PHYSICAL REVIEW A VOLUME 40, NUMBER 8 OCTOBER 15, 1989

Resonance profiles for electron-ion photorecombination at an isolated resonance

S. L. Haan
Department of Physics, Calvin College, Grand Rapids, Michigan 49506
(Received 3 April 1989)

A projection-operator formalism is employed in studying photorecombination at energies close to an autoionizing resonance. A resonance profile is defined, and is presented without approximation for a model system consisting of one electron continuum, one autoionizing state, and one final radiatively stabilized atomic state. Effective line-profile parameters $\hat{\varepsilon}$ and $\hat{q}$ are defined, and the photorecombination resonance profile is shown to the the same as the photoionization resonance profile (for the process in which initial and final atomic states are interchanged from the photorecombination process), provided one-photon spontaneous radiative decay effects are included. The effective line-profile parameters are examined, and are shown to reduce to the standard autoionization line-profile parameters in the limit of no spontaneous radiative decay. Effective line-profile parameters are also defined in the pole approximation for two model systems featuring an isolated autoionizing state. Comparison is made with effective line-profile parameters that have been defined elsewhere in the context of photoionization into coupled electron-continuum channels. The similarity in mathematical formalism for systems supporting multiple continua, regardless of whether these continua are electron or photon continua, is discussed.

I. INTRODUCTION

Several recent investigations[1–5] have pointed out that a rigorous quantum-mechanical theory should not treat radiative and dielectronic recombination as two distinct, noninterfering processes. Alber, Cooper, and Rau,[1] using methods of Davies and Seaton,[6] presented a unified description of the processes for a model system featuring an initially populated electron continuum, one autoionizing state, and one final atomic state with accompanying photon continuum. In their analysis, Alber, Cooper, and Rau made the pole approximation of assuming "flat" continua, so that certain principal-value integrals could be neglected. They showed that the energy dependence of the photorecombination cross section was similar to the energy dependence of "modified Fano profiles" that had previously been introduced[7,8] in studies of the influence of spontaneous radiative decay on weak-field resonant photoionization processes.

The model studied by Alber, Cooper, and Rau[1] has since been generalized by Jacobs, Cooper, and Haan[3] to allow for degenerate magnetic sublevels of the atomic system and for multiple angular-momentum contributions in the partial-wave expansion of the unperturbed eigenstates of the electron continuum. By utilizing scattering-theory techniques that had previously been used[7,9,10] in studies of the decay of a prepared state into coupled continua, they presented an exact, closed-form expression for the photorecombination T matrix for the model system. This exact expression featured the sum of two terms. The first term was the matrix element of a vertex operator, and the second term involved both the vertex operator and the projection of the resolvent operator onto the subspace of the autoionizing states. The first term of the sum was interpreted as representing nonresonant or direct photorecombination, and the second term of the sum was interpreted as the resonance contribution to the photorecombination.

Recent papers[4,5] have presented a projection operator[11–18] approach to the unified treatment of radiative and dielectronic recombination. One of these,[5] hereafter referred to as paper I, considered the transition operator T which describes the photorecombination process, and presented an expression for T which generalized to a model-independent operator form the expression found earlier by Jacobs, Cooper, and Haan[3] for their model system. A similar expression had previously been derived and used by other investigators in other contexts,[19,20] as discussed in paper I.

One feature of the T-operator expression presented in paper I is that it provides a natural separation of resonant and nonresonant processes in the formalism. This separation allows one to compare theoretically the full photorecombination process, when resonances are present, with the photorecombination process in the absence of resonances. In the present work we make such a comparison, and we define and discuss resonance profiles for photorecombination.

In Sec. II of this paper we summarize the relevant formalism of paper I, and in Sec. III we apply the formalism to a model system that is similar to the one studied by Alber, Cooper, and Rau.[1] We present an exact expression for the photorecombination T matrix for this model. In Sec. IV we define a resonance profile for photorecombination in the model system, and we show how effective line-profile parameters, denoted by $\hat{\varepsilon}$ and $\hat{q}$, can be defined so that the resonance profile exhibits the usual Fano form.[21] In Sec. IV B we emphasize that the resonance profile for photorecombination into state $|f\rangle$ is the same as the profile for weak-field photoionization from atomic state $|f\rangle$ when one-photon spontaneous radiative-decay effects are included. In the latter context we also note that one-photon spontaneous radiative-decay effects slow the rate of photoabsorption, and we comment that this change of the transition rate from the initial state is one particular manifestation of the general conclusion that a coupling between final-state continua can change the rate of "decay" of a discrete state, an effect which has been discussed by a number of investigators in many different physical contexts.[7,9,22–27]

In Sec. V we consider the two particular model systems that were studied in paper I. The systems both feature one autoionizing state. In one system, there is only one electron continuum but there are an arbitrary number of photon continua, with each photon continuum corresponding to a different possible final (radiatively stabilized) atomic state. In the second system, there are an arbitrary number of electron continua, but only one photon continuum. We define effective line-profile parameters $\hat{\epsilon}$ and $\hat{q}$ for these systems. We also compare the line-shape-profile parameters defined in this work with those that have been used by other investigators[28,29] for systems featuring an isolated autoionizing resonance and multiple, coupled electron continua. Finally, in Sec. VI we summarize and discuss our results.

II. SUMMARY OF FORMALISM OF PAPER I

As in paper I, 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, where C projects onto the space of continuum eigenstates of H^0, and Q projects onto the space of discrete (autoionizing) eigenstates of H^0. We assume that $(Q+C)V = V(Q+C) = V$, i.e., that the interaction V does not mix the states in the space onto which the sum $Q+C$ projects with states outside that space. The photorecombination process can be described by using the T operator, which is defined as[30]

$$T(z) = V + VG(z)V \;, \tag{2.1}$$

where

$$G(z) = (z - H^0 - V)^{-1} \tag{2.2}$$

is the resolvent or Green's operator. In paper I it is shown that

$$T(z) = \Lambda(z) + \Lambda(z)QG(z)Q\Lambda(z) \;, \tag{2.3}$$

where

$$QG(z)Q = Q\{Q[z - H^0 - \Lambda(z)]Q\}^{-1}Q \;, \tag{2.4}$$

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

$$\Phi(z) = [C(z - H^0 - V)C]^{-1} \;. \tag{2.6}$$

The operator $\Phi(z)$ represents the Green's operator that would be obtained if the system had no discrete (autoionizing) states, and can be thought of as representing the propagator in the continuum space onto which C projects. The operator $\Lambda(z)$ has been frequently referred to as a "level-shift operator" or "vertex operator," and has sometimes been denoted by $R(z)$.[13–17] The projected Green's operator $QG(z)Q$ can be thought of as an effective propagator through the space of discrete states.

As in paper I, we write the continuum projection operator C as the sum of projection operators for electron and photon continua: $C = P + R$, where 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

$$RT(z)P = R\Lambda(z)P + R\Lambda(z)QG(z)Q\Lambda(z)P \;. \tag{2.7}$$

As discussed in paper I, 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 can be said to represent standard, nonresonant radiative recombination. The second term in the sum, $R\Lambda(z)QG(z)Q\Lambda(z)P$, contains all effects of the autoionizing states.

Paper I also presents a general recipe for constructing matrix elements of the photorecombination T operator, based on the equations reproduced above as Eqs. (2.4)–(2.7). In the following section we apply this recipe to a simple model system.

III. APPLICATION OF FORMALISM TO A MODEL SYSTEM

A. Description of model

We begin our study of photorecombination near an isolated resonance with a careful examination of a simple model system which features a single autoionizing state, a single (initially populated) electron continuum, and a single bound atomic state with accompanying photon. This same system has been studied in the pole approximation (which is discussed later in this paper) by Alber, Cooper, and Rau.[1] The system has been studied outside the pole approximation by Jacobs, Cooper, and Haan.[3] The latter work included explicit expressions for the matrix elements of the photorecombination T matrix for the system when degenerate magnetic sublevels were accounted for, and it showed how the expressions simplified when magnetic quantum-number specifications were ignored. In the present section we use the formalism of paper I to rederive the T matrix expressions of Ref. 3 for the case where magnetic sublevels are ignored. Then in Sec. IV we use the formalism to define and to discuss photorecombination profiles and effective profile parameters for the system.

