Interference effects in electron-ion recombination. III. Excited target states and continuum-continuum coupling

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Provision is made for the existence of excited target states and projectile continuum-continuum coupling, within the framework of the interacting resonance theory of electron-ion recombination described previously [Phys. Rev. A **36**, 4662 (1987); **38**, 1820 (1988)]. This "extended" theory makes explicit what was merely implicit in these earlier works. Dielectronic recombination probabilities, which include the effects of interaction and interference between resonances, are derived for two model systems: (a) A target ground state supporting two coupled projectile continua, and one excited target state as a closed channel; (b) a ground and first excited target state, each supporting one projectile continuum, and a second excited target state as a closed channel. Explicit calculations are performed for model (b), wherein are included Rydberg series of fully interacting resonances built on each of the two excited target states. The probability of excitation from the ground to the first excited target state is also obtained for model (b). This probability includes the effect of the interaction and interference between resonances, as well as the interference between resonance and direct excitation processes.

I. INTRODUCTION

In this work, an "extension" of the theory of interference effects in electron-ion recombination is described. That theory was expounded upon in earlier papers of this series (Refs. 1 and 2, to be referred to as I and II, respectively). Provision is now explicitly made in that theory for (i) the existence of more than one singly excited target state; (ii) the coupling among ground and singly excited target states through interaction with the projectile electron, in its several continua; (iii) the coupling between projectile continua due to interaction with the target, in its ground and singly excited states.

These often important parts of any complete treatment of the recombination problem were contained only implicitly in papers I and II, where it was emphasized that wave functions in the (initial-state) P space were assumed to diagonalize the P-space Hamiltonian. However, the implications of this assumption were not fully examined.

The effect of these considerations on calculations of the dielectronic recombination (DR) probability are problematic, and of considerable current interest.[3] Our intent here is to improve the present DR formalism, as exemplified in papers I and II, to the point where such problems can be treated successfully.

The notation and procedures adopted here are identical to those described in detail in paper I. As in that work, we use the Feshbach notation,[4] as adapted for recombination problems by Gau and Hahn.[5]

Our work has implications for the calculation of electron-ion impact excitation probabilities, and in this area, it represents a continuation of the past efforts of many other groups. These prior results have been summarized and discussed in several review articles.[6–8] Our formulation of the excitation probability [Eq. (44)], which includes interacting resonance and interference effects, may be seen as an extension of the work of Pindzola *et al.*[9] Other recent work in the area of resonance excitation, but which does not include the effects of interference, has been reported in Refs. 10–14. Resonance excitation is generally thought to be of significance in the evolution of nonequilibrium plasmas, especially plasmas containing highly charged ions.

In order to implement our program, an explicit separation of the incoming channel (one target state and one continuum partial wave) from all the other relevant P-space channels is performed. That part of the P-space projection operator which projects onto the incoming channel will henceforth be referred to as P_1. All other P-space states will be assigned to the projection operator P_2; i.e., such that

$$P=P_1+P_2 \qquad P_1P_2-P_2P_1=0\ . \tag{1}$$

The P_1 and P_2 spaces are connected via the electron-electron interaction operator $V=\sum_{i<j}(1/r_{ij})$, whenever $P_1VP_2=(P_2VP_1)^{\dagger}\neq 0$. See the remarks following Eq. (2) for a definition of the projection operators and the Hamiltonian governing this electron-ion system.

In Sec. II, the set of relevant Feshbach equations is summarized, and an explicit general solution of these equations is obtained, when P_2 contains just one state. Using these results, in Sec. III two model problems are considered. Explicit forms of the DR probability are obtained for each model, in the "pole approximation" [see discussion preceding Eq. (23)], and when just a single incoming electron linear momentum contributes. These problems feature (a) two coupled continuum partial

waves, each computed in the field of the target ground state, and one target excited state as a closed channel; (b) one continuum partial wave computed in the field of the target ground state, one continuum partial wave computed in the field of the first excited target state, and a second excited target state as a closed channel. As in model (a), the two continua are coupled via interaction with the target.

The excitation probability is also described for model (b). Hence, as in calculations based on multichannel quantum-defect theory (MQDT),[15] predictions of probabilities for both DR and excitation are obtained in a unified theory.

Explicit calculations of both the DR probability P^{DR} and the excitation probability P^{ex} are performed for model (b). "Fully interacting" Rydberg series of closed-channel resonances are included in both calculations. The term "fully interacting" is used here in the sense of paper I; also, see the remarks following Eq. (23) for a definition of this term. Throughout, all quantities are in atomic units.

In Sec. IV, the results of Sec. II are generalized to allow for the existence of more than just two P-space states. The effects of direct radiative coupling between initial and final states, as described in detail in paper II, are then added in an *ex post facto* manner.

II. FORMALISM

As discussed in the Introduction, the full P-space projector P is first divided into two parts. These are P_1, which projects onto the incoming channel (a target state, with N electrons bound, coupled to a projectile electron state of fixed continuum partial wave), and its P-space complement P_2; see Eq. (1). From Eq. (3) of paper I, the coupled Feshbach equations[4,5] for this system become

$$\begin{aligned}
&P_1VP_2\Psi_{P_2}+P_1VQ\Psi_Q=(E-P_1H_0P_1)\Psi_{P_1}\ ,\\
&P_2VP_1\Psi_{P_1}+P_2VQ\Psi_Q=(E-P_2H_0P_2)\Psi_{P_2}\ ,\\
&QVP_1\Psi_{P_1}+QVP_2\Psi_{P_2}+QDR\Psi_R=(E-QH_0Q)\Psi_Q\ ,\\
&RDQ\Psi_Q=(E-RH_0R)\Psi_R\ ,
\end{aligned}\tag{2}$$

where $D\propto\sum_i(\mathbf{r}_i\cdot\boldsymbol{\varepsilon}_i)$ is the electron-photon coupling operator, H_0 is a sum of the kinetic energy operators for all electrons, plus the diagonal (in P_1, P_2, and Q) part of the electron-electron interaction operator V, and E is the total system energy. Subscripts on wave functions denote projected quantities; e.g., $\Psi_{P_1}\equiv P_1\Psi$, $\Psi_{P_2}\equiv P_2\Psi$, etc. We note that Eq. (2) is equivalent to the full Schrödinger equation for this problem.

