# Effect of Interacting Resonances on Dielectronic Recombination in Static Fields

F. Robicheaux,[1] M. S. Pindzola,[1] and D. C. Griffin[2]
[1]*Department of Physics, Auburn University, Auburn, Alabama 36849*
[2]*Department of Physics, Rollins College, Winter Park, Florida 32789*
(Received 28 October 1997)

We find that the static field enhancement of dielectronic recombination may be strongly reduced by the interaction between resonances through common continua. The interaction effect is not limited to a few resonances but extends over whole $n$ manifolds, thus it can significantly reduce the field enhancement of the total recombination rate. The standard lowest order theory is recast using a complex Hamiltonian to include higher order terms usually identified with interaction through common continua. We present calculations for $C^{3+}$ and $Si^{11+}$ using both time independent and time dependent configuration average methods. [S0031-9007(98)05346-0]

PACS numbers: 34.80.Kw, 32.60.+i, 32.80.Dz

The recombination of an electron with an ion through the emission of a photon is an important process in many types of plasmas. This basic phenomenon has been explored experimentally and theoretically for many years [1]. The majority of calculations concerning photorecombination utilize second order perturbation theory. The direct capture of an electron from the continuum (radiative recombination—RR) is described in first order. Capture into a resonance state with subsequent stabilization through the emission of a photon (dielectronic recombination—DR) is a second order effect which is often a larger contribution to the recombination cross section. The resonance state is defined as an eigenstate of the atomic ion Hamiltonian, which for multielectron systems involves the inclusion of configuration interaction. The higher order terms in photorecombination are usually neglected; for example, calculations usually ignore the interaction between two resonances through a common continuum as well as the interference between the direct (RR) and indirect (DR) paths.

There are several circumstances that make this a very good approximation for most practical applications. First, the resonances are usually too sharp in energy to be resolved, so the measurements probe the energy integrated cross section. Also, experiments usually probe total cross sections with a sum over many possible final states and many different incoming directions for the electron; very few measurements exist for photorecombination to a particular final state with the polarization of the photon and the angle between the photon and the incident electron measured. Finally, this is a good approximation for the *total* DR cross section because the interaction through common continua is usually weak, so the resonances need to be closely spaced in energy to be affected; usually, the direct configuration interaction keeps the resonance states too far apart for interaction through the continuum to be important. Despite considerable theoretical effort [2–10], no one has yet found an uncontested case where the total DR cross section changes by more than a few percent when including interactions through the continuum. In this paper, however, we find that the total DR cross section in static fields is strongly affected by these interactions.

Static fields can greatly increase the DR cross section integrated over many $n$ manifolds [11–18]. This increase arises because the electron is captured by the ion in a low-$\ell$ state where the autoionization rate is much larger than the radiative decay rate; in static fields, the electron precesses out of the low-$\ell$ states into high-$\ell$ states where the radiative rate is larger than the autoionization rate thus increasing the photonemission probability. As we show, the effect of interaction through common continua can be substantial. This situation arises because most laboratory fields are very small compared to atomic interactions. Even weak fields can thoroughly mix the states of an $n$ manifold due to the near degeneracy of the energy levels. However, the resulting eigenstates are closely spaced in energy thus opening the possibility of further mixing by interaction through common continua. This interaction serves to reduce the level of mixing from the fields and thus reduce the DR cross section.

There are several important consequences of this reduction in the DR cross section. For example, in calculations without interaction through the continuum, the DR cross section increases with field strength to a saturation value because increasing the field strength cannot mix the states further once they become completely mixed. With this interaction, the saturation value is reached at much larger field strengths since this interaction reduces the mixing. In the cases where the field strength is not known, this circumstance can strongly affect the estimated field strength in an experiment.

For ions in static fields, projection operator theory [19,20] provides the most efficient formulation. The solution $\Psi$ of Schrödinger's equation may be written as three coupled equations:

$$(E - PH_0P)P\Psi = PH_0QQ\Psi\,, \tag{1}$$

$$(E - QH_0Q)Q\Psi = QH_0PP\Psi + QDRR\Psi\,, \tag{2}$$

$$(E - RH_0R)R\Psi = RDQQ\Psi\,, \tag{3}$$

 0031-9007/98/80(7)/1402(4)$15.00 

where the total Hamiltonian $H = H_0 + D$ and the projection operators $P + Q + R = 1$. The Hamiltonian $H_0$ represents electrostatic interactions in the atom and electron interactions with external fields, $D$ is the electron interaction with the radiation field, $P$ projects onto states of $N$ bound electrons, one continuum electron, and no photons, $Q$ projects onto doubly excited states of $N + 1$ bound electrons and no photons, and $R$ projects onto the ground and singly excited states of $N + 1$ bound electrons and one photon. In Eqs. (1) and (3), we have ignored the coupling between two continuum channels through the radiation field. We may formally solve Eq. (2) using $\Psi = P\psi_0^+ + \Lambda$ to find