We will write the electron continuum eigenstates of H^0 as $|\alpha E\rangle$, where α denotes the relevant quantum numbers of the state and E denotes its total energy. We will write the final atomic state as $|f\rangle$, and the accompanying photon continuum eigenstates of H^0 as $|f\omega\rangle$, where ω denotes the total energy. (Throughout this work we take $\hbar = 1$; any photon quantum numbers will be assumed to be absorbed into f.) We will assume that the continuum eigenstates of H^0 have a δ-function normalization with respect to energy, i.e., that $\langle \alpha E|\alpha E'\rangle=\delta(E-E')$, $\langle f\omega|f\omega'\rangle=\delta(\omega-\omega')$, and of course $\langle \alpha E|f\omega\rangle=0$. We will denote the autoionizing state by $|a\rangle$, with $H^0|a\rangle=E_a|a\rangle$, $\langle a|a\rangle=1$, $\langle a|\alpha E\rangle=\langle a|f\omega\rangle=\langle a|f\rangle=0$. We also assume that $\langle \alpha E|V|\alpha E'\rangle=0=\langle f\omega|V|f\omega'\rangle$. For these states the projection operators can be written

$$P=\int dE|\alpha E\rangle\langle\alpha E| \, ,\quad R=\int d\omega|f\omega\rangle\langle f\omega| \, ,\quad Q=|a\rangle\langle a| \, . \tag{3.1}$$

A schematic diagram of the model is shown in Fig. 1.

We take advantage of the separability of the coupling between the two continua[3,7,9] of the model in the dipole approximation, and we write

$$\langle \alpha E|V|f\omega\rangle=d_{\alpha f}(E)g_f(\omega) \, ,\quad \langle f\omega|V|\alpha E\rangle=g_f^*(\omega)d_{f\alpha}(E) \, . \tag{3.2}$$

Here $d_{\alpha f}(E)$ is essentially a dipole matrix element between the electron continuum and the final atomic state $|f\rangle$, and $g(\omega)$ includes the familiar $(\omega_k\alpha_{\rm FS})^{3/2}$ factor, where ω_k denotes the photon energy and $\alpha_{\rm FS}$ the fine-structure constant, as well as multiplicative algebraic factors (we have included the $\alpha_{\rm FS}$ explicitly as an expansion parameter). An exact solution for the matrix elements of the T operator describing photorecombination can be obtained for this model system by following the recipe presented in paper I.

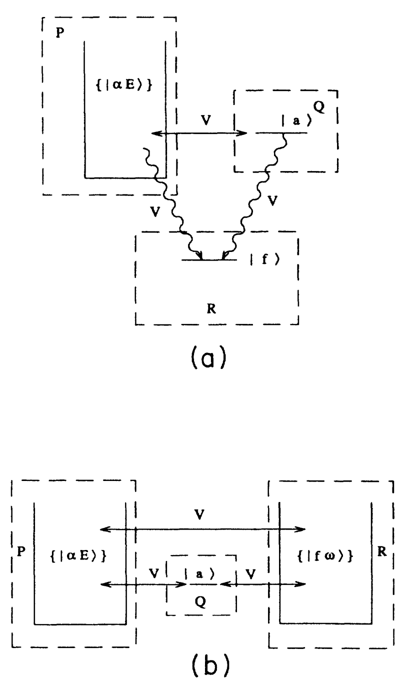

FIG. 1. Schematic diagrams of the model system of Sec. III. In (b), the continuum nature of possible photon energies has been explicitly indicated.

B. Construction of matrix element of $T(z)$

1. Matrix elements of $\Phi(z)$

The first step in the recipe of paper I is to construct matrix elements of $\Phi(z)$. For the interaction described by Eq. (3.2), it is straightforward to show from $C[(z-H^0)\Phi(z)]C=C[1+CVC\Phi(z)]C$ that

$$\langle \alpha E|\Phi(z)|\alpha E'\rangle=\frac{1}{z-E}\left[\delta(E-E')+\frac{d_{\alpha f}(E)}{\psi(z)}\frac{\Sigma^{gg}(z)d_{f\alpha}(E')}{z-E'}\right] ,$$
$$\langle f\omega|\Phi(z)|\alpha E\rangle=\frac{g_f^*(\omega)d_{f\alpha}(E)}{\psi(z)(z-\omega)(z-E)} , \tag{3.3}$$

and, interchanging electron and photon continuum symbols,

$$\langle f\omega|\Phi(z)|f\omega'\rangle=\frac{1}{z-\omega}\left[\delta(\omega-\omega')+\frac{g_f^*(\omega)}{\psi(z)}\frac{\Sigma^{ff}(z)g_f(\omega')}{z-\omega'}\right] , \tag{3.4}$$

$$\langle \alpha E|\Phi(z)|f\omega\rangle=\frac{d_{\alpha f}(E)g_f(\omega)}{\psi(z)(z-E)(z-\omega)} .$$

In these expressions we have introduced the self-energies

$$\Sigma^{gg}(z)=\int d\omega\frac{|g_f(\omega)|^2}{z-\omega} ,\quad \Sigma^{ff}(z)=\int dE\frac{|d_{f\alpha}(E)|^2}{z-E} \tag{3.5a}$$

(where, as throughout this work, it is understood that the integrals are over all continuum energies), and

$$\psi(z)=1-\Sigma^{ff}(z)\Sigma^{gg}(z) . \tag{3.5b}$$

2. Matrix elements of $\Lambda(z)$

The second step of the recipe of paper I is to construct matrix elements of $\Lambda(z)=V+VC\Phi(z)CV$ between the various states of interest. One obtains

$$\langle f\omega|\Lambda(z)|\alpha E\rangle=\frac{g_f^*(\omega)d_{f\alpha}(E)}{\psi(z)}\ ,$$

$$\langle a|\Lambda(z)|\alpha E\rangle=\langle a|V|\alpha E\rangle+\frac{1}{\psi(z)}[\Sigma^{af}(z)\Sigma^{gg}(z)+\Sigma^{ag}(z)]d_{f\alpha}(E)\ ,$$

$$\langle a|\Lambda(z)|a\rangle=\Sigma_{\rm el}^{aa}(z)+\Sigma_{\rm ph}^{aa}(z)+\frac{1}{\psi(z)}[\Sigma^{af}(z)\Sigma^{gg}(z)\Sigma^{fa}(z)+\Sigma^{ag}(z)\Sigma^{ff}(z)\Sigma^{ga}(z)+\Sigma^{af}(z)\Sigma^{ga}(z)+\Sigma^{ag}(z)\Sigma^{fa}(z)]\ , \tag{3.6}$$

$$\langle f\omega|\Lambda(z)|a\rangle=\langle f\omega|V|a\rangle+\frac{g_f^*(\omega)}{\psi(z)}[\Sigma^{ff}(z)\Sigma^{ga}(z)+\Sigma^{fa}(z)]\ ,$$

where the Σ's denote various self-energies:

$$\Sigma^{af}(z)=\int dE\frac{\langle a|V|\alpha E\rangle d_{\alpha f}(E)}{z-E}\ ,$$

$$\Sigma^{ag}(z)=\int d\omega\frac{\langle a|V|f\omega\rangle g_f^*(\omega)}{z-\omega}\ ,$$

$$\Sigma_{\rm el}^{aa}(z)=\int dE\frac{|\langle a|V|\alpha E\rangle|^2}{z-E}\ ,$$

$$\Sigma_{\rm ph}^{aa}(z)=\int d\omega\frac{|\langle a|V|f\omega\rangle|^2}{z-\omega}\ , \tag{3.7}$$

$$\Sigma^{fa}(z)=\int dE\frac{d_{f\alpha}(E)\langle\alpha E|V|a\rangle}{z-E}\ ,$$

$$\Sigma^{ga}(z)=\int d\omega\frac{g_f(\omega)\langle f\omega|V|a\rangle}{z-\omega}\ .$$

Additional simplification occurs if we employ the relationship[3]

$$\langle f\omega|V|a\rangle=g_f^*(\omega)d_{fa}\ , \tag{3.8}$$

where $g_f(\omega)$ is the same function of ω as occurs in Eq. (3.2) and where d_{fa} denotes essentially the dipole matrix element between atomic states $|f\rangle$ and $|a\rangle$. Then

$$\Sigma^{ag}(z)=d_{af}\Sigma^{gg}(z)\ ,$$

$$\Sigma^{ga}(z)=d_{fa}\Sigma^{gg}(z)\ , \tag{3.9}$$

$$\Sigma_{\rm ph}^{aa}(z)=|d_{af}|^2\Sigma^{gg}(z)\ ,$$

and one can write

$$\langle f\omega|\Lambda(z)|\alpha E\rangle=\frac{g_f^*(\omega)d_{f\alpha}(E)}{\psi(z)}\ ,$$

$$\langle f\omega|\Lambda(z)|a\rangle=\frac{g_f^*(\omega)}{\psi(z)}\lambda_{fa}(z)\ ,$$

$$\langle a|\Lambda(z)|a\rangle=\Sigma_{\rm el}^{aa}(z)+\frac{1}{\psi(z)}\Sigma^{gg}(z)\lambda_{af}(z)\lambda_{fa}(z)\ , \tag{3.10}$$

$$\langle a|\Lambda(z)|\alpha E\rangle=\langle a|V|\alpha E\rangle+\lambda_{af}(z)\frac{\Sigma^{gg}(z)d_{f\alpha}(E)}{\psi(z)}\ ,$$

where

$$\lambda_{af}(z)=d_{af}+\Sigma^{af}(z)\ ,$$

$$\lambda_{fa}(z)=d_{fa}+\Sigma^{fa}(z)\ . \tag{3.11}$$

The operator λ represents the level shift operator within a model system which contains one continuum, $\{|\alpha E\rangle\}$, and two discrete states, $|f\rangle$ and $|a\rangle$, and which has Hamiltonian H' such that $\langle f|H'|a\rangle=d_{fa}$, $\langle f|H'|\alpha E\rangle=d_{f\alpha}(E)$, and $\langle a|H'|\alpha E\rangle=\langle a|V|\alpha E\rangle$. When multiplied by the appropriate photon intensity factor, λ represents the level shift operator for the usual Fano[21] or laser-induced autoionization[31] system, in the absence of spontaneous radiative decay.

