Interference effects in electron-ion recombination. II. Resonance and direct channels

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The Feshbach formalism is employed in a study of the effects of interference between direct radiative recombination and dielectronic recombination. A general result is obtained, valid for an arbitrary number of interacting resonances and an arbitrary number of coupled continua. The results of explicit model calculations, based on the pole approximation, are described, and comparison is made with earlier, related work.

INTRODUCTION

A recent flurry of theoretical activity has resulted in an improved understanding of the relationship between dielectronic recombination (DR) and direct radiative recombination (RR). It has been pointed out that, in general, a coupling exists between the probabilities for the decay of doubly excited ionic states d into Auger ($d \rightarrow i$) and radiation ($d \rightarrow f$) channels. This coupling is a consequence of the existence of a direct path from initial to final states; i.e., via the RR channel ($i \rightarrow f$). Several methods have been employed to illustrate these connections,[1-5] and a unified theory of DR and RR has been suggested.[4] Calculations of fluorescence yields modified by interference with the RR channel have been performed for the doubly excited $2l2l'$ states of He-like and Li-like ions.[6] It has been known for some time that similar corrections exist for the photoionization probability.[7]

In this paper (second of a series), we derive the combined probability amplitude for DR and RR, denoted M^{RDR}, using the projection-operator formalism of Feshbach,[8] as adapted for DR calculations by Gau and Hahn.[9] The results of explicit model calculations, based on these formulas and in the pole approximation, will also be presented. This is a continuation of work reported in Ref. 10 (paper I) on interacting resonance effects in DR. In the present work (paper II), underlined quantities reflect an essential coupling between the RR and DR channels.

FORMALISM

In the notation of paper I, the transition between exact initial states $\underline{\Psi}_P$ spanned by the operator P (one electron free, N electrons bound, and no real photons), and asymptotic final states Φ_R spanned by the operator R ($N+1$ electrons bound and one emitted photon), can be mediated directly by the electron-photon dipole-coupling operator D. The RR process proceeds via this mechanism. The RR probability amplitude is

$$\underline{M}^{\mathrm{RR}} = \langle \Phi_R RDP \underline{\Psi}_P \rangle \ , \tag{1}$$

while, from Eq. (8) (paper I), the probability amplitude for DR is

$$\underline{M}^{\mathrm{DR}} = \langle \Phi_R RDQ \underline{\Psi}_Q \rangle \ . \tag{2}$$

Here $\underline{\Psi}_Q$ is an exact intermediate state vector, in a space spanned by the operator Q ($N+1$ electrons in a doubly excited quasibound state and no real photons). The probability amplitude for the combined RR and DR process (labeled RDR) is

$$\underline{M}^{\mathrm{RDR}} = \underline{M}^{\mathrm{RR}} + \underline{M}^{\mathrm{DR}} \ . \tag{3}$$

Equations (1)–(3) are perfectly general. However, $\overline{\Psi}_P$ and $\overline{\Psi}_Q$ remain to be determined. As mentioned earlier, underlined quantities reflect a coupling between the RR and DR channels.

Ignoring all powers of RDP beyond the first in Eq. (1), and all powers of RDP including the first in Eq. (2), one arrives at the weak continuum electron-photon coupling limit for $\underline{M}^{\mathrm{RDR}}$. In this limit, $\underline{\Psi}_P$ and $\underline{\Psi}_Q$ approach Ψ_P and Ψ_Q, respectively, where both Ψ_P and Ψ_Q appear in paper I. For example, when resonances are noninteracting these functions are given by Eqs. (5) (paper I) and (7) (paper I) as

$$\underline{\Psi}_P \approx \Psi_P = \Phi_P + g_P PVQ\Psi_Q \ , \tag{4}$$

$$\underline{\Psi}_Q \approx \Psi_Q = G_Q QVP\Phi_P \ , \tag{5}$$

$$G_Q \equiv (E - QH_0Q - QDRg_R RDQ - QVPg_P PVQ)^{-1} \ , \tag{6}$$

where V is the electron-electron interaction, G_Q is the Q-space propagator, Φ_P is an asymptotic (one free electron at large distances) eigenstate of PH_0P, and the unperturbed P- and R-space propagators are

$$g_p = (E - PH_0P)^{-1} \ , \tag{7}$$

$$g_R = (E - RH_0R)^{-1} \ . \tag{8}$$

If resonances interact, then both Ψ_P and Ψ_Q are altered. In this case Ψ_Q is given by Eq. (15) (paper I).

In order to progress beyond the weak-coupling ($RDP \rightarrow 0$) limit, we return to the Schrödinger equation for the problem, in the form of Eq. (3) (paper I). Upon addition of terms proportional to RDP and PDR, this equation becomes

$$PH_0P\underline{\Psi}_P+PVQ\underline{\Psi}_Q+PDR\underline{\Psi}_R=E\underline{\Psi}_P\ ,$$
$$QVP\underline{\Psi}_P+QH_0Q\underline{\Psi}_Q+QDR\underline{\Psi}_R=E\underline{\Psi}_Q\ , \tag{9}$$
$$RDP\underline{\Psi}_P+RDQ\underline{\Psi}_Q+RH_0R\underline{\Psi}_R=E\underline{\Psi}_R\ ,$$

which leads immediately to an expression for $\underline{\Psi}_R$, the exact final state, in terms of $\underline{\Psi}_P$ and $\underline{\Psi}_Q$; viz.,

$$\underline{\Psi}_R=(E-RH_0R)^{-1}(RDP\underline{\Psi}_P+RDQ\underline{\Psi}_Q)$$
$$=g_R(RDP\underline{\Psi}_P+RDQ\underline{\Psi}_Q)\ . \tag{10}$$

Substituting Eq. (10) back into Eq. (9) yields a pair of coupled equations for $\underline{\Psi}_P$ and $\underline{\Psi}_Q$,

$$(E-PH_0P)\underline{\Psi}_P=PDRg_RRDP\underline{\Psi}_P$$
$$+P(V+DRg_RRD)Q\underline{\Psi}_Q$$
$$=PDRg_RRDP\underline{\Psi}_P+P\underline{V}Q\underline{\Psi}_Q\ , \tag{11}$$
$$(E-QH_0Q)\underline{\Psi}_Q=QDRg_RRDQ\underline{\Psi}_Q$$
$$+Q(V+DRg_RRD)P\underline{\Psi}_P$$
$$=QDRg_RRDQ\underline{\Psi}_Q+Q\underline{V}P\underline{\Psi}_P\ , \tag{12}$$

where

$$\underline{V}\equiv V+DRg_RRD\ . \tag{13}$$

In the following we solve the linked Eqs. (11) and (12) for the P- and Q-space wave functions $\underline{\Psi}_P$ and $\underline{\Psi}_Q$. First we obtain a formal solution, in terms of P-space operators. Matrix elements of these operator expressions are then employed to produce an explicit solution.

FORMAL SOLUTION

From Eq. (11), $\underline{\Psi}_P$ may be written formally in terms of $\underline{\Psi}_Q$ as

$$\underline{\Psi}_P=\underline{\Phi}_P+\underline{g}_PP\underline{V}Q\underline{\Psi}_Q\ , \tag{14}$$

with $\underline{g}_P$, the P-space propagator modified by RDP coupling, given by

$$\underline{g}_P=(E-PH_0P-PDRg_RPDP)^{-1}$$
$$=(1-g_PPDRg_RRDP)^{-1}g_P\ . \tag{15}$$

In Eq. (14), $\underline{\Phi}_P$ denotes an asymptotic (one free electron at large distances) P-space state, modified by RDP coupling, and related to Φ_P by

$$\underline{\Phi}_P=(1-g_PPDRg_RRDP)^{-1}\Phi_P\ . \tag{16}$$

An analogous expression connects $\underline{\Phi}_R$, the asymptotic (one photon at large distances) R-space state modified by RDP coupling, and Φ_R, the asymptotic R-space unmodified by RDP coupling; i.e.,

$$\underline{\Phi}_R=(1-g_RRDPg_PPDR)^{-1}\Phi_R\ . \tag{17}$$

The R-space propagator modified by RDP coupling [analog of Eq. (15)] is

$$\underline{g}_R=(E-RH_0R-RDPg_PPDR)^{-1}$$
$$=(1-g_RRDPg_PPDR)^{-1}g_R\ . \tag{18}$$

Now, using Eq. (14), Eq. (12) becomes

$$(E-QH_0Q)\underline{\Psi}_Q=QDRg_RRDQ\underline{\Psi}_Q$$
$$+Q\underline{V}P(\underline{\Phi}_P+\underline{g}_PP\underline{V}Q\underline{\Psi}_Q)\ , \tag{19}$$

which has a form identical to Eq. (6) (paper I), except that $\underline{g}_P$ replaces g_P, $\underline{V}$ is substituted for V, and $\underline{\Phi}_P$ appears instead of Φ_P.

