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DIELECTRONIC RECOMBINATION THEORY

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INTRODUCTION

A theory now in wide use for the calculation of dielectronic recombination cross sections (σ^{DR}) and rate coefficients (α^{DR}) was one introduced originally by Feshbach[1] for nuclear physics applications, and then later adapted for atomic scattering problems by Hahn[2]. In the following, we briefly review this theory in a very general form, which allows one to account for the effects of overlapping and interacting resonances, as well as continuum-continuum coupling. An extension of our notation will then also allow for the inclusion of the effects of direct radiative recombination, along with a treatment of the interference between radiative and dielectronic recombination. Other approaches to the calculation of σ^{DR} have been described by Fano[3] and by Seaton[4]. We will not consider those theories here.

Calculations of α^{DR} have progressed considerably over the last 25 years, since the early work of Burgess[5]. Advances in the reliability of theoretical predictions have also been promoted recently by a variety of direct laboratory measurements[6-11] of σ^{DR}.

While the measurements of σ^{DR} for $\Delta n \neq 0$ excitations have tended to agree very well with calculations, the case of $\Delta n = 0$ has been much more problematic. However, by invoking a mechanism originally proposed by Jacobs[12], which takes into account the effect of stray electric fields on high Rydberg states (HRS) participating in the DR process, new calculations have improved the agreement between theory and experiment for these cases[6,8,13,14]. Nevertheless, certain discrepancies still remain.

DISCUSSION

We write the hamiltonian for N+1 electrons and an ionic core as

$$H = H_0 + D \tag{1}$$

where H_0 is the hamiltonian for N+1 electrons interacting with each other via $V = \Sigma_{i<j}(1/r_{ij})$, and with a nucleus of charge Z_c through $\Sigma_i(Z_c/r_i)$, and $D \propto \Sigma_i(\vec{r}_i \cdot \vec{\epsilon})$ is the electron-photon interaction. We define the idempotent projection operators P, Q, and R such that $1_{op} = P+Q+R$, where 1_{op} is the unit operator, and $PQ=QP=QR=RQ=RP=PR=0$. The operator P projects onto states of N electrons bound, with one electron in a continuum state of the N electron ion of charge $Z_I = Z_c - N$, and no photons; Q projects onto doubly excited states of N+1 electrons bound and no photons; and R projects onto the ground and singly excited states of

N+1 electrons bound, plus one photon. The wavefunction Ψ satisfies the equation

$$H\Psi = H(P+Q+R)\Psi = E\Psi = E(P+Q+R)\Psi \quad (2)$$

for the total energy E. This single equation may be rewritten as

$$PH_0P\Psi_P + PVQ\Psi_Q = E\Psi_P \quad (3)$$

$$QH_0Q\Psi_Q + QVP\Psi_P + QDR\Psi_R = E\Psi_Q \quad (4)$$

$$RH_0R\Psi_R + RDQ\Psi_Q = E\Psi_R \quad (5)$$

where $\Psi_P \equiv P\Psi$, $\Psi_Q \equiv Q\Psi$, and $\Psi_R \equiv R\Psi$, and we ignore here temporarily the coupling between the R and P states, mediated by D (which gives rise to radiative recombination). Eqn 5 may be rewritten in terms of Ψ_Q as

$$\Psi_R = (E - RH_0R)^{-1}RDQ\Psi_Q \equiv g_RRDQ\Psi_Q \quad (6)$$

which also defines g_R. Similarly, eqn 4 may be rewritten as

$$\Psi_P = \Phi_P + (E - PH_0P)^{-1}PVQ\Psi_Q \equiv \Phi_P + g_PPVQ\Psi_Q \quad (7)$$

upon inclusion of the homogeneous solution Φ_P, for which $(PH_0P - E)\Phi_P = 0$. If eqns 6 and 7 are substituted back into eqn 4, then one obtains an equation for Ψ_Q which is

$$(E - QH_0Q)\Psi_Q = QDRg_RRDQ\Psi_Q + QVP(\Phi_P + g_PPVQ\Psi_Q \quad (8)$$

with the solution

$$\Psi_Q = (E - QH_0Q - QDRg_RRDQ - QVPg_PPVQ)^{-1}QVP\Phi_P \equiv G_QQVP\Phi_P \quad (9)$$

which also defines the operator G_Q.

Since $\Psi_Q = Q\Psi$ is the projection onto doubly excited states of the exact wavefunction Ψ, then the matrix element describing the DR probability amplitude is

$$T^{DR} = <\Phi_RRDQ\Psi_Q> = <\Phi_RRDQG_QQVP\Phi_P> \quad (10)$$

where $(RH_0R - E)\Phi_R = 0$. Expanding Q in eigenstates of QH_0Q as

$$Q = \Sigma_\alpha|\alpha><\alpha| \quad (11)$$

where

$$QH_0Q|\alpha> \equiv \epsilon_\alpha|\alpha> \quad (12)$$

the DR probability $P^{DR} \equiv |T^{DR}|^2$ becomes

$$P^{DR} = |<\Phi_RRD\Sigma_\alpha|\alpha><\alpha|G_Q\Sigma_{\alpha'}|\alpha'><\alpha'|VP\Phi_P>|^2 \quad (13)$$

where integration over incoming electron and outgoing photon momenta is understood. In a region of energies where resonances are nonoverlapping and/or interactions between resonances are ignored, eqn 13 may be written as

$$P^{DR} = \Sigma_\alpha|<\Phi_RRD|\alpha>G_{Q\alpha}<\alpha|VP\Phi_P>|^2 \quad (14)$$

where $G_{Q\alpha} \equiv <\alpha|G_Q|\alpha> = (E - \epsilon_\alpha - <\alpha|DRg_RRD|\alpha> - <\alpha|VPg_PPV|\alpha>)^{-1}$, which is the usual form of the DR probability in the isolated resonance approximation (IRA).