On inspection of Eq. (3.10) we notice two relations that will be useful later:

$$\langle f\omega|\Lambda(z)|a\rangle=\frac{\lambda_{fa}(z)}{d_{f\alpha}(E)}\langle f\omega|\Lambda(z)|\alpha E\rangle\ , \tag{3.12a}$$

and

$$\langle a|\Lambda(z)|a\rangle=\Sigma_{\rm el}^{aa}(z)+\left[\frac{\langle\alpha|\Lambda(z)|\alpha E\rangle-\langle a|V|\alpha E\rangle}{d_{f\alpha}(E)}\right]\lambda_{fa}(z)\ . \tag{3.12b}$$

3. *Matrix elements of $RT(E+i0)P$*

For our simple one-discrete state system, the projected Green's operator $QG(z)Q$ of Eq. (2.4) is given by

$$QG(z)Q=\frac{|a\rangle\langle a|}{z-E_a-\langle a|\Lambda(z)|a\rangle}\ . \tag{3.13}$$

It follows that the matrix element of the T operator coupling the initial state $|\alpha E\rangle$ with the final state $|f\omega\rangle$ can be written

$$\langle f\omega|T(z)|\alpha E\rangle=\langle f\omega|\Lambda(z)|\alpha E\rangle+\frac{\langle f\omega|\Lambda(z)|a\rangle\langle a|\Lambda(z)|\alpha E\rangle}{z-E_a-\langle a|\Lambda(z)|a\rangle}\ . \tag{3.14}$$

Equation (3.14), with the matrix elements of $\Lambda(z)$ given in Eqs. (3.6) and (3.12), is the same as Eq. (87) of Ref. 3.[32] Setting $z=E+i0$ in Eq. (3.14) and using Eq. (3.12), we obtain

$$\langle f\omega|T(E+i0)|\alpha E\rangle=\frac{\langle f\omega|\Lambda(E+i0)|\alpha E\rangle}{E-E_a-\langle a|\Lambda(E+i0)|a\rangle}\left[E-E_a-\langle a|\Lambda(E+i0)|a\rangle+\frac{\lambda_{fa}(E+i0)\langle a|\Lambda(E+i0)|\alpha E\rangle}{d_{fa}(E)}\right], \tag{3.15a}$$

which is equivalent to Eq. (94) of Ref. 3. In anticipation of defining resonance profile parameters, we use Eq. (3.12b) for $\langle a|\Lambda(E+i0)|a\rangle$ to rewrite Eq. (3.15a) as

$$\langle f\omega|T(E+i0)|\alpha E\rangle=\frac{\langle f\omega|\Lambda(E+i0)|\alpha E\rangle}{E-E_a-\mathrm{Re}[\Lambda_{aa}(E+i0)]-i\,\mathrm{Im}[\Lambda_{aa}(E+i0)]}\times\left[\{E-E_a-\mathrm{Re}[\Lambda_{aa}(E+i0)]\}+\left[\mathrm{Re}[\Lambda_{aa}(E+i0)]-\Sigma_{\rm el}^{aa}(E+i0)+\frac{\langle a|V|\alpha E\rangle\lambda_{fa}(E+i0)}{d_{fa}(E)}\right]\right]. \tag{3.15b}$$

IV. PHOTORECOMBINATION RESONANCE PROFILE

A. Definition and derivation

If the autoionizing state $|a\rangle$ were not present, then the T matrix for photorecombination would be given simply by

$$\langle f\omega|T(E+i0)|\alpha E\rangle=\langle f\omega|\Lambda(E+i0)|\alpha E\rangle . \tag{4.1}$$

Thus all effects of the autoionizing state can be described in terms of the "photorecombination resonance profile," which we define as

$$L_{fa}(E)=\left|\frac{\langle f\omega|T(E+i0)|\alpha E\rangle}{\langle f\omega|\Lambda(E+i0)|\alpha E\rangle}\right|^2\Bigg|_{\omega=E} . \tag{4.2}$$

The expression (3.15) can be rewritten in the form

$$\langle f\omega|T(E+i0)|\alpha E\rangle=\langle f\omega|\Lambda(E+i0)|\alpha E\rangle\times\left[\frac{\hat{\varepsilon}(E)+\hat{q}(E)}{\hat{\varepsilon}(E)+i}\right] \tag{4.3}$$

by defining $\hat{\varepsilon}$ and $\hat{q}$ as appropriate functions of E. Then the resonance profile of Eq. (4.2) can be written

$$L_{fa}(E)=\frac{|\hat{\varepsilon}+\hat{q}|^2}{1+\hat{\varepsilon}^2} \tag{4.4}$$

(where we have suppressed the argument E in $\hat{\varepsilon}$ and $\hat{q}$), which has the same form as the familiar line-profile introduced by Fano,[21] except for the substitutions of $\hat{\varepsilon}$ for ε and $\hat{q}$ for q. We show below that the quantities $\hat{\varepsilon}$ and $\hat{q}$ are straightforward generalizations of the ε and q parameters introduced by Fano.

We define

$$\hat{\varepsilon}(E)\equiv\frac{E-E_a-\mathrm{Re}[\langle a|\Lambda(E+i0)|a\rangle]}{-\mathrm{Im}[\langle a|\Lambda(E+i0)|a\rangle]} . \tag{4.5}$$

If one thinks of $\mathrm{Re}\Lambda_{aa}$ as an energy shift of state $|a\rangle$ due to interactions with the continua and of $-\mathrm{Im}\Lambda_{aa}$ as the half-width of state $|a\rangle$, then, to the extent to which we can neglect the E dependence of the matrix elements of $\Lambda(E+i0)$, $\hat{\varepsilon}$ can be thought of as representing a dimensionless continuum energy parameter, giving the energy relative to the energy of the autoionizing state in units of the half-width of the state. It is clearly equivalent to the ε defined by Fano[21] and other investigators.[28,29]

For the case in which $\langle a|V|\alpha E\rangle$ and the matrix elements of d are real, we define the effective lineshape parameter $\hat{q}$ by

$$\hat{q}(E)\equiv\frac{\mathrm{Re}[\Lambda_{aE}(E+i0)\lambda_{fa}(E+i0)]}{-\mathrm{Im}[\Lambda_{aE}(E+i0)\lambda_{fa}(E+i0)]} . \tag{4.6}$$

That this definition gives the result (4.3) can easily be demonstrated by noting that

$$\mathrm{Im}\left[\frac{\langle a|V|\alpha E\rangle\lambda_{fa}(E+i0)}{d_{fa}(E)}\right]=\mathrm{Im}\left[-\Sigma_{\rm el}^{aa}(E+i0)\right]=\pi|\langle a|V|\alpha E\rangle|^2 \tag{4.7}$$

[where the last equality follows from Eq. (4.21) below], so that, in Eq. (3.15),

$$\mathrm{Re}[\Lambda_{aa}(E+i0)]-\Sigma_{\rm el}^{aa}(E+i0)+\frac{\langle a|V|\alpha E\rangle\lambda_{fa}(E+i0)}{d_{fa}(E)}=\mathrm{Re}\left[\Lambda_{aa}(E+i0)-\Sigma_{\rm el}^{aa}(E+i0)+\frac{\langle a|V|\alpha E\rangle\lambda_{fa}(E+i0)}{d_{fa}(E)}\right] \tag{4.8}$$

$$=\mathrm{Re}\left[\frac{\Lambda_{aE}(E+i0)\lambda_{fa}(E+i0)}{d_{fa}(E)}\right], \tag{4.9}$$

and by also noting from Eqs. (4.7) and (3.12b) that

$$\mathrm{Im}[\langle a|\Lambda(E+i0)|a\rangle]=\mathrm{Im}\left[\frac{\Lambda_{aE}(E+i0)\lambda_{fa}(E+i0)}{d_{fa}(E)}\right]. \tag{4.10}$$

The parameter $\hat{q}(E)$ will be studied in Sec. IV C.

B. Equivalence of photorecombination and photoionization profiles

In this section we show that the photorecombination profile of Eq. (4.4) is the same as the weak-field resonance profile for photoionization from $|f\rangle$, provided that single-photon spontaneous radiative decay to the continuum $\{|f\omega\rangle\}$ is included in the analysis. We also show that the generalized line-shape parameters $\hat{\epsilon}$ and $\hat{q}$ apply to both situations.

