V_{PR}G_R^0(1+\xi+\xi^2+\xi^3+\cdots)\\&=G_P^0V_{PR}G_R^0\left[\frac{1}{1-\xi}\right]\\&=G_P^0V_{PR}G_R^0\left[\frac{1}{\psi}\right] \ ,\end{aligned} \tag{5.20}$$

where

$$\psi=1-\xi=1+\pi^2\sum_{f'}|V_{\alpha f'}|^2 \ . \tag{5.21}$$

Thus if one thinks in terms of the V appearing in the infinite "perturbation series" as representing virtual transitions, then ψ can be thought of as arising from multiple

virtual transitions between the two spaces of continua. We note that one could draw Feynman-like diagrams for the various terms in the perturbation series, indicating propagation through the various intermediate continua.

A useful expression analogous to Eq. (5.18) is

$$G_P^0 V_{PR} G_R^0 V_{RP} G_P^0 = \sum_f (-i\pi)^3 |\alpha E_p\rangle V_{\alpha f} V_{f\alpha} \langle \alpha E_p| = -i\pi |\alpha E_p\rangle \xi \langle \alpha E_p| = G_P^0 \xi \ . \tag{5.22}$$

However,

$$G_R^0 V_{RP} G_P^0 V_{PR} G_R^0 = \sum_f \sum_{f'} (-i\pi)^3 |f\omega_p\rangle V_{f\alpha} V_{\alpha f'} \langle f'\omega_p|$$

allows for propagation from one photon continuum (with atomic state $|f'\rangle$) to a different photon continuum (with atomic state $|f\rangle$), and cannot be written as $G_R^0 \xi$.

Expressions analogous to Eq. (5.20) for other projections of Φ can be derived from their series expansions using the relations (5.18) and (5.22). One finds

$$P\Phi P = G_P^0 \left[\frac{1}{\psi}\right] , \tag{5.23a}$$

$$R\Phi R = G_R^0 + G_R^0 V_{RP} G_P^0 V_{PR} G_R^0 \left[\frac{1}{\psi}\right] , \tag{5.23b}$$

$$R\Phi P = G_R^0 V_{RP} G_P^0 \left[\frac{1}{\psi}\right] . \tag{5.23c}$$

One can now write expressions for the various projections or matrix elements of Λ that are of interest. For example,

$$R\Lambda P = R(V + VC\Phi CV)P = V_{RP} + V_{RP}\Phi_{PR} V_{RP} = V_{RP} + \frac{1}{\psi} V_{RP} G_P^0 V_{PR} G_R^0 V_{RP} \tag{5.24}$$

and

$$\langle f\omega|\Lambda(E_p + i0)|\alpha E_p\rangle = \langle f\omega|V|\alpha E_p\rangle + \frac{1}{\psi}\langle f\omega|V_{RP} G_P^0 V_{PR} G_R^0 V_{RP}|\alpha E_p\rangle \ . \tag{5.25}$$

Next it is straightforward to show, using (5.15), (5.16), and (5.19) that

$$\langle f\omega_p|V_{RP} G_P^0 V_{PR} G_R^0 V_{RP}|\alpha E_p\rangle = \xi V_{f\alpha} \tag{5.26}$$

so that Eq. (5.25) gives, in the approximation $\langle f\omega|V|\alpha E_p\rangle = \langle f\omega_p|V|\alpha E_p\rangle = V_{f\alpha}$

$$\langle f\omega|\Lambda(E_p + i0)|\alpha E_p\rangle = V_{f\alpha} + \frac{\xi}{\psi} V_{f\alpha} = \frac{1}{\psi} V_{f\alpha} \ . \tag{5.27}$$

