# Direct solution for projected $T$ operators with application to photorecombination in an external electric field

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(Received 27 April 1990)

A projection operator formalism is employed in considering the $T$ operator for describing a scattering or reaction event in which a system evolves from one continuum channel into another continuum channel. The formalism is based upon projections of the Lippmann-Schwinger equations for $T$ and an operator generalization of Gauss's reduction for linear algebraic equations. A formal solution of the projected Lippmann-Schwinger equation is presented for the case in which the couplings involving the final-state continua satisfy a chosen separability condition. The simplifications that occur when the pole approximation is made on the final-state continua or on both the initial- and final-state continua are presented. The formalism is employed in considering the effects of an external dc electric field in photorecombination processes in a model atomic system which features two autoionizing states, two electron continua (one of which contains the initial state), and two photon continua (corresponding to radiatively stabilized atomic states). Particular attention is paid to the effects of the coupling between the two electron continua.

## I. INTRODUCTION

Projection operators have been used effectively within a number of contexts for describing scattering and decay processes. Feshbach[1] used projection-operator techniques in the context of nuclear reaction theory to separate resonance states from asymptotic continua. His techniques have been extended in the context of electron-ion dielectronic-recombination processes to separate also the various scattering channels or sets of asymptotic continua.[2] Projection operators have also been very useful in discussing photoionization and the decay of prepared systems.[3] Recently several papers[4–6] have used projection operators to give a unified treatment of "radiative recombination" and "dielectronic recombination" in atomic physics. One of these [Haan and Jacobs[5] (hereafter HJ)] has presented an expression for the $T$ operator, given previously by other authors[7] in other contexts, which separates naturally into a term describing direct, or nonresonant, transitions and a term describing the resonance contribution. Such a separation can be useful in situations in which one is especially interested in knowing the effects of the resonances.[6] However, if one is only interested in calculating the matrix element of the $T$ operator between the initial and final states of interest, there may be other, more direct methods one can use. One purpose of the present paper is to present such a method.

In this paper we consider processes in systems featuring two sets of orthogonal asymptotic continuum channels and a set of resonances. We assume that the interaction of interest couples the continuum channels to each other and to the resonances. We allow for coupling between the resonances, and for coupling within individual continuum channels. We look specifically at the projection of the $T$ operator appropriate for describing a scattering or reaction event in which a system evolves from one continuum channel into the other continuum channel. The method, based upon projections of the Lippmann-Schwinger equations for $T$ and an operator generalization of Gauss's reduction for linear algebraic equations, provides us with a relatively simple final expression for the $T$ operator. Although the expression does not separate naturally into resonant and nonresonant parts, it has the advantage of providing a simple, basic equation to use in calculating the matrix element of the $T$ operator for the initial and final states of interest.

We emphasize that the results of this paper are useful in a wide variety of physical situations, and are by no means limited to discussions of electron-ion photorecombination processes.

We begin by assuming that the Hamiltonian $H$ for the system of interest has been decomposed as $H=H^0+V$, where the scattering eigenstates of $H^0$ are known, and where $V$ is the interaction of interest. We further assume that the multichannel $T$ operator which describes the scattering event of interest can be written[8] in the form

$$T(z)=V+VG(z)V \tag{1.1a}$$

$$=V+VG^0(z)V+VG^0(z)VG^0(z)V+\cdots \tag{1.1b}$$

$$=V+VG^0(z)T(z) \tag{1.1c}$$

$$=V+T(z)G^0(z)V\ , \tag{1.1d}$$

where

$$G(z)=(z-H)^{-1} \tag{1.2a}$$

and

$$G^0(z)=(z-H^0)^{-1} \tag{1.2b}$$

represent the full and unperturbed resolvents, respectively. A direct solution for matrix elements of the $T$ opera-

 

tor based on Eqs. (1.1c) or (1.1d), which are the Lippmann-Schwinger equations for $T$, will be developed in this paper.

In reactions, the initial state is a projectile incident on a bound target. This initial state is a continuum eigenstate of $H^0$ asymptotically. Similarly, the final state, with unbound reaction products and bound residual system is a continuum eigenstate of $H^0$ asymptotically. In addition to a direct process leading from the initial state to the final state, reactions are mediated by resonances of the combined system. Indeed, the resonance process frequently dominates the reaction. The resonances can be considered to be discrete eigenstates of $H^0$.

This provides motivation for partitioning state space into disjoint eigenspaces of $H^0$. The partitioning is effected by defining projection operators $P$, $R$, and $Q$ onto the following three spaces, respectively:

(1) $P$ space—the continuum states $\{p\}$ to which the initial state naturally belongs;

(2) $R$ space—the continuum states $\{r\}$ describing all possible reaction channels orthogonal to $\{p\}$;

(3) $Q$ space—the discrete eigenstates $\{q\}$ of $H^0$.

The three projection operators satisfy

$$P_i P_j = P_i \delta_{ij} ,$$
$$P_i H^0 P_j = P_i H^0 \delta_{ij} = H^0 P_i \delta_{ij} \tag{1.3}$$

(where the indices $i$ and $j$ are used to distinguish between the three projection operators $P$, $R$, and $Q$). The projection operators are thus as used in other works that have studied electron-ion photorecombination.[2,4–6] A schematic diagram of the partitioning is shown in Fig. 1.

In Sec. II we develop a formal expression for $RT(z)P$ which is based upon Eq. (1.1c). Several operators are defined in the development, and they are discussed briefly at the end of the section. In Sec. III we consider the matrix elements of $RT(z)P$ within the context of photorecombination, and present a formal solution for the matrix elements of $T(z)$ for the case in which the couplings to $R$ space satisfy a separability condition. We conclude the section with a discussion of the form of the matrix elements of the operators needed in order to calculate matrix elements of $T(z)$; we consider especially the cases in which the couplings within the $P$ space are separable or zero. In Sec. IV we discuss the simplifications which occur if one makes the pole approximation on the $R$-space continua only or on both the $R$- and $P$-space continua. In Sec. V we employ the formalism to study photorecombination processes in a model system featuring two autoionizing states in an external dc electric field. We consider especially the effects that the couplings between the various $\{p\}$ states have on the photorecombination process. In Sec. VI we present the parallel formalism that can be obtained using Eq. (1.1d) instead of (1.1c). Finally, in Sec. VII we summarize our results.

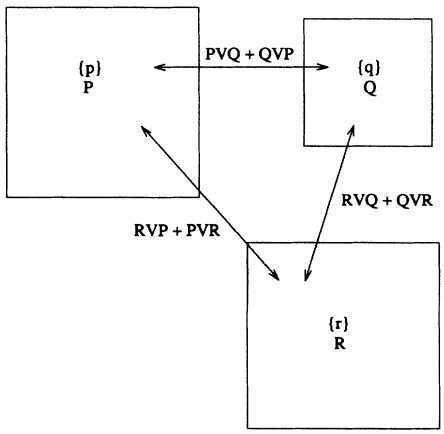


FIG. 1. Schematic diagram of the partitioning of the eigenstates of $H^0$ into three disjoint eigenspaces. The interaction $V$ not only couples the eigenspaces to each other, but also $PVP$, $QVQ$, and $RVR$ couple various states within each space.

## II. FORMAL EQUATIONS FOR THE PROJECTED $T$ OPERATOR

Matrix elements of the projected $T$ operator RTP are of primary interest in this paper. Using Eq. (1.1c) gives

$$RT(z)P = RVP + RVRG^0(z)RT(z)P + RVPG^0(z)PT(z)P + RVQG^0(z)QT(z)P , \tag{2.1a}$$

which will be written using the more succinct notation

$$T_{RP} = V_{RP} + V_{RR}G_R^0 T_{RP} + V_{RP}G_P^0 T_{PP} + V_{RQ}G_Q^0 T_{QP} . \tag{2.1b}$$

Similar independent equations for the projected $T$ operators $T_{PP}$ and $T_{QP}$ permit a unique solution for $T_{RP}$. These are

$$T_{PP} = V_{PP} + V_{PR}G_R^0 T_{RP} + V_{PP}G_P^0 T_{PP} + V_{PQ}G_Q^0 T_{QP} , \tag{2.2}$$

$$T_{QP} = V_{QP} + V_{QR}G_R^0 T_{RP} + V_{QP}G_P^0 T_{PP} + V_{QQ}G_Q^0 T_{QP} . \tag{2.3}$$

The three linear equations in the three unknown projected $T$ operators will be solved using an operator generalization of Gauss's reduction for linear algebraic equations.[9]

Rearranging the equations gives

$$(P - V_{PP}G_P^0)T_{PP} - V_{PR}G_R^0 T_{RP} - V_{PQ}G_Q^0 T_{QP} = V_{PP} , \tag{2.4}$$

$$-V_{QP}G_P^0 T_{PP} - V_{QR}G_R^0 T_{RP} + (Q - V_{QQ}G_Q^0)T_{QP} = V_{QP} , \tag{2.5}$$

$$-V_{RP}G_P^0 T_{PP} + (R - V_{RR}G_R^0)T_{RP} - V_{RQ}G_Q^0 T_{QP} = V_{RP} . \tag{2.6}$$

In Gauss's reduction, the "less desirable" unknowns are eliminated sequentially. $T_{PP}$ is eliminated by first multiplying Eq. (2.4) on the left by $V_{QP}G_P^0(P - V_{PP}G_P^0)^{-1}$, an inverse in $P$ space only, and then adding the result to Eq.

(2.5). After defining

$$\lambda^P(z) \equiv V + VG_P^0(z)[P - V_{PP}G_P^0(z)]^{-1}PV \ , \tag{2.7}$$

one obtains

$$-\lambda_{QR}^P G_R^0 T_{RP} + (Q - \lambda_{QQ}^P G_Q^0)T_{QP} = \lambda_{QP}^P \ . \tag{2.8}$$

The form of $\lambda^P$ and the $P$-space operator inversion which must be carried out to find $\lambda^P$ are discussed at the end of this section, in Sec. III C, and in Sec. IV B.