$$(E - \tilde{H})Q\Lambda = QH_0P|\psi_0^+\rangle, \tag{4}$$

where the complex Hamiltonian $\tilde{H}$ is given by

$$\tilde{H} = QH_0Q + QH_0P(E - PH_0P)^{-1}PH_0Q + QDR(E - RH_0R)^{-1}RDQ, \tag{5}$$

and $|\psi_0^+\rangle$ is the homogeneous solution of Eq. (1). The matrix element for DR is given by

$$\mathcal{M} = \langle\chi|RDQ|Q\Lambda\rangle, \tag{6}$$

where $|\chi\rangle$ is a homogeneous solution of Eq. (3). Combining Eqs. (4) and (6) yields

$$\mathcal{M} = \langle\chi|RDQ(E - \tilde{H})^{-1}QH_0P|\psi_0^+\rangle. \tag{7}$$

This is the main working equation of this paper. $|\mathcal{M}|^2$ is directly proportional to a DR cross section which includes provision for interacting resonance structures.

The complex Hamiltonian $\tilde{H}$ of Eq. (5) may be analyzed in a basis of states $|\phi_\alpha\rangle$ which are homogeneous solutions of Eq. (2). In the pole approximation

$$\langle\phi_\alpha|\tilde{H}|\phi_\beta\rangle \equiv \tilde{H}_{\alpha\beta} = E_\alpha\delta_{\alpha\beta} - \frac{i}{2}(\Gamma^a_{\alpha\beta} + \Gamma^r_{\alpha\beta}), \tag{8}$$

where $E_\alpha$ is the real energy of state $|\phi_\alpha\rangle$ and

$$\Gamma^a_{\alpha\beta} = \frac{4}{k}\langle\phi_\alpha|QH_0P|\psi_0^+\rangle\langle\psi_0^+|PH_0Q|\phi_\beta\rangle \tag{9}$$

is a generalization of the autoionization rate and

$$\Gamma^r_{\alpha\beta} = 2\pi\langle\phi_\alpha|QDR|\chi\rangle\langle\chi|RDQ|\phi_\beta\rangle \tag{10}$$

is a generalization of the radiative decay rate. The diagonal elements of $\Gamma^a_{\alpha\beta}$ and $\Gamma^r_{\alpha\beta}$ are the usual autoionization and radiative rates in atomic units. In these formulas $k$ is the linear momentum of the Auger electron, continuum normalization is chosen as 1 times a sine function, $D = \sqrt{2\omega^3/3\pi c^3}\sum_i \vec{r}_i$ is the dipole radiation field interaction, $\omega$ is the frequency of the emitted radiation, and $c$ is the speed of light. The isolated resonance approximation neglects interaction through the continua by using $\Gamma^a_{\alpha\beta} = \Gamma^a_\alpha\delta_{\alpha\beta}$ and $\Gamma^r_{\alpha\beta} = \Gamma^r_\alpha\delta_{\alpha\beta}$. This approximation becomes problematic when $\Gamma^a_{\alpha\beta} + \Gamma^r_{\alpha\beta} \geq |E_\alpha - E_\beta|$.

The DR cross section to go from channel $i$ to state $f$ may be written as

$$\sigma^{f\leftarrow i}_{\rm DR} = \frac{8\pi^2}{k_i^3}\left|\sum_{\alpha\beta} D_{f\alpha}[(E - \tilde{H})^{-1}]_{\alpha\beta}V_{\beta i}\right|^2, \tag{11}$$

where $D_{f\alpha} = \langle\chi_f|RDQ|\phi_\alpha\rangle$ and $V_{\beta i} = \langle\phi_\beta|QH_0P|\psi^+_{0,i}\rangle$. This equation is formally equivalent to that derived in Ref. [14] and used in Ref. [6], but is in a form more amenable for investigating energy averaged cross sections. Equation (11) is somewhat awkward in practical applications since often energy resolutions are *much* larger than the widths of the resonances. The matrix $\tilde{H}_{\alpha\beta}$ is complex symmetric so we can use its eigenvectors and values to simplify the expression, Eq. (11). Using

$$\sum_\beta \tilde{H}_{\alpha\beta}U_{\beta\rho} = U_{\alpha\rho}\tilde{E}_\rho \quad \text{and} \quad \sum_\beta U_{\beta\rho}U_{\beta\rho'} = \delta_{\rho\rho'}, \tag{12}$$