As per the development leading up to Eq. (15) (paper I), the general (formal) solution of Eq. (19), when resonances are allowed to interact, and for a Q-space state labeled by α, is

$$\langle\alpha\mid\underline{\Psi}_Q\equiv\underline{\Psi}_{Q\alpha}=\sum_\beta(\underline{\Omega}^{-1})_{\alpha\beta}\underline{G}_{Q\beta}\langle\beta\mid\underline{V}P\underline{\Phi}_P\ , \tag{20}$$

where the Q-space propagator $\underline{G}_{Q\beta}$ is defined as

$$\underline{G}_{Q\beta}\equiv(E-\langle\beta\mid QH_0Q\mid\beta\rangle-\langle\beta\mid QDRg_RRDQ\mid\beta\rangle$$
$$-\langle\beta\mid Q\underline{V}P\underline{g}_PP\underline{V}Q\mid\beta\rangle)^{-1}\ . \tag{21}$$

Note that $\underline{G}_{Q\beta}\neq\langle\beta\mid G_Q\mid\beta\rangle$, where G_Q was defined in Eq. (6). The Q-space operator $\underline{\Omega}^{-1}$ is the inverse of an operator $\underline{\Omega}$ with elements

$$\underline{\Omega}_{\alpha\beta}=\delta_{\alpha\beta}-(1-\delta_{\alpha\beta})\underline{G}_{Q\alpha}\underline{\Lambda}_{\alpha\beta}\ . \tag{22}$$

In Eq. (22), $\delta_{\alpha\beta}$ is the Kronecker δ and the operator $\underline{\Lambda}$ is given by

$$\underline{\Lambda}=QDRg_RRDQ+Q\underline{V}P\underline{g}_PP\underline{V}Q\ . \tag{23}$$

From the form of Eqs. (22) and (23) it is clear that $\underline{\Omega}$ mixes Q-space states via interaction with the P and/or R space. In this context, recall that the Q-space states are assumed to already diagonalize the Q-space Hamiltonian QH_0Q.

The Q-space propagator $\underline{G}_{Q\beta}$ [Eq. (21)] can be rearranged to read, in a more symmetrical form,

$$\underline{G}_{Q\beta}=(E-\langle\beta\mid QH_0Q\mid\beta\rangle-\langle\beta\mid QDR\underline{g}_RRDQ\mid\beta\rangle$$
$$-\langle\beta\mid QVP\underline{g}_PPVQ\mid\beta\rangle$$
$$-\langle\beta\mid QDRg_RRDP\underline{g}_PPVQ\mid\beta\rangle$$
$$-\langle\beta\mid QVPg_PPDR\underline{g}_RRDQ\mid\beta\rangle)^{-1}\ . \tag{24}$$

EXPLICIT SOLUTION

Returning to Eq. (11), we now discretize the continuum electron momentum. Then, instead of Eq. (14), one has for the (ith element of the) vector $\underline{\Psi}_P$

$$\langle i\mid\underline{\Psi}_P\equiv\underline{\Psi}_{Pi}=\sum_j(\underline{\omega}^{-1})_{ij}(\underline{\Phi}_{Pj}+\underline{g}_{Pj}\langle j\mid\underline{V}Q\underline{\Psi}_Q)\ , \tag{25}$$

in terms of the still unknown function $\underline{\Phi}_{Pj}=\langle j\mid\underline{\Phi}_P$ [given by Eq. (16)] and the as yet unknown vector $\underline{\Psi}_Q$ [solution of Eq. (12)], where the P-space operator $\underline{\omega}$ has

the elements

$$\underline{\omega}_{ij}=\delta_{ij}-(1-\delta_{ij})\underline{g}_{Pi}\underline{\lambda}_{ij} . \tag{26}$$

The operator $\underline{\lambda}$ is given by

$$\underline{\lambda}=PDRg_RRDP \tag{27}$$

and

$$\underline{g}_{Pi}\equiv(E-\langle i\mid PH_0P\mid i\rangle-\langle i\mid PDRg_RPDR\mid i\rangle)^{-1} . \tag{28}$$

Note that, in general, $\underline{g}_{Pi}\neq\langle i\mid \underline{g}_P\mid i\rangle$. In Eqs. (25) and (26), i labels both the target state (there may be more than one) and the discretized momentum of the continuum electron.

From the form of Eqs. (26) and (27), it is clear that $\underline{\omega}$ mixes P-space states via interaction with the R space. We emphasize that the P-space states are assumed to already diagonalize the P-space Hamiltonian PH_0P.

We can now easily solve Eq. (16) and obtain for the asymptotic P-space wave function modified by RDP coupling

$$\underline{\Phi}_{Pi}=\sum_j(\underline{\omega}^{-1})_{ij}\underline{g}_{Pj}g_{Pj}^{-1}\Phi_{Pj} , \tag{29}$$

where $g_{Pi}=\langle i\mid g_P\mid i\rangle$, $\Phi_{Pi}=\langle i\mid\Phi_P$, and both g_P and Φ_P are free of RDP coupling; g_P was defined in Eq. (7), while Φ_P was defined following Eq. (5). A similar expression exists for $\underline{\Phi}_{Rf}=\langle f\mid\underline{\Phi}_R$, the solution of Eq. (17),

$$\underline{\Phi}_{Rf}=\sum_h(\underline{\nu}^{-1})_{fh}\underline{g}_{Rh}g_{Rh}^{-1}\Phi_{Rh} , \tag{30}$$

where $g_{Rh}=\langle h\mid g_R\mid h\rangle$, $\Phi_{Rh}=\langle h\mid\Phi_R$, g_R was defined in Eq. (8), and Φ_R was defined preceding Eq. (17). Note that Eq. (30) implies a discretization of the emitted photon momentum. The R-space propagator $\underline{g}_{Rh}$ is defined as

$$\underline{g}_{Rh}=(E-\langle h\mid RH_0R\mid h\rangle-\langle h\mid RDPg_PPDR\mid h\rangle)^{-1} . \tag{31}$$

The elements of the matrix $\underline{\nu}$ are

$$\underline{\nu}_{fh}=\delta_{fh}-(1-\delta_{fh})\underline{g}_{Rf}\underline{\mu}_{fh} , \tag{32}$$

where

$$\underline{\mu}=RDPg_PPDR . \tag{33}$$

Now Eq. (19) becomes

$$(E-QH_0Q)\underline{\Psi}_Q=QDRg_RRDQ\underline{\Psi}_Q+\sum_i\sum_j\underline{QVP}\mid i\rangle(\underline{\omega}^{-1})_{ij}\times(\underline{\Phi}_{Pj}+\underline{g}_{Pj}\langle j\mid P\underline{VQ}\underline{\Psi}_Q) , \tag{34}$$

with solution

$$\underline{\Psi}_{Q\alpha}=\sum_\beta(\underline{\Omega}^{-1})_{\alpha\beta}\underline{G}_{Q\beta}\langle\underline{QVP}\underline{\omega}^{-1}\underline{\Phi}_P , \tag{35}$$

where the Q-space propagator is now [a generalization of Eq. (21)]

$$\underline{G}_{Q\beta}=\left[E-\langle\beta\mid QH_0Q\mid\beta\rangle-\langle\beta\mid QDRg_RRDQ\mid\beta\rangle-\sum_i\sum_j\langle\beta\mid\underline{QVP}\mid i\rangle(\underline{\omega}^{-1})_{ij}\underline{g}_{Pj}\langle j\mid P\underline{VQ}\mid\beta\rangle\right]^{-1} \tag{36}$$

and the Q-space mixing operator $\underline{\Omega}$, corrected for RDP coupling and coupling between P-space states, has the elements

$$\underline{\Omega}_{\alpha\beta}=\delta_{\alpha\beta}-(1-\delta_{\alpha\beta})\underline{G}_{Q\alpha}\underline{\Lambda}_{\alpha\beta} . \tag{37}$$

In Eq. (37), the operator $\underline{\Lambda}$ is given by

$$\underline{\Lambda}=QDRg_RRDQ+\sum_i\sum_j\underline{QVP}\mid i\rangle(\underline{\omega}^{-1})_{ij}\underline{g}_{Pj}\langle j\mid P\underline{VQ} . \tag{38}$$

From Eqs. (25) and (35), the general solution for $\underline{\Psi}_P$ is now

$$\underline{\Psi}_{Pi}=\sum_j(\underline{\omega}^{-1})_{ij}\left[\underline{\Phi}_{Pj}+\underline{g}_{Pj}\langle j\mid P\underline{VQ}\sum_\alpha\sum_\beta\mid\alpha\rangle(\underline{\Omega}^{-1})_{\alpha\beta}\times\underline{G}_{Q\beta}\langle\beta\mid\underline{QVP}\underline{\omega}^{-1}\underline{\Phi}_P\right] , \tag{39}$$

with $\underline{\Phi}_{Pj}$ given by Eq. (29).