Interacting Resonances

If resonances are interacting, then we have recourse to the following procedure. We rewrite eqn 8 as an explicit q-component equation, where q is the dimension of the Q-space, as

$$(E - \epsilon_\alpha)\Psi_{Q\alpha} = <\alpha|VP\Phi_P> + \Sigma_\beta[<\alpha|DRg_RRD|\beta> + <\alpha|VPg_PPV|\beta>]\Psi_{Q\beta} \quad (15)$$

where β and α ranges from 1 to q. Then eqn 9 becomes

$$\Psi_{Q\alpha} = (E - \epsilon_\alpha - <\alpha|DRg_RRD|\alpha> - <\alpha|VPg_PPV|\alpha>)^{-1} \quad (16)$$

$$.[<\alpha|VP\Phi_P> + \Sigma_{\beta\neq\alpha}(<\alpha|VPg_PPV|\beta> + <\alpha|DRg_RRD|\beta>)\Psi_{Q\beta}]$$

or, in a condensed notation,

$$\Psi_{Q\alpha} \equiv G_{Q\alpha}(<\alpha|VP\Phi_P> + \Sigma_{\beta\neq\alpha}\Lambda_{\alpha\beta}\Psi_{Q\beta}) \quad (17)$$

which defines $\Lambda_{\alpha\beta}$. The solution of eqn 17 is

$$\Psi_{Q\alpha} = \Sigma_\beta(\Omega^{-1})_{\alpha\beta}G_{Q\beta} <\beta|VP\Phi_P> \quad (18)$$

where Ω^{-1} is the inverse of the matrix Ω with elements

$$\Omega_{\alpha\beta} = \delta_{\alpha\beta} - (1 - \delta_{\alpha\beta})G_{Q\alpha}\Lambda_{\alpha\beta} \quad (19)$$

and $\delta_{\alpha\beta}$ is the Kronecker δ. The DR probability is then

$$P^{DR} = |\Sigma_\alpha\Sigma_\beta <\Phi_R RD|\alpha> (\Omega^{-1})_{\alpha\beta}G_{Q\beta} <\beta|VP\Phi_P>|^2 \quad (20)$$

We refer to this last equation, which includes the effects of interactions between resonances, but does not take into account radiative recombination, nor explicit continuum-continuum coupling, as the "multiple interacting resonance approximation" (MIRA).

We point out that the interactions between resonances being discussed here occur entirely through the coupling of distinct doubly excited states (eigenstates of QH_0Q)), as these make *virtual* transitions into the electron and photon continua; see eqn 16. For the purpose of this discussion, we assume that the Q-space, as well as the P and R-spaces states, have been prediagonalized. However, the subject of configuration interaction (CI) among the Q-space states alone is a significant one in its own right, and effects of this "restricted" CI have been computed for select ions[15]. Similar remarks are presumably true also for CI among the P-space states alone.

Eqn 20 can be reduced analytically for certain model problems; see ref. 16 for details. In the following, we consider three special cases.

(i) If the Q-space states do not couple through either the P or R-spaces, then $\Lambda_{\alpha\beta} = 0$ for all α and β. Consequently, $\Omega_{\alpha\beta} = \delta_{\alpha\beta}$, and eqn 20 reduces to eqn 14, which is the isolated resonance approximation (IRA). This is the trivial case.

(ii) Suppose instead that the $\Lambda_{\alpha\beta}$ are identical and nonzero for all α and β. Then eqn 20 becomes

$$P^{DR} = A_a A_r|G_{Q0}|^2|\Sigma_\alpha\Sigma_\beta(\Omega^{-1})_{\alpha\beta}|^2 \quad (21)$$

having assumed a complete degeneracy in energy of the states labeled by α, where $G_{Q0} \equiv G_{r_\alpha}$ for all α, and where we have defined the autoionization and radiative rates as

$$A_a \equiv -2Im <\alpha|VPg_PPV|\alpha> \quad (22)$$

$$A_r \equiv -2Im <\alpha|DRg_RRD|\alpha>$$

which, in this example, are the same for all α. Under these conditions, one has that

$$\Omega_{\alpha\beta} = \delta_{\alpha\beta} + \mu(1 - \delta_{\alpha\beta}) \quad (23)$$

where the complex variable μ is given by

$$\mu \equiv [i(A_a + A_r)/2]G_{Q0} \quad (24)$$

$$= [i(A_a + A_r)/2]/[E - \epsilon + i(A_a + A_r)/2]$$

so that, after a considerable amount of algebra,

$$(\Omega^{-1})_{\alpha\beta} = ([1 + (N - 2)\mu]\delta_{\alpha\beta} - \mu[1 - \delta_{\alpha\beta}])/(1 + [N - 2]\mu - [N - 1]\mu^2) \quad (25)$$

where N is the dimension of the Q-space and, in the preceding, we have ignored the real part of $\Lambda_{\alpha\beta}$. The double sum in eqn 21 becomes

$$\Sigma_\alpha \Sigma_\beta (\Omega^{-1})_{\alpha\beta} = N/[1 + (N-1)\mu] \tag{26}$$

which implies for the DR probability

$$P^{DR} = N^2 A_a A_r / |(E - \epsilon) + iN(A_a + A_r)/2|^2 \tag{27}$$

$$\sim 2\pi N A_a A_r \delta(E - \epsilon)/(A_a + A_r)$$

which is the same, for this example as the IRA result, given by eqn 14.