We summarize the characteristics of the projectors P_1, P_2, Q, and R as follows. (1) Together they form a set of mutually orthogonal and idempotent operators covering the space of physically meaningful wave-function solutions of Eq. (2). The construction of such a set of operators is possible in principle, albeit sometimes difficult in practice, especially for target ions containing two or more electrons.[9,16] (2) Q projects onto the space of wave functions with $N+1$ (all) electrons bound, and no photons; R projects onto the space of wave functions with $N+1$ electrons bound and one photon; $P=P_1+P_2$ projects onto the space or wave functions with N electrons bound, one electron in the continuum, and no photons. Other possibilities are ignored; i.e., one or more photons in the Q and P spaces, two or more photons in the R space, and more than one electron in the P-space continuum. For recombination and excitation problems, the most important states in the Q space are doubly excited, while the most important electronic states in the R space are singly excited. The bound component of the P space is usually limited to ground and singly excited states.

The second and fourth equations in Eq. (2) can be solved formally in terms of Ψ_{P_1} and Ψ_Q to give

$$\Psi_{P_2}=g_{P_2}(P_2VP_1\Psi_{P_1}+P_2VQ\Psi_Q)\ ,\tag{3}$$

$$\Psi_R=g_RRDQ\Psi_Q\ ,\tag{4}$$

where

$$g_{P_2}=(E-P_2H_0P_2)^{-1}\ ,\tag{5}$$

and as in Eq. (4) (of paper I)

$$g_R=(E-RH_0R)^{-1}\ .\tag{6}$$

A formal solution for Ψ_{P_1} may be obtained in terms of Ψ_Q as

$$\begin{aligned}
\Psi_{P_1}&=\tilde{\Phi}'_{P_1}+\tilde{g}'_{P_1}P_1(V+VP_2g_{P_2}P_2V)Q\Psi_Q\\
&=\tilde{\Phi}'_{P_1}+\tilde{g}'_{P_1}P_1\tilde{V}'Q\Psi_Q\ ,
\end{aligned}\tag{7}$$

where

$$\tilde{V}'\equiv V+VP_2g_{P_2}P_2V\ ,\tag{8}$$

and where $\tilde{\Phi}'_{P_1}$ is the P_1-space solution of the equation

$$(E-P_1H_0P_1-P_1VP_2g_{P_2}P_2VP_1)\tilde{\Phi}'_{P_1}=0\ .\tag{9}$$

The tilde indicates an operator or function modified by coupling between the P spaces, while the prime reflects the influence of the P_2 space on the P_1-space functions, or vice versa. At this point in the development, the prime may be considered to be a redundant label.

The corresponding P_1-space propagator is given formally by

$$\tilde{g}'_{P_1}=(E-P_1H_0P_1-P_1VP_2g_{P_2}P_2VP_1)^{-1}\ .\tag{10}$$

As per the development leading up to Eq. (15) (of paper I), the individual Q-space wave functions $\Psi_{Q_\alpha}\equiv\langle\alpha|\Psi_Q$ are then given (but still formally) by

$$\Psi_{Q_\alpha}=\sum_\beta(\Omega^{-1})_{\alpha\beta}G_{Q\beta}\langle\beta|\tilde{V}'P_1\tilde{\Phi}'_{P_1}\ ,\tag{11}$$

where the $\langle\alpha|$ are eigenstates of QH_0Q, such that $\langle\alpha|QH_0Q=\langle\alpha|\varepsilon_\alpha$, and the Q-space propagator is

$$G_{Q\alpha}\equiv(E-\varepsilon_\alpha-\langle\alpha|DRg_RRD|\alpha\rangle-\langle\alpha|VP_2g_{P_2}P_2V|\alpha\rangle$$
$$-\langle\alpha|\tilde{V}'P_1\tilde{g}'_{P_1}P_1\tilde{V}'|\alpha\rangle)^{-1}\ . \tag{12}$$

The Q-space mixing operator Ω has the elements

$$\Omega_{\alpha\beta}=\delta_{\alpha\beta}-(1-\delta_{\alpha\beta})G_{Q\alpha}\Lambda_{\alpha\beta}\ , \tag{13}$$

which depend upon the interaction Λ, with elements

$$\Lambda_{\alpha\beta}\equiv\langle\alpha|DRg_RRD|\beta\rangle+\langle\alpha|VP_2g_{P_2}P_2|\beta\rangle$$
$$+\langle\alpha|\tilde{V}'P_1\tilde{g}'_{P_1}P_1\tilde{V}'|\beta\rangle\ . \tag{14}$$

The formal DR probability amplitude, from Eq. (8) (of paper I), is then

$$M^{\rm DR}=\langle\Phi_RRDQ\Psi_Q\rangle$$
$$=\sum_\alpha\langle\Phi_RRD|\alpha\rangle\Psi_{Q\alpha}$$
$$=\sum_\alpha\langle\Phi_RRD|\alpha\rangle\sum_\beta(\Omega^{-1})_{\alpha\beta}G_{Q\beta}\langle\beta|\tilde{V}'P_1\tilde{\Phi}'_{P_1}\rangle\ . \tag{15}$$

In order to facilitate actual calculations based on Eq. (15), it is first necessary to construct explicit solutions for $\tilde{\Phi}'_{P_1}$, the coupled asymptotic state in the incoming channel, and $\tilde{g}'_{P_1}$, the coupled P_1-space propagator. To this purpose, the momentum in the incoming channel is discretized. Of equal importance, generally, the P_2-space projection operator P_2 and propagator g_{P_2}, must be defined more carefully. However, if the P_2 space contains just a single state, then these operators need no further definition. This simplest case will be considered next. In Sec. IV results obtained here will be generalized to include an arbitrary number of P_2-space states. With these stipulations, Eq. (9) becomes

$$(E-\varepsilon_{P_i}-\langle i|VP_2g_{P_2}P_2V|i\rangle)\tilde{\Phi}'_{P_1i}$$
$$=\sum_{j\neq i}\langle i|VP_2g_{P_2}P_2V|j\rangle\tilde{\Phi}'_{P_1j}\ , \tag{16}$$

where i (or j) labels the initial target state, incoming continuum partial wave, and a particular value of the incoming continuum electron linear momentum. The total energy in the incoming channel is $\varepsilon_{P_1i}\equiv\langle i|P_1H_0P_1|i\rangle$, and $\tilde{\Phi}'_{P_1i}\equiv\langle i|\tilde{\Phi}'_{P_1}\rangle$. The solution of Eq. (16) is

$$\tilde{\Phi}'_{P_1i}=\sum_j(\omega^{-1})_{ij}\tilde{\Phi}_{P_1j}\ , \tag{17}$$

where $\tilde{\Phi}_{P_1i}$ (no prime) is the single-momentum P_1-space asymptotic wave function which solves

$$(E-\varepsilon_{P_1i}-\langle i|VP_2g_{P_2}P_2V|i\rangle)\tilde{\Phi}_{P_1i}=0\ , \tag{18}$$

and the P-space mixing operator ω has the elements

$$\omega_{ij}=\delta_{ij}-(1-\delta_{ij})\tilde{g}_{P_1i}\lambda_{ij}\ . \tag{19}$$