The probability amplitude for RDR, corrected for interacting resonances, interacting continua, and RDP coupling, is given by Eqs. (1)–(3), with $\underline{\Psi}_P$ taken from Eq. (39) and $\underline{\Psi}_Q$ from Eq. (35); i.e., in this most general case, $\underline{M}^{\mathrm{RDR}}$ is the sum of the probability amplitudes for RR and DR, given individually by

$$\underline{M}^{\mathrm{RR}}=\langle\Phi_RRDP\underline{\omega}^{-1}\underline{\Phi}_P\rangle+\sum_i\sum_j\sum_\alpha\sum_\beta\langle\Phi_RRDP\mid i\rangle(\underline{\omega}^{-1})_{ij}\underline{g}_{Pj}\times\langle j\mid P\underline{VQ}\mid\alpha\rangle\times(\underline{\Omega}^{-1})_{\alpha\beta}\underline{G}_{Q\beta}\langle\beta\mid\underline{QVP}\underline{\omega}^{-1}\underline{\Phi}_P\rangle , \tag{40}$$

$$\underline{M}^{\mathrm{DR}}=\sum_\alpha\sum_\beta\langle\Phi_RRDQ\mid\alpha\rangle(\underline{\Omega}^{-1})_{\alpha\beta}\underline{G}_{Q\beta}\times\langle\beta\mid\underline{QVP}\underline{\omega}^{-1}\underline{\Phi}_P\rangle , \tag{41}$$

where $\underline{\Omega}$ is an operator [Eq. (37)] which mixes the Q-space states among themselves via interaction with the P and/or R spaces, and $\underline{\omega}$ [Eq. (26)] mixes the P-space states among themselves via interaction with the R space. Again, we point out that the Q-space states and the P-space states are assumed to already diagonalize the Q and P space Hamiltonians QH_0Q and PH_0P, respectively. The propagators $\underline{g}_P$ and $\underline{g}_R$, both modified by RDP coupling, will be discussed further in the following section.

If only one resonance participates in the RDR process, then $\underline{\Omega}=\underline{\Omega}^{-1}=\delta$, where δ is the Kronecker δ. However, even if just one P-space target state participates, then still, in general, $\underline{\omega}\neq\delta$, since the continuum electron

momentum has been discretized. It is only if one makes the approximation that just a single continuum electron momentum participates, as well as a single target state, that $\omega=\omega^{-1}=\delta$. We remind the reader that if $RDP=0$, then $\underline{\omega}=\delta$, also as in paper I.

DISCUSSION

We begin by pointing out some of the more important features of the formulas derived in the preceding section. Transition rates for autoionization, stabilizing radiative decay, radiative recombination, and photoionization are defined. Then the pole approximation is introduced, and several explicit examples are considered. Finally, the results of a model calculation are described.

If $RDP=0$, then from Eq. (18) (paper I), the full-width $\Gamma_{\rm tot}(\alpha)$ of an isolated resonance state labeled by α may be defined as

$$\begin{aligned}\Gamma_{\rm tot}(\alpha)&=2\,{\rm Im}\langle\alpha\mid G_Q^{-1}\mid\alpha\rangle\\&=-2\,{\rm Im}(\langle\alpha\mid DRg_RRD\mid\alpha\rangle+\langle\alpha\mid VPg_PPV\mid\alpha\rangle)\\&\equiv\Gamma_r(\alpha)+\Gamma_a(\alpha)\ ,\end{aligned}\tag{42}$$

where Γ_r and Γ_a are the total radiative and autoionization transition rates, respectively, defined as

$$\begin{aligned}\Gamma_r(\alpha)&=\sum_f A_r(\alpha\to f)\ ,\\\Gamma_a(\alpha)&=\sum_i A_a(\alpha\to i)\ ,\end{aligned}\tag{43}$$

with the state-to-state radiative and autoionization widths being given by

$$\begin{aligned}A_r(\alpha\to f)&=k_\gamma^2\mid\langle f\mid D\mid\alpha\rangle\mid^2\equiv k_\gamma^2D_{\alpha f}^2\ ,\\A_a(\alpha\to i)&=k_i\mid\langle i\mid V\mid\alpha\rangle\mid^2\equiv k_iV_{\alpha i}^2\ .\end{aligned}\tag{44}$$

Physical rates are obtained from Eq. (42) by taking the on-shell limit; i.e., $E\to E_i=E_f$, where E_i and E_f are the total initial- and final-state energies. However, if $RDP\neq0$, then from Eq. (24) the full width of the resonance, modified by RDP coupling, becomes

$$\begin{aligned}\underline{\Gamma}_{\rm tot}(\alpha)=&-2\,{\rm Im}(\langle\alpha\mid DR\underline{g}_RRD\mid\alpha\rangle+\langle\alpha\mid VP\underline{g}_PPV\mid\alpha\rangle)\\&-2\,{\rm Im}(\langle\alpha\mid DRg_RRDP\underline{g}_PPV\mid\alpha\rangle\\&+\langle\alpha\mid VPg_PPDR\underline{g}_RRD\mid\alpha\rangle)\ ,\end{aligned}\tag{45}$$

See Eqs. (53), (62), and (64) for a definition of the radiative and autoionization widths modified by RDP coupling, $\underline{\Gamma}_r$ and $\underline{\Gamma}_a$, respectively.

Now, due to the RDP coupling, both $\underline{g}_P$ and $\underline{g}_R$ have finite imaginary parts; viz., from Eqs. (7), (8), (15), and (18),

$$\begin{aligned}\underline{g}_P=&[\,E-PH_0P-PDR({\rm Re}g_R)RDP\\&+i\pi PDR\,\delta(E-RH_0R)RDP]^{-1}\ ,\\\underline{g}_R=&[\,E-RH_0R-RDP({\rm Re}g_P)PDR\\&+i\pi RDP\delta(E-PH_0P)PDR]^{-1}\ .\end{aligned}\tag{46}$$

The imaginary part of $\underline{g}_P$ is proportional to $\Gamma_{\rm RR}$, the total RR transition rate correct to second order in RDP, while the imaginary part of $\underline{g}_R$ is proportional to $\Gamma_{\rm PI}$, the total direct photoionization transition rate, with an identical limitation. That is, for a P-space state labeled by i, and an R-space state labeled by f,

$$\begin{aligned}\Gamma_{\rm RR}(i)&=2\pi\langle i\mid DR\delta(E-RH_0R)RD\mid i\rangle\\&=2\pi\sum_f\int d\mathbf{k}_\gamma\langle i\mid D\mid f\rangle\delta(E-\varepsilon_f)\langle f\mid D\mid i\rangle\\&=\sum_f k_\gamma^2D_{if}^2\\&\equiv\sum_f A_{\rm RR}(i\to f)\ ,\end{aligned}\tag{47}$$

$$\begin{aligned}\Gamma_{\rm PI}(f)&=2\pi\langle f\mid DP\delta(e-PH_0P)PD\mid f\rangle\\&=2\pi\sum_i\int d\mathbf{k}_i\langle f\mid D\mid i\rangle\delta(E-\varepsilon_i)\langle i\mid D\mid f\rangle\\&\equiv\sum_i k_iD_{fi}^2\\&\equiv\sum_i A_{\rm PI}(f\to i)\ ,\end{aligned}\tag{48}$$

where $k_i=[2(E-\varepsilon_i)]^{1/2}$ and $k_\gamma=(E-\varepsilon_f)$ are the electron and photon wave vectors, respectively, with ε_i and ε_f denoting the initial- and final-state ion energies.

A detailed balance relationship connects the state-to-state transition rates $A_{\rm RR}$ and $A_{\rm PI}$; viz.,

$$k_iA_{\rm RR}(i\to f)=k_\gamma^2A_{\rm PI}(f\to i)\ .\tag{49}$$

Similarly, the total transition rates are connected by

$$\sum_i k_i\Gamma_{\rm RR}(i)=\sum_f k_\gamma^2\Gamma_{\rm PI}(f)\ .\tag{50}$$

For later convenience, we now define the generalized transition rates $\Gamma_{\rm RR}(i,j)$ and $\Gamma_{\rm PI}(f,g)$ as

$$\begin{aligned}\Gamma_{\rm RR}(i,j)&\equiv\sum_f k_\gamma^2D_{if}D_{fj}\ ,\\\Gamma_{\rm PI}(f,g)&=\sum_i k_iD_{fi}D_{ig}\ ,\end{aligned}\tag{51}$$

and the "normalized" transition rates according to

$$\begin{aligned}W_{\rm RR}(i,i)&\equiv k_i\Gamma_{\rm RR}(i)\ ,\\W_{\rm PI}(f,f)&\equiv k_\gamma^2\Gamma_{\rm PI}(f)\ ,\\W_{\rm RR}(i,j)&\equiv k_i\Gamma_{\rm RR}(i,j)\ ,\\W_{\rm PI}(f,g)&\equiv k_\gamma^2\Gamma_{\rm PI}(f,g)\ .\end{aligned}\tag{52}$$