Eq. (11) may be written as

$$\sigma^{f\leftarrow i}_{DR} = \frac{8\pi^2}{k_i^3}\left|\sum_\rho D_{f\rho}(E - \tilde{E}_\rho)^{-1}V_{\rho i}\right|^2, \tag{13}$$

where $D_{f\rho} = \sum_\beta D_{f\beta}U_{\beta\rho}$ and $V_{\rho i} = \sum_\beta V_{\beta i}U_{\beta\rho}$. If the cross section is convolved with a weight function $W(E, E_0)$ that has an energy width much greater than the imaginary parts of $\tilde{E}_\rho$ then

$$\langle\sigma^{f\leftarrow i}_{\rm DR}\rangle(E_0) = \int \sigma^{f\leftarrow i}_{\rm DR}(E)W(E, E_0)\,dE \simeq \frac{16\pi^3 i}{k_i^3}\sum_{\rho\rho'} D_{f\rho}V_{\rho i}D^*_{f\rho'}V^*_{\rho' i} \times W(\tfrac{1}{2}\ {\rm Re}[\tilde{E}_\rho + \tilde{E}_{\rho'}], E_0)/(\tilde{E}^*_{\rho'} - \tilde{E}_\rho). \tag{14}$$

We have examined the effect of interacting resonances using a configuration average type approximation that simplifies the atomic structure but preserves the effect from the fields and the interaction through the continuum. In this approximation, the core angular momenta are ignored and the $\alpha$ states are simply labeled by $n\ell m$ of the Rydberg electron. The Rydberg orbital is generated from the configuration-average Hartree-Fock equations with the core orbitals frozen. The mass-velocity term is included through first order perturbation theory. Finally, we ignore the *zero field* interaction through the continuum since this has little effect on the cross section. For the systems considered below, the fields are too weak to mix states from different $n$ manifolds so the interaction of states through the fields is incorporated by diagonalizing within each $n$ manifold separately.

In terms of the Rydberg orbital $|n\ell m\rangle$ of each doubly excited configuration, the complex Hamiltonian is approximately given by

$$\langle n\ell' m'|\tilde{H}|n\ell m\rangle = \left(E_{n\ell} - \frac{i}{2}\Gamma_{n\ell}\right)\delta_{\ell' m',\ell m} + \langle n\ell' m'|H_{\rm field}|n\ell m\rangle, \tag{15}$$

where $E_{n\ell}$ is the configuration-average energy and $\Gamma_{n\ell}$ is the sum of the configuration-average autoionization and radiative rates. The external field Hamiltonian is given by $H_{\rm field} = F \cdot z$ when $B = 0$ and $H_{\rm field} = F \cdot x + B \cdot L_z$ in the crossed field configuration. The $B = 0$ Hamiltonian conserves $m$, thus the diagonalization for each

TABLE I. Total DR cross section in perpendicular electric and magnetic fields integrated over an energy range including all states of the $n = 25-38$ manifolds for $C^{3+}$. The $\sigma^r$ ($\sigma^c$) are cross sections obtained by ignoring (including) interaction through the continuum.

| | $B = 0$ G | | $B = 30$ G | |
|---|---|---|---|---|
| $F$ (V/cm) | $\sigma^r$ (Mb eV) | $\sigma^c$ (Mb eV) | $\sigma^r$ (Mb eV) | $\sigma^c$ (Mb eV) |
| 0 | 0.50 | 0.50 | 0.50 | 0.50 |
| 2 | 2.18 | 1.05 | 2.96 | 1.06 |
| 4 | 2.21 | 1.43 | 3.51 | 1.60 |
| 6 | 2.22 | 1.65 | 3.54 | 1.97 |
| 8 | 2.23 | 1.79 | 3.44 | 2.21 |
| 10 | 2.24 | 1.88 | 3.29 | 2.32 |
| 15 | 2.25 | 2.02 | 2.97 | 2.41 |
| 20 | 2.26 | 2.09 | 2.79 | 2.41 |

$m$ is performed separately. The crossed field Hamiltonian commutes with the $z$-inversion operator, $z \longrightarrow -z$, thus the diagonalization for states with $\ell + m =$ even and $\ell + m =$ odd are performed separately.