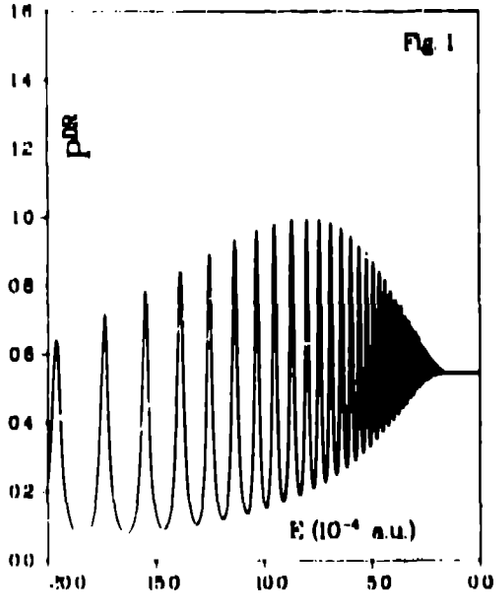
(iii) More interestingly, we suppose again that N states in the Q-space are completely degenerate in energy, the $< \alpha|VPg_PPV|\alpha >$ are again identical for all α, but now the $Im < \alpha|DRg_RRD|\beta >$ are instead proportional to $A_r\delta_{\alpha\beta}$. This choice of parameters mimics the case of DR in single, or few times charged ions, where large numbers of high Rydberg states participate. For such systems, one has that $Im < n|VPg_PPV|n' > \propto 1/(nn')^{3/2}$, where n labels the HRS principal quantum number. But since radiative stabilization, for such an ion, involves the inner (non-Rydberg) electron only, one has also that $< \alpha|DRg_RRD|\beta > \propto \delta_{nn'}$. Procedures similar to those described in the last example lead now to

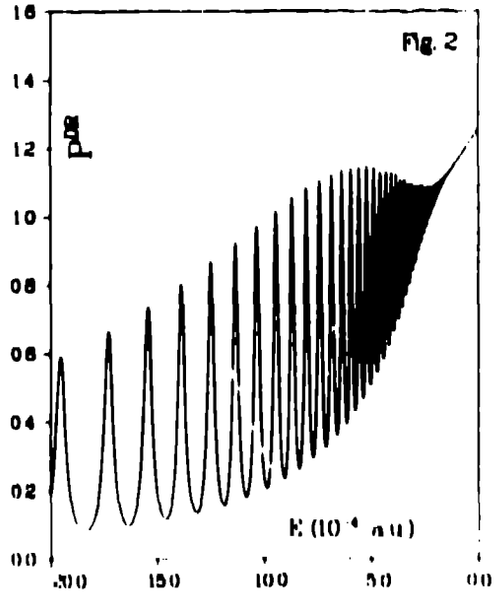
$$P^{DR} = NA_a A_r / |(E - \epsilon) + i(NA_a + A_r)/2|^2 \tag{28}$$

$$\sim 2\pi N A_a A_r \delta(E - \epsilon)/(NA_a + A_r)$$

This "multiple interacting resonance" (MIRA) calculation approaches the IRA prediction only in the limit in which $A_r >> NA_a$. However, if $A_r << NA_a$, then $P^{DR}(MIRA)/P^{DR}(IRA) \sim 1/N$. Note, however, that this result holds only if the resonances are strictly degenerate in energy, a rather unrealistic condition.

(iv) Elaborating on the previous example, where the Q-space states are again labeled by n, we now choose specific values for the widths: $Im < n|VPg_PPV|n' > \equiv -2A_{a0}/(nn')^{3/2} \equiv -0.4/(nn')^{3/2}$, and $Im < n|DRg_RRD|n' > \equiv -2A_r\delta_{nn'} \equiv -2x10^{-5}\delta_{nn'}$, with resonance energies $\epsilon_n = -0.5/n^2$, all in atomic units (a.u.), and for the range of n-values $2 \leq n \leq 100$. In natural units, the choice of atomic parameters made here corresponds to a radiative rate of $1x10^{11}$/sec, and an autoionization rate of $3x10^{14}$/sec (for n=3). Then, a numerical evaluation of eqn 20, for this choice of parameters, yields the results depicted in Fig. 1 (for $n \geq 16$).





For comparison, we plot in Fig. 2 the IRA prediction (from eqn 14), for the same choice of parameters. The two results are virtually indistinguishable, until P^{DR} exceeds ≈ 0.5. For larger values, the IRA prediction becomes increasingly unreliable, eventually even rising beyond total probability equal to 1, as $E \to 0$, when resonances become completely overlapped. For this example, one can show that $P^{DR} \to 2\pi A_{a0}$, as $E \to 0$.

Continuum-Continuum Coupling

In the following, we will extend the formalism of the preceding sections, in order to include the effect on P^{DR} of the coupling between distinct projectile continua, due to their interaction with the target in its ground and singly excited states. This extension also has implications for the calculation of electron-ion impact (resonance) excitation probabilities. Our formulation of the excitation probability, which includes interacting resonance and interference effects, represents a continuation of previous work by other authors[17-19]. Resonance excitation is generally thought to be of importance in the evolution of nonequilibrium plasmas.

We begin by dividing the P-space into two subspaces: P_1 projects onto the incoming state; the remainder of the P-space will be denoted by P_2; i.e.,

$$P = P_1 + P_2 \tag{29}$$

such that

$$P_1 P_2 = P_2 P_1 = 0 \tag{30}$$

Then, eqns 3-5 become

$$P_1 V P_2 \Psi_{P_2} + P_1 V Q \Psi'_Q = (E - P_1 H_0 P_1)\Psi_{P_1} \tag{31}$$

$$P_2 V P_1 \Psi_{P_1} + P_2 V Q \Psi'_Q = (E - P_2 H_0 P_2)\Psi_{P_2} \tag{32}$$

$$Q V P_1 \Psi_{P_1} + Q V P_2 \Psi_{P_2} + Q D R \Psi'_R = (E - Q H_0 Q)\Psi'_Q \tag{33}$$

$$R D Q \Psi'_Q = (E - R H_0 R)\Psi'_R \tag{34}$$

Where necessary, primes have been included to distinguish functions modified by continuum-continuum coupling from their unmodified versions which have appeared in earlier sections.