The stabilizing radiative and autoionization rates modified by RDP coupling, $\underline{\Gamma}_r$ and $\underline{\Gamma}_a$, may now be defined. However, it is first necessary to rewrite Eq. (45), so that the asymptotic initial and final states modified by RDP coupling ($\underline{\Phi}_{Pi}$ and $\underline{\Phi}_{Rf}$) appear explicitly. This amounts to a unitary transformation on the basis states Φ_{Pi} and Φ_{Rf}, contained in the P and R spaces. We will denote these "diagonalized" state spaces as $\underline{P}$ and $\underline{R}$; i.e., $\underline{P}$ projects onto the $\underline{\Phi}_{Pi}$ and $\underline{R}$ projects onto the $\underline{\Phi}_{Rf}$. Using Eqs. (15)–(18), Eq. (45) becomes

$$\begin{aligned}\underline{\Gamma}_{\rm tot}(\alpha)=&-2\,{\rm Im}(\langle\alpha\mid D\underline{R}g_R\underline{R}D\mid\alpha\rangle-\langle\alpha\mid VPg_PPD\underline{R}g_R\underline{R}DPg_PPV\mid\alpha\rangle)\\&-2\,{\rm Im}(\langle\alpha\mid V\underline{P}g_P\underline{P}V\mid\alpha\rangle-\langle\alpha\mid DRg_RRD\underline{P}g_P\underline{P}DRg_RRD\mid\alpha\rangle)\\&-2\,{\rm Im}(\langle\alpha\mid VPg_PPD\underline{R}g_R\underline{R}D\mid\alpha\rangle-\langle\alpha\mid DRg_RRDPg_PPD\underline{R}g_R\underline{R}DPg_PPV\mid\alpha\rangle)\\&-2\,{\rm Im}(\langle\alpha\mid DRg_RRD\underline{P}g_P\underline{P}V\mid\alpha\rangle-\langle\alpha\mid VPg_PPDRg_RRD\underline{P}g_P\underline{P}DRg_RRD\mid\alpha\rangle)\\=&\underline{\Gamma}_r(\alpha)+\underline{\Gamma}_a(\alpha)\ .\end{aligned}\tag{53}$$

The stabilizing radiative width modified by *RDP* coupling $\underline{\Gamma}_r$ is given by the first and third lines of Eq. (53) (where the $\underline{R}$-space states appear explicitly); the autoionization width modified by *RDP* coupling $\underline{\Gamma}_a$ is given by the second and fourth lines of Eq. (53) (where the $\underline{P}$-space states appear). In the following section we evaluate these functions in the pole approximation.

We conclude this discussion by noting that evaluation of Eqs. (40) and (41) for $\underline{M}^{\rm RDR}$ is complicated by the fact that matrix elements of the electron self-energy operator DRg_RRD have a formally infinite real part. The removal of this unphysical singularity will require careful treatment, with techniques borrowed from quantum electrodynamics;[11] e.g., subtraction of a mass counter term and the effective introduction of a cutoff in photon momenta due to virtual pair creation. Therefore the actual evaluation of $\underline{M}^{\rm RDR}$ for a specific case must either be deferred until the QED issues have been resolved, or invoke the "pole approximation," as per the work of Refs. 3–6 and 12. In the pole approximation, we set to zero the real part of the P- and R-space propagators g_P, $\underline{g}_P$, g_R, and $\underline{g}_R$.

POLE APPROXIMATION

In the following, we mean by the "pole approximation" that the real parts of all P- and R-space propagators are set equal to zero. Also, as in the preceding section, the continuum electron momentum is understood to have been discretized.

We begin by considering the matrix elements of the P- and R-space propagators modified by *RDP* coupling $\underline{g}_P$ and $\underline{g}_R$. From Eqs. (7), (8), (15), and (18), and using a Lippmann-Schwinger equation, we can write

$$\langle i\mid\underline{g}_P\mid j\rangle=g_{pi}\delta_{ij}+g_{Pi}\sum_f D_{if}g_{Rf}\sum_k D_{fk}\langle k\mid\underline{g}_P\mid j\rangle\ ,\tag{54}$$

$$\langle f\mid\underline{g}_R\mid g\rangle=g_{Rf}\delta_{fg}+g_{Rf}\sum_i D_{fi}g_{Pi}\sum_h D_{ih}\langle h\mid\underline{g}_R\mid g\rangle\ .$$

Then, using Eqs. (51) and (52), and in the pole approximation,

$$\langle i\mid\underline{g}_P\mid j\rangle=(-ik_i/2)\delta_{ij}-(\tfrac{1}{4})W_{\rm RR}(i,i)\langle i\mid\underline{g}_P\mid j\rangle-\tfrac{1}{4}\sum_k(1-\delta_{ki})W_{\rm RR}(i,k)\langle k\mid\underline{g}_P\mid j\rangle\ ,\tag{55}$$

with solution

$$\langle i\mid\underline{g}_P\mid j\rangle=(-ik_j/2)(\underline{\omega}^{-1})_{ij}/[1+W_{\rm RR}(j,j)/4]\ ,\tag{56}$$

where $\underline{\omega}$ was given in Eq. (26). In the pole approximation, $\underline{\omega}$ becomes

$$\omega_{ij}=\delta_{ij}+(\tfrac{1}{4})(1-\delta_{ij})W_{\rm RR}(i,j)/[1+W_{\rm RR}(i,i)/4]\ .\tag{57}$$

An analogous expression exists for $\langle f\mid\underline{g}_R\mid g\rangle$; viz.,

$$\langle f\mid\underline{g}_R\mid g\rangle=(-ik_\gamma^2/2)(\underline{\nu}^{-1})_{fg}/[1+W_{\rm PI}(f,f)/4]\ ,\tag{58}$$

with $\underline{\nu}$ being given by Eq. (32). In the pole approximation, one has that

$$\underline{\nu}_{fg}=\delta_{fg}+(\tfrac{1}{4})(1-\delta_{fg})W_{\rm PI}(f,g)/[1+W_{\rm PI}(g,g)/4]\ .\tag{59}$$

Alternately, one may make use of relationships between $\underline{g}_P$ and $\underline{g}_R$,

$$\begin{aligned}\underline{g}_R&=g_R+g_RRDPg_PPDRg_R\ ,\\ \underline{g}_P&=g_P+g_PPDRg_RRDPg_P\ ,\end{aligned}\tag{60}$$

to write

$$\begin{aligned}\langle f\mid\underline{g}_R\mid g\rangle&=g_{Rf}\left[\delta_{fg}+\sum_i D_{fi}\langle i\mid\underline{g}_P\mid j\rangle D_{jg}\right]g_{Rg}\ ,\\ \langle i\mid\underline{g}_P\mid j\rangle&=g_{Pi}\left[\delta_{ij}+\sum_f D_{if}\langle f\mid\underline{g}_R\mid g\rangle D_{gj}\right]g_{Pj}\ ,\end{aligned}\tag{61}$$

so that the matrix elements of $\underline{g}_R$ may be obtained from those of $\underline{g}_P$, or vice versa.

Now, for the autoionization width modified by *RDP* coupling, one finds from Eq. (53), in the pole approximation, that

$$\begin{aligned}\underline{\Gamma}_a(\alpha)=&-2\,{\rm Im}(\langle\alpha\mid V\underline{P}g_P\underline{P}V\mid\alpha\rangle-\langle\alpha\mid DRg_RRD\underline{P}g_P\underline{P}DRg_RRD\mid\alpha\rangle)\\=&\sum_i\sum_j V_{\alpha j}M_j(\underline{\omega}^{-1})_{ji}k_i\sum_k(\underline{\omega}^{-1})_{ik}M_kV_{k\alpha}\\&+\tfrac{1}{4}\sum_i\sum_f k_\gamma^2D_{\alpha f}\sum_j D_{fj}M_j(\underline{\omega}^{-1})_{ji}k_i\sum_k(\underline{\omega}^{-1})_{ik}M_k\sum_g k_\gamma^2D_{kg}D_{g\alpha}\end{aligned}\tag{62}$$

[the fourth term in Eq. (53) is zero in the pole approximation], where

$$M_i\equiv 1/[1+W_{\rm RR}(i,i)/4]\ .\tag{63}$$

Similarly, for the stabilizing radiative width, one has from Eq. (53) that

$$\begin{aligned}\underline{\Gamma}_r(\alpha)&=-2\,\mathrm{Im}(\langle\alpha\mid D\underline{R}g_R\underline{R}D\mid\alpha\rangle-\langle\alpha\mid VPg_PPD\underline{R}g_R\underline{R}DPg_PPV\mid\alpha\rangle)\\&=\sum_f\sum_g D_{\alpha g}N_g(\underline{\nu}^{-1})_{gf}k_\gamma^2\sum_h(\underline{\nu}^{-1})_{fh}N_hD_{h\alpha}\\&\quad+\tfrac{1}{4}\sum_f\sum_i k_iV_{\alpha i}\sum_g D_{ig}N_g(\underline{\nu}^{-1})_{gf}k_\gamma^2\sum_h(\underline{\nu}^{-1})_{fh}N_h\sum_j k_jD_{hj}V_{j\alpha}\end{aligned}\tag{64}$$