Multiplying Eq. (2.4) on the left by $V_{RP}G_P^0(P - V_{PP}G_P^0)^{-1}$ and adding the result to Eq. (2.6) gives

$$(R - \lambda_{RR}^P G_R^0)T_{RP} - \lambda_{RQ}^P G_Q^0 T_{QP} = \lambda_{RP}^P \ . \tag{2.9}$$

Equation (2.8) is solved for $T_{QP}$ by multiplying on the left by $(Q - \lambda_{QQ}G_Q^0)^{-1}$, an inverse in $Q$ space only:

$$T_{QP} = (Q - \lambda_{QQ}G_Q^0)^{-1}(\lambda_{QP} + \lambda_{QR}G_R^0 T_{RP}) \ . \tag{2.10}$$

The operator $Q - \lambda_{QQ}G_Q^0$ is a square matrix of dimensionality equal to the number of important resonances, and the operator inversion is an elementary matrix calculation.

Substituting Eq. (2.10) into Eq. (2.9) and defining the operators

$$G_Q^P(z) \equiv Q[Q(z - H^0)Q - \lambda_{QQ}^P]^{-1} \tag{2.11a}$$

$$= G_Q^0(Q - \lambda_{QQ}^P G_Q^0)^{-1} \tag{2.11b}$$

and

$$t^P(z) = \lambda^P(z) + \lambda^P(z)G_Q^P(z)\lambda^P(z) \ , \tag{2.12}$$

one obtains

$$(R - t_{RR}^P G_R^0)T_{RP} = t_{RP}^P \ . \tag{2.13}$$

Equation (2.13) represents the final result of the general formalism based on Eq. (1.1c). We defer seeking its solution to Sec. III. We conclude the present section with a brief discussion of how various operators defined above relate to the operators discussed in HJ, and we consider the operator $\lambda^P$ in detail.

It follows from the relationship

$$G_P^0(P - V_{PP}G_P^0)^{-1} = [P(z - H^0 - V)P]^{-1}P$$

that $\lambda^P$ can be written as

$$\lambda^P(z) = V + V[P(z - H^0 - V)P]^{-1}PV \ . \tag{2.14}$$

Here $[P(z - H^0 - V)P]^{-1}P$ represents a propagator in $P$ space. The operator $\lambda^P(z)$ features only $P$-space intermediate states and corresponds to the level shift operator [denoted by $\Lambda(z)$ in HJ] for a system which features $P$-space continua, but no $R$-space continua. For the systems of interest in this paper, it represents the level shift operator for $P+Q$ space, i.e., for the limited Hilbert space featuring states onto which $P$ and $Q$ project, but lacking the continua onto which $R$ projects.

The operator $G_Q^P(z)$ defined in Eq. (2.11) is the $Q$-space propagator when $P$-space intermediate states are allowed for. It corresponds to $QG(z)Q$ in the limited Hilbert space onto which $P+Q$ projects:

$$G_Q^P(z) = Q[(P+Q)(z - H^0 - V)(P+Q)]^{-1}Q$$

$$= Q\{Q[z - H^0 - \lambda^P(z)]Q\}^{-1}Q \ , \tag{2.15}$$

where the last equality follows from Eq. (2.6) of HJ. It follows from the relation $T(z) = \Lambda(z) + \Lambda(z)QG(z)Q\Lambda(z)$ presented in HJ and from Eq. (2.12) that $t^P(z)$ denotes the transition or $T$ operator within this limited $P+Q$ space.

Solution of Eq. (2.13) for $T_{RP}$ or its matrix elements requires knowledge first of all of $\lambda^P(z)$, and then of $t^P(z)$. We thus consider briefly the operator $\lambda^P(z)$. One can easily show from the definition of $\lambda^P$, Eq. (2.7), that

$$P\lambda^P = PV + (V_{PP}G_P^0 - P + P)(P - V_{PP}G_P^0)^{-1}PV$$

$$= P(P - V_{PP}G_P^0)^{-1}PV \ , \tag{2.16}$$

and thus that

$$\lambda^P = V + VG_P^0\lambda^P \ . \tag{2.17}$$

Similarly, one can easily show that

$$\lambda^P P = V(P - G_P^0 V_{PP})^{-1}P \tag{2.18}$$

and

$$\lambda^P = V + \lambda^P G_P^0 V \ . \tag{2.19}$$

Matrix elements of $\lambda^P$ can be constructed from matrix element of $P\lambda^P$ using Eq. (2.17), or from matrix elements of $\lambda^P P$ using Eq. (2.19). The latter method is more useful in solving Eq. (2.13) for the matrix elements of $T_{RP}$, since one can use the matrix elements of $\lambda^P P$ and $\lambda^P$ along with Eq. (2.12) to construct the matrix elements of $t_{RP}$ and $t_{RR}$ which are needed in Eq. (2.13).

## III. DIRECT SOLUTIONS FOR MATRIX ELEMENTS OF $T_{RP}$

### A. Equations for matrix elements of $T_{RP}$

An algebraic realization of Eq. (2.13) will be developed for a problem of current interest in atomic physics: an unbound electron is captured by a positive ion and a photon is emitted. Our notation will be similar to that used in HJ and Ref. 6. The initial state is $|\alpha E\rangle$, where $E$ is the energy of the electron, and $\alpha$ denotes all discrete quantum numbers needed to specify the unbound electron-ion state completely. The final state is $|f\omega\rangle$, where $\omega$ is the energy of the state, and $f$ denotes all discrete quantum numbers needed to specify the bound electron-ion plus photon state completely. We assume that these orthogonal eigenstates of $H^0$ have a $\delta$-function normalization with respect to energy: $\langle \alpha E|\alpha' E'\rangle = \delta_{\alpha\alpha'}\delta(E - E')$, $\langle f\omega|f'\omega'\rangle = \delta_{ff'}\delta(\omega - \omega')$, $\langle f\omega|\alpha E\rangle = 0$. The projection operators $P$ and $R$ are, neglecting all other reaction channels,

$$P = \sum_\alpha \int dE|\alpha E\rangle\langle \alpha E| \ , \tag{3.1a}$$

$$R = \sum_f \int d\omega|f\omega\rangle\langle f\omega| \ . \tag{3.1b}$$

The projection operator $Q$ is

$$Q=\sum_a |a\rangle\langle a| \ , \tag{3.2}$$

where $a$ denotes all quantum numbers needed to specify the resonant (autoionizing) electron-ion state completely, and $\langle a|a'\rangle=\delta_{aa'}$, $\langle a|f\omega\rangle=\langle a|\alpha E\rangle=0$, $H^0|a\rangle=E_a|a\rangle$.

It should be emphasized that although the context of the discussion is photorecombination, the formalism can also be applied to other scattering situations for which similar projection operators $P$, $Q$, and $R$ can be defined.

Taking the matrix element of Eq. (2.13) and using Eq. (3.1b) gives

$$\langle f\omega|T(z)|\alpha E\rangle=\langle f\omega|t^P(z)|\alpha E\rangle+\sum_{f'}\int d\omega'\langle f\omega|t^P(z)G_R^0(z)|f'\omega'\rangle\langle f'\omega'|T(z)|\alpha E\rangle \tag{3.3a}$$

$$=\langle f\omega|t^P(z)|\alpha E\rangle+\sum_{f'}\int d\omega'\frac{\langle f\omega|t^P(z)|f'\omega'\rangle\langle f'\omega'|T(z)|\alpha E\rangle}{z-\omega'} \ . \tag{3.3b}$$

The matrix elements of $t^P$ are obtained by substituting Eq. (3.2) into Eq. (2.12):

$$\begin{aligned}\langle f\omega|t^P(z)|\alpha E\rangle&=\langle f\omega|\lambda^P(z)|\alpha E\rangle+\sum_{a,a'}\langle f\omega|\lambda^P(z)|a\rangle\langle a|G_Q^P(z)|a'\rangle\langle a'|\lambda^P(z)|\alpha E\rangle \ ,\\ \langle f\omega|t^P(z)|f'\omega'\rangle&=\langle f\omega|\lambda^P(z)|f'\omega'\rangle+\sum_{a,a'}\langle f\omega|\lambda^P(z)|a\rangle\langle a|G_Q^P(z)|a'\rangle\langle a'|\lambda^P(z)|f'\omega'\rangle \ .\end{aligned} \tag{3.4}$$

Approaches to the calculations of the matrix elements of $\lambda^P$ which appear in Eq. (3.4) for various situations will be considered in Secs. III C and IV B.

### B. Solution of equations for separable *RVP* potentials

We consider systems for which the matrix elements of $V$ between the $\{r\}$ states and the $\{p\}$ and $\{q\}$ states satisfy the separability condition:

$$\begin{aligned}&\langle f\omega|V|\alpha E\rangle=b_f^*(\omega)d_{f\alpha}(E) \ ,\\ &\langle \alpha E|V|f\omega\rangle=d_{\alpha f}(E)b_f(\omega) \ ,\\ &\langle f\omega|V|a\rangle=b_f^*(\omega)d_{fa} \ ,\\ &\langle a|V|f\omega\rangle=d_{af}b_f(\omega) \ .\end{aligned} \tag{3.5}$$

This condition is met, for example, by the spontaneous radiative decay coupling of electron-ion photorecombination. (This separability has been exploited in HJ and in Refs. 6 and 10.) Then $b_f$ is proportional to photon energy to the three-halves power, and $d$ represents essentially the electric dipole operator. For the spontaneous radiative decay coupling, matrix elements of $RVR$ are diagonal in photon quantum numbers, including frequency. We set

$$RVR=0 \ , \tag{3.6}$$

thereby accounting for this diagonality and also assuming that an adequate description of electron-ion bound states is given by eigenstates of $H^0$.