One can also find the matrix elements of Λ that involve discrete states. Simplifying relationships which can be easily demonstrated are

$$G_P^0 V_{PR} G_R^0 V_{RP}|\alpha E_p\rangle = |\alpha E_p\rangle \xi \tag{5.28a}$$

and

$$\langle \alpha E_p|V_{PR} G_R^0 V_{RP} G_P^0 = \xi \langle \alpha E_p| \ . \tag{5.28b}$$

One then finds

$$\langle a|\Lambda(E_p + i0)|\alpha E_p\rangle = \langle a|V|\alpha E_p\rangle + \langle a|V_{QR}\Phi_{RR} V_{RP}|\alpha E_p\rangle + \langle a|V_{QP}\Phi_{PR} V_{RP}|\alpha E_p\rangle \ , \tag{5.29}$$

which, using (5.23b), (5.23c), and (5.28) gives

$$\Lambda_{a\alpha} = \frac{1}{\psi}(\langle a|V|\alpha E_p\rangle + \langle a|V_{QR} G_R^0 V_{RP}|\alpha E_p\rangle) \ . \tag{5.30a}$$

Using similar methods,

$$\Lambda_{aa} = \langle a|V_{QR} G_R^0 V_{RQ}|a\rangle + \frac{1}{\psi}(\langle a|V_{QR} G_R^0 V_{RP} G_P^0 V_{PR} G_R^0 V_{RQ}|a\rangle + \langle a|V_{QP} G_P^0 V_{PR} G_R^0 V_{RQ}|a\rangle + \langle a|V_{QR} G_R^0 V_{RP} G_P^0 V_{PQ}|a\rangle + \langle a|V_{QP} G_P^0 V_{PQ}|a\rangle) \ , \tag{5.30b}$$

$$\Lambda_{fa} = \langle f\omega_p|V_{RQ}|a\rangle + \frac{1}{\psi}(\langle f\omega_p|V_{RP} G_P^0 V_{PR} G_R^0 V_{RQ}|a\rangle + \langle f\omega_p|V_{RP} G_P^0 V_{PQ}|a\rangle) \ . \tag{5.30c}$$

When the explicit forms (5.15) and (5.16) are used for G_P^0 and G_R^0, one promptly reproduces Eqs. (5.4). Terms in (5.30) that feature an even number of intermediate state propagators contribute to the real parts of the matrix elements of Λ, and terms that feature an odd number of intermediate states contribute to the imaginary parts of the matrix elements.

C. Second application: multiple electron continua, one photon continuum

As a second application of the general recipe of Sec. IV, we consider a system featuring multiple electron continua, but only a single photon continuum $|f\omega\rangle$. As in the first application, we make the pole approximation on all the continua. For the present case of interest, $\tilde{\sigma}$ is a scalar, and we define

$$\psi' \equiv 1 - \tilde{\sigma} = 1 + \pi^2 \sum_{\alpha'} |\langle \alpha' E_p|V|f\omega_p\rangle|^2 \ . \tag{5.31}$$

Matrix elements of $\Phi(E_p + i0)$ can be obtained from Eq. (5.2) through a simple symbol interchange

$$\langle \alpha E|\Phi(E_p+i0)|\alpha' E'\rangle = -i\pi\delta(E-E_p)\delta(E'-E_p)\left[\delta_{\alpha\alpha'}-\frac{\pi^2\langle \alpha E|V|f\omega_p\rangle\langle f\omega_p|V|\alpha' E'\rangle}{\psi'}\right], \tag{5.32a}$$

$$\langle f\omega|\Phi(E_p+i0)|f\omega'\rangle = \left[\frac{-i\pi}{\psi'}\right]\delta(\omega-E_p)\delta(\omega'-E_p), \tag{5.32b}$$

$$\langle \alpha E|\Phi(E_p+i0)|f\omega\rangle = \frac{-\pi^2}{\psi'}\delta(E-E_p)\delta(\omega-E_p)\langle \alpha E|V|f\omega\rangle, \tag{5.32c}$$

$$\langle f\omega|\Phi(E_p+i0)|\alpha E\rangle = \frac{-\pi^2}{\psi'}\delta(\omega-E_p)\delta(E-E_p)\langle f\omega|V|\alpha E\rangle . \tag{5.32d}$$