(the third term is zero in the pole approximation), where

$$N_f\equiv 1/[1+W_{\mathrm{PI}}(f,f)/4]\ .\tag{65}$$

For certain kinds of problems it may be that the P space is effectively much smaller than the R space, or vice versa. In the first instance, it would be expedient to rewrite Eq. (64) in terms of $\underline{\omega}$ instead of $\underline{\nu}$. That is, using Eqs. (45), (51), and (53), Eq. (64) may be written as

$$\begin{aligned}\underline{\Gamma}_r(\alpha)=&\sum_f k_\gamma^2D_{\alpha f}^2+\tfrac{1}{4}\sum_i k_iV_{\alpha i}\sum_f k_\gamma^2D_{if}\sum_j k_jD_{fj}V_{j\alpha}-\tfrac{1}{2}\sum_f k_\gamma^2D_{\alpha f}\sum_i D_{fi}k_iM_i\sum_j(\underline{\omega}^{-1})_{ij}\sum_g k_\gamma^2D_{jg}D_{g\alpha}\\&-\tfrac{1}{8}\sum_i k_iV_{\alpha i}\sum_f k_\gamma^2D_{if}\sum_j\sum_k D_{fj}(\underline{\omega}^{-1})_{jk}M_kk_j\sum_g D_{kg}k_\gamma^2\sum_l k_lD_{gl}V_{l\alpha}\\&+\tfrac{1}{16}\sum_f k_\gamma^2D_{\alpha f}\sum_i D_{fi}k_iM_i\sum_j(\underline{\omega}^{-1})_{ij}\sum_g D_{jg}k_\gamma^2\sum_k D_{gk}k_kM_k\sum_l(\underline{\omega}^{-1})_{kl}\sum_h k_\gamma^2D_{lh}D_{h\alpha}\\&+\tfrac{1}{64}\sum_i k_iV_{\alpha i}\sum_f k_\gamma^2D_{if}\sum_j D_{fj}k_jM_j(\underline{\omega}^{-1})_{jk}\sum_g k_\gamma^2D_{kg}\sum_l D_{gl}k_lM_l\sum_m(\underline{\omega}^{-1})_{lm}\sum_h D_{mh}k_\gamma^2\sum_n D_{hn}k_nV_{n\alpha}\ .\end{aligned}\tag{66}$$

Similarly, Eq. (62) may be rewritten in terms of $\underline{\nu}$ instead of $\underline{\omega}$.

FIRST WORKED EXAMPLE

We proceed to evaluate the full RDR probability amplitude $\underline{M}^{\mathrm{RDR}}$, as given by Eqs. (3), (40), and (41), for a single P-space state, a single Q-space state ($\Omega=\delta$), and in the pole approximation. In addition, we assume for simplicity that only a single continuum electron momentum participates. We point out that, in this simple case, sums over i reduce to a single term ($\underline{\omega}=\delta$). The various terms appearing in $\underline{M}^{\mathrm{RDR}}$ can now be evaluated as follows.

From Eq. (29), the initial state modified by RDP coupling is

$$\underline{\Phi}_P=\underline{\Phi}_{Pi}=\Phi_{Pi}M_i\ .\tag{67}$$

The P- and R-space propagators are

$$\begin{aligned}&\langle i\mid\underline{g}_P\mid i\rangle=(-ik_i/2)M_i\ ,\\&\langle f\mid\underline{g}_R\mid g\rangle=(-ik_\gamma^2/2)[\delta_{fg}-(k_i/4)M_ik_\gamma^2D_{fi}D_{ig}]\ .\end{aligned}\tag{68}$$

From Eq. (62), one has for the autoionization width that

$$\underline{\Gamma}_a(\alpha)=[A_a(\alpha\to i)+(\tfrac{1}{4})k_i\Gamma_{Rr}(\alpha,i)^2]M_i^2\ ,\tag{69}$$

where

$$\Gamma_{Rr}(\alpha,i)\equiv\sum_f k_\gamma^2D_{\alpha f}D_{fi}\ .\tag{70}$$

For the radiative width, from Eq. (66),

$$\begin{aligned}\underline{\Gamma}_r(\alpha)=&\,\Gamma_r(\alpha)+k_i\Gamma_{Rr}(\alpha,i)^2(M_i^2-1)/W_{\mathrm{RR}}(i,i)\\&+\tfrac{1}{4}A_a(\alpha\to i)W_{\mathrm{RR}}(i,i)M_i^2\ .\end{aligned}\tag{71}$$

Matrix elements of the interaction operator $\underline{V}$, defined in Eq. (13) and appearing in Eqs. (13), (40), and (41), become

$$\begin{aligned}\langle\alpha\mid\underline{V}\mid i\rangle&=\langle\alpha\mid V+DRg_RRD\mid i\rangle\\&=V_{\alpha i}-\sum_f(ik_\gamma^2/2)D_{\alpha f}D_{fi}\\&=V_{\alpha i}-i\Gamma_{Rr}(i,\alpha)/2\\&\equiv\underline{V}_{\alpha i}\ .\end{aligned}\tag{72}$$

The total decay width in the Q-space state α is, from Eqs. (69) and (71),

$$\begin{aligned}\underline{\Gamma}_{\mathrm{tot}}(\alpha)&=\underline{\Gamma}_r(\alpha)+\underline{\Gamma}_a(\alpha)\\&=\{A_a(\alpha\to i)+\Gamma_r(\alpha)+\tfrac{1}{4}[\Gamma_r(\alpha)W_{\mathrm{RR}}(i,i)\\&\qquad-k_i\Gamma_{Rr}(i,\alpha)^2]\}M_i\ .\end{aligned}\tag{73}$$

$\underline{M}^{\mathrm{RR}}$ and $\underline{M}^{\mathrm{DR}}$ can now be written down immediately as

$$\underline{M}^{\mathrm{RR}}=D_{fi}M_i-(ik_i/2)D_{fi}\underline{V}_{i\alpha}\underline{G}_{Q\alpha}\underline{V}_{\alpha i}M_i^2\ ,\tag{74}$$

$$\underline{M}^{\mathrm{DR}}=D_{f\alpha}\underline{G}_{Q\alpha}\underline{V}_{\alpha i}M_i\ ,\tag{75}$$

where the Q-space propagator is

$$\underline{G}_{Q\alpha}=[E-\underline{\varepsilon}_\alpha+(i/2)\underline{\Gamma}_{\mathrm{tot}}(\alpha)]^{-1}\tag{76}$$

and the shifted eigenvalue $\underline{\varepsilon}_\alpha$ is, in the pole approximation, from Eqs. (23) and (70),

$$\begin{aligned}\underline{\varepsilon}_\alpha&=\varepsilon_\alpha-(k_i/2)V_{\alpha i}M_i\sum_f k_\gamma^2D_{if}D_{f\alpha}\\&=\varepsilon_\alpha-(\tfrac{1}{2})[k_iA_a(\alpha\to i)]^{1/2}M_i\Gamma_{Rr}(i,\alpha)\ .\end{aligned}\tag{77}$$

The RDR probability for this example is then

$$\underline{P}^{\mathrm{RDR}}(i\to\alpha)=\sum_f (2\pi)^{-4}\int d\mathbf{k}_\gamma\int d\mathbf{k}_i \mid \underline{M}^{\mathrm{RR}}+\underline{M}^{\mathrm{DR}} \mid^2 \delta(E-\varepsilon_i)\delta(E-\varepsilon_f)$$
$$=k_i\sum_f k_\gamma^2 \mid \underline{M}^{\mathrm{RR}}+\underline{M}^{\mathrm{DR}} \mid^2$$
$$=k_i M_i^2 \mid \underline{G}_{Q\alpha} \mid^2 \sum_f k_\gamma^2 \mid D_{fi}\{E-\underline{\varepsilon}_\alpha+(i/2)[\underline{A}_a(\alpha\to i)+\underline{\Gamma}_r(\alpha)]\}+D_{fi}(-ik_i/2)\underline{V}_{\alpha i}\underline{V}_{\alpha i}M_i+D_{f\alpha}\underline{V}_{\alpha i} \mid^2 . \tag{78}$$

This expression can be rearranged to read

$$\underline{P}^{\mathrm{RDR}}(i\to\alpha)=M_i^2 \mid \underline{G}_{Q\alpha} \mid^2(\{W_{\mathrm{RR}}(i,i)(E-\varepsilon_\alpha)^2+2\Gamma_{Rr}(i,\alpha)[k_i A_a(\alpha\to i)]^{1/2}(E-\varepsilon_\alpha)+A_a(\alpha\to i)\Gamma_r(\alpha)\}$$
$$+\tfrac{1}{4}\Gamma_r(\alpha)[W_{\mathrm{RR}}(i,i)\Gamma_r(\alpha)-k_i\Gamma_{Rr}^2(i,\alpha)]) . \tag{79}$$

Note that, in Eq. (79), ε_α appears and not $\underline{\varepsilon}_\alpha$. Equation (79) is the final form of the *RDR* probability, as determined in the pole approximation, for the case of a single Q-space state, a single P-space state (and a single continuum electron momentum), but an arbitrary number of R-space states.