To establish the equivalence of the photorecombination and weak-field photoionization profiles, we begin by generalizing Eqs. (3.2) and (3.8) to

$$\langle f\omega|V=g_f^*(\omega)\langle f|d\ , \tag{4.11}$$

and writing[3]

$$\langle f\omega|T(E+i0)|\alpha E\rangle=\langle f\omega|V[1+G(E+i0)V]|\alpha E\rangle \tag{4.12}$$

$$=g_f^*(\omega)\langle f|d[1+G(E+i0)V]|\alpha E\rangle$$

$$=g_f^*(\omega)\langle f|d|\alpha E+\rangle \tag{4.13}$$

where

$$|\alpha E+\rangle\equiv\Omega_+|\alpha E\rangle=[1+G(E+i0)V]|\alpha E\rangle \tag{4.14}$$

(with, as in paper I, Ω_+ denoting the Møller operator of scattering theory).[30] The ket $|\alpha E+\rangle$ is a continuum eigenstate of H^0+V with eigenvalue E, and it corresponds to a scattering eigenstate when the interaction V, representing both configuration interaction and spontaneous radiative decay, is included in the Hamiltonian. It corresponds asymptotically to a free-electron continuum, but in the vicinity of the atom is a linear combination[33] of the continua $\{|\alpha E\rangle\}$ and $\{|f\omega\rangle\}$ as well as the discrete state $|a\rangle$.

The photorecombination profile (4.2) can be written using Eq. (4.14) as

$$L_{fa}(E)=\left|\frac{g_f^*(\omega)\langle f|d|\alpha E+\rangle}{g_f^*(\omega)\langle f|d|\alpha E\rangle/\psi(E+i0)}\right|^2$$

$$=\left|\psi(E+i0)\frac{\langle f|d|\alpha E+\rangle}{\langle f|d|\alpha E\rangle}\right|^2. \tag{4.15}$$

We now will show that this same profile is obtained when one considers photoabsorption from $|f\rangle$ while allowing for single photon spontaneous radiative decay back to $|f\rangle$.

A schematic diagram of the system of interest for discussing photoabsorption from $|f\rangle$, when $|f\rangle$ is the initially populated state, is shown in Fig. 2. The interaction responsible for photoabsorption from $|f\rangle$ can be written in the dipole approximation as $\sqrt{I}d$, where I is a photon intensity parameter and d is the same dipole operator that appears above. The rate of photoabsorption from $|f\rangle$ into the asymptotic electron continuum $\{|\alpha E+\rangle\}$ for weak fields is, by Fermi's golden rule, $r_+=2\pi I|\langle f|d|\alpha E+\rangle|^2$ (evaluated at the continuum energy E which is one photon in energy above state $|f\rangle$). Previous discussions of the effects of spontaneous radiative decay on Fano profiles[7,8] have compared the rate r_+ with the photoabsorption rate in the absence of both the autoionizing state and spontaneous radiative decay. The latter rate is simply $2\pi I|\langle f|d|\alpha E\rangle|^2$. However, in considering the effects of the autoionizing state on the photoabsorption rate, one would want to compare the rate r_+ with the rate r that would be obtained in the absence of the autoionizing state, but still including spontaneous radiative decay from the electron continuum to the photon continuum $|f\omega\rangle$, as shown in Fig. 3. This rate can be obtained from the matrix element of d between the initial atomic state $|f\rangle$ and the diagonalized electron continuum in the two-continuum space onto which C projects:

$$r=2\pi I|\langle f|dC\{1+[C(z-H^0-V)C]^{-1}CVC\}|\alpha E\rangle|^2\Big|_{z=E+i0}$$

$$=2\pi I|\langle f|d+dC\Phi(E+i0)CVC|\alpha E\rangle|^2\ . \tag{4.16}$$

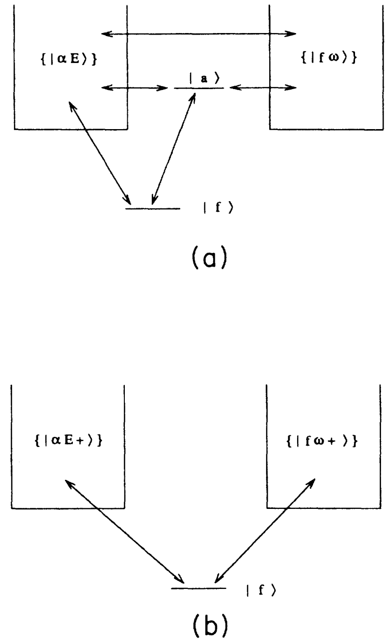

FIG. 2. Schematic of system for studying photoabsorption from $|f\rangle$, when spontaneous radiative decay to the one photon continuum $\{|f\omega\rangle\}$ is included. In (b), the $\{|\alpha E\rangle\}-|a\rangle-\{|f\omega\rangle\}$ system has been diagonalized, using the Møller operator Ω_+, into the two orthogonal, uncoupled continua $\{|\alpha E+\rangle\}$ and $\{|f\omega+\rangle\}$. The quantity r_+ represents the transition rate from $|f\rangle$ to $\{|\alpha E+\rangle\}$.

In (4.16), we have used the projection operator C to exclude the autoionizing state. The rate r can be rewritten using Eqs. (4.11) and (2.5) as

$$r=\frac{2\pi I}{|g(\omega)|^2}|\langle f\omega|\Lambda(E+i0)|\alpha E\rangle|^2$$
$$=\frac{2\pi I}{\psi(E+i0)|^2}|\langle f|d|\alpha E\rangle|^2\ . \qquad (4.17)$$

The photoabsorption profile when single-photon spontaneous decay effects are considered is then the ratio of the two rates, and is given by

$$\frac{r_+}{r}=\frac{I|\langle f|d|\alpha E+\rangle|^2}{I|\langle f|d|\alpha E\rangle|^2/|\psi(E+i0)|^2}\ , \qquad (4.18)$$

which is equal to the profile of Eq. (4.15). This establishes the equivalence of the profiles for photorecombination and for photoionization, when one-photon spontaneous radiative-decay processes are taken into account.

The result (4.17) for r is worthy of brief discussion. It indicates that the coupling between the final-state continua $\{|\alpha E\rangle\}$ and $\{|f\omega\rangle\}$ changes the transition rate from $|f\rangle$ to the asymptotic electron continuum. The total rate of depopulation of the initial state for this system is $2\pi I\{|\langle f|d|\alpha E+\rangle|^2+|\langle f|d|f\omega+\rangle|^2\}$, and can be shown to be $2\pi I|\langle f|d|\alpha E\rangle|^2/\psi$. This is one particular manifestation of the general conclusion that a separable coupling between final-state continua can change the rate of "decay" of a discrete state. This result has been discussed previously in the context of the decay of autoionizing states by Armstrong, Theodosiou, and Wall[22] and others.[7,9] The result has been discussed in the context of intense field multiphoton ionization by Deng and Eberly,[23] who also indicated that similar conclusions had been drawn in the study of decay processes and multiphoton excitation in polyatomic molecules by Lefebvre and Beswick[24] and others.[25] In addition, the result has been discussed in the context of photodecomposition of molecules by Druger,[26] and in a general context by Robinson.[27] Even though the contexts of these discussions have been very different, the mathematics and the conclusions are nonetheless similar.[34]

C. Discussion of the effective line-shape parameter $\hat{q}$

We begin our examination of the effective line-shape parameter $\hat{q}$ defined in Eq. (4.6) by writing out Λ_{aE} using Eq. (3.10):

$$\hat{q}(E)=\frac{\mathrm{Re}\left[\left[V_{aE}+\frac{\Sigma^{gg}(E+i0)d_{fa}(E)}{\psi(E+i0)}\lambda_{af}(E+i0)\right]\lambda_{fa}(E+i0)\right]}{-\mathrm{Im}\left[\left[V_{aE}+\frac{\Sigma^{gg}(E+i0)d_{fa}(E)}{\psi(E+i0)}\lambda_{af}(E+i0)\right]\lambda_{fa}(E+i0)\right]}\ . \qquad (4.19)$$

In the limit of vanishingly small spontaneously radiative decay, i.e., $\lim g(\omega)\to 0$, we have $\Sigma^{gg}\to 0$ and (assuming V_{aE} real)

$$\hat{q}(E)\to\frac{\mathrm{Re}[\lambda_{fa}(E+i0)]}{-\mathrm{Im}[\lambda_{fa}(E+i0)]}=\frac{d_{fa}+\mathrm{P}\int dE'\frac{d_{fE'}V_{E'a}}{E-E'}}{\pi d_{fE}V_{Ea}}\ , \qquad (4.20)$$

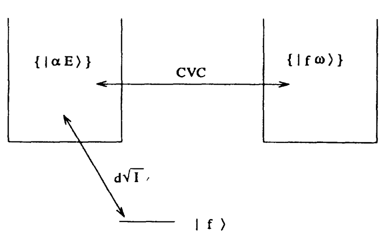

FIG. 3. In the absence of a discrete (autoionizing) state, the initial state $|f\rangle$ "decays" through photoabsorption into the coupled continua $\{|\alpha E\rangle\}$ and $\{|f\omega\rangle\}$. The quantity r represents the transition rate from $|f\rangle$ to the asymptotic electron continuum that is obtained when the $\{|\alpha E\rangle-\{|f\omega\rangle\}$ system has been diagonalized into two orthogonal, uncoupled continua.

which is the usual Fano line-shape parameter.[21] In writing Eq. (4.20) we have used the well-known relationship

$$\frac{1}{E+i0-E'}=\mathrm{P}\left[\frac{1}{E-E'}\right]-i\pi\delta(E-E')\ , \qquad (4.21)$$

where P represents the principal part.