In the same approximations as led to Eq. (5.4), the matrix elements of $\Lambda(E_p+i0)$ can be obtained from (5.4) through symbol interchanges and using the relation $\Lambda^\dagger(z)=\Lambda(z^*)$ [which gives, for example, $\langle a|\Lambda(z)|\alpha E\rangle = \langle \alpha E|\Lambda^\dagger(z)|a\rangle^* = \langle \alpha E|\Lambda(z^*)|a\rangle^* = \langle \alpha E|\Lambda(z)|a\rangle$],

$$\langle f\omega|\Lambda(E_p+i0)|\alpha E\rangle = \frac{1}{\psi'}V_{f\alpha}, \tag{5.33a}$$

$$\langle a|\Lambda(E_p+i0)|\alpha E\rangle = V_{a\alpha}-\frac{\pi^2}{\psi'}\sum_{\alpha'}V_{a\alpha'}V_{\alpha' f}V_{f\alpha}-\frac{i\pi}{\psi'}V_{af}V_{f\alpha}, \tag{5.33b}$$

$$\langle f\omega|\Lambda(E_p+i0)|a\rangle = \frac{1}{\psi'}\left[V_{fa}-i\pi\sum_{\alpha}V_{f\alpha}V_{\alpha a}\right], \tag{5.33c}$$

$$\langle a|\Lambda(E_p+i0)|a\rangle = \frac{-2\pi^2}{\psi'}\sum_{\alpha}V_{a\alpha}V_{\alpha f}V_{fa}-\frac{i\pi}{\psi'}\left[V_{af}^2+\psi'\sum_{\alpha}V_{a\alpha}^2-\pi^2\sum_{\alpha}\sum_{\alpha'}V_{a\alpha}V_{\alpha f}V_{f\alpha'}V_{\alpha' a}\right]. \tag{5.33d}$$

Defining

$$\gamma_f = 2\pi V_{af}^2, \tag{5.34a}$$

$$q_{f\alpha} = \frac{V_{fa}}{\pi V_{f\alpha}V_{\alpha a}}, \tag{5.34b}$$

$$\Gamma_\alpha = 2\pi V_{a\alpha}^2, \tag{5.34c}$$

$$\frac{1}{q} = \sum_{\alpha}\frac{1}{q_{f\alpha}}$$

$$\Gamma = \sum_{\alpha}\Gamma_\alpha, \tag{5.34d}$$

so that

$$\pi V_{f\alpha} = \frac{1}{q_{f\alpha}}\left[\frac{\gamma_f}{\Gamma_\alpha}\right]^{1/2} \tag{5.35}$$

and

$$\psi' = 1+\sum_{\alpha}\frac{\gamma_f}{q_{f\alpha}^2\Gamma_\alpha}, \tag{5.36}$$

one obtains

$$\Lambda_{f\alpha} = \frac{1}{\pi\psi'}\frac{1}{q_{f\alpha}}\left[\frac{\gamma_f}{\Gamma_\alpha}\right]^{1/2}, \tag{5.37a}$$

$$\Lambda_{a\alpha} = \left[\frac{\Gamma_\alpha}{2\pi}\right]^{1/2}\left[1-\left[\frac{1}{\psi'}\right]\frac{\gamma_f}{\Gamma_\alpha q_{f\alpha}}\left[\frac{1}{q}\right]-\frac{i}{\psi'}\frac{\gamma_f}{\Gamma_\alpha q_{f\alpha}}\right], \tag{5.37b}$$

$$\Lambda_{fa} = \frac{1}{\psi'}\left[\frac{\gamma_f}{2\pi}\right]^{1/2}\left[1-\frac{i}{q}\right], \tag{5.37c}$$