If, in addition to these restrictions on the Q and P spaces, we stipulate that the R space contains just one state (labeled by f_α), then the last line of Eq. (79) reduces to zero, and Eq. (79) becomes

$$\underline{P}^{\mathrm{RDR}}(i\to\alpha)=M_i^2 \mid \underline{G}_{Q\alpha} \mid^2\{W_{\mathrm{RR}}(i,i)(E-\varepsilon_\alpha)^2+2[k_i A_{\mathrm{RR}}(i\to f_\alpha)A_r(\alpha\to f_\alpha)A_a(\alpha\to i)]^{1/2}(E-\varepsilon_\alpha)$$
$$+A_a(\alpha\to i)A_r(\alpha\to f_\alpha)\} . \tag{80}$$

Now Eq. (80) agrees exactly with the result quoted in Eq. (5a) of Ref. 4, which was based on a model calculation, with one initial, one intermediate, and one final state. Similarly, the autoionization and stabilizing radiative probabilities modified by *RDP* coupling [Eqs. (62) and (66), respectively] reduce in this limit to the results quoted in Eqs. (12a) and (12b) of Ref. 3 and Eqs. (81) and (82) of Ref. 12. The asymptotic P- and R-space states modified by *RDP* coupling, Eqs. (29) and (30), also appear in Eq. (5a) of Ref. 3.

A real *RDR* process well described (in the pole approximation) by Eq. (80) is

$$1s+k_c(l_c=1)\leftrightarrow 2pns\to 1sn's+\gamma ,$$
$$1s+k_c(l_c=1)\to 1sn's+\gamma \tag{81}$$

for $n\geq 2$, provided that n values are small enough, so that resonances are truly isolated, and if $n=n'$. If $n\neq n'$, then Eq. (79) must be employed. It seems worth reemphasizing that even though the $2pns$ intermediate states in Eq. (81) carry single particle labels, the states are assumed to be configuration-interaction (CI) states which diagonalize QH_0Q. Similar remarks apply to the $1sn's$ final states which are assumed to diagonalize RH_0R, and to the $1s+k_cl_c$ initial states which are assumed to diagonalize PH_0P.

The total *RDR* probability for the process of Eq. (81), when resonances do not interact and do not overlap, is obtained then as

$$\underline{P}^{\mathrm{RDR}}(i)=\sum_\alpha \underline{P}^{\mathrm{RDR}}(i\to\alpha) , \tag{82}$$

where $\underline{P}^{\mathrm{RDR}}(i\to\alpha)$ is given by Eq. (80) if R contains just one state, and by Eq. (79) otherwise. This is a generalization to the *RDR* process of the so-called isolated resonance approximation (IRA), familiar from pure DR calculations [see Eq. (12), paper I].

In the special case where resonances *are* overlapping while being at the same time strictly *non*interacting, then instead of Eqs. (79) or (80) one has that

$$\underline{P}^{\mathrm{RDR}}(i)=k_i M_i^2\sum_f k_\gamma^2 \mid D_{fi}M_i$$
$$+(-ik_i/2)D_{fi}M_i^2\sum_\alpha \underline{V}_{i\alpha}^2\underline{G}_{Q\alpha}$$
$$+\sum_\alpha D_{f\alpha}\underline{G}_{Q\alpha}\underline{V}_{\alpha i}M_i \mid^2 . \tag{83}$$

SECOND WORKED EXAMPLE

If resonances are interacting, then the analog of Eq. (79) for $\underline{P}^{\mathrm{RDR}}$ can be obtained from Eqs. (3), (40), and (41). For this purpose, matrix elements of the Q-space mixing operator $\underline{\Omega}$, from Eq. (22), are required. In the pole approximation, and for a single P-space state and a single continuum electron momentum ($\omega=\delta$), these matrix elements are

$$\underline{\Omega}_{\alpha\beta}=\delta_{\alpha\beta}+(1-\delta_{\alpha\beta})(i/2)\underline{G}_{Q\alpha}$$
$$\times\left[\sum_f k_\gamma^2 D_{\alpha f}D_{f\beta}+k_i\underline{V}_{\alpha i}M_i\underline{V}_{i\beta}\right] , \tag{84}$$

which becomes, for the process of Eq. (81),

$$\underline{\Omega}_{\alpha\beta}=\delta_{\alpha\beta}+(1-\delta_{\alpha\beta})(ik_i/2)\underline{G}_{Q\alpha}\underline{V}_{\alpha i}M_i\underline{V}_{i\beta} , \tag{85}$$

where

$$\underline{V}_{\alpha i}=V_{\alpha i}-(i/2)[A_{\mathrm{RR}}(i\to f_\alpha)A_r(\alpha\to f_\alpha)]^{1/2} , \tag{86}$$

with a similar expression holding for $\underline{V}_{i\beta}$.

The probability amplitudes for RR and DR are now

$$\underline{M}^{\mathrm{RR}}=D_{fi}M_i \times\left[1+(-ik_i/2)\sum_{\beta}\sum_{\alpha}\underline{V}_{i\beta}(\underline{\Omega}^{-1})_{\beta\alpha}\underline{G}_{Q\alpha}\underline{V}_{\alpha i}M_i\right], \tag{87}$$

$$\underline{M}^{\mathrm{DR}}=\sum_{\beta}\sum_{\alpha}D_{f\beta}(\underline{\Omega}^{-1})_{\beta\alpha}\underline{G}_{Q\alpha}\underline{V}_{\alpha i}M_i , \tag{88}$$

where the Q-space propagator $\underline{G}_{Q\alpha}$ appears in Eq. (76). The *RDR* probability, for the ith initial state, is therefore

$$\begin{aligned}\underline{P}^{\mathrm{RDR}}(i)&=\sum_f(2\pi)^{-4}\int d\mathbf{k}_\gamma\int d\mathbf{k}_i\,|\,\underline{M}^{\mathrm{RR}}+\underline{M}^{\mathrm{DR}}\,|^2\delta(E-\varepsilon_i)\delta(E-\varepsilon_f)\\&=k_i\sum_f k_\gamma^2\,|\,\underline{M}^{\mathrm{RR}}+\underline{M}^{\mathrm{DR}}\,|^2 ,\end{aligned} \tag{89}$$

with $\underline{M}^{\mathrm{RR}}$ given by Eq. (87) and $\underline{M}^{\mathrm{DR}}$ given by Eq. (88).

We now model this example by defining the unperturbed stabilizing radiative, autoionization, and first-order normalized radiative recombination transition rates, such that (a) $A_{r0}\equiv A_r(2pns\rightarrow 1sn's)\delta_{nn'}$; (b) $A_{a0}/n^3\equiv A_a(2pns\rightarrow 1s+k_cl_c)$; and (c) $W_{\mathrm{RR0}}/n^3\equiv k_iA_{\mathrm{RR}}(1s+k_cl_c\rightarrow 1sns)$; where A_{r0}, A_{a0}, and W_{RR0} are all constants which characterize the model. When $W_{\mathrm{RR0}}=0$, the model leads to the values of the DR probability displayed in Fig. 1 of paper I. We referred to the method of paper I as the multiple interacting resonance approximation (MIRA). It did not include the effects of the RR channel.

Now from Eq. (89), and for the arbitrary modeling constants A_{r0}, A_{a0}, and W_{RR0}, the *RDR* probability becomes, for the single initial state i,

$$\underline{P}^{\mathrm{RDR}}(i)=M_0^2\sum_n\left|\,(W_{\mathrm{RR0}}/n^3)^{1/2}+A_{r0}^{1/2}V_0\zeta_n-(iM_0V_0^2/2)(W_{\mathrm{RR0}}/n^3)^{1/2}\times\sum_{n'}n'^{-3/2}\zeta_{n'}\,\right|^2 , \tag{90}$$

where the quantities appearing in Eq. (90) are defined according to

$$\begin{aligned}M_0&\equiv 1\Big/\left[1+(1/4)\sum_{n=1}^{\infty}W_{\mathrm{RR0}}/n^3\right]\\&\cong 1/(1+0.30W_{\mathrm{RR0}}) ,\\V_0&\equiv A_{a0}^{1/2}-(i/2)(W_{\mathrm{RR0}}A_{r0})^{1/2} ,\\\zeta_n&\equiv\sum_{n'}(\underline{\Omega}^{-1})_{nn'}\underline{G}_{Qn'}n'^{-3/2} ,\end{aligned} \tag{91}$$

$$\underline{G}_{Qn}=[E-\varepsilon_n+(M_0/2n^3)(A_{r0}A_{a0}W_{\mathrm{RR0}})^{1/2}+(iM_0/2)(A_{r0}+A_{a0}/n^3)]^{-1} , \tag{92}$$

where $\varepsilon_n\equiv -Z^2/2n^2$ is the unshifted energy of the captured electron in the Q state labeled by n. For simplicity, the energy of the excited (struck) electron in the Q state is set equal to zero. This only serves to shift the zero of total energy E. From Eq. (85), matrix elements of the Q-space mixing operator are

$$\underline{\Omega}_{nn'}=\delta_{nn'}+(1-\delta_{nn'})(i/2)\underline{G}_{Qn}V_0^2M_0n^{-3/2}n'^{-3/2} . \tag{93}$$

Results of calculations based on this model are displayed in Figs. 1–2, for $2\le n\le 7$. In generating this data we interacted states with n between 2 and 11. As in paper I, we assigned the values $A_{a0}=0.2$ and $A_{r0}=2.0\times 10^{-5}$ a.u., for $Z=1$. In order to illustrate the dependence on W_{RR0}, we examined the very wide range, $0\le W_{\mathrm{RR0}}\le 40$ a.u. However, for the values of A_{a0} and A_{r0} chosen, a physical choice for W_{RR0} would be $\sim 10^{-10}$ a.u. See the Appendix for a discussion of the connection between A_a, A_r, and W_{RR}.