Eqns 32 and 34 may be solved formally in terms of Ψ_{P_1} and Ψ'_Q to give

$$\Psi_{P_2} = g_{P_2}(P_2 V P_1 \Psi_{P_1} + P_2 V Q \Psi'_Q) \tag{35}$$

and

$$\Psi'_R = g_R R D Q \Psi'_Q \tag{36}$$

where

$$g_{P_2} = (E - P_2 H_0 P_2)^{-1} \tag{37}$$

and g_R is given as in eqn 6. Then, a formal solution for Ψ_{P_1} can be obtained in terms of Ψ'_Q as

$$\begin{aligned} \Psi_{P_1} &= \Phi'_{P_1} + g'_{P_1} P_1 (V + V P_2 g_{P_2} P_2 V) Q \Psi'_Q \\ &= \Phi'_{P_1} + g'_{P_1} P_1 V' Q \Psi'_Q \end{aligned} \tag{38}$$

where

$$V' \equiv V + V P_2 g_{P_2} P_2 V \tag{39}$$

and where Φ'_{P_1} is the solution of

$$(E - P_1 H_0 P_1 - P_1 V P_2 g_{P_2} P_2 V P_1)\Phi'_{P_1} = 0 \tag{40}$$

The modified P_1-space propagator is given by

$$g'_{P_1} = (E - P_1 H_0 P_1 - P_1 V P_2 g_{P_2} P_2 V P_1)^{-1} \tag{41}$$

As per the development leading up to eqn 16, the Q-space wavefunctions satisfy the equation

$$\Psi'_{Q\alpha} = \Sigma_\beta (\Omega'^{-1})_{\alpha\beta} G'_{Q\beta} < \beta | V' P_1 \Phi'_{P_1} > \quad (42)$$

where the Q-space Green's functions are

$$G'_{Q\alpha} = (E - \epsilon_\alpha - < \alpha | DRg_R RD | \alpha > - < \alpha | V' P_2 g_{P_2} P_2 V' | \alpha > - < \alpha | V' P_1 g'_{P_1} P_1 V' | \alpha >)^{-1} \quad (43)$$

The Q-space mixing operator is now

$$\Omega'_{\alpha\beta} = \delta_{\alpha\beta} - (1 - \delta_{\alpha\beta}) G'_{Q\alpha} \Lambda'_{\alpha\beta} \quad (44)$$

where the operator Λ' has the elements

$$\Lambda'_{\alpha\beta} = < \alpha | DRg_R RD | \beta > + < \alpha | V' P_2 g_{P_2} P_2 V' | \beta > + < \alpha | V' P_1 g'_{P_1} P_1 V' | \beta > \quad (45)$$

The DR probability amplitude is then

$$T'^{DR} = \Sigma_\alpha < \Phi_R RD | \alpha > \Sigma_\beta (\Omega'^{-1})_{\alpha\beta} G'_{Q\beta} < \beta | V' P_1 \Phi'_{P_1} > \quad (46)$$

In order to facilitate actual computations based on eqn 46, it is first necessary to construct explicit solutions for the coupled asymptotic state in the incoming channel Φ'_{P_1}, and the coupled P_1-space propagator g'_{P_1}. Accordingly, we discretize the momentum in the incoming channel. Further, and for purposes of exposition, we assume that the P_2-space consists of just one state. Generalization is straightforward, and is discussed in a prior publication[20]. Eqn 40 becomes

$$(E - \epsilon_{P_i} - < i | V' P_2 g_{P_2} P_2 V' | i > \Phi'_{P_1 i} = \Sigma_{j \neq i} < i | V' P_2 g_{P_2} P_2 V' | j > \Phi'_{P_1 j} \quad (47)$$

where i (or j) labels the initial target state, incoming continuum partial wave, and a particular value of the incoming momentum. The total energy in the incoming channel is $\epsilon_{P_i} \equiv < i | P_1 H_0 P_1 | i >$, and $\Phi'_{P_1 i} \equiv < i | \Phi'_{P_1} >$. The solution of eqn 47 is

$$\Phi'_{P_1 i} = \Sigma_j (\omega^{-1})_{ij} \Phi_{P_1 j} \quad (48)$$

where $\Phi_{P_1 i}$ is the single-momentum P_1-space asymptotic wavefunction which solves the equation

$$(E - \epsilon_{P_1 i} - < i | V' P_2 g_{P_2} P_2 V' | i >) \Phi_{P_1 i} = 0 \quad (49)$$

and the P-space mixing operator ω has the elements

$$\omega_{ij} = \delta_{ij} - (1 - \delta_{ij}) g_{P_1 i} \lambda_{ij} \quad (50)$$

The single momentum P_1-space propagator g_{P_1} has the form

$$g_{P_1 i} = (E - \epsilon_{P_1 i} - < i | V' P_2 g_{P_2} P_2 V' | i >)^{-1} \quad (51)$$

and the P-space interaction operator λ has the elements

$$\lambda_{ij} = < i | V' P_2 g_{P_2} P_2 V' | j > \quad (52)$$

Elements of the full P_1-space propagator are obtainable as

$$< i | g'_{P_1} | j > = (\omega^{-1})_{ij} g_{P_1 j} \quad (53)$$

For a two channel problem, and if only a single electron (continuum) momentum participates, then $\lambda_{ij} = 0$, for $i \neq j$, so that $\omega_{ij} = \delta_{ij}$.