In Eq. (19), the single (linear) -momentum P_1-space propagator is given by

$$\tilde{g}_{P_1i}=(E-\varepsilon_{P_1i}-\langle i|VP_2g_{P_2}P_2V|i\rangle)^{-1}\ , \tag{20}$$

(no prime) and the P-space interaction λ has the elements

$$\lambda_{ij}=\langle i|VP_2g_{P_2}P_2V|j\rangle\ . \tag{21}$$

By the same means, the full P_1-space propagator is obtained as

$$\langle i|\tilde{g}'_{P_1}|j\rangle=(\omega^{-1})_{ij}\tilde{g}_{P_1j}\ . \tag{22}$$

in Eqs. (17), (19), and (21), if only a single continuum electron linear momentum participates, then $\omega=\delta$. In general, Eqs. (11), (12), and (14) for the Q-space wave functions, and mixing operators Ω and Λ are valid, but now Eqs. (17) and (22) describe the relevant coupled P_1-space functions. This completes the explicit solution of the coupled (P, Q, and R spaces) channel recombination problem, for two P-space states, and without direct radiative coupling between initial (P space) and final (R space) states. Both the generalization to more than two P-states, and the inclusion of direct radiative coupling can be performed *ex post facto*. See Sec. IV.

III. MODEL PROBLEMS

In this section, two model problems will be considered. In both models, the pole approximation will be invoked, and a single continuum electron linear momentum will be assumed ($\omega=\delta$). Formulas derived in Sec. II will be employed. As described in paper II, by the pole approximation we mean that the real parts of all P- and R-space propagators are set equal to zero.

(a) In the first model, a target ground state with two coupled continuum partial waves, one singly excited target state, and a set of fully interacting resonances in the (closed) excitation channel is assumed. For example, a process of the form

$$2p+k_{i1}(l_{i1}=0)\leftrightarrow 3dnp\rightarrow 2pn'p+\gamma$$
$$\leftrightarrow 3dnp\rightarrow 2p+k_{i2}(l_{i2}=2)\quad(n\geq 3)\ , \tag{23}$$

in LSJ coupling ($L=1$), is such a case.

In Eq. (23), the ground and first excited target states are labeled by $2p$ and $3d$, respectively, while $l_{i1}=0$ denotes the incoming electron continuum partial wave. A similar equation holds when $L=1$ with the roles of i_1 and i_2 reversed; i.e., in which the incoming continuum partial wave is $l_{i1}=2$. For $L=3$, an analogous equation holds in which $l_{i1}=2$ and $l_{i2}=4$ (or $l_{i1}=4$ and $l_{i2}=2$) are coupled.

The Rydberg series of resonances $3dnp$ ($n\geq 3$) is fully interacting in the sense of paper I. To recapitulate, by fully interacting Q-space states we mean the following: (i) First, the individual Q-space states (labled by $nLSJ$) are assumed to already diagonalize the Q-space Hamiltonian. Thus n is intended to be only an effective principle quantum number. (ii) Second, these Q-space states interact further via coupling to the P and R spaces, through the mixing operator Ω [Eq. (13)]. Note that, in analogy to (i), we intend $2pn'p$ to represent one of a set of R-space states which already diagonalizes the R-space Hamiltonian.

Thus n' is also an effective principal quantum number.

For this example, the full P_1-space propagator, from Eqs. (20) and (22), is

$$\begin{aligned}\langle i|\tilde{g}'_{P_1}|i\rangle &= \langle i|\tilde{g}_{P_1}|i\rangle \\ &\equiv \tilde{g}_{P_1 i} \\ &= (1-g_{P_1 i}\langle i|P_1 V P_2 g_{P_2} P_2 V P_1|i\rangle)^{-1} g_{P_1 i} ,\end{aligned} \tag{24}$$

where $g_{P_1 i}$ is given by

$$g_{P_1 i} = (E-\varepsilon_{P_1 i})^{-1} . \tag{25}$$

Then, in the pole approximation,

$$\tilde{g}'_{P_1 i} = (1+k_{i1}k_{i2}V_{12}^2/4)^{-1} g_{P_1 i} \equiv U_{12} g_{P_1 i} , \tag{26}$$

which defines U_{12}, and where

$$V_{12} \equiv \langle i_1|V|i_2\rangle \tag{27}$$

and

$$\begin{aligned}k_{i1} &= (2E)^{1/2} , \\ k_{i2} &= [2(E-\Delta_{12})]^{1/2} .\end{aligned} \tag{28}$$

In Eq. (28), the target ground-state energy is set equal to zero and the target excitation energy is denoted by $\Delta_{12}=\varepsilon_{3d}-\varepsilon_{2p}$ ($\Delta_{12}>0$).

Continuing, from Eqs. (17), (18), and (26), the full asymptotic incoming wave is

$$\tilde{\Phi}'_{P_1 i} = \tilde{\Phi}_{P_1 i} = U_{12}\Phi_{P_1 i} , \tag{29}$$

where the uncoupled asymptotic initial state $\Phi_{P_1 i}$ solves

$$(E-\varepsilon_{P_1 i})\Phi_{P_1 i} = 0 . \tag{30}$$

Then, from Eqs. (7) and (8), the exact incoming wave is

$$\begin{aligned}\Psi_{P_1 i} &= U_{12}\Phi_{P_1 i} + U_{12} g_{P_1 i} \sum_\alpha \langle i_1|\tilde{V}'|\alpha\rangle \Psi_{Q\alpha} \\ &\equiv U_{12}\Phi_{P_1 i} + U_{12} g_{P_1 i} \sum_\alpha \tilde{V}'_{1\alpha}\Psi_{Q_\alpha} ,\end{aligned}$$

$$\begin{aligned}\Psi_{P_1 i} &= U_{12}\Phi_{P_1 i} \\ &\quad + U_{12} g_{P_1 i} \sum_\alpha [V_{1\alpha} - (ik_{i2}/2)V_{12}V_{2\alpha}]\Psi_{Q\alpha} ,\end{aligned} \tag{31}$$

having inserted a set of Q-space states labeled by α; i.e., where, from Eq. (23), α enumerates the states $3d3p$, $3d4p$, $3d5p$, ...