We also used this model to simulate *RDR* for He^{+1} and Li^{+2} ground-state targets. In Fig. 3 we plot $\underline{P}^{\mathrm{PDR}}$ versus E, for $2\le n\le 5$, when $A_{a0}=0.2$, $A_{r0}=1\times 10^{-8}$, $W_{\mathrm{RR0}}=3\times 10^{-7}$ a.u., and $Z=1$. These are physically reasonable parameter choices for the He^{+1} ion. For comparison, a plot at $W_{\mathrm{RR0}}=0$ also appears. In Fig. 4 we plot again $\underline{P}^{\mathrm{RDR}}$ versus E for He^{+1}, but confine our attention to details of the $2p2s$ resonance. Four plots appear in this figure: one describing the isolated resonance approximation (IRA), one describing the MIRA (paper I), one describing the *RDR* process without interacting resonances, and one describing the full *RDR* process including interacting resonances. Since this was a model calculation, we did not undertake a diagonalization of the QH_0Q and RH_0R Hamiltonians in the $2pns$ and $1sn's$ bases.

To illustrate the Z dependence, in Fig. 5 we plot cases analogous to those displayed in Fig. 4, but for the Li^{+2} ion. Parameter values were taken to be $A_{a0}=0.2$, $A_{r0}=5\times 10^{-8}$, $W_{\mathrm{RR0}}=6\times 10^{-7}$ a.u., and $Z=2$.

From the figures it seems clear that the RR process produces significant alternations in the DR spectrum only at very low n and very low Z, for this $\Delta n\neq 0$ excita-

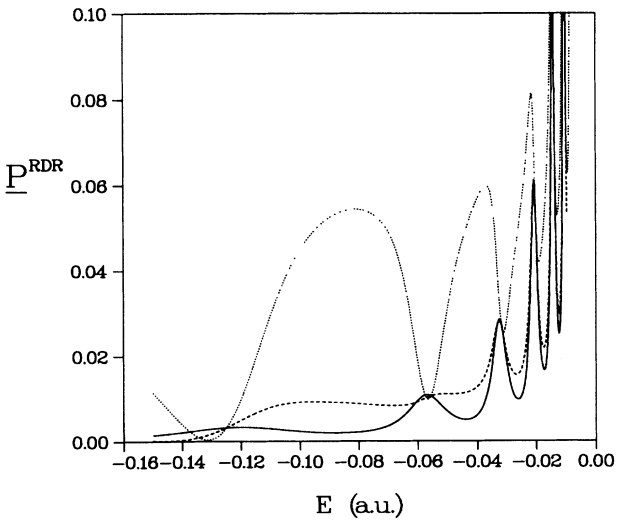

FIG. 1. $\underline{P}^{\mathrm{RDR}}$ vs E for the model described in example 2, where $Z=1$, $A_{a0}=0.2$, $A_{r0}=2.0\times 10^{-5}$; $W_{\mathrm{RR0}}=0$ (——), $W_{\mathrm{RR0}}=2\times 10^{-3}$ (— — —), and $W_{\mathrm{RR0}}=2\times 10^{-2}$ (. . . .). Resonances $2pns$, with $2\le n\le 7$, appear.

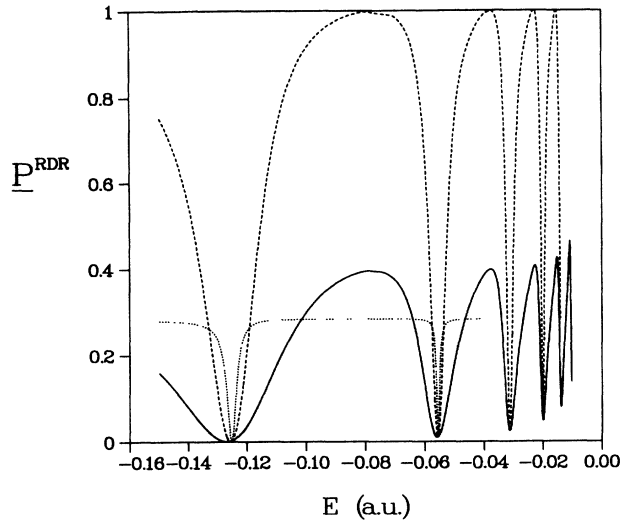

FIG. 2. Same as Fig. 1, but for $W_{RR0}=0.2$ (——), $W_{RR0}=2$ (— — —), and $W_{RR0}=20$ (· · · ·).

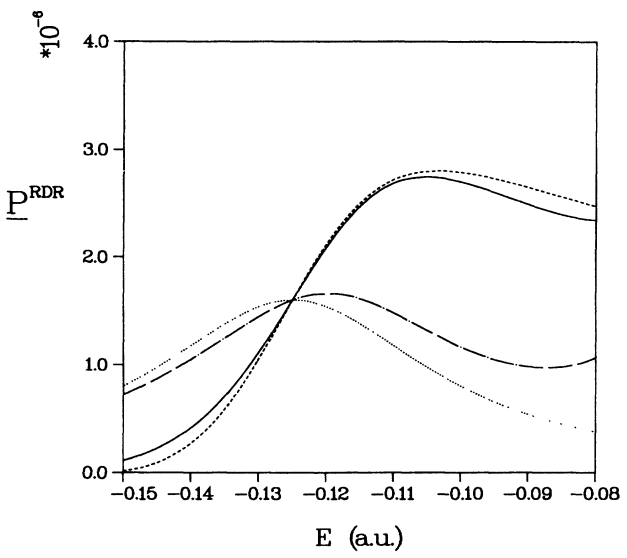

FIG. 4. $\underline{P}^{RDR}$ vs E for the $2p2s$ resonance of the model described in example 2, where $Z=1$, $A_{a0}=0.2$, $A_{r0}=1\times10^{-8}$, $W_{RR0}=3\times10^{-7}$: *RDR* with interacting resonances (——), *RDR* without interacting resonances (— — —), MIRA (· · · ·), and IRA (—·—·—·).

tion. In this region of parameter space, however, the effects can be rather large. At the same time, complications introduced by interacting resonances are at a minimum for low n.

THIRD WORKED EXAMPLE

Of course, our general results also apply to cases involving more than one P-space partial wave (when $\omega\neq\delta$); i.e., the process

$$\begin{aligned} &1s+k_c(l_c=1,3)\leftrightarrow 2pnd\rightarrow 1sn'd+\gamma\ , \\ &1s+k_c(l_c=1,3)\rightarrow 1sn'd+\gamma \end{aligned} \tag{94}$$

for $n\geq 3$. Here our description includes the effects of interference between the P-space states of $l_c=1$ and $l_c=3$, via interaction with the R-space, as well as interference between the Q-space states via interaction with the P space. Equations (3), (40), and (41) are still valid, but now the operators $\underline{\Omega}$ and $\underline{\omega}$ appearing in those equations are all nondiagonal in the i, f, α basis. Again we draw attention to the fact that, in spite of single particle labels in Eq. (94), the intermediate states $2pnd$ are assumed to diagonalize QH_0Q, the final states $1sn'd$ should diagonalize RH_0R, and the initial states $1s+k_cl_c$ should diagonalize

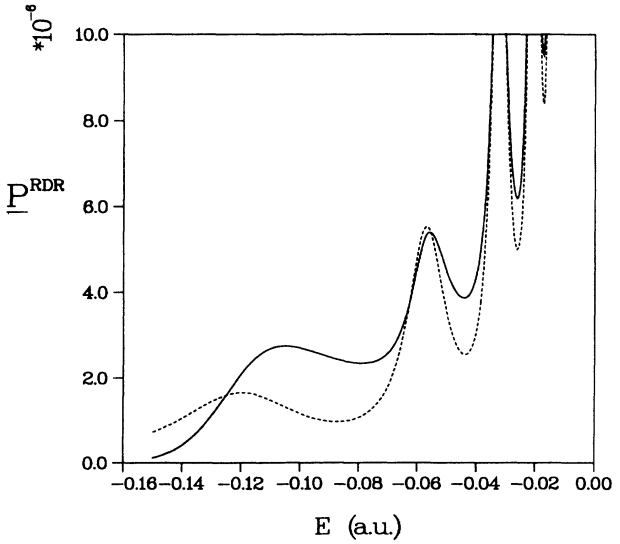

FIG. 3. $\underline{P}^{RDR}$ vs E for the model described in example 2, where $Z=1$, $A_{a0}=0.2$, $A_{r0}=1\times10^{-8}$, $W_{RR0}=3\times10^{-7}$ (——), and $W_{RR0}=0$ (— — —). Resonances $2pns$, with $2\leq n\leq 5$, appear.