Because $\Sigma^{gg}(E+i0)$, $\psi(E+i0)$, and $\lambda_{fa}(E+i0)$ are all complex, explicit forms for the real and imaginary parts of the quantity in square brackets in Eq. (4.19) are algebraically messy. However, if one makes the approximation of neglecting all principal-value integrals that arise when Eq. (4.21) is applied to various quantities in Eq. (4.19) (we will refer to this approximation throughout this work as the pole approximation), a simple expression for $\hat{q}$ is obtained. In this approximation, and assuming $V_{a\alpha}$, d_{fa}, and $d_{f\alpha}$ real and constant in energy (hence the subscript α rather than E in $V_{a\alpha}=\langle a|V|\alpha E\rangle$), $\hat{q}$ can be written

$$\hat{q}=\frac{V_{a\alpha}d_{fa}(1-\pi^2|g_f|^2d_{f\alpha}^2)}{\pi d_{f\alpha}(|g_f|^2d_{af}^2+V_{a\alpha}^2)} \qquad (4.22a)$$

$$=\left[\frac{d_{fa}}{\pi d_{f\alpha}V_{a\alpha}}\right]\left[\frac{1-\pi^2|g_f|^2d_{f\alpha}^2}{1+|g_f|^2d_{af}^2/V_{a\alpha}^2}\right]\ . \qquad (4.22b)$$

In this approximation $\hat{q}$ is independent of energy. We note that the first term in parentheses in Eq. (4.22b) is the usual pole approximation q parameter. If we define

$$\Gamma=2\pi V_{aa}^2 ,\quad \gamma=2\pi V_{af}^2=2\pi|g|^2 d_{af}^2 ,\quad q=\frac{d_{fa}}{\pi d_{fa} V_{aa}} , \tag{4.23}$$

where Γ and γ represent the lowest-order unperturbed autoionization and radiative decay rates (or widths), respectively, and q is the usual Fano line-profile parameter[21] in the pole approximation, then

$$\hat{q}=q\frac{1-\gamma/(\Gamma q^2)}{1+\gamma/\Gamma} \tag{4.24}$$

We note from this expression that $|\hat{q}|\le|q|$, and that $|\hat{q}|$ decreases monotonically with increasing γ. Since the peak value of the resonance profile is $\hat{q}^2+1$, it follows that spontaneous radiative decay decreases the maximum height of the resonance profile. For $q^2 \gg \gamma/\Gamma$, as is often the case in systems for which photorecombination is an important process,[34,35] we have

$$\hat{q}\simeq q\frac{1}{1+\gamma/\Gamma} , \tag{4.25}$$

which is the generalized q value given by Bell and Seaton.[2]

In the pole approximation, the quantity Λ_{aa} can be written

$$\Lambda_{aa}=\frac{\Gamma}{2}(\Delta_a-i\eta) , \tag{4.26a}$$

where

$$\Delta_a=-\left[\frac{2}{\psi}\right]\frac{\gamma_f}{\Gamma q_f} ,\quad \eta=\frac{1}{\psi}\left[1+\frac{\gamma_f}{\Gamma}\right] ,\quad \psi=1+\pi^2|g_f|^2 d_{fa}^2=1+\frac{\gamma}{\Gamma q^2} . \tag{4.26b}$$

As discussed elsewhere,[7,9,22] the quantity $(\Gamma/2)\Delta_a$ can be thought of as an energy shift of the discrete autoionizing state induced by the interaction with the coupled continua, and $\eta\Gamma$ can be thought of as the total width or decay rate of the state. [We note again the factor of ψ, which arises from the continuum-continuum coupling, and which acts[7,9,22] to decrease the rate of decay of state $|a\rangle$ from $\Gamma+\gamma$ to $(1/\psi)(\Gamma+\gamma)$.] In terms of the parameters of Eq. (4.26), we can write

$$\hat{\varepsilon}=\frac{\varepsilon-\Delta_a}{\eta} ,\quad \hat{q}=\frac{q+\Delta_a}{\eta} , \tag{4.27}$$

where ε denotes the usual continuum energy parameter in the pole approximation,

$$\varepsilon=\frac{E-E_a}{\Gamma/2} . \tag{4.28}$$

The profile can then be written in either of the two forms

$$L_{fa}=\frac{(\hat{\varepsilon}+\hat{q})^2}{1+\hat{\varepsilon}^2}=\frac{(\varepsilon+q)^2}{(\varepsilon-\Delta_a)^2+\eta^2} \tag{4.29}$$

The latter form is the "modified Fano profile" presented in earlier works,[7,8] except for a factor of ψ^2 which arose because those works defined the profile differently, as discussed above Eq. (4.16).

An alternative to neglecting all the principal value integrals in Eq. (4.19) is to neglect only the principal value integral appearing in $\Sigma^{gg}(E+i0)$, i.e., to make the pole approximation only on the photon continuum. In this "partial pole approximation,"

$$\psi(E+i0)=1+\pi^2|g_f|^2|d_{f\alpha}(E)|^2+i\pi|g_f|^2 \mathrm{P}\int\frac{|d_{f\alpha}(E')|^2}{E-E'}dE' , \tag{4.30}$$

which we write as

$$\psi(E+i0)=\psi_0+i\chi ,$$

where ψ_0 is the value of ψ when the pole approximation is made on both continua [as given in Eq. (4.26b)], and where ψ_0 and χ are real. It is then straightforward to show

$$\hat{q}(E)=\frac{V_{aE}d'_{af}(E)[1+\chi^2-\pi^4|g|^4 d_{f\alpha}(E)^4]+\pi\chi|g|^2 d_{f\alpha}(E)[V_{Ea}^2\pi^2 d_{\alpha f}(E)^2+d'_{af}(E)^2]}{\pi d_{\alpha f}(E)[V_{aE}^2(\psi_0+\chi^2)+|g|^2 d'^2_{af}(E)\psi_0-2\chi\pi|g|^2 d_{f\alpha}(E)d'_{af}(E)V_{aE}]} \tag{4.31}$$

$$=\left[\frac{d'_{af}(E)}{\pi d_{af}(E)V_{aE}}\right]\left[\frac{1+\chi^2-\pi^4|g|^4 d_{f\alpha}(E)^4+\pi\chi|g|^2 d_{f\alpha}(E)[V_{Ea}\pi^2 d_{\alpha f}(E)/d'_{af}(E)+d'_{af}(E)/V_{aE}]}{\psi_0+\chi^2+|g|^2 d'_{af}(E)\psi_0/V_{aE}^2-2\chi\pi|g|^2 d_{f\alpha}(E)d'_{af}(E)/V_{aE}}\right] , \tag{4.32}$$

where

$$d'_{af}(E)=\mathrm{Re}[\lambda_{af}(E+i0)]=V_{af}+\mathrm{Re}[\Sigma^{af}(E+i0)] \ , \tag{4.33}$$

and where we have again assumed V_{aE} and all matrix elements of d real. The first term in parentheses in Eq. (4.32) represents the usual Fano q parameter.

V. EFFECTIVE LINE-PROFILE PARAMETERS FOR MODEL SYSTEMS OF PAPER I

In paper I photorecombination processes within two particular model systems were studied in the pole approximation, and expressions for the T matrix were written in terms of the usual line-profile parameters q and ε. The systems studied both featured one autoionizing state. In one system, there was only one electron continuum but an arbitrary number of photon continua, with each photon continuum corresponding to a different possible final (radiatively stabilized) atomic state. In the other system, there were an arbitrary number of electron continua, but only one photon continuum.