As indicated above, the operator $\lambda^P$ is the level shift operator for $P+Q$ space. However, its matrix elements are defined in the entire $P+Q+R$ Hilbert space. It follows from the separability condition (3.5) that matrix elements of $\lambda^P(z)$ which involve the $R$-space states can be written in the form

$$\begin{aligned}&\langle f\omega|\lambda^P(z)|\alpha E\rangle=b_f^*(\omega)\tilde{\lambda}_{f\alpha}^P(z,E) \ ,\\ &\langle f\omega|\lambda^P(z)|a\rangle=b_f^*(\omega)\tilde{\lambda}_{fa}^P(z) \ ,\\ &\langle f\omega|\lambda^P(z)|f'\omega'\rangle=b_f^*(\omega)b_{f'}(\omega')\tilde{\lambda}_{ff'}^P(z) \ ,\\ &\langle a|\lambda^P(z)|f\omega\rangle=b_f(\omega)\tilde{\lambda}_{af}^P(z) \ ,\end{aligned} \tag{3.7}$$

for some $\omega$-independent $\tilde{\lambda}$.

We can similarly define $\omega$-independent matrix elements $\tilde{t}_{f\alpha}^P(z,E)$ and $\tilde{t}_{ff'}^P(z)$ such that

$$\langle f\omega|t^P(z)|\alpha E\rangle=b_f^*(\omega)\tilde{t}_{f\alpha}^P(z,E)$$

and

$$\langle f\omega|t^P(z)|f'\omega'\rangle=b_f^*(\omega)b_{f'}(\omega')\tilde{t}_{ff'}^P(z) \ . \tag{3.8}$$

In these equations $\tilde{\lambda}^P$ and $\tilde{t}^P$ represent operators in a system which features discrete states $\{|f\rangle\}$ (i.e., characterized by quantum numbers $f$) rather than photon continua $\{|f\omega\rangle\}$. This $\{|f\rangle\}+\{|a\rangle\}+\{|\alpha E\rangle\}$ system features the Hamiltonian $\tilde{H}=\tilde{H}^0+\tilde{V}$, where

$$\begin{aligned}\tilde{H}^0&=\sum_f E_f|f\rangle\langle f|+\sum_a E_a|a\rangle\langle a|+\sum_\alpha\int dE E|\alpha E\rangle\langle \alpha E| \ ,\\ \tilde{V}&=\left[\sum_{f,a}|f\rangle d_{fa}\langle a|+\sum_{f,\alpha}\int dE|f\rangle d_{f\alpha}(E)\langle \alpha E|+\sum_{a,\alpha}\int dE|a\rangle\langle a|V|\alpha E\rangle\langle \alpha E|\right]+\text{H.c.}\\ &\quad+\sum_{\alpha,\alpha'}\int dE\int dE'|\alpha E\rangle\langle \alpha E|V|\alpha' E'\rangle\langle \alpha' E'| \ .\end{aligned} \tag{3.9}$$

We shall denote the space of this limited system, which features only one set of continua, but two sets of discrete states, by $\tilde{S}$. $\tilde{\lambda}^P$ is the level shift operator in space $\tilde{S}$,

$$\tilde{\lambda}^P(z)=\tilde{V}+\tilde{V}[P(z-H^0-\tilde{V})P]^{-1}P\tilde{V} , \tag{3.10a}$$

$$=\tilde{V}+\tilde{V}(P-G_P^0\tilde{V}_{PP})^{-1}G_P^0\tilde{V} , \tag{3.10b}$$

and

$$\tilde{\lambda}^P(z)P=\tilde{V}(P-G_P^0\tilde{V}_{PP})^{-1}P .$$

Matrix elements of $\tilde{\lambda}^P$ include

$$\tilde{\lambda}^P_{f\alpha}(z,E)=\sum_{\alpha'}\int dE' d_{f\alpha'}(E')\langle\alpha'E'|[P-G_P^0(z)\tilde{V}_{PP}]^{-1}|\alpha E\rangle \tag{3.11a}$$

and

$$\tilde{\lambda}^P_{a\alpha}(z,E)=\sum_{\alpha'}\int dE'\langle a|V|\alpha'E'\rangle\langle\alpha'E'|[P-G_P^0(z)\tilde{V}_{PP}]^{-1}|\alpha E\rangle . \tag{3.11b}$$

Other matrix elements of $\tilde{\lambda}^P$ can be constructed from $\tilde{\lambda}^P=\tilde{V}+\tilde{\lambda}^P G_P^0\tilde{V}$. The operator $\tilde{t}^P$ has matrix elements

$$\tilde{t}^P_{f\alpha}(z,E)=\tilde{\lambda}^P_{f\alpha}(z,E)+\sum_{a,a'}\tilde{\lambda}^P_{fa}(z)\langle a|G_Q^P(z)|a'\rangle\tilde{\lambda}^P_{a'\alpha}(z,E) \tag{3.12a}$$

and

$$\tilde{t}^P_{ff'}(z)=\tilde{\lambda}^P_{ff'}(z)+\sum_{a,a'}\tilde{\lambda}^P_{fa}(z)\langle a|G_Q^P(z)|a'\rangle\tilde{\lambda}^P_{a'f'}(z) , \tag{3.12b}$$

where $\langle a|G_Q^P(z)|a'\rangle$ are the various matrix elements of the inverse of the matrix

$$\langle a|G_Q^P(z)^{-1}|a'\rangle=\langle a|(z-H^0-\tilde{\lambda}^P)|a'\rangle=(z-E_a)\delta_{aa'}-\tilde{\lambda}^P_{aa'} . \tag{3.13}$$

The matrix elements in Eq. (3.12) are matrix elements of the operator

$$\tilde{t}^P(z)=\tilde{\lambda}^P(z)+\tilde{\lambda}^P(z)G_Q^P(z)\tilde{\lambda}^P(z) , \tag{3.14}$$

which differs from the $T$ operator in the space $\tilde{S}$ only in that $G_Q^P(z)$ allows for propagation only through the $Q$ ($\{|a\rangle\}$) states, and not through the $\{|f\rangle\}$ states.

Equation (3.3) can now be written

$$\langle f\omega|T(z)|\alpha E\rangle=b_f^*(\omega)\tilde{t}^P_{f\alpha}(z,E)+b_f^*(\omega)\sum_{f'}\tilde{t}^P_{ff'}(z)\int d\omega'\frac{b_{f'}(\omega')\langle f'\omega'|T(z)|\alpha E\rangle}{z-\omega'} . \tag{3.15}$$

Next, we note that we can write

$$\langle f\omega|T(z)=b_f^*(\omega)\langle f|[\tilde{V}+\tilde{V}G(z)V] , \tag{3.16}$$

so that Eq. (3.15) can be written

$$b_f^*(\omega)\langle f|[\tilde{V}+\tilde{V}G(z)V]|\alpha E\rangle=b_f^*(\omega)\tilde{t}^P_{f\alpha}(z,E)+b_f^*(\omega)\sum_{f'}\tilde{t}^P_{ff'}(z)\sigma_{f'}(z)\langle f'|[\tilde{V}+\tilde{V}G(z)V]|\alpha E\rangle , \tag{3.17a}$$

where

$$\sigma_f(z)=\int d\omega'\frac{|b_f(\omega')|^2}{z-\omega'} . \tag{3.17b}$$

Equation (3.17a) can be solved to obtain

$$\langle f\omega|T(z)|\alpha E\rangle=b_f^*(\omega)\sum_{f'}[L^{-1}_{ff'}(z)\tilde{t}^P_{f'\alpha}(z,E)] , \tag{3.18a}$$

where $L$ is a matrix such that

$$L_{ff'}(z)=\delta_{ff'}-\tilde{t}^P_{ff'}(z)\sigma_{f'}(z) . \tag{3.18b}$$

Equation (3.18) presents a formal solution for the matrix element of $T$ in terms of $\tilde{t}^P$ for systems satisfying the separability condition (3.5). In order to find explicit forms for the matrix elements of $\tilde{t}^P$, one can first find explicit forms for the matrix elements of $\tilde{\lambda}^P$, and construct the matrix elements of $\tilde{t}^P$ from them using Eq. (3.12). The form of the $\tilde{\lambda}^P$ matrix elements will depend on the particulars of the *PVP* coupling. Explicit forms can be constructed using Eq. (3.11), or, if the matrix elements of $\lambda^P$ are known, using Eq. (3.7).

### C. Form of $\lambda^P$ for *PVP* separable or zero

The operator $\lambda^P$, which is defined in Eq. (2.6) and also given in Eq. (2.14), is the level shift operator in $P+Q$ space. The specific forms which its matrix elements take

depend upon the nature of the coupling between the $P$ states. In this section, we consider the two special cases in which $PVP$ is separable or zero, and we present expressions for $\lambda^P$ for these cases. A third case, in which we make the so-called pole approximation on the $PVP$ coupling, will be considered in Sec. IV. The results of this section do not require $RVR=0$ except where explicitly indicated.