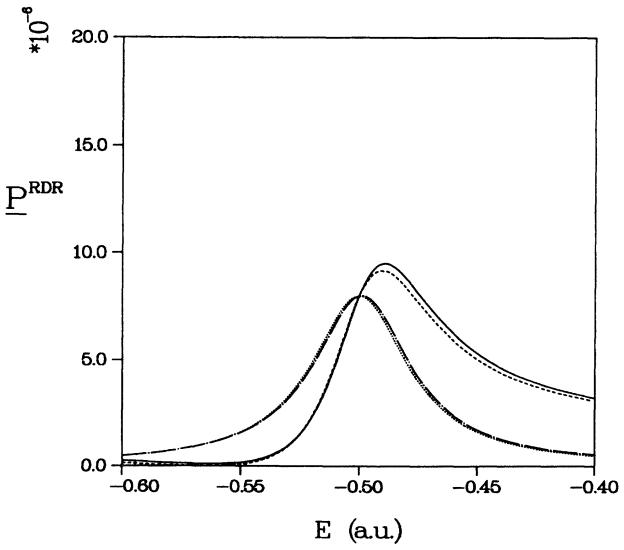

FIG. 5. Same as Fig. 4 but for $Z=2$, $A_{a0}=0.2$, $A_{r0}=5\times10^{-8}$, and $W_{RR0}=6\times10^{-7}$.

PH_0P.

Matrix elements of the P-space mixing operator $\underline{\omega}$, in the pole approximation, appear in Eq. (57). The asymptotic P-space states perturbed by *RDP* coupling $\underline{\Phi}_P$ are related to the unperturbed states Φ_P in the pole approximation by Eq. (29).

Altogether, then one has for the total *RDR* probability, in this general case, but in the pole approximation,

$$\underline{P}^{\mathrm{RDR}}=\sum_i k_i \sum_f k_\gamma^2 \Big| \sum_j \sum_k D_{fj}(\underline{\omega}^{-1})_{jk}(\underline{\omega}^{-1})_{ki}M_i + \sum_\alpha \sum_\beta \sum_j \sum_k \sum_l \sum_m \sum_n [D_{fj}(\underline{\omega}^{-1})_{jk}(\underline{\omega}^{-1})_{kl}(-ik_kM_k)\underline{V}_{l\alpha}(\underline{\Omega}^{-1})_{\alpha\beta}\underline{G}_{Q\beta}\underline{V}_{\beta m}(\underline{\omega}^{-1})_{mn}(\underline{\omega}^{-1})_{ni}M_i] + \sum_\alpha \sum_\beta \sum_j \sum_k D_{f\alpha}(\underline{\Omega}^{-1})_{\alpha\beta}\underline{G}_{Q\beta}\underline{V}_{\beta j}(\underline{\omega}^{-1})_{jk}(\underline{\omega}^{-1})_{ki}M_i \Big|^2 , \tag{95}$$

where $\underline{G}_{Q\alpha}$ and $\underline{\Omega}_{\alpha\beta}$ are given by Eqs. (36) and (37). Note that Eq. (95) has a sufficiently general form that a solution may be constructed which includes a full discretization of the continuum electron momentum. In Eq. (95), for the example being considered, α and β range from 2 to ∞, while $i,j,\ldots,n$ take on the values 1 and 2. The results of explicit calculations for real systems, based on Eq. (95), will be described at a later date.

SUMMARY

We have described here a comprehensive formalism for the calculation of the combined radiative recombination (RR) and dielectronic recombination (DR) probability amplitude, for the case of a continuum electron interacting with an isolated ion. The combined recombination process was labeled RDR. Feshbach notation was employed throughout. This is a continuation of studies of interfering resonance effects in DR begun in paper *I*.[10]

The formalism explicitly includes the effects of interacting continuum channels, as well as interacting resonances. To this extent, it represents a complete solution of the single electron, single ion recombination problem. However, important QED questions such as electron self-energy and other relativistic effects are not addressed. In this sense, the solution is still incomplete.

General results, in the form of matrix elements of functions of operators, are contained in Eqs. (3), (40), and (41). An explicit reduction of these general expressions is obtained in the pole approximation, and appears as a formula for the *RDR* probability (P^{RDR}), in Eq. (95). Values of P^{RDR} for the relatively simple case of a single continuum channel are derived and given, in the pole approximation, in Eqs. (87)–(89). A model calculation is described, the results of which may be found in Figs. 1–5.

Examination of the structure of the *RDR* equations, and the results of our model calculations, suggest that interference between the RR and DR channels leads to important changes in the *RDR* probability only for low-lying intermediate states, and only for small Z values, for $\Delta n \neq 0$ excitations. On the other hand, interfering resonance effects are expected to be important only for relatively high-lying resonance states. The situation is quite different for $\Delta n = 0$ excitations. See the Appendix for further discussion.

Part of the approach described herein properly falls under the heading of configuration-interaction (CI) theory. However, as emphasized throughout this paper, and in paper I, the CI we invoke mixes resonance states solely via interaction with the initial- (continuum electron) and/or final- (emitted photon) state spaces. Similarly, the initial states are mixed only through interaction with the final-state space. Thus the Ci we describe is akin to that introduced by Fano.[7] The apparent equivalence of our approach to that of multichannel quantum-defect theory[13] has been discussed in paper I.

APPENDIX

We summarize here essential information concerning the relationship between A_a, A_r, and W_{RR}. In an *LS* averaged approximation, and for the reaction of Eq. (81), one has for the stabilizing radiative probability

$$A_r(2p \rightarrow 1s+\gamma)=(4\alpha^3/3)(r_{2p,1s})^2(\varepsilon_{2p}-\varepsilon_{1s})^3 , \tag{A1}$$

as obtained from Eq. (44), where α is the fine structure constant, $r_{2p,1s}$ is the dipole matrix element, and ε_{2p} and ε_{1s} are the energies of the electron before and after the transition. All quantities are in a.u.

The autoionization probability, in the Bethe approximation, is

$$\begin{aligned} A_a(2pns \rightarrow 1s+k_cl_c) &= (4k_c/3)(r_{2p,1s})^2 \\ &\quad \times |\langle ns \,|\, r^{-2} \,|\, k_cl_c\rangle|^2 \\ &\approx (4k_c/3\tau_0)(r_{2p,1s})^2Z^{-2} \\ &\quad \times (0.5k_c^2-\varepsilon_{ns})^4(r_{kclc,ns})^2 \end{aligned} \tag{A2}$$

from Eq. (44), where Z is the target charge and, at the second step, we have made use of an exact relationship between matrix elements of Coulomb functions.[14] In Eq. (A2), and in the following, the continuum wave functions possess plane-wave normalization.

The normalized state-to-state radiative recombination probability, correct to second order in *RDP*, is

$$W_{\mathrm{RR}}(k_cl_c \rightarrow ns+\gamma)=(4k_c\alpha^3/3)(r_{kclc,ns})^2(0.5k_c^2-\varepsilon_{ns})^3 \tag{A3}$$

from Eqs. (47) and (52).

One then has the following approximate relationship between the normalized state-to-state radiative recombination, stabilizing radiative, and autoionization probabilities,

$$W_{\mathrm{RR}}=(4\alpha^6Z^2/3)(\varepsilon_{2p}-\varepsilon_{1s})^3(0.5k_c^2-\varepsilon_{ns})^{-1}(A_a/A_r)\ . \tag{A4}$$

Now, from Eq. (A4), if we take $A_a=0.2/n^3$, $A_r=10^{-8}$, $Z=1$, $n=2$, and $k_c\approx 1$, then $W_{\mathrm{RR}}\approx 3\times 10^{-7}$; i.e., in this case $W_{\mathrm{RR}}\gg A_r$, so that presumably W_{RR} has a relatively large effect on the *RDR* probability. However, since A_r scales as Z^4 [see Eq. (A1)], whereas W_{RR} scales only as Z^2 [see Eq. (A3)], then at $Z\approx 6$, A_r and W_{RR} are of comparable size, and the relative effect of W_{RR} on $\underline{P}^{\mathrm{RDR}}$ diminishes. For an identical choice of parameters, except that now $n=3$, then $W_{\mathrm{RR}}\approx 10^{-7}$ at $Z=1$. Hence, as n increases, the effect of W_{RR} on $\underline{P}^{\mathrm{RDR}}$ may also be expected to decrease. We emphasize that this discussion pertains to so-called $\Delta n\neq 0$ transitions. By contrast, for $\Delta n=0$ transitions, A_r scales as Z, so that as Z increases the effect of W_{RR} on $\underline{P}^{\mathrm{RDR}}$ may be expected to increase.

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