and

$$\Lambda_{aa} = \frac{\Gamma}{2}(\Delta_a'-i\eta'), \tag{5.37d}$$

where

$$\Delta_a' = -\left[\frac{2}{\psi'}\right]\frac{\gamma_f}{\Gamma q}, \tag{5.38a}$$

$$\eta' = 1+\frac{\gamma_f}{\psi'\Gamma}(1-1/q^2). \tag{5.38b}$$

It is straightforward to show that for the case of only one autoionizing state $|a\rangle$,

$$\langle f\omega|T(E_p+i0)|\alpha E\rangle = \frac{1}{E_p-E_a-\Lambda_{aa}}\left[\frac{1}{\psi'}\right]\left[(E_p-E_a)V_{f\alpha}+V_{fa}V_{a\alpha}-i\pi\sum_{\alpha'}(V_{f\alpha'}V_{\alpha' a}V_{a\alpha}-V_{f\alpha}V_{a\alpha'}^2)\right] \tag{5.39a}$$

$$= \frac{1}{\pi\psi' q_{f\alpha}}\left[\frac{\gamma_f}{\Gamma_\alpha}\right]^{1/2}\left[\frac{\epsilon'+q_{f\alpha}\Gamma_\alpha/\Gamma+i[1-(q_{f\alpha}/q)(\Gamma_\alpha/\Gamma)]}{\epsilon'-\Delta_a'+i\eta'}\right], \tag{5.39b}$$

$$\epsilon' = \frac{E_p - E_a}{\Gamma/2} \ . \tag{5.40}$$

For the case in which only one electron continuum is initially populated, the electron-ion photorecombination cross section is proportional to

$$|\langle f\omega|T(E_p+i0)|\alpha E\rangle|^2 = \left[\frac{1}{\pi\psi' q_{f\alpha}}\right]^2 \left[\frac{\gamma_f}{\Gamma_\alpha}\right] \left[\frac{(\epsilon'+q_{f\alpha}\Gamma_\alpha/\Gamma)^2+[1-(q_{f\alpha}/q)(\Gamma_\alpha/\Gamma)]^2}{(\epsilon'-\Delta_a')^2+\eta'^2}\right] . \tag{5.41}$$

Thus we note that the additional electron continua in general prevent the recombination profile from exhibiting any zeroes.

VI. DISCUSSION AND CONCLUSIONS

In this paper we have used a projection-operator formalism to obtain a general recipe for constructing matrix elements of the T operator for electron-ion photorecombination processes in model systems featuring a limited number of discrete states and continua. In Sec. II of this paper we have presented the basic projection-operator formalism, and we have derived Eq. (2.10) for the transition or T operator. This equation, preveously derived by others in different contexts, provides the foundation for the later sections of the paper. In Sec. III we have applied Eq. (2.10) to electron-ion photorecombination processes, and have observed that it separates naturally into a direct term, representing radiative recombination, and a resonance term, which incorporates all effects of the autoionizing states and which can be thought of as providing a general description of dielectronic recombination.

In Sec. III A we have presented the general recipe for constructing the required matrix elements of the T operator. Implementation of the general recipe requires knowledge of projections of the matrix elements of the combined electron and photon continuum-space propagator $\Phi(z)$, defined in Eq. (2.3), and in Sec. IV we have addressed the problem of finding the required matrix elements of this operator. Our results for the electron-space–electron-space (P-P) projection and photon-space–photon-space (R-R) projection of the propagators are presented in Eqs. (4.10) and (4.18b), for the case in which we have made the pole approximation on the photon continua but not on the electron continua. Because of our having made the pole approximation on the photon continua, evaluation of (4.10) and (4.18b) requires the inversion of only finite dimensional matrices, provided the model system of interest features either a finite number of electron continua or a finite number of photon continua. Matrix elements of the propagators leading from one continuum subspace to the other (electron to photon and vice versa) can subsequently be constructed using Eqs. (3.5a) and (3.7b). In Sec. IV C we have presented the simplification of Eqs. (4.10) and (4.18b) that occurs when one makes the pole approximation on the electron continua as well as the photon continua. We have also noted that symmetry considerations indicate that alternative expressions for the propagators can be obtained through a simple symbol interchange; the results of such an interchange are given in Eq. (4.21).