Effective line-profile parameters for isolated autoionizing states in photoionizing systems which feature multiple electron continua but no photon continua have been defined by other investigators. Fano and Cooper[28] have shown how the line-shape parameters originally defined by Fano[21] can be extended to such systems, and Starace[29] has studied the behavior of partial cross sections and branching ratios for such systems. The generalized lineshape parameters used by these investigators for multiple electron continuum systems can be written very simply in terms of the operator Λ used in the present paper. Their electron energy parameter ε is equivalent to our $\hat{\varepsilon}$ for such systems, and can be written as in Eq. (4.5) [where $\Lambda(z)$ is as defined in Eq. (2.5), with $\Phi(z)$ given in Eq. (2.6) and with C representing the projection operator onto the set of continua]. The line-shape profile parameter $q(E)$ which these investigators define in describing photoionization can be written (for initial state $|f\rangle$, in the absence of spontaneous radiative decay, and assuming all matrix elements of the Hamiltonian to be real)

$$q(E)=\frac{\mathrm{Re}[\langle f|\Lambda(E+i0)|a\rangle]}{-\mathrm{Im}[\langle f|\Lambda(E+i0)|a\rangle]} \ . \tag{5.1}$$

In the present work we wish to allow for the possibility of one or more spontaneous radiative decay continua, and we emphasize that there is a mathematical as well as a physical distinction between photon and electron continua. In particular, the coupling responsible for radiative decay satisfies the relationships (3.2) and (3.8), while the couplings that may arise between electron continua in general will not. In such situations the parameter $\hat{q}(E)$ of Eq. (4.6) may be more useful than the $q(E)$ of Eq. (5.1).

In this work we shall define the effective line-shape parameters $\hat{q}_f$ for multiple-continuum systems so that the T matrix for photorecombination from electron continuum $|\alpha E\rangle$ into atomic state $|f\rangle$ can be written as

$$\langle f\omega|T(E+i0)|\alpha E\rangle=\langle f\omega|\Lambda(E+i0)|\alpha E\rangle\frac{\hat{\varepsilon}+\hat{q}_f}{\hat{\varepsilon}+i} \ , \tag{5.2}$$

where $\hat{\varepsilon}$ is given in Eq. (4.5) and is real, but where $\hat{q}_f$ may be complex.

For a system featuring only one electron continuum $\{|\alpha E\rangle\}$ but an arbitrary number of photon continua $\{|f'\omega\rangle\}$ [such that $\langle f\omega|f'\omega'\rangle=\delta_{ff'}\delta(\omega-\omega')$ and $\langle f\omega|V|f'\omega'\rangle=0$], paper I gave the results

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

where

$$\begin{aligned}\Delta_a&=-\left[\frac{2}{\psi}\right]\sum_{f'}\frac{\gamma_{f'}}{\Gamma q_{f'}} \ ,\\ \eta&=\frac{1}{\psi}\left[1+\sum_{f'}\frac{\gamma_{f'}}{\Gamma}+\sum_{f',f''}\frac{\gamma_{f'}\gamma_{f''}}{\Gamma^2 q_{f''}}\left[\frac{1}{q_{f''}}-\frac{1}{q_{f'}}\right]\right]\\ &=\frac{1}{\psi}\left\{1+\psi\sum_{f'}\frac{\gamma_{f'}}{\Gamma}-\left[\sum_{f'}\frac{1}{q_{f'}}\left[\frac{\gamma_{f'}}{\Gamma}\right]\right]^2\right\} \ ,\end{aligned} \tag{5.3}$$

and where

$$\begin{aligned}\Gamma&=2\pi V_{a\alpha}^2 \ ,\\ \gamma_f&=2\pi V_{af}^2 \ ,\\ q_f&=\frac{V_{fa}}{\pi V_{f\alpha}V_{\alpha a}} \ ,\\ \psi&=1+\sum_f\frac{\gamma_f}{\Gamma q_f^2} \ .\end{aligned} \tag{5.4}$$

These expressions for Δ_a, η, and ψ are generalizations of those presented in Eq. (4.26b) for systems featuring a single electron continuum and a single photon continua.

Using Eqs. (4.5) and (5.2), one obtains

$$\hat{\varepsilon}=\frac{\varepsilon-\Delta_a}{\eta} \tag{5.5}$$

and

$$\hat{q}_f=\frac{q_f+\Delta_a+i\sum_{f'}(1-q_f/q_{f'})(\gamma_{f'}/\Gamma)}{\eta} \ . \tag{5.6}$$

We note that the imaginary part of $\hat{q}_f$, which arose due to the additional possible final states, in general prevents the profile from exhibiting any zeroes. We also note that it does not provide a simple, flat "background," but rather $(\mathrm{Im}\hat{q})^2/(1+\hat{\varepsilon}^2)$, when considered as a function of the dimensionless continuum energy parameter $\hat{\varepsilon}$, is Lorentzian, with width 1 and height $(\mathrm{Im}\hat{q})^2$. A "total photorecombination profile" can be obtained by summing over final states: $L_\alpha(\hat{\varepsilon})=\sum_f L_{f\alpha}(\hat{\varepsilon})$.

Some graphs of $L_{f\alpha}$ versus energy for various atomic parameters are drawn in Figs. 4 and 5. In order to maintain a consistent energy scale while varying the atomic parameters, the horizontal axes give energy, relative to

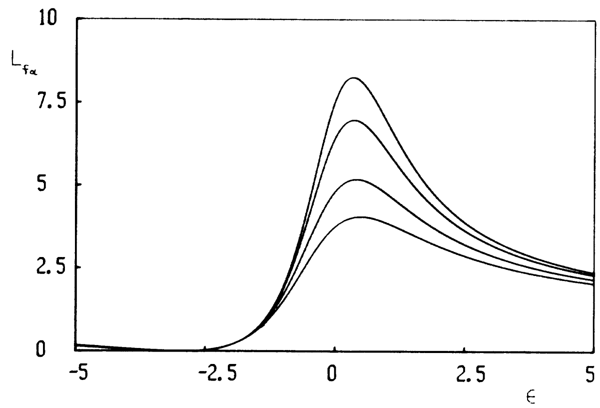

FIG. 4. Resonance profile for photorecombination to the photon continuum $\{|f'\omega\rangle\}$ for a system featuring one electron continuum and one autoionizing state. The uppermost curve gives the profile when only the one photon continuum is available, while the other curves give the profile for photorecombination to the same state when a second photon continuum $\{|f'\omega\rangle\}$ is accessible. In all cases $\gamma_f/\Gamma=0.1$ and $q_f=3$. For the lower curves, $q_{f'}=3$ and, in order of decreasing profile height, $\gamma_{f'}/\Gamma=0.1$, 0.3, and 0.5. All the curves are drawn as functions of ε, not $\hat{\varepsilon}$, so that the energy units are consistent for all curves.

E_a, in units of $\Gamma/2$ [i.e., $L_{f\alpha}$ is actually graphed as a function of the ε of Eq. (4.28) rather than as a function of $\hat{\varepsilon}$]. Figure 4 shows the smoothing of the resonance profile that can occur when a second final atomic (radiatively stabilized) state is available. The topmost curve in the diagram shows a profile when only one state $|f\rangle$ is available, while each of the lower curves gives the resonance profile for photorecombination to $|f\rangle$ when a second state $|f'\rangle$ is accessible. For the values of the atomic parameters of Fig. 4, the height of the resonance profile decreases as $\gamma_{f'}$ increases. A simple physical interpretation of this smoothing is that some of the population which goes from $|\alpha E\rangle$ to $|a\rangle$ nows decays to $|f'\rangle$ rather than to $|f\rangle$. In Fig. 4, $q_f=q_{f'}$, so that $\text{Im}\hat{q}=0$, and the minimum is retained. The curves thus all show the usual Fano line shape (although they are graphed versus ε rather than $\hat{\varepsilon}$).

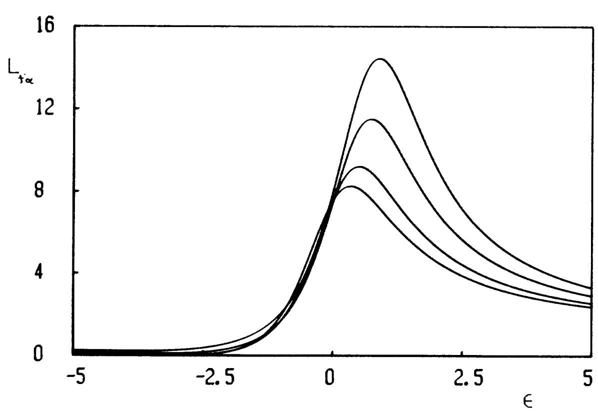

FIG. 5. Resonance profile for photorecombination to the photon continuum $\{|f\omega\rangle\}$ as a function of ε as in Fig. 4, again with $\gamma_f/\Gamma=0.1$, $q_f=3$, but now with $q_{f'}=-1$. The top three curves correspond, in order of decreasing height, to $\gamma_{f'}=0.5$, 0.3, and 0.1, respectively. The lowest curve shows the profile when only one photon continuum is present, and reproduces part of Fig. 4. As $\gamma_{f'}\to\infty$, the peak height increases without bound (as $\gamma_{f'}^2$).