In order to illustrate the results of this section, we consider the example of two coupled channels, each made up of a Rydberg series of resonances, when just one continuum momentum participates in the incoming channel. Such a case might be described by the transitions

$$1s + k_1(l_1 = 1) \rightarrow 2s\,or\,p(n \geq 2) \rightarrow 1s2s + \gamma$$

$$1s + k_1(l_1 = 1) \rightarrow 2pn's(n' \geq 3) \rightarrow 1sn's + \gamma$$
$$2s + k_2(l_2 = 1) \rightarrow 2pn's(n' \geq n_x)$$

where P_1 projects onto $1s + k_1(l_1 = 1)$, and P_2 projects onto $2s + k_2(l_2 = 1)$. The threshold value of n', beyond which the process $2pn's \rightarrow 2s + k_2 l_2$ is allowed is denoted n_x. If the difference in energy between the 1s and 2s target states is labeled $\Delta_{12} \equiv \epsilon_{2s} - \epsilon_{1s}$, then on-shell, $k_1^2/2 = k_2^2/2 + \Delta_{12}$, if the 2s channel is open. In this example, we assume that the total energy ranges from below to above the threshold for 2s excitation, but always remains below the 2p threshold, thus justifying the assumption of just two participating P-space states.

From eqn 46, the DR probability becomes

$$P^{DR} = U_{12}^2 k_1 \Sigma_f |\Sigma_\alpha \Sigma_\beta k_\gamma D_{f\alpha} (\Omega'^{-1})_{\alpha\beta} G'_{Q\beta} V'_{1\beta}|^2 \tag{55}$$

where f enumerates the "final" states 1s2s, 1s3s, 1s4s, ..., and α labels the Q-space states 2s2p, 2s3p, 2s4p, ..., as well as 2p3s, 2p4s, 2p5s, ... The function U_{12} is

$$U_{12} = (1 + k_1 k_2 V_{12}^2/4)^{-1} \tag{56}$$

which also appears in the expression for the modified P_1-space propagator according to

$$g'_{P_1} = U_{12} g_{P_1} \tag{57}$$

and where V_{12} is the matrix element of the electron-electron interaction between the ground (1s) and first excited (2s) target states, with one electron in the continuum: i.e., the $1s \rightarrow 2s$ excitation matrix element. In deriving these formulas, the "pole approximation" has been invoked everywhere; i.e., all Green's functions have been reduced to their imaginary parts. If the continuum energy is held below the 2s threshold, then $k_2^2 < 0$ so that, all quantities proportional, in the preceding equations, to k_2 would be set to zero; e.g., $U_{12} = 1$; $g'_{P_1} = g_{P_1}$; $V' = V$; etc.

Defining the autoionization and radiative widths as

$$A_{a1}(\alpha) \equiv k_1 V_{1\alpha}^2$$
$$A_{a2}(\alpha) \equiv k_2 V_{2\alpha}^2 \tag{58}$$
$$A_\gamma(\alpha) \equiv \Sigma_f k_\gamma^2 D_{\alpha f}^2$$

we constructed a model problem in analogy to example *(iv)* in the last Section. Specifically, we chose

$$k_1 V^2(2snp \rightarrow 1s + k_1 l_1) \equiv A_{aI}/n^3 (n \geq 2)$$
$$k_1 V^2(2pn's \rightarrow 1s + k_1 l_1) \equiv A_{aII}/n'^3 (n' \geq 3) \tag{59}$$
$$k_2 V^2(2pn's \rightarrow 2s + k_2 l_2) \equiv A_{aIII}/n'^3 (n' \geq n_x)$$

and

$$k_\gamma^2 D^2(2snp \rightarrow 1s2s + \gamma) \equiv A_{\gamma 0}/n^3$$
$$k_\gamma^2 D^2(2pn's \rightarrow 1sn's + \gamma) \equiv A_{\gamma 0} \tag{60}$$

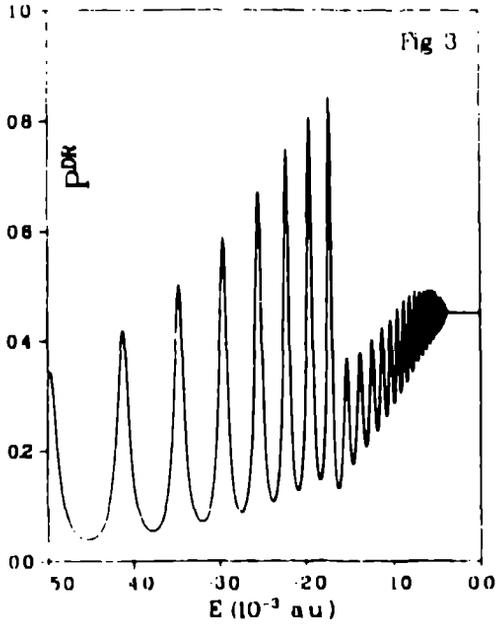
We chose the values $A_{\gamma 0} = 2x10^{-5}$, $n_x = 18$, and $\epsilon_{2p} - \epsilon_{2s} = 1.54x10^{-3}$, all in a.u. The range of Rydberg states included was $10 \leq n \leq 40$, $10 \leq n' \leq 65$, and the zero of total energy was set at the 2p threshold. In Fig. 3 we plot values of P^{DR} vs E when $A_{aI} = 0.0$, and $A_{aII} = A_{aIII} = 0.2$ a.u., while in Fig. 4 we plot P^{DR} when $A_{aI} = 0.2$ a.u., and $A_{aII} = A_{aIII} = 0.0$. The complete P^{DR} appears in Fig. 5, where $A_{aI} = A_{aII} = A_{aIII} = 0.2$ a.u.