In Sec. V we have applied the formalism to two different model systems featuring an isolated autoionizing state. The first system studied features one electron continuum but an arbitrary number of photon continua, and the second system studied features one photon continuum but an arbitrary number of electron continua. Equations (5.12) and (5.41) give our final results for the modulus squared of the appropriate matrix element of the T operator. In Sec. V B we have shown, for the first model system, how the matrix elements of the continuum space propagator Φ and the "vertex operator" Λ can be interpreted, within the context of a perturbation series, in terms of multiple virtual transitions.

The formalism presented in this paper may prove useful for a variety of studies. Because of the natural separation of the direct and resonance behavior, the formalism will likely prove useful in theoretical studies investigating effects of resonances. In this context one could, for example, define a resonance profile as $|\langle f\omega|T(E+i0)|\alpha E\rangle|^2/|\langle f\omega|\Lambda(E+i0)|\alpha E\rangle|^2$, and one could define effective resonance profile parameters. The results of such a study will be reported in a separate publication.

Possible extensions of the model systems studied in this paper include allowing explicitly for angular momentum degeneracies and simultaneously allowing for multiple electron and photon continua. Other extensions include studies of overlapping resonances and of recombination processes in external fields. For application to electron-ion photorecombination in high-density plasmas, the analysis should be extended to allow for the effects of collisional dephasing processes and plasma electric microfields. For such studies, it will likely be desirable to develop a density-matrix description of the electron-ion photorecombination processes.

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APPENDIX

In this appendix we show how the formalism of multichannel scattering theory[27] can be applied to the pho-

torecombination process is such a way that some of the interactions can be absorbed into the "unperturbed Hamiltonian," and so that Eq. (2.9) can be used to describe the scattering due to the interaction of primary interest. The total Hamiltonian for the electron and target system can be written as

$$H = H_T + H_e + H_F + V_{e\text{-}T} + V_{A\text{-}F} \tag{A1}$$

where H_T denotes the Hamiltonian of the positive-ion target, H_e the Hamiltonian of a freely moving electron, H_F the Hamiltonian of the free radiation field, $V_{e\text{-}T}$ the atomic interaction between the electron and target, and V_{AF} the interaction between atom (target plus electron) and field. The channel featuring an asymptotic free electron is characterized by channel Hamiltonian

$$H^{\text{el}} = H_T + H_e + H_F \tag{A2a}$$

and scattering potential

$$V^{\text{el}} = V_{e\text{-}T} + V_{A\text{-}F} \ . \tag{A2b}$$

The channel featuring an emitted photon, with the electron bound to the ion, is characterized by the channel Hamiltonian

$$H^{\text{ph}} = H_T + H_e + H_F + V_{e\text{-}T} \tag{A3a}$$

and scattering potential

$$V^{\text{ph}} = V_{A\text{-}F} \ . \tag{A3b}$$

The full T operator for scattering from the electron channel to the photon channel can be written as either

$$\tilde{T}^{\,\text{ph}\leftarrow\text{el}}(z) = V^{\text{el}} + V^{\text{ph}} G(z) V^{\text{el}} \tag{A4a}$$

or

$$T^{\text{ph}\leftarrow\text{el}}(z) = V^{\text{ph}} + V^{\text{ph}} G(z) V^{\text{el}} \ , \tag{A4b}$$

where $G(z) = (z - H)^{-1}$ denotes the full Green's operator. Although in general $\tilde{T}^{\,\text{ph}\leftarrow\text{el}} \neq T^{\text{ph}\leftarrow\text{el}}$, they both lead to the same on-shell T matrix,[27] and either can be used to describe the scattering process. We shall use the latter form.