From Eq. (11), the Q-space states become

$$\Psi_{Q_\alpha} = U_{12} \sum_\beta (\Omega^{-1})_{\alpha\beta} G_{Q_\beta} \tilde{V}'_{\beta 1} , \tag{32}$$

where, from Eq. (13), the matrix elements of the Q-space mixing operator are

$$\Omega_{\alpha\beta} = \delta_{\alpha\beta} + (1-\delta_{\alpha\beta})(i/2) G_{Q\alpha}\Gamma(\alpha,\beta) , \tag{33}$$

the Q-space propagator is

$$\begin{aligned}G_{Q_\alpha} &= \{E-\varepsilon_{Q\alpha} + U_{12}[k_{i1}k_{i2}V_{12}^2 A_{a1}(\alpha)A_{a2}(\alpha)]^{1/2} \\ &\quad + (i/2)[\Gamma_r(\alpha) + U_{12}A_{a1}(\alpha) + U_{12}A_{a2}(\alpha)]\}^{-1} ,\end{aligned} \tag{34}$$

and the Q-space "widths" are given by

$$\Gamma(\alpha,\beta) = \sum_f k_\gamma^2 D_{\alpha f} D_{f\beta} + k_{i2}V_{\alpha 2}V_{2\beta} + U_{12}k_{i1}\tilde{V}'_{\alpha 1}\tilde{V}'_{1\beta} , \tag{35}$$

$$\begin{aligned}A_{a1}(\alpha) &= k_{i1}V_{\alpha 1}^2 , \\ A_{a2}(\alpha) &= k_{i2}V_{\alpha 2}^2 , \\ \Gamma_r(\alpha) &= \sum_f k_\gamma^2 D_{\alpha f}^2 .\end{aligned} \tag{36}$$

From Eq. (17) in paper I, the DR probability is then, for the process of Eq. (23),

$$\begin{aligned}P_{i1}^{\mathrm{DR}} &= U_{12}^2 k_{i1} \sum_{n''} \Big| \sum_n \sum_{n'} k_\gamma D_{n''n}(\Omega^{-1})_{nn'} G_{Qn'} \tilde{V}'_{n'i1} \Big|^2 \\ &= U_{12}^2 A_{r0} k_{i1} \sum_{n''} \Big| \sum_{n'} (\Omega^{-1})_{n''n'} G_{Qn'} \\ &\quad \times [V_{n'1} - (ik_{i2}/2)V_{n'2}V_{21}] \Big|^2\end{aligned} \tag{37}$$

for the partial wave labeled by i_1; a similar expression holds for P_{i2}^{DR}, but with the roles of 1 and 2 reversed. In Eq. (37), $A_{r0}=k_\gamma^2\langle D\rangle^2$ is the $3d\rightarrow 2p$ radiative probability, assumed independent of n, the principal quantum number of the spectator electron; i.e., $D_{n''n}=\langle D\rangle\delta_{n''n}$. Note that in Eq. (17) of paper I, the factors k_{i1} and k_γ did not appear explicitly, but were "understood" to occur. See Eq. (78) of paper II for a more complete understanding of the origin of these factors.

(b) Next, an example of DR is treated in which two singly excited target states exist, but in which the total energy is below the threshold for impact excitation of the uppermost state. Just one projectile electron-continuum partial wave is assumed to occur in both the initial (ground) and first excited-target-state channels. The two channels exhibit continuum-continuum coupling in the sense of Eq. (9). Two series of fully interacting (through the P space) resonances are included; e.g.,

$$\begin{aligned}&1s+k_{i1}(l_{i1}=1) \leftrightarrow 2snp \rightarrow 1s2s+\gamma \quad (n\geq 2) , \\ &1s+k_{i1}(l_{i1}=1) \leftrightarrow 2pn's \rightarrow 1sn''s+\gamma \quad (n'\geq 3) , \\ &1s+k_{i1}(l_{i1}=1) \leftrightarrow 2pn's \rightarrow 2s+k_{i2}(l_{i2}=1) \quad (n'\geq n_x) ,\end{aligned} \tag{38}$$

where P_1 projects onto $1s+k_{i1}(l_{i1}=1)$, P_2 projects onto $2s+k_{i2}(l_{i2}=1)$, and LSJ coupling is assumed. The ground and first two excited target states are labeled $1s$, and $2s$ and $2p$, respectively. The threshold value of n', at or above which the process $2pn's\rightarrow 2s+k_{i2}l_{i2}$ is energetically allowed, is denoted n_x. The minimum energy required to make the $1s\rightarrow 2s$ transition is denoted $\Delta_{12}=\varepsilon_{2s}-\varepsilon_{1s}$ ($\Delta_{12}>0$), so that on the energy shell one has that $k_{i2}^2=k_{i1}^2-2\Delta_{12}>0$, when the $2s$ channel is open.

The minimum energy required to make the $1s \rightarrow 2p$ transition is denoted $\Delta_{13} = \varepsilon_{2p} - \varepsilon_{1s}$. In all of what follows, we assume that the $2p$ channel remains closed ($k_{i1}^2 < 2\Delta_{13}$).

Now, Eqs. (31)–(36) remain valid. From Eq. (37), the DR probability is

$$P^{\mathrm{DR}} = U_{12}^2 k_{i1} \sum_f \left| \sum_\alpha \sum_\beta k_\gamma D_{f\alpha} (\Omega^{-1})_{\alpha\beta} G_{Q\beta} \tilde{V}'_{\beta i1} \right|^2 , \quad (39)$$

where f enumerates the states $1s2s, 1s3s, 1s4s, \ldots$, and α labels the states $2s2p, 2s3p, 2s4p, \ldots$, and $2p3s, 2p4s, 2p5s, \ldots$. Note that if the continuum energy is at or below the first excited-state threshold ($2s$ channel closed) $k_{i1}^2 \leq 2\Delta_{12}$, then in the pole approximation all quantities proportional to k_{i2} are zero; e.g., in Eq. (34), $A_{a2} = 0$, $U_{12} = 1$; in Eq. (35), $\tilde{V}' = V$; etc.