### 1. PVP separable

We consider here the case in which the $PVP$ coupling satisfies the separability condition

$$\langle \alpha E|V|\alpha' E'\rangle = A^*_\alpha(E)B_{\alpha'}(E') \tag{3.19}$$

for some functions $A$ and $B$. In order to find matrix elements of $\lambda^P$, we consider first the matrix elements of $(P-G_P^0V_{PP})^{-1}$. Starting from the expression

$$(P-G_P^0V_{PP})^{-1}=P+G_P^0V_{PP}(P-G_P^0V_{PP})^{-1}\ ,$$

it is straightforward to show, using methods similar to those used in obtaining Eq. (3.18),

$$\langle \alpha E|(P-G_P^0V_{PP})^{-1}|\alpha' E'\rangle = \delta_{\alpha\alpha'}\delta(E-E')+\frac{A^*_\alpha(E)B_{\alpha'}(E')}{(z-E)[1-\beta(z)]}\ , \tag{3.20}$$

where

$$\beta(z)=\sum_\alpha \int dE \frac{B_\alpha(E)A^*_\alpha(E)}{z-E}\ . \tag{3.21}$$

It then follows from (2.18) that

$$\langle a|\lambda^P(z)|\alpha E\rangle = \langle a|V|\alpha E\rangle + \sum_{\alpha'}\int dE' \frac{\langle a|V|\alpha' E'\rangle A^*_{\alpha'}(E')}{z-E'}\frac{B_\alpha(E)}{1-\beta(z)}\ ,$$

$$\langle f\omega|\lambda^P(z)|\alpha E\rangle = \langle f\omega|V|\alpha E\rangle + \sum_{\alpha'}\int dE' \frac{\langle f\omega|V|\alpha' E'\rangle A^*_{\alpha'}(E')}{z-E'}\frac{B_\alpha(E)}{1-\beta(z)}\ ,$$

and from Eq. (2.19) that

$$\langle f\omega|\lambda^P(z)|a\rangle = \langle f\omega|V|a\rangle + \sum_{\alpha'}\int dE' \frac{\langle f\omega|V|\alpha' E'\rangle\langle \alpha' E'|V|a\rangle}{z-E'} + \frac{1}{1-\beta(z)}\sum_{\alpha'}\int dE' \frac{\langle f\omega|V|\alpha' E'\rangle A^*_{\alpha'}(E')}{z-E'}\sum_{\alpha''}\int dE'' \frac{B_{\alpha''}(E'')\langle \alpha'' E''|V|a\rangle}{z-E''}\ ,$$

$$\langle f\omega|\lambda^P(z)|f'\omega'\rangle = \langle f\omega|V|f'\omega'\rangle + \sum_{\alpha'}\int dE' \frac{\langle f\omega|V|\alpha' E'\rangle\langle \alpha' E'|V|f'\omega'\rangle}{z-E'} + \frac{1}{1-\beta(z)}\sum_{\alpha'}\int dE' \frac{\langle f\omega|V|\alpha' E'\rangle A^*_{\alpha'}(E')}{z-E'}\sum_{\alpha''}\int dE'' \frac{B_{\alpha''}(E'')\langle \alpha'' E''|V|f'\omega'\rangle}{z-E''}\ . \tag{3.22}$$

### 2. PVP zero

If $PVP=0$, then the full $P$-space propagator $[P(z-H^0-V)P]^{-1}P$ is equal to the free $P$-space propagator $G_P^0(z)=[P(z-H^0)P]^{-1}P$. We then have from Eq. (2.18) $\lambda^P P=VP$, and the level shift operator is simply

$$\lambda^P(z)=V+VG_P^0(z)V\ . \tag{3.23}$$

The required matrix elements of $t^P$ then reduce to

$$\langle f\omega|t^P(z)|\alpha E\rangle = \langle f\omega|V|\alpha E\rangle + \langle f\omega|[V+VG_P^0(z)V]G_Q^P V|\alpha E\rangle\ , \tag{3.24a}$$

$$\langle f\omega|t^P(z)|f'\omega'\rangle = \langle f\omega|V|f'\omega'\rangle + \langle f\omega|VG_P^0(z)V|f'\omega'\rangle + \langle f\omega|[V+VG_P^0(z)V]G_Q^P(z)[V+VG_P^0(z)V]|f'\omega'\rangle\ , \tag{3.24b}$$

where, since $PVP=0$,

$$G_Q^P(z)=[Q(z-H^0-V-VG_P^0V)Q]^{-1}Q\ . \tag{3.25}$$

For the case in which $PVP=0$, $RVR=0$, and $RVP$ is separable [so that Eq. (3.5) is satisfied], $\tilde{\lambda}^P$ can be written

$$\tilde{\lambda}^P(z)=\tilde{V}+\tilde{V}G_P^0(z)\tilde{V}\ ,$$

and its matrix elements, as well as those of $\tilde{t}$, can easily be constructed.

## IV. POLE APPROXIMATION

### A. Pole approximation on the *R* continuum only

Matrix elements of the scattering matrix $S$ are related to matrix elements of $T$ by $\langle f\omega_0|S|\alpha E\rangle=-2\pi i\delta(\omega_0-E)\langle f\omega_0|T(\omega_0+i0)|\alpha E\rangle$. Thus the argument of $T$ that is of interest is $\omega_0+i0$, i.e., $\lim_{\epsilon\to 0+}(\omega_0+i\epsilon)$. For this argument one can use the well-known relation

$$\frac{1}{\omega_0+i0-E}=\mathrm{P}\left[\frac{1}{\omega_0-E}\right]-i\pi\delta(\omega_0-E)\ , \tag{4.1}$$

where P represents the principal part, to write, for some function $\phi(\omega)$,

$$\int\frac{\phi(\omega)}{\omega_0+i0-\omega}d\omega=\mathrm{P}\int\frac{\phi(\omega)}{\omega_0-\omega}d\omega-i\pi\phi(\omega_0)\ . \tag{4.2}$$

If $\phi$ is slowly varying, then one can make the "pole approximation" of neglecting the principal value integral in Eq. (4.2). This approximation has been widely discussed in the literature. We emphasize that in what follows in this section we make the pole approximation only on the photon continua, and not on the electron continua.

We begin by noting that we may write $\langle f'\omega'|T(z)|\alpha E\rangle=\langle f'\omega'|V[1+G(z)V]|\alpha E\rangle$ as $\langle f'\omega'|V|N(z,E)\rangle$ for some ket $N$; this matrix element of $V$ is a slowly varying function of $\omega'$ (although it may be a rapidly varying function of $E$). Similarly, it follows from Eqs. (3.4) and (2.7) that we can write $\langle f\omega|t^P(z)|f'\omega'\rangle$ as $\langle M(z,\omega)|V|f'\omega'\rangle$ for some $M$; this matrix element will also be a slowly varying function of $\omega'$. Equation (3.3b) can then be written, taking $\omega=\omega_0$,

$$\langle f\omega_0|T(\omega_0+i0)|\alpha E\rangle=\langle f\omega_0|t^P(\omega_0+i0)|\alpha E\rangle+\int d\omega'\left[\frac{\sum_{f'}\langle M(\omega_0+i0,\omega_0)|V|f'\omega'\rangle\langle f'\omega'|V|N(\omega_0+i0,E)\rangle}{\omega_0+i0-\omega'}\right]\ . \tag{4.3}$$

We now make the pole approximation in the integral over $\omega'$, and solve the resulting equation to obtain

$$\langle f\omega_0|T(\omega_0+i0)|\alpha E\rangle=\sum_{f'}K^{-1}_{ff'}(\omega_0+i0)\langle f'\omega_0|t^P(\omega_0+i0)|\alpha E\rangle\ , \tag{4.4}$$

where

$$K_{ff'}(\omega_0+i0)=\delta_{ff'}+i\pi\langle f\omega_0|t^P(\omega_0+i0)|f'\omega_0\rangle\ . \tag{4.5}$$

The right-hand side of Eq. (4.4) is a simple matrix product.

An equivalent expression for the matrix element of $T$ can be obtained by applying the pole approximation to the results of Sec. III B, in which the coupling to the $\{r\}$ continua was assumed separable. For this case one writes

$$\sigma_f(\omega_0+i0)=-i\pi|b_f(\omega_0)|^2\ . \tag{4.6a}$$

One can assume without loss of generality that $b_{f'}(\omega_0)=1$ for all $f'$ [since one can absorb any constant multiplicative factors into $d$ in Eq. (3.5) as needed]. Equation (4.6a) then becomes

$$\sigma_f(\omega_0+i0)=-i\pi\ , \tag{4.6b}$$

and Eq. (3.18a) gives (setting $\omega=\omega_0$ in the bra of $T$)

$$\langle f\omega_0|T(\omega_0+i0|\alpha E\rangle=\sum_{f'}[L^{-1}_{ff'}(\omega_0+i0)\tilde{t}^P_{f'\alpha}(\omega_0+i0,E)]\ , \tag{4.7}$$

with [froms Eqs. (3.8) and (3.18b)]

$$\begin{aligned}&\tilde{t}^P_{f'\alpha}(\omega_0+i0,E)=\langle f'\omega_0|t^P(\omega_0+i0)|\alpha E\rangle\ ,\\ &\tilde{t}^P_{ff'}(\omega_0+i0)=\langle f\omega_0|t^P(\omega_0+i0)|f'\omega_0\rangle\ ,\\ &L_{ff'}(\omega_0+i0)=K_{ff'}(\omega_0+i0)\ .\end{aligned} \tag{4.8}$$

The matrix elements of $t^P(\omega_0+i0)$ appearing in Eq. (4.8) are the same as those appearing in Eq. (4.4).

### B. $\lambda^P$ in pole approximation on the *PVP* couplings

The limited Hilbert-space level shift operator $\lambda^P$ allows for $P$-space intermediate states and takes into account to all orders the couplings between the $P$-space states. Explicit forms for it can be obtained in several different ways. We could, for example, follow a procedure similar to that used for separable $PVP$ coupling in order to find an expression for the matrix elements of $\lambda^P$. Instead, we examine the operator $\lambda^P$ in the pole approximation by taking a perturbation series expansion. The analysis uses the methods of Sec. V B of HJ.