In the present work we wish to concentrate on the effects that the interactions responsible for spontaneous radiative decay and for autoionization have on the scattering, rather than studying the full scattering problem. Accordingly, we wish to define an alternative T operator which describes the effects of the interactions of primary interest. As a first step, we split $V_{e\text{-}T}$ into two parts,

$$V_{e\text{-}T} = V_1 + V_2 \ , \tag{A5}$$

where V_1 provides a close approximation to $V_{e\text{-}T}$, and where V_2 is the interaction of primary interest in H^{el}. We define

$$H^0 = H_T + H_e + H_F + V_1 \ , \tag{A6}$$

and we assume that the eigenstates of H^0 include stable doubly excited states. We further assume that the only effect of V_2 is to couple these doubly excited states with electron continuum eigenstates of H^0, so that the doubly excited states become autoionizing states. The other interaction of interest, the atom-field interaction $V_{A\text{-}F}$, will couple these doubly excited states, as well as the electron-continuum states, with the eigenstates of H^0 in which the electron is bound to the target and a photon has been emitted. We assume that V_2 does not couple these final, bound atomic states to any other states, so that they are eigenstates not only of H^0, but also of H^{ph}.

If we let $|\psi_E^\alpha\rangle$ denote an eigenstate of H^{el} (with quantum numbers α and energy E), then, defining

$$V = V_2 + V_{A\text{-}F} \ , \tag{A7a}$$

we have

$$\begin{aligned} T^{\text{ph}\leftarrow\text{el}}(z)|\psi_E^\alpha\rangle &= V_{A\text{-}F}[1 + G(z)(V_{e\text{-}T} + V_{A\text{-}F})]|\psi_E^\alpha\rangle \\ &= V_{A\text{-}F}[1 + G(z)(V_1 + V)]|\psi_E^\alpha\rangle \ . \end{aligned} \tag{A7b}$$

The Green's operator can be written as $G(z) = (z - H^{\text{el}} - V_1 - V)^{-1}$, and it is straightforward to show from $G(z)(z - H^{\text{el}} - V_1) = 1 + G(z)V$ that

$$1 + G(z)(V_1 + V) = [1 + G(z)V][1 + G^1(z)V_1] \ , \tag{A8a}$$

where

$$G^1(z) = (z - H^{\text{el}} - V_1)^{-1} \ . \tag{A8b}$$

Thus,

$$T^{\text{ph}\leftarrow\text{el}}(E + i0)|\psi_E^\alpha\rangle = V_{A\text{-}F}[1 + G(E + i0)V]|\alpha E\rangle \ , \tag{A9a}$$

where

$$|\alpha E\rangle = \Omega_+^1 |\psi_E^\alpha\rangle = [1 + G^1(E + i0)V_1]|\psi_E^\alpha\rangle \ . \tag{A9b}$$

Here Ω_+^1 denotes the Møller scattering operator for the potential V_1. The scattering state $|\alpha E\rangle$ is a continuum eigenstate of $H^{\text{el}} + V_1$, with energy eigenvalue E. In the present work $RV_{A\text{-}F} = RV$, and

$$RT^{\text{ph}\leftarrow\text{el}}(E + i0)|\psi_E^\alpha\rangle = RT(E + i0)|\alpha E\rangle \ , \tag{A10a}$$

where

$$T(z) \equiv V + VG(z)V \ . \tag{A10b}$$

The T operator of Eq. (A10) is the transition operator that we use throughout this paper; also, our "unperturbed" Green's operator $G^0(z)$ is equal to the $G^1(z)$ of Eq. (A8). The unperturbed continuum eigenstates $|\alpha E\rangle$ that we use correspond to the scattering eigenstates denoted by the same symbol.

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