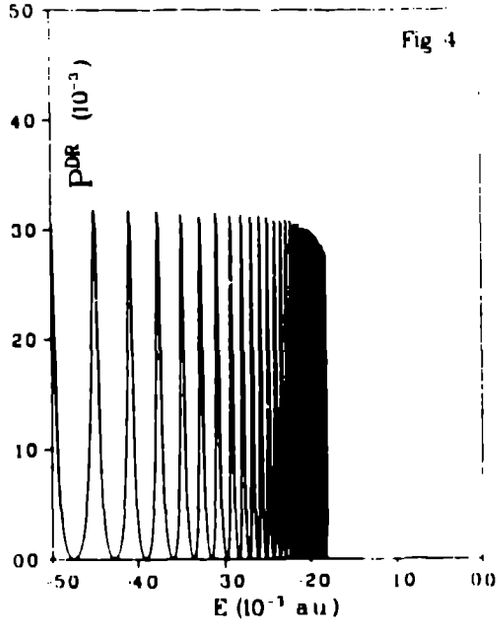
Note that, although the $2snp$ series (Fig. 4) does not contribute greatly to P^{DR} when considered in isolation from the $2pn's$ series (Fig. 3), its effect on the total P^{DR} (Fig. 5) is profound. The interaction between the $2snp$ and $2pn's$ series of resonances has been discussed recently[41] in the context of calculations performed of the photoionization rates for neutral helium, in the resonance region. The occurrence of especially sharp structures in the cross

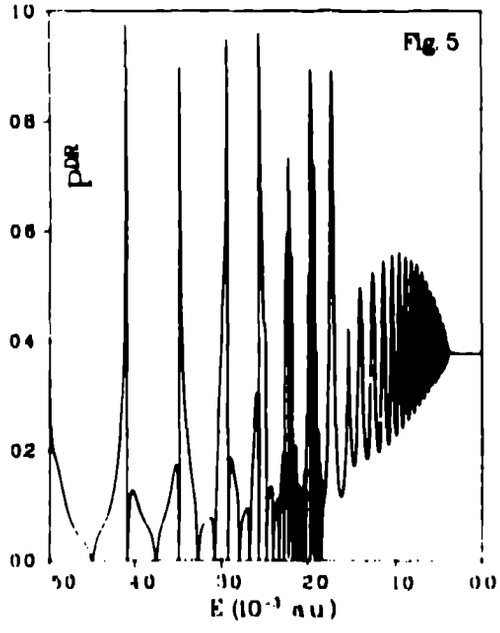
section was noted in that work, and is also apparent here in our model calculation.

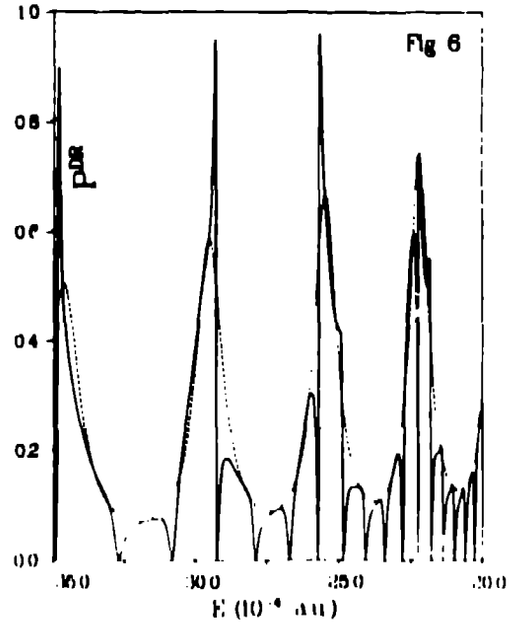
In order to emphasize this last point, we plot in Fig. 6 an expanded version of the total P^{RDR}, for a restricted range of energies (solid line). The corresponding values from Fig. 3 are also plotted for comparison (dashed line). The very sharp peaks arise from the $2pn'$s series of Q-space states, modified by QVP coupling to the $2snp$ series. Only resonances for which $12 \leq n' \leq 15$ are displayed.

The IRA prediction, for this choice of atomic parameters, exceeds the probability bound ($P^{DR} > 1$), for energies just below the excitation threshold; see ref. 20 for further details.









From the foregoing, the $1s - 2s$ excitation probability can be easily constructed. The probability amplitude for this process can be divided into two parts: The amplitude for direct excitation is

$$T^{DE} = < \Phi_{P_2} P_2 V P_1 \Psi_{P_1} > \tag{61}$$

while the amplitude for resonance excitation (through $1s + k_1 l_1 - 2pn'l' - 2s + k_2 l_2$) is given by

$$T^{RE} = < \Phi_{P_2} P_2 V Q \Psi_Q > \tag{62}$$

where the asymptotic final state function Φ_{P_2} satisfies

$$(E - P_2 H_0 P_2)\Phi_{P_2} = 0 \tag{63}$$

The total excitation probability is then

$$P^{EX} = k_1 k_2 |T^{DE} + T^{RE}|^2 \tag{64}$$

The amplitude for direct excitation can be written in a more explicit form as

$$T^{DE} = U_{12} V_{21} [1 + (-ik_1/2)\Sigma_\alpha V'_{1\alpha}]\Psi_{Q\alpha} \tag{65}$$

while the amplitude for resonance excitation can also be expressed as

$$T^{RE} = \Sigma_\alpha V_{2\alpha} \Psi_{Q\alpha} \tag{66}$$

where $\Psi_{Q\alpha}$ appears in eqn 44. This formulation of P^{EX} conserves total probability in that $0 \leq P^{EX} + P^{DR} < 1$. We refer the reader to ref. 20 for further information.