Figure 5 shows one type of behavior the profiles can exhibit when $q_{f'}\neq q_f$. Here we have chosen $q_{f'}$ small and of opposite sign from q_f. For this case the zero is lost, and increasing $\gamma_{f'}$ increases the height of the resonance profile. Mathematically the increased height of the profile comes about because $\text{Re}\hat{q}>q$ (for $q_{f'}<0$ and $|\gamma_{f'}/\Gamma q_{f'}|>|\gamma_f/\Gamma q_f|$, Δ_a is positive). A more physical picture can be obtained if one thinks in terms of perturbation series, such as were discussed in Sec. 5.B of paper I. Now the second photon continuum provides additional pathways leading from the initial state to the final atomic state (such as $|\alpha E\rangle\to|f'\omega'\rangle\to|a\rangle\to|f\omega\rangle$). The strong coupling to the second photon continuum which is implied by large $\gamma_{f'}$ and small q acts for the present parameters to enhance the sum of the amplitudes for the pathways that lead through the autoionizing state relative to the sum of the amplitude for the pathways that bypass the autoionizing state.

The second system studied in paper I featured an arbitrary number of electron continua for which $\langle\alpha E|V|\alpha' E'\rangle=0$, but only one photon continuum $\{|f\omega\rangle\}$. For this system, it was indicated that

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

where

$$\Delta_a'=-\left[\frac{2}{\psi'}\right]\frac{\gamma_f}{\Gamma q} , \qquad \eta'=\left[1+\frac{\gamma_f}{\psi'\Gamma}(1-1/q^2)\right] \tag{5.7}$$

with

$$\gamma_f=2\pi V_{af}^2 , \quad q_{f\alpha}=\frac{V_{fa}}{\pi V_{f\alpha}V_{\alpha a}} , \quad \Gamma_\alpha=2\pi V_{\alpha a}^2 , \quad \frac{1}{q}=\sum_\alpha\frac{1}{q_{f\alpha}}, \quad \Gamma=\sum_\alpha\Gamma_\alpha , \quad \psi'=1+\sum_\alpha\frac{\gamma_f}{q_{f\alpha}^2\Gamma_\alpha} . \tag{5.8}$$

The q parameter defined in Eq. (5.8) is the generalized q parameter used by other investigators[28,29] and given in Eq. (5.1), evaluated in the pole approximation. This equivalence follows directly from the pole approximation expression for Λ_{fa} given in Eq. (5.37c) of I:

$$\Lambda_{fa} = \frac{1}{\psi'} \sqrt{\gamma_f/2\pi} \left[1 - \frac{i}{q} \right] . \tag{5.9}$$

The line-profile for this system can be written down using Eq. (5.41) of paper I:

$$L_{f\alpha}(\varepsilon') = \frac{(\varepsilon' + q_{f\alpha}\Gamma_\alpha/\Gamma)^2 + [1 - (q_{f\alpha}/q)(\Gamma_\alpha/\Gamma)]^2}{(\varepsilon' - \Delta'_a)^2 + \eta'^2} . \tag{5.10}$$

where

$$\varepsilon' = \frac{E - E_a}{\Gamma/2} = \varepsilon \left[\frac{\Gamma_\alpha}{\Gamma} \right] . \tag{5.11}$$

Effective line-profile parameters for photorecombination from the electron continuum $|\alpha E\rangle$ to the photon continuum $|f\omega\rangle$ can be defined by

$$\hat{\varepsilon} = \frac{\varepsilon' - \Delta'_a}{\eta'} , \tag{5.12a}$$

$$\hat{q}_{f\alpha} = \frac{q_{f\alpha}\Gamma_\alpha/\Gamma + \Delta'_a + i[1 - (q_{f\alpha}/q)(\Gamma_\alpha/\Gamma)]}{\eta'} . \tag{5.12b}$$

Once again the effective q parameter, $\hat{q}_{f\alpha}$, is complex, preventing the profile from exhibiting zeros.

Photorecombination profiles given by Eq. (5.10) are presented in Figs. 6 and 7. Figure 6 shows the smoothing of the profile that can occur when a second electron continuum channel is present. As for the situation of Fig. 4, this smoothing can be thought of as occurring because population in the autoionizing state can decay into the other electron continuum rather than to state $|f\rangle$. Figure 7 shows the enhancement of the profile that can occur when the second electron continuum is present. The enhancement occurs in the figure when the line-shape parameter $q_{f\alpha'}$ is small. In this case, the parameter q of Eq. (5.8) is smaller than $q_{f\alpha}$; thus the ratio $q_{f\alpha}/q$ appearing in (5.12b) is greater than 1.

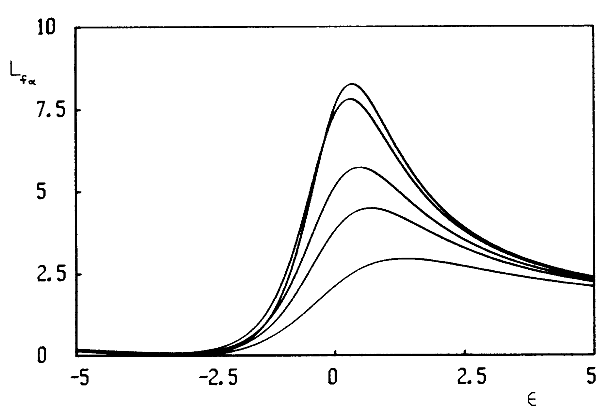

FIG. 6. Photorecombination profiles for a system featuring one or two distinct electron continua. The curve with the highest peak shows the profile when only one electron continuum is present, for $\gamma_f/\Gamma_\alpha = 0.1$ and $q_{f\alpha} = 3$. The other curves include the second electron continuum; all have $q_{f\alpha'} = 3$. In order of decreasing profile height, $\Gamma_{\alpha'}/\Gamma_\alpha = 0.1$, 0.3, 0.5, and 1.0. To maintain a consistent energy scale, the profiles are drawn as functions of ε rather than ε' or $\hat{\varepsilon}$.

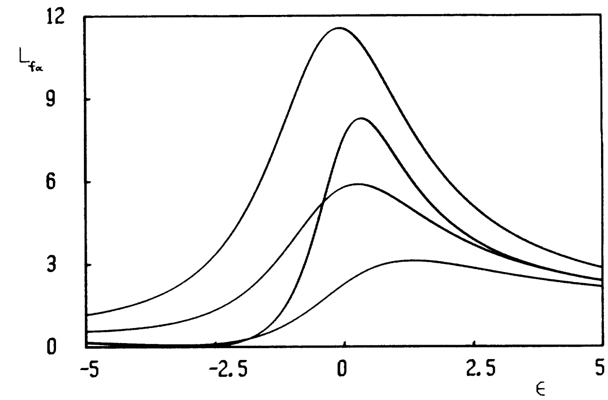

FIG. 7. Photorecombination profile vs ε for a system featuring one or two distinct electron continua. In this figure, the second tallest curve shows the profile when only one electron continuum is present, again for $\gamma_f/\Gamma_\alpha = 0.1$ and $q_{f\alpha} = 3$. The others have $\Gamma_{\alpha'}/\Gamma_\alpha = 1$, and from highest to lowest, $q_{f\alpha'} = 0.5$, 0.7, and 100.

VI. DISCUSSION AND CONCLUSIONS

In this paper we have used the projection operator formalism and recipe that was presented in an earlier paper[5] to construct matrix elements of the T operator for electron-ion photorecombination for a model system containing a single electron continuum, one autoionizing state, and a single photon continuum. The result is presented in Eqs. (3.14) and (3.15). The natural separation between the direct and resonant processes that is provided by the formalism has led us to define in Eq. (4.2) a "resonance profile" for photorecombination. This resonance profile is characterized by the parameters $\hat{\varepsilon}(E)$ and $\hat{q}(E)$, defined in Eqs. (4.5) and (4.6) respectively, which are generalizations of the familiar weak-field photoionization profile parameters $\varepsilon(E)$ and $q(E)$ that were introduced by Fano.[21] We have shown that the resonance profile, when written in terms of $\hat{\varepsilon}$ and $\hat{q}$, has the same form as the usual Fano profile has in terms of ε and q: $L_{f\alpha} = (\hat{\varepsilon} + \hat{q})^2/(1 + \hat{\varepsilon})^2$.

In Sec. IV B we have shown that the photorecombination profile is the same as the profile for photoionization, if one-photon spontaneous radiative-decay processes are allowed for in the latter process. In this context we have also noted that the radiative coupling between the final-state continua slows the rate of photoabsorption, and we have commented that this slowing is one particular manifestation of a more general effect which has been discussed in a number of different contexts.[7,9,22–27] In Sec. IV C, we have discussed the effective line-shape parameter $\hat{q}$. We have shown that it reduces to the usual Fano q

parameter in the limit of no spontaneous radiative decay. We also have shown that in the pole approximation $|\hat{q}|$ is always less than $|q|$, and that in the appropriate limiting case our $\hat{q}$ parameter reduces to that introduced by Bell and Seaton.[2]

In Sec. V we have defined effective line-shape parameters and studied resonance profiles for the model systems studied in paper I. For both cases it was noted that the presence of additional channels can wash out the Fano minimum. We have also discussed how the effective line-shape parameters of the present work relate to those that have been used by other investigators in the context of multiple electron continua. We have emphasized that the spontaneous radiative decay situation of interest in this paper and indicated in Fig. 3 is mathematically different from a two-electron continuum situation because the coupling responsible for radiative decay satisfies the relationships (3.2) and (3.8).