With reference to Eq. (39), one sees that our formulation of P^{DR} includes the effects of (a) an interaction between resonances, mediated by the generally nondiagonal mixing operator Ω (Ω mixes Q-space states via interaction with the P and R spaces); (b) a further shifting of the positions and widths of individual responces due to a coupling between the P_1 and P_2 spaces [as reflected, in Eq. (34), by the presence of U_{12}]; (c) the interference between resonances mandated by the coherent sum of resonant amplitudes appearing in Eq. (39). This formulation of P^{DR} conserves probability; see the remarks following Eq. (47).

Based on Eq. (39), we performed calculations with this model when

$$(k_{i1})^{1/2} V(2snp \rightarrow 1s + k_{i1} l_{i1}) \equiv (A_{a01}/n^3)^{1/2} \quad \text{for } n \geq 2 ,$$

$$(k_{i1})^{1/2} V(2pn's \rightarrow 1s + k_{i1} l_{i1}) \equiv (A_{a02}/n'^3)^{1/2} \quad \text{for } n' \geq 3 ,$$

$$(k_{i2})^{1/2} V(2pn's \rightarrow 2s + k_{i2} l_{i2}) \equiv (A_{a03}/n'^3)^{1/2} \quad \text{for } n' \geq n_x ,$$

and

$$k_\gamma D(2snp \rightarrow 1s2s + \gamma) \equiv (8A_{r0}/n^3)^{1/2} ,$$

$$k_\gamma D(2pn's \rightarrow 1sn''s + \gamma) \equiv (A_{r0})^{1/2} \delta_{n'n''} .$$

The dependence on principal quantum n of Auger and bound-bound radiative transition probabilities described here is consistent with the well-known behavior of these quantities.[17]

Results of these calculations appear in Figs. 1–4. In all cases, we chose $A_{r0} = 2.0 \times 10^{-5}$, $n_x = 18$, and $\Delta_{23} \equiv \Delta_{13} - \Delta_{12} = \varepsilon_{2p} - \varepsilon_{2s} = 1.54 \times 10^{-3}$ (parameters which are appropriate, approximately, for a C^{5+} target ion). The range of included Rydberg states was always $10 \leq n \leq 40$ and $10 \leq n' \leq 65$, and the zero of total energy E was placed at the $2s$ threshold. Because of the upper n' cutoff, values of P^{DR} obtained for $E > 1.4 \times 10^{-3}$ may be inaccurate (Figs. 1, 3, and 5); because of the upper n cutoff, values of P^{DR} obtained for $-0.27 \times 10^{-3} < E < 0.0$ are also suspect (Figs. 2 and 3). For the purpose of evaluating Rydberg state energies, and in order to facilitate comparison with results appearing in paper I, we choose $Z = 1$.

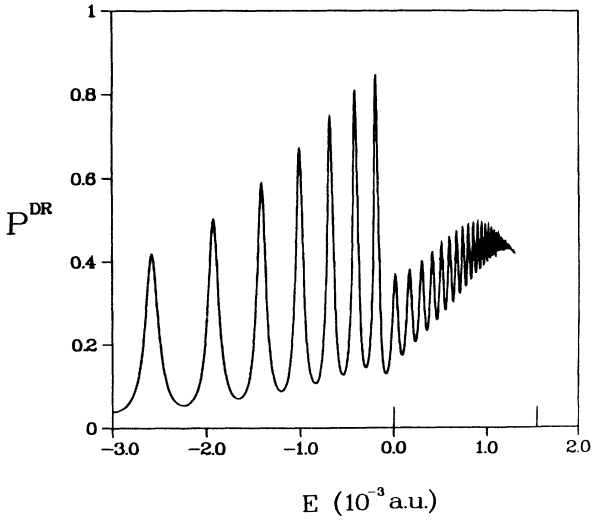

FIG. 1. P^{DR} vs E; for model (b), when $A_{a01} = 0.0$, $A_{a02} = A_{a03} = 0.2$, and $A_{r0} = 2.0 \times 10^{-5}$; the zero of E is set at the $2s$ threshold; both the $2s$ and $2p$ thresholds are indicated by vertical lines.

In Fig. 1, we plot P^{DR} versus E when $A_{a01} = 0.0$ and $A_{a02} = A_{a03} = 0.2$; in Fig. 2, we plot P^{DR} when $A_{a01} = 0.2$ and $A_{a02} = A_{a03} = 0.0$; and in Fig. 3, we plot P^{DR} when $A_{a01} = A_{a02} = A_{a03} = 0.2$. An overlay of Figs. 1 and 3 appears in Fig. 4, for a limited range of energies. Note from Fig. 4 that the effect of the $2snp$ resonances on P^{DR} is not negligible. For example, the integral of P^{DR} over $-2.0 \times 10^{-3} \leq E \leq -0.4 \times 10^{-3}$ is equal to 4.17×10^{-4} if $A_{a01} = 0.0$ (dashed curve in Fig. 4), while the corresponding quantity is equal to 3.54×10^{-4} when $A_{a01} = 0.2$ (solid curve in Fig. 4). This is in spite of the fact that the $2snp$ resonances themselves make only a very few small contribution to P^{DR}, when considered in isolation from the $2pn's$ resonances (see Fig. 2). The limits on the range of n and n' in these models are $10 \leq n \leq 40$ and $10 \leq n' \leq 65$.

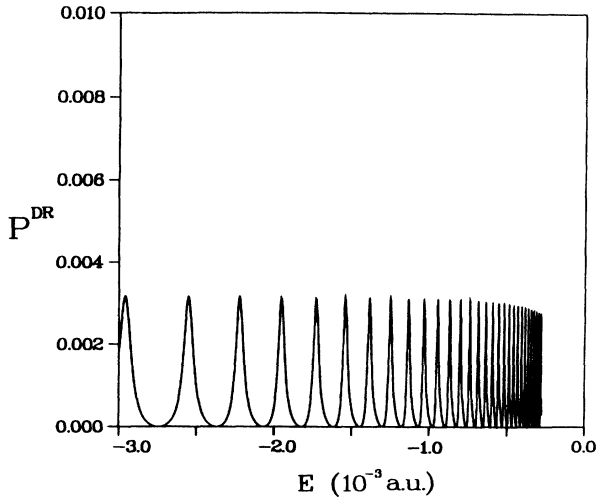

FIG. 2. Same as Fig. 1, except $A_{a01} = 0.2$ and $A_{a02} = A_{a03} = 0.0$.