Radiative Recombination

The effect of radiative recombination (RR) on DR has been discussed lately, with increasing frequency[22-25], although no direct experimental tests of theoretical predictions have as yet emerged. Usually, RR is of importance at very low energies of the incident electron, while DR rates become appreciable only at elevated energies. Consequently, the opportunity for interference between the two processes would seem to be limited. Nevertheless, we recapitulate here our approach to the formulation of this problem, building on the work described in the previous Sections.

The total probability amplitude for electron-ion recombination can be written as a sum of two terms

$$T^{RDR} \equiv \underline{T}^{RR} + \underline{T}^{DR} \tag{67}$$

where we refer to the joint process as "radiative dielectronic recombination" (RDR), and where the underscore signifies a function modified by coupling between the RR and DR channels. The amplitude for RR (in the presence of DR) can be described by

$$\underline{T}^{RR} = < \Phi_R R D P \underline{\Psi}_{P_1} > \tag{68}$$

while the amplitude for DR (in the presence of RR) may be expressed as

$$\underline{T}^{DR} = < \Phi_R R D Q \underline{\Psi}_Q > \tag{69}$$

where in eqn 68 $\underline{\Psi}_{P_1}$ is the exact wavefunction describing the incoming state. As in the previous Section, we assume that the P-space has been divided into two parts; P_1 projects onto the incoming channel and P_2 projects onto all other states of N electrons bound and one electron in the continuum.

Upon addition of the terms $P_1 D R \underline{\Psi}_R$, $P_2 D R \underline{\Psi}_R$, and $R D P_1 \underline{\Psi}_{P_1} + R D P_2 \underline{\Psi}_{P_2}$ to the left-hand-sides of eqns 31, 32, and 34, respectively, with all wavefunctions underscored to denote RDP coupled quantities, an analogous set of (four) equations results which can be reduced

by the procedures already described. For example, we note that the asymptotic P_1 space wavefunction $\underline{\Phi}'_{P_1}$ now satisfies

$$(E - P_1 H_0 P_1 - P_1 DRg_R RDP_1 - P_1 \underline{V} P_2 \underline{g}_{P_2} P_2 \underline{V} P_1)\underline{\Phi}'_{P_1} \tag{70}$$

where

$$\underline{V} \equiv V + DRg_R RD \tag{71}$$

and

$$\underline{g}_{P_2} \equiv (E - P_2 H_0 P_2 - P_2 DRg_R RDP_2)^{-1} \tag{72}$$

instead of eqn 40, in which RDP coupling was not included. The R-space propagator g_R is still given by eqn 6. Similarly, instead of eqn 43, the Q-space propagator is now

$$\underline{G}'_{Q\alpha} \equiv (E - \epsilon_{Q\alpha} - <\alpha|DRg_R RD|\alpha> - <\alpha|\underline{V}' P_1 \underline{g}'_{P_1} P_1 \underline{V}'|\alpha> - <\alpha|\underline{V} P_2 \underline{g}_{P_2} P_2 \underline{V}|\alpha>)^{-1} \tag{73}$$

where

$$\underline{V}' \equiv \underline{V} + \underline{V} P_2 \underline{g}_{P_2} P_2 \underline{V} \tag{74}$$

which generalizes eqn 39, and

$$\underline{g}'_{P_1} \equiv (E - P_1 H_0 P_1 - P_1 DRg_R RDP_1 - P_1 \underline{V} P_2 \underline{g}_{P_2} P_2 \underline{V} P_1)^{-1} \tag{75}$$

which generalizes eqn 41. Further reduction of these equations is somewhat complex, and the reader is referred to ref. 23 for details.

In general, the effects of RR on DR (or viceversa) should be most apparent when the RR rate alone is roughly comparable to, or greater than, the rate of stabilizing radiative decay in DR. Since the RR rate scales approximately as Z_I^2, where Z_I is the net ionic charge, while the stabilizing radiative rate varies as Z_I^4 for $\Delta n \neq 0$ transitions, and as Z_I for $\Delta n = 0$ decays, it is most promising to look for interference effects at low Z_I for $\Delta n \neq 0$ transitions, and at high Z_I for $\Delta n = 0$ decays. Also, since RR rates are relatively large at the lowest continuum energies, it is best to confine oneself to the region of energies corresponding to the lowest lying DR resonances. In accordance with these ideas, in the following we examine the results of calculations of P^{RDR} performed for the two RDR processes

$$1s + k_i l_i \rightarrowtail 2pns(n \geq 2) \rightarrow 1sn's + \gamma \tag{76}$$

$$1s + k_i l_i \rightarrowtail\!\!\!\rightarrow 1sn's(n' \geq 2) + \gamma$$

for ground state He^+ targets, involving a $\Delta n \neq 0$ stabilizing radiative transition, and

$$3s + k_i l_i \rightarrowtail 3pnl(n \geq 3) \rightarrow 3sn'l + \gamma \tag{77}$$

$$3s + k_i l_i \rightarrowtail\!\!\!\rightarrow 3sn'l(n' \geq 3) + \gamma$$

for ground state sodium-like targets, involving a $\Delta n = 0$ stabilizing radiative decay. We assume that, in each case, only one target state participates in the RDR process, so that $P_2 = 0$ and $P_1 \equiv P$. In addition, since we will confine our attention entirely to the region of energies around the lowest lying DR resonance (which is usually well seperated from the resonance next highest in energy) we make the isolated resonance approximation (IRA).