Equation (2.18) for $\lambda^P P$ can be expanded in an infinite series as

$$\begin{aligned}\lambda^P P&=VP+VG^0_PV_{PP}+VG^0_PVG^0_PV_{PP}+\cdots\\ &=\sum_{n=0}^{\infty}(VG^0_P)^nVP\ .\end{aligned} \tag{4.9}$$

One can draw Feynman-like diagrams for the various terms in (4.9); each $G^0_P$ can be thought of as representing unperturbed propagation in one intermediate $P$-space continuum. If the various $P$-space eigenstates of $H^0$ are denoted by $|\alpha E\rangle$, then in the pole approximation,

$$VG^0_P(E_0+i0)V|\alpha E_0\rangle=-i\pi\sum_{\alpha'}V|\alpha' E_0\rangle\underline{V}_{\alpha'\alpha}\ , \tag{4.10a}$$

where

$$\underline{V}_{\alpha'\alpha} \equiv \langle \alpha' E_0 | V | \alpha E_0 \rangle \ . \tag{4.10b}$$

$\underline{V}$ is a square matrix with dimensionality equal to the number of continua in $P$ space. It follows that

$$\begin{aligned} & VG_P^0(E_0+i0)VG_P^0(E_0+i0)V|\alpha E_0\rangle \\ & \quad = \sum_{\alpha',\alpha''} V|\alpha'' E_0\rangle(-i\pi\underline{V}_{\alpha''\alpha'})(-i\pi\underline{V}_{\alpha'\alpha}) \\ & \quad = \sum_{\alpha'} V|\alpha' E_0\rangle[(-i\pi\underline{V})^2]_{\alpha'\alpha} \ . \end{aligned} \tag{4.11}$$

Generalizing for all $n \geq 0$,

$$[VG_P^0(E_0+i0)]^n V|\alpha E_0\rangle = \sum_{\alpha'} V|\alpha' E_0\rangle[(-i\pi\underline{V})^n]_{\alpha'\alpha} \ , \tag{4.12}$$

and from (4.9)

$$\lambda^P(E_0+i0)|\alpha E_0\rangle = \sum_{\alpha'} \left[ V|\alpha' E_0\rangle \left[ \sum_{n=0}^{\infty} (-i\pi\underline{V})^n_{\alpha'\alpha} \right] \right] \tag{4.13a}$$

$$= \sum_{\alpha'} V|\alpha' E_0\rangle(\underline{1}+i\pi\underline{V})^{-1}_{\alpha'\alpha} \ , \tag{4.13b}$$

where $\underline{1}$ denotes the unity matrix with dimensionality equal to that of $\underline{V}$. Thus the matrix which needs to be inverted in Eq. (4.13) has dimensionality equal to the number of electron continua in $P$ space.

Finally, Eq. (2.19) gives

$$\lambda^P(E_0+i0) = V - i\pi \sum_{\alpha,\alpha'} V|\alpha' E_0\rangle(\underline{1}+i\pi\underline{V})^{-1}_{\alpha'\alpha}\langle \alpha E_0|V \ . \tag{4.14}$$

Equations (4.13) and (4.14) can now be used to write explicit expressions for the various matrix elements of $\lambda^P(E_0+i0)$. The results can then be used to find matrix elements of $t^P_{RP}$, $K_{RR}$, and $G^P_Q$. The calculations are simplified if we assume matrix elements of $PVP$ are slowly varying enough that we can write

$$\langle \alpha E|V|\alpha' E'\rangle = \langle \alpha E_0|V|\alpha' E_0\rangle = \underline{V}_{\alpha\alpha'} \ , \tag{4.15}$$

i.e., if we neglect totally the energy dependence of the matrix elements of $PVP$.

## V. SAMPLE APPLICATION: PHOTORECOMBINATION IN AN EXTERNAL dc ELECTRIC FIELD

As an example of the use of the above formalism, we will consider photorecombination processes within the model system that is depicted in Figs. 2(a) and 2(b). The $P$ space consists of two electron continua $\{|\alpha E\rangle\}$ and $\{|\beta E\rangle\}$, the $Q$ space consists of two discrete states $|a\rangle$ and $|b\rangle$ with energies $E_a$ and $E_b$, respectively, and the $R$ space consists of two final atomic states with their corresponding photon continua. The two $R$-space continua are $\{|f\omega\rangle\}$ and $\{|g\omega\rangle\}$.

We shall assume that the matrix elements of $V$ which

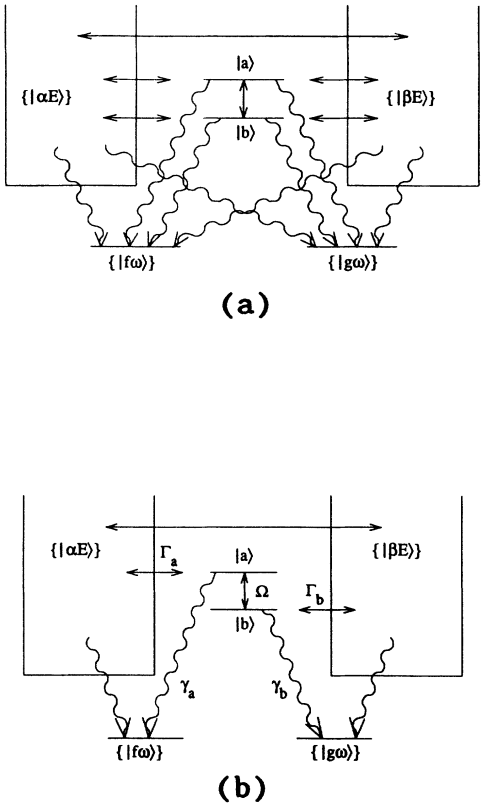


FIG. 2. Schematic diagram of the model systems of Sec. V.

involve continuum states are slowly varying functions of continuum energy, so that we may apply the pole approximation in the analysis and so that we may write the couplings shown in Fig. 2(a) as

$$\begin{aligned} & \langle f\omega|V|\alpha E\rangle = V_{f\alpha}, \quad \langle f\omega|V|\beta E\rangle = V_{f\beta} \ , \\ & \langle g\omega|V|\alpha E\rangle = V_{g\alpha}, \quad \langle g\omega|V|\beta E\rangle = V_{g\beta} \ , \\ & \langle a|V|\alpha E\rangle = V_{a\alpha}, \quad \langle a|V|\beta E\rangle = V_{a\beta} \ , \\ & \langle b|V|\alpha E\rangle = V_{b\alpha}, \quad \langle b|V|\beta E\rangle = V_{b\beta} \ , \\ & \langle \alpha E|V|\beta E'\rangle = V_{\alpha\beta} \ , \end{aligned} \tag{5.1}$$

and

$$\langle a|V|b\rangle = V_{ab} \ .$$

Their Hermitian conjugates are written similarly. We assume $RVR = 0$ (thus $\langle f\omega|V|g\omega'\rangle = 0$), and that the couplings other than those listed above or their Hermitian conjugates are zero. Because we neglect the energy dependence of the matrix elements of $V$, there is no need to distinguish $\underline{V}$, which was used in the previous section to identify matrix elements of $V$ at a particular continuum energy, from $V$.

Under these assumptions, Eqs. (4.13) and (4.14) give, using an obvious matrix notation (and denoting the transpose of a matrix by superscript $T$),

$$
R\lambda^P P=(1/\psi_{\alpha\beta})\begin{bmatrix} V_{f\alpha}-i\pi V_{f\beta}V_{\beta\alpha} & V_{f\beta}-i\pi V_{f\alpha}V_{\alpha\beta} \\ V_{g\alpha}-i\pi V_{g\beta}V_{\beta\alpha} & V_{g\beta}-i\pi V_{g\alpha}V_{\alpha\beta} \end{bmatrix},
$$

$$
R\lambda^P Q=\begin{bmatrix} V_{fa} & V_{fb} \\ V_{ga} & V_{gb} \end{bmatrix}-(1/\psi_{\alpha\beta})\begin{bmatrix} \pi^2(V_{f\alpha}V_{\alpha\beta}V_{\beta a}+V_{f\beta}V_{\beta\alpha}V_{\alpha a}) & \pi^2(V_{f\alpha}V_{\alpha\beta}V_{\beta b}+V_{f\beta}V_{\beta\alpha}V_{\alpha b}) \\ +i\pi(V_{f\alpha}V_{\alpha a}+V_{f\beta}V_{\beta a}) & +i\pi(V_{f\alpha}V_{\alpha b}+V_{f\beta}V_{\beta b}) \\ \pi^2(V_{g\alpha}V_{\alpha\beta}V_{\beta a}+V_{g\beta}V_{\beta\alpha}V_{\alpha a}) & \pi^2(V_{g\alpha}V_{\alpha\beta}V_{\beta b}+V_{g\beta}V_{\beta\alpha}V_{\alpha b}) \\ +i\pi(V_{g\alpha}V_{\alpha a}+V_{g\beta}V_{\beta a}) & +i\pi(V_{g\alpha}V_{\alpha b}+V_{g\beta}V_{\beta b}) \end{bmatrix},
$$

$$
Q\lambda^P P=(1/\psi_{\alpha\beta})\begin{bmatrix} V_{a\alpha}-i\pi V_{a\beta}V_{\beta\alpha} & V_{a\beta}-i\pi V_{a\alpha}V_{\alpha\beta} \\ V_{b\alpha}-i\pi V_{b\beta}V_{\beta\alpha} & V_{b\beta}-i\pi V_{b\alpha}V_{\alpha\beta} \end{bmatrix}, \tag{5.2}
$$

$$
Q\lambda^P Q=(1/\psi_{\alpha\beta})\begin{bmatrix} -\pi^2(V_{a\alpha}V_{\alpha\beta}V_{\beta a}+V_{a\beta}V_{\beta\alpha}V_{\alpha a}) & V_{ab}\psi_{\alpha\beta}-\pi^2(V_{a\alpha}V_{\alpha\beta}V_{\beta b}+V_{a\beta}V_{\beta\alpha}V_{\alpha b}) \\ -i\pi(|V_{a\alpha}|^2+|V_{a\beta}|^2) & -i\pi(V_{a\alpha}V_{\alpha b}+V_{a\beta}V_{\beta b}) \\ V_{ab}\psi_{\alpha\beta}-\pi^2(V_{a\alpha}V_{\alpha\beta}V_{\beta b}+V_{a\beta}V_{\beta\alpha}V_{\alpha b}) & -\pi^2(V_{b\alpha}V_{\alpha\beta}V_{\beta b}+V_{b\beta}V_{\beta\alpha}V_{\alpha b}) \\ -i\pi(V_{b\alpha}V_{\alpha a}+V_{b\beta}V_{\beta a}) & -i\pi(|V_{b\alpha}|^2+|V_{b\beta}|^2) \end{bmatrix},
$$

$$
\psi_{\alpha\beta}=1+\pi^2|V_{\alpha\beta}|^2 .
$$

Matrix elements of $Q\lambda^P R$ can be obtained from $R\lambda^P Q$ by taking the transpose and interchanging the order of the subscripts.