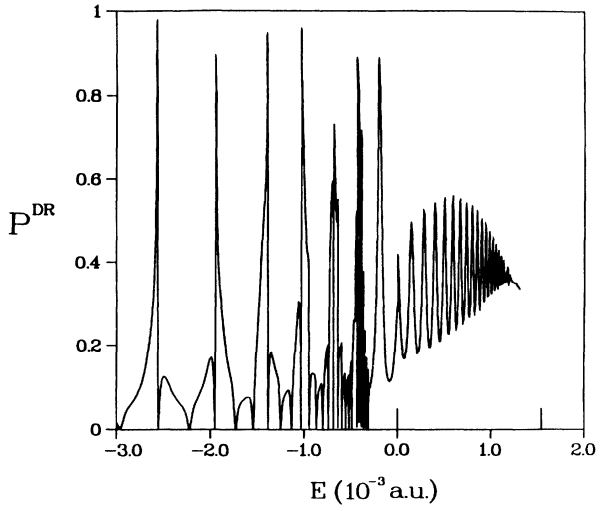

FIG. 3. Same as Fig. 1, except $A_{a01}=A_{a02}=A_{a03}=0.2$.

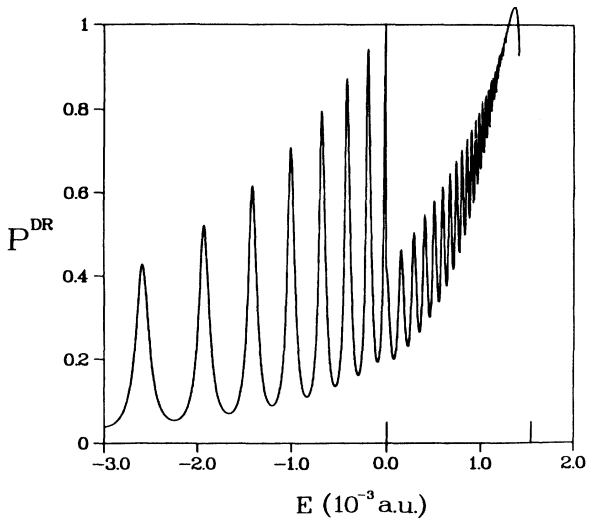

FIG. 5. Same as Fig. 1, except P^{DR} obtained in the isolated resonance approximation.

For further comparison, in Fig. 5 we plot P^{DR} computed in the isolated resonance approximation (IRA; see paper I), when $A_{a01}=0.0$ and $A_{a02}=A_{a03}=0.2$. Figure 5 should be compared with Fig. 1. As remarked previously in paper I, the IRA is especially bad when resonances interact, since it does not conserve probability; i.e., P^{DR} can be greater than 1 in the IRA. We note, finally, that the case $A_{a01}=A_{a03}=0.0$, $A_{a02}=0.2$ has already been considered; see Fig. 1 of paper I.

(c) Lastly in this section, we consider the excitation process allowed in model (b). For this model, a direct excitation must follow the path

$$1s+k_{i1}l_{i1}\rightarrow 2s+k_{i2}l_{i2}\ , \tag{40}$$

with the probability amplitude being given by

$$M^{DE}=\langle \Phi_{P_2}P_2VP_1\Psi_{P_1}\rangle\ . \tag{41}$$

A resonance excitation follows the path

$$1s+k_{i1}l_{i1}\rightarrow 2pn's\rightarrow 2s+k_{i2}l_{i2} \tag{42}$$

and has the probability amplitude

$$M^{RE}=\langle \Phi_{P_2}P_2VQ\Psi_Q\rangle\ . \tag{43}$$

The total probability for excitation is then

$$P^{ex}=k_{i1}k_{i2}|M^{DE}+M^{RE}|^2\ , \tag{44}$$

when $k_{i2}^2=k_{i1}^2-2\Delta_{12}>0$, where $\Delta_{12}=\varepsilon_{2s}-\varepsilon_{1s}$. In Eqs. (41) and (43), Φ_{P_2} solves the equation

$$(E-P_2H_0P_2)\Phi_{P_2}=0\ . \tag{45}$$

Then, from Eqs. (31)–(36),

$$\begin{aligned} M^{DE}&=U_{12}V_{21}+U_{12}V_{21}(-ik_{i1}/2)\sum_\alpha \tilde{V}'_{1\alpha}\Psi_{Q\alpha}\ ,\\ M^{RE}&=\sum_\alpha V_{2\alpha}\Psi_{Q\alpha}\ , \end{aligned} \tag{46}$$

where

$$\Psi_{Q\alpha}=\sum_\beta(\Omega^{-1})_{\alpha\beta}G_{Q\beta}\tilde{V}'_{\beta 1}U_{12}\ , \tag{47}$$

and, from Eq. (23), α (and β) enumerate the resonance states $2pn_xs,2p(n_x+1)s,2p(n_x+2)s,\ldots$. More precisely, α (and β) may be said to enumerate all of the $2snp$ and the $2pn's$ ($n<n_x$) states as well. The effect of these "far from resonance" states on P^{ex} may not be small.

With reference to Eqs. (44) and (46), and as per the remarks following Eq. (39), we point out that our formulation of P^{ex} includes the effects of (a) interaction between resonances, as mediated by Ω (Ω mixes Q-space states via interaction with the P and R spaces); (b) further shifting of the positions and widths of individual resonances due

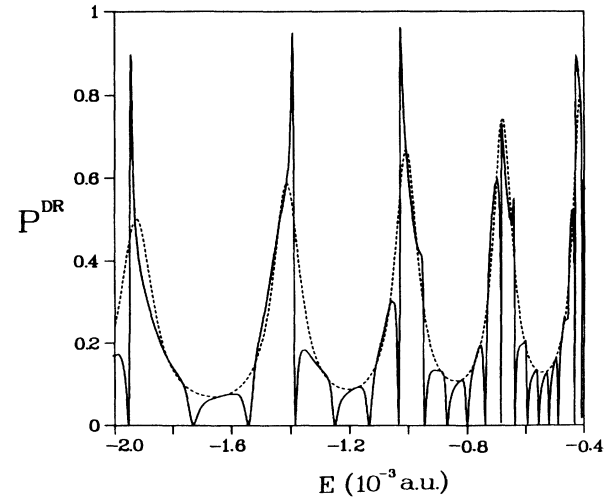

FIG. 4. P^{DR} vs E; for model (b), when $A_{r0}=2.0\times10^{-5}$ and $A_{a01}=A_{a02}=A_{a03}=0.2$ (solid curve); $A_{a01}=0.0$, $A_{a02}=A_{a03}=0.2$ (dashed curve).

to coupling between the P_1 and P_2 spaces [as reflected, in Eq. (34), by the presence of U_{12}]; (c) interference between resonances, and between resonant and direct scattering processes, mandated by the coherent sum of scattering amplitudes in Eq. (44). This formulation of P^{ex} (and P^{DR}) conserves probability; i.e., $0 \le P^{ex}+P^{DR} < 1$.