From eqns 67-75 and the results of ref. 21, the RDR probability for the processes of eqns 76 and 77 is

$$P^{RDR} = M^2 \Sigma_{n'} |W_{RRn'}^{1/2}[1 - (iM/2)\Sigma_n \underline{G}_{Qn} \underline{A}_a(n)] + \Sigma_n \underline{G}_{Qn} \underline{A}_a^{1/2}(n) A_r^{1/2} \delta_{nn'}|^2 \tag{78}$$

where A_r is the stabilizing radiative decay rate: $2p \rightarrow 1s + \gamma$, in the case of eqn 76, and $3p \rightarrow 3s + \gamma$ for eqn 77. The direct radiative recombination rate to Rydberg state n is[24]

$$W_{RRn} = 7.5x10^{-6} Z_I^2/(n^3[1/n^2 + 2(E + \Delta\epsilon)/Z_I^2]) \tag{79}$$

all in a.u., where $\Delta\epsilon$ is the excitation energy, and E is the total energy (adjusted so that E=0 at the excitation threshold). The prefactor M is defined as

$$M \equiv 1/(1 + \Sigma_n W_{RRn}/4) \tag{80}$$

the autoionization rate modified by RDP coupling is

$$\underline{A}_a(n) = [A_a^{1/2}(n) - (i/2)W_{RRn}^{-1/2}A_r^{1/2}]^2 \tag{81}$$

and the modified Q-space propagator is given by

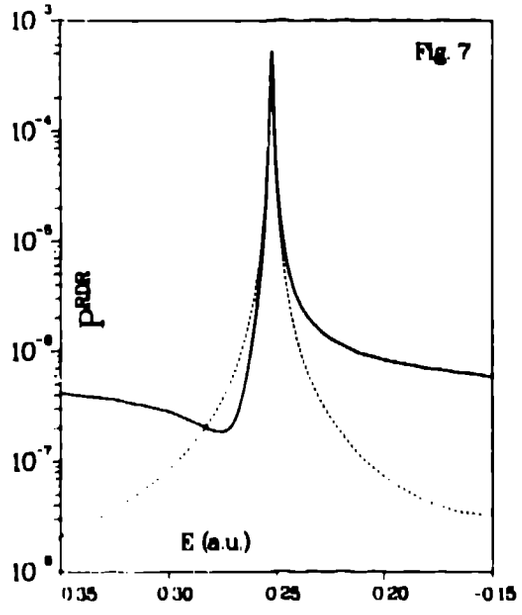
$$\underline{G}_{Qn} = (E - \epsilon_n + (i/2)[A_r + M\underline{A}_a(n)])^{-1} \tag{82}$$

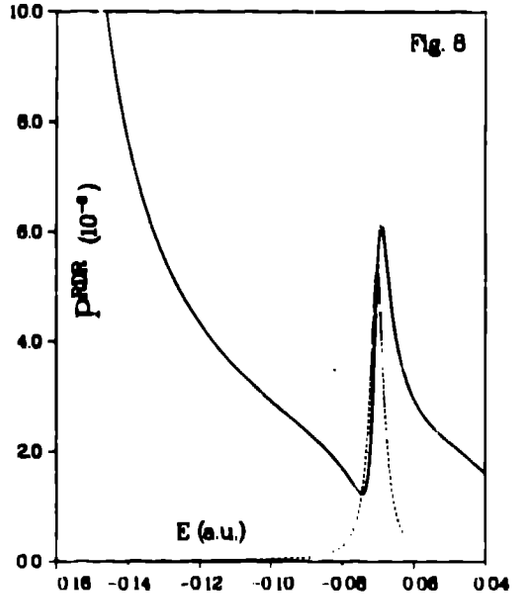
Fig. 7, we plot values of P^{RDR} for the process of eqn 76, with $A_a(n) = 9.5x10^{-3}/n^3$ a.u., and $A_r = 1.6x10^{-7}$ a.u., for $Z_I = 1$ (ground state He^+ targets). In Fig. 8, we plot values of P^{RDR} for the process of eqn 77, with $A_a(n) = 1.2x10^{-1}/n^3$ a.u., and $A_r = 6.1x10^{-9}$ a.u., for $Z_I = 1$ (ground state Mg^+ targets). For comparison, in both Figs. 7 and 8 we include plots of the DR component alone (dashed line).

The lack of any significant effect of the RR process on the RDR probability, for $\Delta n \neq 0$ excitations, is demonstrated by the result displayed in Fig. 7, at $Z_I = 1$. For larger Z_I, the effect is even smaller. However, for the $\Delta n = 0$ excitation described by Fig. 8, there is a perceptible effect of RR at $Z_I = 1$; and this effect increases somewhat, as Z_I increases. However, since larger Z_I-values lead to larger values for the minimum accessible n-value, this effect seems to disappear for Z_I greater than two or three.

Electric Field Effects

The enhancement of calculated σ^{DR} values, for $\Delta n = 0$ excitations, due to Stark mixing of participating high Rydberg states by stray electric fields, has been remarked on frequently over the past 5-10 years. Measurements of these cross sections by several different groups have confirmed the reality of this effect[6-14].





It is now well-known that field induced enhancements of DR probabilities result from an increase in the number of angular momentum states accessible to dielectronic capture. Ordinarily, capture only occurs with an appreciable probability to states of orbital angular momentum $l < 5 - 10$, even for very high Rydberg states $n >> 10$. However, in an externally applied electric field, states of high angular momentum acquire low angular momentum character due to Stark mixing. Thus, captures to very high Rydberg states are promoted by the presence of an electric field. More detailed arguments may be found in ref. 26.

Agreement between DR theory and experiment, for $\Delta n = 0$ excitations, exists now generally to within a factor of ~ 2. Discrepancies remain, however, and work should continue in order to resolve these problems[7,8,27]. The application of interacting resonance theory, as described earlier in this review, should be attempted. And the effect of angular factors, peculiar to the geometry of any given DR measurement, needs to be looked at very carefully. Nevertheless, the situation is today much improved from that which obtained in the early 1980's, when measured DR cross sections were an order of magnitude larger than the theoretical predictions.

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