These expressions may be used to find $G_Q^P$, $t_{RP}$ and $K_{RR}$, as outlined in Sec. IV. However, rather than proceeding with the general case, we shall narrow our focus and describe photorecombination processes within the simplified system depicted in Fig. 2(b). This model system represents a positive ion having two discrete states of opposite parity, each of which can decay by either autoionization or photon emission. The states $|a\rangle$, $\{|\alpha E\rangle\}$, and $|g\rangle$ have one parity, and the states $|b\rangle$, $\{|\beta E\rangle\}$, and $|f\rangle$ have the opposite parity. Configuration interaction couples $|a\rangle$ to the continuum $\{|\alpha E\rangle\}$ and $|b\rangle$ to the continuum $\{|\beta E\rangle\}$. The model also features parity-mixing matrix elements $V_{ab}$ and $V_{\alpha\beta}$ representing an external dc electric field. This system is similar to that studied by Ravi and Agarwal[11] (hereafter RA), but generalizes theirs to include the coupling $V_{\alpha\beta}$ between the electron continua. Equations (5.2) then simplify to

$$
\begin{aligned}
R\lambda^P P&=(1/\psi_{\alpha\beta})\begin{bmatrix} V_{f\alpha} & -i\pi V_{f\alpha}V_{\alpha\beta} \\ -i\pi V_{g\beta}V_{\beta\alpha} & V_{g\beta} \end{bmatrix}, \\
R\lambda^P Q&=(1/\psi_{\alpha\beta})\begin{bmatrix} V_{fa}\psi_{\alpha\beta}-i\pi V_{f\alpha}V_{\alpha a} & -\pi^2 V_{f\alpha}V_{\alpha\beta}V_{\beta b} \\ -\pi^2 V_{g\beta}V_{\beta\alpha}V_{\alpha a} & V_{bg}\psi_{\alpha\beta}-i\pi V_{g\beta}V_{\beta b} \end{bmatrix}, \\
Q\lambda^P P&=(1/\psi_{\alpha\beta})\begin{bmatrix} V_{a\alpha} & -i\pi V_{a\alpha}V_{\alpha\beta} \\ -i\pi V_{b\beta}V_{\beta\alpha} & V_{b\beta} \end{bmatrix}, \\
Q\lambda^P Q&=(1/\psi_{\alpha\beta})\begin{bmatrix} -i\pi|V_{a\alpha}|^2 & V_{ab}\psi_{\alpha\beta}-\pi^2 V_{a\alpha}V_{\alpha\beta}V_{\beta b} \\ V_{ab}\psi_{\alpha\beta}-\pi^2 V_{a\alpha}V_{\alpha\beta}V_{\beta b} & -i\pi|V_{b\beta}|^2 \end{bmatrix}.
\end{aligned} \tag{5.3}
$$

Equations (5.3) can then be combined with Eqs. (2.11), (2.12), and (4.5) to find $G_Q^P$, $t_{RP}^P$, and $K_{RR}$. We define linewidth parameters

$$
\Gamma_a=2\pi|V_{a\alpha}|^2,\quad \Gamma_b=2\pi|V_{b\beta}|^2,\quad \gamma_a=2\pi|V_{fa}|^2,\quad \gamma_b=2\pi|V_{gb}|^2,\quad \Omega=\frac{4|V_{ab}|^2}{\Gamma_a^2},\quad \xi=\pi V_{\alpha\beta} , \tag{5.4a}
$$

dimensionless energy parameters

$$
\epsilon=\frac{2}{\Gamma_a}(E-E_a),\quad \Delta=\frac{2}{\Gamma_a}(E_b-E_a) , \tag{5.4b}
$$

and line-shape parameters

$$
\begin{aligned}
&q_f=\frac{1}{\pi V_{f\alpha}}\left[\frac{\gamma_a}{\Gamma_a}\right]^{1/2},\quad q_g=\frac{1}{\pi V_{g\beta}}\left[\frac{\gamma_b}{\Gamma_b}\right]^{1/2},\quad \eta=\left[\frac{\Omega\Gamma_b}{\Gamma_a}\right]^{1/2}, \\
&\mu_f=1+\pi^2|V_{f\alpha}|^2+\pi^2|V_{\alpha\beta}|^2,\quad \mu_g=1+\pi^2|V_{g\beta}|^2+\pi^2|V_{\alpha\beta}|^2 , \\
&\psi_{f\alpha}=1+\pi^2|V_{f\alpha}|^2,\quad \psi_{g\beta}=1+\pi^2|V_{g\beta}|^2 .
\end{aligned} \tag{5.4c}
$$

Then assuming that the discrete state-continuum matrix elements of $V$ are real and positive, and that $V_{\alpha\beta}$ is real, we find using Eq. (2.12) that the matrix elements of $t^P_{RP}(E+i0)$ are

$$\langle f\omega|t^P|\alpha E\rangle=\frac{(\gamma_a/\Gamma_a)^{1/2}}{\pi q_f}\frac{(\epsilon+q_f)(\epsilon-\Delta)-\Omega+i\left[\frac{\Gamma_b}{\Gamma_a}(\epsilon+q_f)-q_f\eta\xi\right]}{[\epsilon(\epsilon-\Delta)-\Omega]\psi_{\alpha\beta}+2\eta\xi-\frac{\Gamma_b}{\Gamma_a}+i\left[\epsilon\left[1+\frac{\Gamma_b}{\Gamma_a}\right]-\Delta\right]},$$

$$\langle f\omega|t^P|\beta E\rangle=\frac{(\gamma_a/\Gamma_a)^{1/2}}{\pi q_f}\frac{q_f\eta-i[(\epsilon+q_f)(\epsilon-\Delta)\xi-\Omega\xi+\eta]}{[\epsilon(\epsilon-\Delta)-\Omega]\psi_{\alpha\beta}+2\eta\xi-\frac{\Gamma_b}{\Gamma_a}+i\left[\epsilon\left[1+\frac{\Gamma_b}{\Gamma_a}\right]-\Delta\right]},$$

$$\langle g\omega|t^P|\alpha E\rangle=\frac{(\gamma_b/\Gamma_b)^{1/2}}{\pi q_g}\frac{q_g\eta-i\{\epsilon[\epsilon-\Delta+q_g(\Gamma_b/\Gamma_a)]\xi-\Omega\xi+\eta\}}{[\epsilon(\epsilon-\Delta)-\Omega]\psi_{\alpha\beta}+2\eta\xi-\frac{\Gamma_b}{\Gamma_a}+i\left[\epsilon\left[1+\frac{\Gamma_b}{\Gamma_a}\right]-\Delta\right]},\tag{5.5}$$

$$\langle g\omega|t^P|\beta E\rangle=\frac{(\gamma_b/\Gamma_b)^{1/2}}{\pi q_g}\frac{\epsilon[\epsilon-\Delta+q_g(\Gamma_b/\Gamma_a)]-\Omega+i[\epsilon-\Delta+q_g(\Gamma_b/\Gamma_a)-q_g\eta\xi]}{[\epsilon(\epsilon-\Delta)-\Omega]\psi_{\alpha\beta}+2\eta\xi-\frac{\Gamma_b}{\Gamma_a}+i\left[\epsilon\left[1+\frac{\Gamma_b}{\Gamma_a}\right]-\Delta\right]}.$$

The matrix elements of $K_{RR}$ can now be constructed from Eq. (4.5), and are presented in Eq. (5.6) on the following page.

It is now a straightforward matrix calculation to use Eq. (4.4) to construct matrix elements of $RT(E+i0)P$. Because of the algebraic length of the results, we do not write out the final, algebraic expressions for the matrix elements.

The probability of photorecombination from initial continuum state $|\alpha E\rangle$ to the final photon continuum $\{|f\omega\rangle\}$ can be calculated as $4\pi^2|\langle f\omega|T(E+i0)|\alpha E\rangle|^2$, where by conservation of energy $\omega=E$. Figure 3 shows this probability as a function of the electron energy parameter $\epsilon$ for varying dc field strengths. The various atomic parameters were chosen so as to match those of Fig. 2 of RA, except that we have included the coupling between the two electron continua. In order to show clearly the effects which this latter coupling can have, we have made it comparable in size to the coupling between the discrete states. In the absence of the field, the problem reduces to the well-understood case of a single resonance imbedded in a continuum, and demonstrates the expected single resonance profile. As noted by RA, increasing the dc field causes the resonances to exhibit a doublet structure. In this case the electric field mixes the autoionizing states to form dressed states, each of which can decay to the photon continuum $|f\omega\rangle$. For our case,

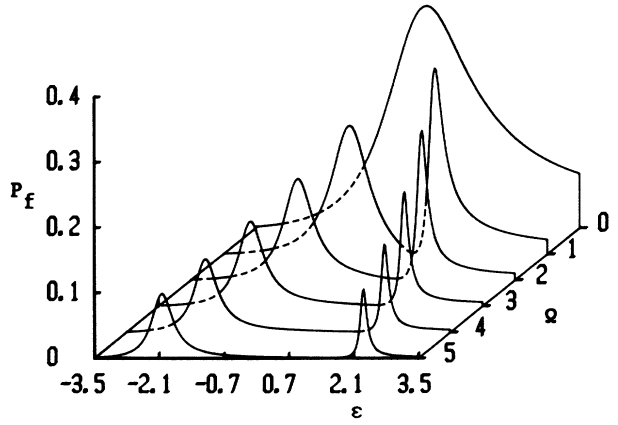


FIG. 3. Probability $P_f$ of photorecombination into continuum $\{|f\omega\rangle\}$ from initial state $|\alpha E\rangle$ vs incident electron energy parameter $\epsilon$ for various values of the external electric field. Fixed parameters are $\Gamma_b/\Gamma_a=0.07$, $\gamma_a/\Gamma_a=0.1$, $\gamma_b/\Gamma_a=0.1$, $q_f=5$, $q_g=1$, and $\Delta=0.3$. The third axis gives $\Omega$, which is dimensionless and proportional to the square of the electric field. In this figure, the electron continuum-electron continuum coupling is related to the coupling between the autoionizing states by $V_{\alpha\beta}=V_{ab}/\Gamma_a=\sqrt{\Omega}/2$, or $\xi=(\pi/2)\sqrt{\Omega}$.