We have indicated in Sec. IV C that the $\hat{q}$ parameter defined in Eq. (4.6) simplifies to the usual q parameter in the limit of $|g_f|^2$ going to zero, i.e., in the limit of no spontaneous radiative decay. It is also natural to ask about the limiting behavior of the effective q parameters defined in Sec. V, where we considered multiple continua in the pole approximation. For the first system studied, which featured multiple-photon continua, Eq. (5.6) gives $\hat{q}_f \rightarrow q_f$ in the limit of $\gamma_{f'} \rightarrow 0$, just as one would expect for a system in which the additional continua arose only through spontaneous radiative decay. For the second system, featuring multiple electron continua, Eq. (5.12b) gives, in the limit $\gamma_f \rightarrow 0$,

$$\hat{q}_{f\alpha} \rightarrow q_{f\alpha}\Gamma_\alpha/\Gamma + i[1-(q_{f\alpha}/q)(\Gamma_\alpha/\Gamma)] \ . \tag{6.1}$$

We conclude this paper with some additional comments concerning similarities in formalisms for systems supporting multiple continua. We have already indicated that the system shown in Fig. 3 for photoionization is mathematically distinct from a system featuring two electron continua. However, we wish to emphasize that in many cases there is considerable similarity between formalisms dealing with systems supporting spontaneous radiative decay and formalisms dealing with systems supporting several electron channels. Physically, the photon and electron continua are very different, but in the formalisms the couplings are often written only in terms of matrix elements between discrete states and continua. In such a situation, the mathematical formalisms are equivalent, regardless of whether one is dealing with electron or photon continua. For example, in the context of laser-induced autoionization,[31] there have been several studies in which the autoionization state could "decay" into a continuum other than the autoionization continuum which was coupled to the initial state. "Decay" mechanisms have included spontaneous radiative decay,[36] autoionization into a second electron continuum,[37] and photoabsorption into a different electron continuum.[38] The first two are formally equivalent for the case where spontaneous radiative decay from the electron continuum is ignored, except that in the second case one can define a "total electron spectrum." (This spectrum is just the sum of the electron and photon spectra of the spontaneous radiative-decay case, once thresholds are properly taken into account.) The third case is also formally equivalent, except that the coupling strength between the autoionizing state and the additional decay continuum would in this case be proportional to laser intensity.

Of course, the similarity of formalisms for describing physically different phenomena is well documented in the literature. To cite just a few examples, Armstrong, Beers, and Feneuille[39] stressed the equivalence of the formalisms for autoionization and for multiphoton ionization. Agarwal *et al.*[40] have discussed the isomorphism between studies of laser-induced effects in autoionization of dc-field-induced interferences in autoionization. Knight[41] has also pointed out the parallels between studies of population trapping phenomena in laser-induced autoionization and the theory of K-meson decay. There are likely many other examples that could be referenced.

ACKNOWLEDGMENTS

I acknowledge the contributions of V. L. Jacobs, A. J. Kromminga, and P. S. DeVos. This work has been financially supported by Calvin College and by the National Science Foundation through Grant No. 8711639 to Calvin College.

[1]G. Alber, J. Cooper, and A. R. P. Rau, Phys. Rev. A **30**, 2845 (1984).

[2]R. H. Bell and M. J. Seaton, J. Phys. B **18**, 1589 (1985).

[3]V. L. Jacobs, J. Cooper, and S. L. Haan, Phys. Rev. A **36**, 1093 (1987).

[4]K. J. LaGattuta, Phys. Rev. A **36**, 4662 (1987); **38**, 1820 (1988).

[5]S. L. Haan and V. L. Jacobs, Phys. Rev. A **40**, 80 (1989).

[6]P. C. W. Davies and M. J. Seaton, J. Phys. B **2**, 757 (1969).

[7]S. L. Haan and G. S. Agarwal, in *Spectral Line Shapes,* edited by K. Burnett (de Gruyter, Berlin, 1983), Vol. 2, p. 1013.

[8]G. S. Agarwal, S. L. Haan, and J. Cooper, Phys. Rev. A **29**, 2552 (1984).

[9]S. L. Haan and J. Cooper, Phys. Rev. A **28**, 3349 (1983).

[10]V. L. Jacobs, Phys. Rev. A **31**, 383 (1985).

[11]H. Feshbach, Ann. Phys. (N.Y.) **5**, 357 (1958).

[12]H. Feshbach, Ann. Phys. (N.Y.) **19**, 287 (1962).

[13]M. L. Goldberger and K. M. Watson, *Collision Theory* (Wiley, New York, 1964).

[14]L. Mower, Phys. Rev. **142**, 799 (1966).

[15]L. Mower, Phys. Rev. **165**, 145 (1968).

[16]Y. Gontier and M. Trahin, in *Multi-photon Ionization of Atoms,* edited by S. L. Chin and P. Lambropoulos (Academic, Orlando, 1986).

[17]S. L. Haan and G. S. Agarwal, Phys. Rev. A **35**, 4592 (1987).

[18]J. Gau and Y. Hahn, J. Quant. Spectrosc. Radiat. Transfer **23**, 121 (1980).

[19]L. S. Rodberg, Phys. Rev. **137**, 210 (1961).

[20]B. W. Shore, Rev. Mod. Phys. **39**, 439 (1967).

[21]U. Fano, Phys. Rev. **124**, 1866 (1961).

[22]L. Armstrong, Jr., C. E. Theodosiou, and M. J. Wall, Phys. Rev. A **18**, 2538 (1978).

[23]Z. Deng and J. H. Eberly, Phys. Rev. Lett. **53**, 1810 (1984).

[24]L. Lefebvre and J. Beswick, Mol. Phys. **23**, 1223 (1972).

[25]See, for example, B. Carmeli, I. Schek, A. Nitzan, and J. Jortner, J. Chem. Phys. **72**, 1928 (1980).

[26]S. D. Druger, J. Chem. Phys. **73**, 2287 (1980).

[27]E. J. Robinson, Phys. Rev. Lett. **57**, 1281 (1986); **60**, 472(E) (1988).

[28]U. Fano and J. W. Cooper, Phys. Rev. **137**, A1364 (1965).

[29]A. F. Starace, Phys. Rev. A **16**, 231 (1977).

[30]See, for example, J. R. Taylor, *Scattering Theory* (Wiley, New York, 1972), and the Appendix of paper I (Ref. 5).

[31]See, for example, K. Rzazewski and J. H. Eberly, Phys. Rev. Lett. **47**, 408 (1981) and Ref. 8 (as well as references therein).

[32]We note a typographical error in Eq. (87) of Ref. 3, in that a plus sign has been omitted between $\Sigma^{fa}(z)$ and $\Sigma^{af}(z)$ in the third line of the equation.

[33]For a discussion of the use of Møller operators and continuum-continuum mixing see Ref. 9.

[34]We comment that there is no change in decay rate arising from continuum-continuum couplings of the form $\langle \alpha E|V|f\omega\rangle = v_{\alpha f}\delta(E-\omega)$. This result can easily be shown using the formalism of Sec. III. It has also been shown in, for example, P. R. Fontana, *Atomic Radiative Processes* (Academic, New York, 1982).

[35]V. L. Jacobs, J. E. Rogerson, M. H. Chen, and R. D. Cowan, Phys. Rev. A **32**, 3382 (1985).

[36]G. S. Agarwal, S. L. Haan, K. Burnett, and J. Cooper, Phys. Rev. Lett. **48**, 1164 (1982); Phys. Rev. A **26**, 2277 (1982).

[37]J. Zakrzewski, J. Phys. B **17**, 719 (1984).

[38]A. I. Andryushin, M. V. Federov, and A. E. Kazakov, J. Phys. B **15**, 2851 (1982); A. I. Andryushin, A. E. Kazakov, and M. V. Federov, Zh. Eksp. Teor. Fiz. **82**, 91 (1982) [Sov. Phys.–JETP **55**, 53 (1982)].

[39]L. Armstrong, Jr., B. L. Beers, and S. Feneuille, Phys. Rev. A **12**, 1903 (1975).

[40]G. S. Agarwal, J. Cooper, S. L. Haan, and P. L. Knight, Phys. Rev. Lett. **56**, 2586 (1986).

[41]P. L. Knight, Comments At. Mol. Phys. **15**, 193 (1984).