In Fig. 6, we plot P^{ex} versus E for the set of parameters adopted in model (b) and when $A_{a01}=0.0$, $A_{a02}=A_{a03}=0.2$ (solid curve); for comparison, P^{DR} appears (dashed curve), as well as the total inelastic probability $P^{DR}+P^{ex}$ (dotted curve). In Fig. 7, P^{ex} is plotted when $A_{a01}=A_{a02}=A_{a03}=0.2$ (solid curve); for comparison again, P^{DR} appears (dashed curve), as well as the total inelastic probability $P^{DR}+P^{ex}$ (dotted curve). In both Figs. 6 and 7, the elastic scattering probability is $1-P^{DR}-P^{ex}$, for $k_{i1}^2 < 2\Delta_{13}$; i.e., below the threshold for $2p$ excitation.

A comparison of Figs. 6 and 7 shows that, for this choice of model parameters, the effect of the resonance $2pns$ states on P^{ex} is not small. For example, the value of P^{ex} integrated over the range $\Delta_{12} \le E \le \Delta_{13}$ is 3.3×10^{-4} when $A_{a01}=0.0$ (resonance excitation only; the solid curve in Fig. 6), while the corresponding quantity obtained when $A_{a01}=0.2$ is 8.5×10^{-4} (resonance plus direct excitation; the solid curve in Fig. 7). Recall that the zero of total energy has been set at the $2s$ threshold. Limitations on the range of n and n' are as was described previously for model (b). Values of P^{ex} for $1.42\times10^{-3} < E < 1.54\times10^{-3}$ are therefore suspect since resonances $2pn's$ for $n' > 65$ have been omitted from the calculation.

We note that our prediction of the direct excitation probability, in the absence of resonances (in the pole approximation and when only a single continuum electron linear momentum contributes), is

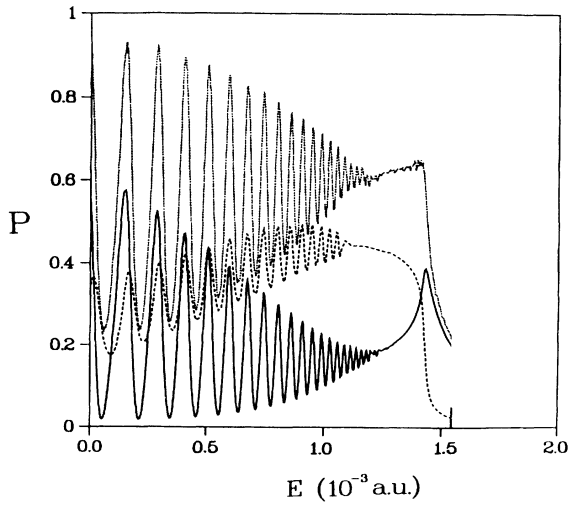

FIG. 6. P^{ex} (solid curve), P^{DR} (dashed curve), and $P^{ex}+P^{DR}$ (dotted curve), all vs E; for model (c), when $A_{a01}=0.0$, $A_{a02}=A_{a03}=0.2$, and $A_{r0}=2.0\times10^{-5}$.

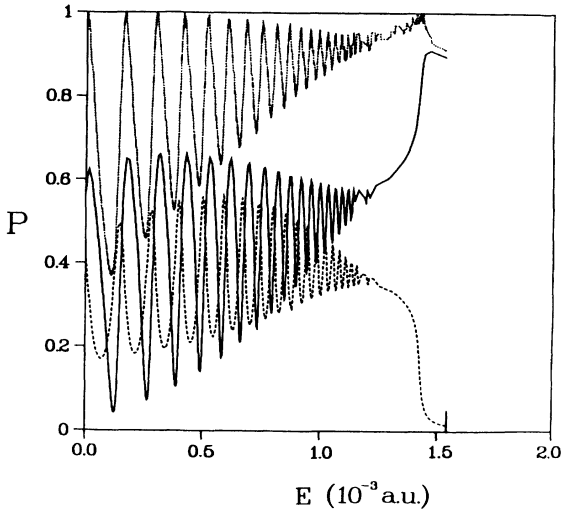

FIG. 7. Same as Fig. 6, except $A_{a01}=A_{a02}=A_{a03}=0.2$.

$$P^{DE}=k_{i1}k_{i2}|M^{DE}|^2=k_{i1}k_{i2}U_{12}^2V_{12}^2$$
$$=k_{i2}k_{i2}V_{12}^2/(1+k_{i1}k_{i2}V_{12}^2/4)^2 , \quad (48)$$

having used Eqs. (26), (44), and (46). This prediction agrees with the MQDT result for this model, only up to terms of order V_{12}^4, the MQDT result being given by[18]

$$P^{DE}=1-\exp(-k_{i1}k_{i2}V_{12}^2) . \quad (49)$$

The reason for this discrepancy is not yet apparent.

IV. GENERALIZATIONS

We made the two following generalizations.