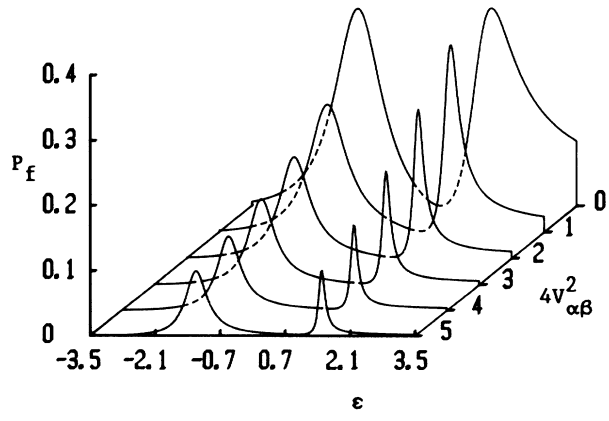


FIG. 4. $P_f$ vs $\epsilon$ for various values of the electron continuum-electron continuum coupling, but with fixed discrete state-discrete state coupling parameter $\Omega=2$. The values of the coupling between the electron continua are quoted along the third axis as multiples of $4V^2_{\alpha\beta}=4\xi^2/\pi^2$. Other parameters are the same as in Fig. 3.

in which changing the dc field strength changes both the discrete state-discrete state coupling parameter $\Omega$ and the continuum-continuum coupling parameter $\xi$, increasing field strength corresponds to a significant decrease in peak height.

In Fig. 4 we consider only the effect of the electron continuum-continuum couplings—the discrete state couplings are held constant. It is clear from the curves that large continuum-continuum coupling suppresses the transitions into the $\{|f\omega\rangle\}$ continuum and narrows the linewidth of the resonances. We also note that the coupling between the electron continua has little effect on the separation of the resonances.

In Fig. 5 we present the probability of photoemission into the second photon continuum, $\{|g\omega\rangle\}$, for the same conditions as in Fig. 3. If there is no dc field, no transitions into the $\{|g\omega\rangle\}$ continuum occur. When the field is present, the couplings it introduces allow the population to reach the $\{|g\omega\rangle\}$ continuum. When the *PVP* coupling is nonzero, the population need not pass through the autoionizing states in order to reach the $\{|g\omega\rangle\}$ continuum—it can go from electron continuum $\{|\alpha E\rangle\}$ to electron continuum $\{|\beta E\rangle\}$, and then directly to $\{|g\omega\rangle\}$. Thus the curves in Fig. 5 exhibit sizable probability $P_g$ even far from resonance. We notice that the effect of the autoionizing states is indeed to inhibit rather than to enhance the probability near the energies of the dressed states.

Figures 6(a), 6(b), and 6(c) show the effects of increasing the coupling between the two electron continua while keeping the coupling between the resonances at a constant value. At zero *PVP* coupling, the dressed state energies correspond to peaks in the curves, but as the coupling increases the dressed state energies begin to correspond to dips in the curves.

Our results clearly show that the *PVP* coupling can strongly influence the photorecombination process, and the magnitude and importance of the *PVP* coupling will need to be considered in any study of real systems featuring photorecombination in an external field.

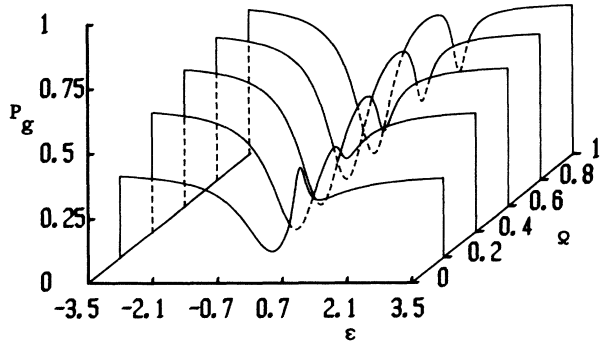


FIG. 5. Probability $P_g$ of photorecombination into continuum $\{|g\omega\rangle\}$ from initial state $|\alpha E\rangle$ vs $\epsilon$ for the same conditions as in Fig. 3. The total photorecombination probabilities can be obtainied by summing these curves with those of Fig. 3.

$$\langle f\omega|K|f\omega'\rangle = K_{ff} = \frac{\mu_f[\epsilon(\epsilon-\Delta)-\Omega]+\dfrac{2\gamma_a}{q_f\Gamma_a}(\epsilon-\Delta)+2\eta\xi-\dfrac{\Gamma_b}{\Gamma_a}\left|1+\dfrac{\gamma_a}{\Gamma_a}\right|+i\left|\dfrac{\Gamma_b}{\Gamma_a}\epsilon\psi_{f\alpha}+(\epsilon-\Delta)\left|1+\dfrac{\gamma_a}{\Gamma_a}\psi_{\alpha\beta}\right|+\dfrac{2\gamma_a}{q_f\Gamma_a}\left|\dfrac{\Gamma_b}{\Gamma_a}-\eta\right|\right|}{[\epsilon(\epsilon-\Delta)-\Omega]\psi_{\alpha\beta}+2\eta\xi-\dfrac{\Gamma_b}{\Gamma_a}+i\left|\epsilon\left|1+\dfrac{\Gamma_b}{\Gamma_a}\right|-\Delta\right|},$$

$$\langle f\omega|K|g\omega'\rangle = \langle g\omega'|K|f\omega\rangle = K_{fg} = K_{gf} = \frac{1}{q_f q_g}\left|\frac{\gamma_a\gamma_b}{\Gamma_a\Gamma_b}\right|^{1/2}\frac{(q_f+q_g)\eta-i\{(\epsilon+q_f)[\epsilon-\Delta+(\Gamma_b/\Gamma_a)q_g]\xi-\Omega\xi+\eta(1+q_fq_g\psi_{\alpha\beta})\}}{[\epsilon(\epsilon-\Delta)-\Omega]\psi_{\alpha\beta}+2\eta\xi-\dfrac{\Gamma_b}{\Gamma_a}+i\left|\epsilon\left|1+\dfrac{\Gamma_b}{\Gamma_a}\right|-\Delta\right|},$$

$$\langle g\omega|K|g\omega'\rangle = K_{gg} = \frac{\mu_g[\epsilon(\epsilon-\Delta)-\Omega]+\eta\xi+\dfrac{2\gamma_b}{q_g\Gamma_a}\epsilon+2\eta\xi-\dfrac{\Gamma_b}{\Gamma_a}\left|1+\dfrac{\gamma_b}{\Gamma_b}\right|+i\left|\dfrac{\Gamma_b}{\Gamma_a}\epsilon\left|1+\dfrac{\gamma_b}{\Gamma_b}\psi_{\alpha\beta}\right|+(\epsilon-\Delta)\psi_{g\alpha}-\dfrac{2\gamma_b}{q_g\Gamma_b}\left|\dfrac{\Gamma_b}{\Gamma_a}-\eta\xi\right|\right|}{[\epsilon(\epsilon-\Delta)-\Omega]\psi_{\alpha\beta}+2\eta\xi-\dfrac{\Gamma_b}{\Gamma_a}+i\left|\epsilon\left|1+\dfrac{\Gamma_b}{\Gamma_a}\right|-\Delta\right|}.$$

(5.6)

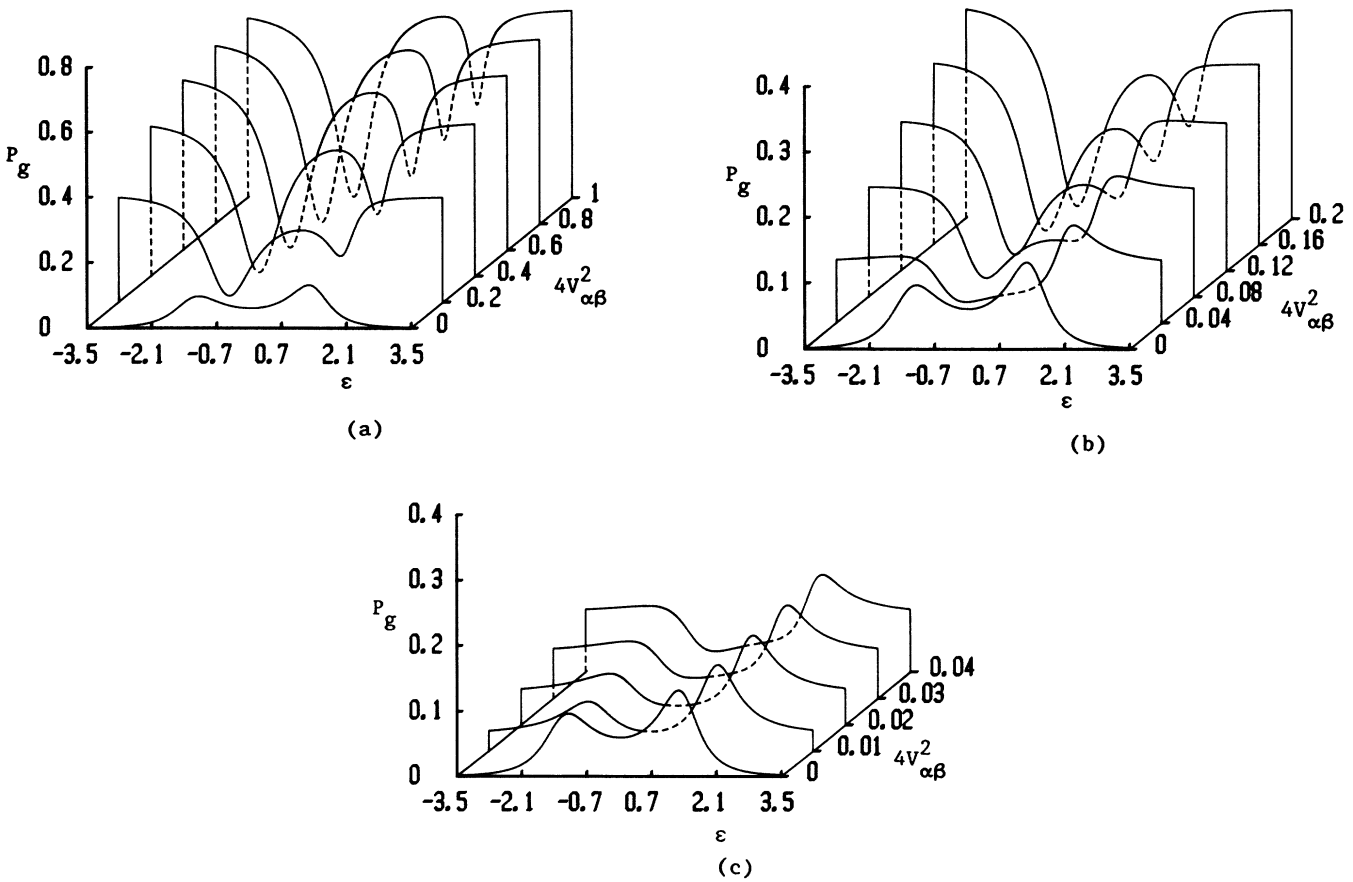


FIG. 6. $P_g$ vs $\epsilon$ for various values of $4V^2_{\alpha\beta}$ and for $\Omega=2$. The total photorecombination probabilities can be obtained by summing these curves with those of Fig. 4.

## VI. ALTERNATIVE EQUATIONS FOR THE PROJECTED $T$ OPERATOR

Alternative equations for the projected $T$ operator, based on Eq. (1.1d) rather than Eq. (1.1c), will be displayed in this section. Analogs to all final equations in Secs. II, III A, and III B will be presented. The alternative formulation is particularly useful when the couplings satisfy a separability condition in which the initial-state energy can be separated out in a manner analogous to the way that the final-state energy separates out in Eq. (3.5). Since this "initial-state separability" condition is met in, for example, photoionization, in which the initial state is a photon continuum state, we shall in this section solve for $T_{PR}$ instead of $T_{RP}$. Then $R$ can continue to represent the photon continuum projection operator and $P$ the electron continuum projection operator. Of course, the formalism can also be applied to other situations in which $R$ and $P$ represent projection operators onto other appropriate initial- and final-state continua.

The equation for $T_{PR}$ which follows from Eq. (1.1d) is

$$T_{PR}=V_{PR}+T_{PR}G^0_R V_{RR}+T_{PP}G^0_P V_{PR}+T_{PQ}G^0_Q V_{QR}\ . \tag{6.1}$$

The equations for the required projected $T$ operators $T_{PQ}$ and $T_{PP}$ can be written down by inspection. The entire calculation is then carried out in a manner analogous to that of Secs. I–IV. The main difference is that most operator multiplications are performed from the right. The formal solution is

$$T_{PR}(R-G^0_R t^P_{RR})=t^P_{PR}\ , \tag{6.2}$$

where the operator $t^P$ is defined in Eq. (2.12).

It follows from Eq. (6.2) that the matrix element of $T_{PR}$ solves

$$\langle \alpha E|T(z)|f\omega\rangle=\langle \alpha E|t^P(z)|f\omega\rangle+\sum_{f'}\int d\omega'\frac{\langle \alpha E|T(z)|f'\omega'\rangle\langle f'\omega'|t^P(z)|f\omega\rangle}{z-\omega'}\ , \tag{6.3}$$

where the matrix elements of $t^P$ are obtained from Eq. (3.4). It can be seen from Eqs. (6.3) and (3.4) that matrix elements of $P\lambda^P$ are needed rather than of $\lambda^P P$. Accordingly, in a systematic approach to solving Eq. (6.3) one first uses (2.16) to find matrix elements of $P\lambda^P$. Then (2.17) is used to construct all additional matrix elements of $\lambda^P$. These are substituted into Eq. (2.12) to obtain all necessary matrix elements of $t^P$. Finally, these are substituted into Eq. (6.3), an integral equation that involves initial states. Because we are considering $T_{PR}$ these are the continuum states $\{r\}$.

The solution is facilitated if all matrix elements coupling the $\{r\}$ continua satisfy the separability condition

$$\begin{aligned}
&\langle f\omega|V|\alpha E\rangle=\phi_f(\omega)d_{f\alpha}(E)\ ,\\
&\langle \alpha E|V|f\omega\rangle=d_{\alpha f}(E)\phi_f^*(\omega)\ ,\\
&\langle f\omega|V|a\rangle=\phi_f(\omega)d_{fa}\ ,\\
&\langle a|V|f\omega\rangle=d_{af}\phi_f^*(\omega)\ .
\end{aligned} \tag{6.4}$$

The function $\phi_f(\omega)$ is the same throughout Eq. (6.4). This condition is met for reactions induced by a single photon and provides motivation for considering $T_{PR}$ rather than $T_{RP}$. In this context, $\phi_f(\omega)$ corresponds to the square root of the spectral density function for the incident radiation, and $d$ is essentially the electric dipole operator. The solution to Eq. (6.3) for separable potentials as described by Eq. (6.4) is

$$\langle \alpha E|T(z)|f\omega\rangle=\sum_{f'}\tilde{t}^P_{\alpha f'}(z,E)J^{-1}_{f'f}(z)\phi_f^*(\omega)\ , \tag{6.5}$$

where $J$ is a matrix such that

$$J_{f'f}(z)=\delta_{f'f}-s_{f'}(z)\tilde{t}^P_{f'f}(z)\ , \tag{6.6a}$$

with

$$s_f(z)=\int d\omega\frac{|\phi_f(\omega)|^2}{z-\omega}\ , \tag{6.6b}$$

and $\tilde{t}^P_{f'f}(z)$ being given by Eq. (3.12).

The matrix element $\tilde{t}^P_{\alpha f}(z,E)$ is

$$\tilde{t}^P_{\alpha f}(z,E)=\tilde{\lambda}^P_{\alpha f}(z,E)+\sum_{a,a'}\tilde{\lambda}^P_{\alpha a}(z,E)\langle a|G^P_Q(z)|a'\rangle\tilde{\lambda}^P_{a'f}(z)\ , \tag{6.7}$$

with

$$\begin{aligned}
\tilde{\lambda}^P_{\alpha f}(z,E)&=\sum_{\alpha'}\int dE'\langle \alpha E|(P-\tilde{V}_{PP}G^0_P)^{-1}|\alpha' E'\rangle d_{\alpha' f}(E')\ ,\\
\tilde{\lambda}^P_{\alpha a}(z,E)&=\sum_{\alpha'}\int dE'\langle \alpha E|(P-\tilde{V}_{PP}G^0_P)^{-1}|\alpha' E'\rangle\langle \alpha' E'|V|a\rangle\ .
\end{aligned} \tag{6.8}$$

Other matrix elements of $\tilde{\lambda}^P$ can be constructed from

$$\tilde{\lambda}^P=\tilde{V}+\tilde{V}G^0_P\tilde{\lambda}^P\ . \tag{6.9}$$

Application of this formalism will not be presented in the present work.

## VII. SUMMARY AND CONCLUSIONS

We have presented a formalism for finding projections of the $T$ operator. The formalism is based upon the projected Lippmann-Schwinger equations for $T$, given in Eq. (2.1), and an operator generalization of Gauss's reduction for linear algebraic equations. The projection operators we have used are $P$, which projects onto the set of continua in which the initial state naturally belongs, $Q$, which represents resonances (or discrete eigenstates of the unperturbed Hamiltonian), and $R$, which represents a set of reaction channels orthogonal to $P$. In Sec. II we have developed a formal equation for $T_{RP}(z)$, Eq. (2.13), which is based on the Lippmann-Schwinger equation, Eq. (1.1c). The equation for $T_{RP}$ involves the operator $t^P(z)$, which is defined in Eq. (2.12) in terms of the operator $\lambda^P(z)$ of Eqs. (2.7) and (2.14) and of the operator $G^P_Q(z)$ of Eq. (2.11). We have identified $\lambda^P(z)$ as the level shift operator for a system which features $P$-space continua, but no $R$-space continua; we have also identified $G^P_Q(z)$ as the $Q$-space to $Q$-space propagator in the same limited Hilbert space.

In Sec. III we have developed an algebraic realization of Eq. (2.13) for systems in which the projection operators $P$, $Q$, and $R$ can be written as in Eqs. (3.1) and (3.2). For the case in which the final-state continua (the $R$-space continua) satisfy the separability condition (3.5) and satisfy $RVR=0$, considerable simplification occurs, and the matrix elements of $T_{RP}(z)$ are given by Eq. (3.18) [see also (3.12) and (3.17)]. In Sec. III C we have considered the level shift operator $\lambda^P(z)$, and we have shown how it can be written when the $PVP$ coupling satisfies the separability condition (3.19) or when $PVP$ is zero.

In Sec. IV we have shown how the results simplify if one makes the pole approximation on the $R$-space continua, with the results (4.4) and (4.10). We also show how the $P$-space propagator and $\lambda^P$ simplify when the pole approximation is made on the $PVP$ coupling.

As a sample application, we have considered photorecombination processes in a model atomic system which features two autoionizing states, two electron continua (one of which contains the initial state), and two photon continua (corresponding to radiatively stabilized atomic states). We have made the pole approximation throughout the analysis. The model is similar to the one studied by Ravi and Agarwal,[11] but includes coupling between the two electron continua. We have shown that this $PVP$ (electron continuum-electron continuum) coupling can have a dramatic effect on the photorecombina-

tion processes. These effects are shown clearly in Figs. 3–6.

Finally, in Sec. VI we have sketched the derivation of matrix elements of $T_{PR}$ based on the Lippmann-Schwinger equation (1.1d). This formulation simplifies for the case in which initial-state continua satisfy the separability condition (6.4), such as in photoionization.

Although we have used the formalism only in one case of present interest in atomic physics, the formalism may prove useful in a wide variety of problems involving very different physical situations.

## ACKNOWLEDGMENTS

This work was supported by the National Science Foundation through Grant No. PHY-8711639, and by Calvin College.

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