(1) We consider the generalization of the preceding results to more than two P-space states. Specifically, for the case of three P-space states, one has the following. The propagator for the P_3 space satisfies an equation analogous to Eq. (5); i.e.,

$$g_{P_3}=(E-P_3H_0P_3) , \quad (50)$$

while now the P_2-space propagator satisfies an equation similar to Eq. (9):

$$\tilde{g}'_{P_2}=(E-P_2VP_3g_{P_3}P_3VP_2)^{-1} . \quad (51)$$

The P_1-space propagator is then, instead of Eq. (9),

$$\tilde{g}''_{P_1}=(E-P_1VP_3g_{P_3}P_3VP_1-P_1\tilde{V}'P_2\tilde{g}'_{P_2}P_2\tilde{V}'P_1)^{-1} , \quad (52)$$

where

$$\tilde{V}'=V+VP_3g_{P_3}P_3V . \quad (53)$$

The full P_1-space wave function is given by, instead of Eq. (7),

$$\Psi_{P_1}=\tilde{\Phi}''_{P_1}+\tilde{g}''_{P_1}P_1\tilde{V}''Q\Psi_Q , \quad (54)$$

where $\tilde{\Phi}''_{P_1}$ is the solution of

$$(E-P_1H_0P_1-P_1VP_3g_{P_3}P_3VP_1 - P_1\tilde{V}'P_2\tilde{g}'_{P_2}P_2\tilde{V}'P_1)\tilde{\Phi}''_{P_2}=0 , \quad (55)$$

and where

$$\tilde{V}''=\tilde{V}'+\tilde{V}'P_2\tilde{g}'_{P_2}P_2\tilde{V}' . \quad (56)$$

The full Q-space propagator is, instead of Eq. (12),

$$G_{Q\alpha}=(E-\varepsilon_{Q\alpha}-\langle\alpha|DRg_RRD|\alpha\rangle-\langle\alpha|VP_3g_{P_3}P_3V|\alpha\rangle - \langle\alpha|\tilde{V}'P_2\tilde{g}'_{P_2}P_2\tilde{V}'|\alpha\rangle - \langle\alpha|\tilde{V}''P_1\tilde{g}''_{P_1}P_1\tilde{V}''|\alpha\rangle)^{-1} . \quad (57)$$

From Eq. (14), the Q-space interaction now has the elements

$$\Lambda_{\alpha\beta}=\langle\alpha|DRg_RRD|\beta\rangle+\langle\alpha|VP_3g_{P_3}P_3V|\beta\rangle + \langle\alpha|\tilde{V}'P_2\tilde{g}'_{P_2}P_2\tilde{V}'|\beta\rangle + \langle\alpha|\tilde{V}''P_1\tilde{g}''_{P_1}P_1\tilde{V}''|\beta\rangle , \quad (58)$$

and, from Eq. (15), the DR probability amplitude is now

$$M^{\mathrm{DR}}=\sum_\alpha\langle\Phi_RRD|\alpha\rangle\sum_\beta(\Omega^{-1})_{\alpha\beta}G_{Q\beta}\langle\beta|\tilde{V}''P_1\tilde{\Phi}''_{P_1}\rangle . \quad (59)$$

This completes the description of the three-state P-space case. Formulas for the case of four or more P-space states can be obtained from Eqs. (48)–(57) by induction.

(ii) Finally, as per the transition from the formulas of paper I to those of paper II, in which relevant operators and functions were modified to take account of direct radiative coupling between initial (target plus continuum) and final (recombined) states, the formulas of the present work can be correspondingly altered in order to include these effects. For example, when the P space contains just two states, so that Eqs. (2)–(22) hold, then the effect of RDP coupling is to modify the preceding formulas as follows. The asymptotic P_1-space wave function solves, instead of Eq. (9), the equation

$$(E-P_1H_0P_1-P_1DRg_RRDP_1 - P_1\underline{V}P_2\underline{g}_{P_2}P_2\underline{V}P_1)\tilde{\underline{\Phi}}'_{P_1}=0 , \quad (60)$$

where, as in Eqs. (13) and (15), respectively, of paper II,

$$\underline{V}=V+DRg_RRD , \quad (61)$$

$$\underline{g}_{P_2}=(E-P_2H_0P_2-P_2DRg_RRDP_2)^{-1} , \quad (62)$$

and g_R is still given by Eq. (6). In Eq. (60), $\tilde{\underline{\Phi}}'_{P_1}$ has been underlined in order to denote the RDP coupling. Similarly, the propagator in the Q space is now, instead of Eq. (12),

$$\underline{G}_{Q\alpha}=(E-\varepsilon_{Q\alpha}-\langle\alpha|DRg_RRD|\alpha\rangle-\langle\alpha|\underline{V}P_2\underline{g}_{P_2}P_2\underline{V}|\alpha\rangle - \langle\alpha|\tilde{\underline{V}}'P_1\underline{\tilde{g}}'_{P_1}P_1\tilde{\underline{V}}'|\alpha\rangle)^{-1} , \quad (63)$$

and where, instead of Eq. (8) for $\tilde{V}'$, one has that

$$\tilde{\underline{V}}'=\underline{V}+\underline{V}P_2\underline{g}_{P_2}P_2\underline{V} , \quad (64)$$

and instead of Eq. (10) for $\tilde{g}'_{P_1}$,

$$\underline{\tilde{g}}'_{P_1}=(E-P_1H_0P_1-P_1DRg_RRDP_1 - P_1\underline{V}P_2\underline{g}_{P_2}P_2\underline{V}P_1)^{-1} . \quad (65)$$

The formulas appearing in Eqs. (2)–(59) can now all be modified to take account of RDP coupling by making the following two changes throughout: (1) $P_jH_0P_j \rightarrow P_j(H_0+DRg_RRD)P_j$, for each of the P-space states labeled by j; and (2) $V\rightarrow\underline{V}$, where $\underline{V}$ appears in Eq. (61). Details will be deferred to a future publication.

V. SUMMARY

The results described in this paper may facilitate calculations of DR probabilities and excitation probabilities, which are more accurate than those available today. These formulas can account for the effects of interaction and interference between resonances, and interference between resonance and direct processes, in the case of both excitation and recombination. They can self-consistently describe the effects of autoionization into an excited target state during both recombination[3] and excitation, including the effects of interference. They can describe the effect of radiation damping on the excitation process.[19,20] The effect of radiation damping on recombination alone has been discussed in paper II.

One concludes from this work that the effects of interchannel coupling on P^{DR} will not always be negligible. In model (b), P^{DR}, integrated over a range of energies, was reduced by $\sim 15\%$ when such coupling (between $2s$ and $2p$ excitation channels, and the Q-space states) was included. Nor can the effects of interchannel coupling be neglected, generally, in calculations of P^{ex}. In model (c), approximately 40% of P^{ex} arose from resonance excitation.

Recall that, in paper I, a demonstration of the importance of coupling among the Q-space states (via interaction with a single P-space state) in calculations of P^{DR} was given; and in paper II, the importance of a proper inclusion of direct radiative coupling between initial and final states was discussed. In the light of these results, it seems reasonable to expect that future accurate calculations of P^{DR} and P^{ex} for real systems, should include many, if not all, of these interaction and interference effects.

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