Within these approximations, the total DR rates integrated over energy for a particular $n$ manifold can be obtained from Eq. (13) in the form

$$\langle \sigma_{\mathrm{DR}}^{\mathrm{n,TOT}} \rangle = \frac{2\pi^2 i}{k_i^2} \sum_{\rho\rho'} \Gamma^a_{\rho\rho'} \Gamma^r_{\rho\rho'} / (\tilde{E}^*_{\rho'} - \tilde{E}_\rho) \qquad (16)$$

with the generalized rates defined as

$$\Gamma^{a,r}_{\rho\rho'} = \sum_{\ell m} \Gamma^{a,r}_{n\ell} U_{n\ell m,\rho} U_{n\ell m,\rho'} . \qquad (17)$$

The effects of interacting resonances are examined for contributions to the DR cross section from all of the states from the $n = 25-38$ manifolds. Calculations have been performed for DR in the Li-like ions $C^{3+}$ and $Si^{11+}$. The results of these calculations are presented in Tables I and II; the cross sections are integrated over an energy range covering the $n = 25-38$ manifolds. The $\sigma^r$ is from a calculation using the isolated resonance approximation (i.e., ignoring interaction through the continuum) and the $\sigma^c$ is from a calculation using the complex Hamiltonian (i.e., including the interaction through the continuum). In Figs. 1 and 2, these integrated cross sections are presented in graphical form. Notice that the cross section summed over 14 000 states can dramatically depend on whether or not the higher order terms are included in the calculations of the DR cross section. As can be seen from these tables and figures, the effect of the interaction through the continuum is to reduce the energy integrated cross section. The largest effect is at the smallest fields; as the fields increase, the states become spread by a larger amount and thus become less susceptible to interaction through continua. The reduction is larger for $B \neq 0$ since the density of states is larger; however, the cross section *is* still enhanced for $B \neq 0$. The structure of the core increases the separation of the Rydberg states in zero field; thus the interaction through the continuum will be somewhat less when the configuration approximation is lifted, but we still expect a sizable effect.

We suggest the following qualitative explanation for the effects seen in these calculations. In the isolated resonances approximation, the states are mixed by the field to the extent that the field can overcome the difference in energy from the change in quantum defect with $\ell$. By adding a complex term to the Hamiltonian, Eq. (5), the states become further separated in the complex energy plane and thus are less mixed for a given field strength. This effect can be seen in a simple two state case. Suppose two states have exactly the same real energy but wildly different decay rates. If a small coupling between the states is introduced, the isolated resonance approximation gives two states that are equal mixtures of the two original states and thus each of the eigenstates decays with a rate equal to the average of the rates of the unmixed states. Using interacting resonance theory, the mixing between the states becomes appreciable only when the coupling matrix element becomes comparable to the difference in decay rates.

TABLE II. Same as Table I but for $Si^{11+}$.

| | $B = 0$ G | | $B = 300$ G | |
|---|---|---|---|---|
| $F$ (V/cm) | $\sigma^r$ (Mb eV) | $\sigma^c$ (Mb eV) | $\sigma^r$ (Mb eV) | $\sigma^c$ (Mb eV) |
| 0 | 1.25 | 1.25 | 1.25 | 1.25 |
| 10 | 1.51 | 1.39 | 1.80 | 1.42 |
| 20 | 1.95 | 1.64 | 2.37 | 1.69 |
| 30 | 2.31 | 1.89 | 2.90 | 1.97 |
| 40 | 2.57 | 2.12 | 3.37 | 2.26 |
| 50 | 2.77 | 2.31 | 3.76 | 2.53 |
| 75 | 3.09 | 2.67 | 4.45 | 3.11 |
| 100 | 3.27 | 2.90 | 4.84 | 3.56 |
| 150 | 3.46 | 3.18 | 5.15 | 4.12 |

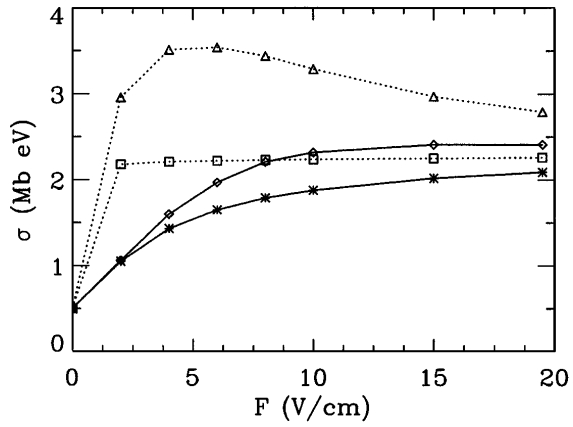


FIG. 1. Plot of the numbers in Table I. The dotted lines with squares ($B = 0$) and triangles ($B = 30$ G) are the isolated resonance approximation results, while the solid lines with asterisks ($B = 0$) and diamonds ($B = 30$ G) include the interaction through the continuum.

The time independent implementation of this theory rests on the ability to diagonalize complex symmetric matrices. For ions in static electric fields the matrices are moderately large. The number of states that participate in $\tilde{H}$ becomes so large in crossed electric and magnetic fields that even present day supercomputers are pushed to the limit [21]. For this reason, we have developed a time dependent method that offers interesting possibilities. We note that the time dependent function

$$D_{fi}(t) = \sum_{\rho} D_{f\rho} e^{-i\tilde{E}_{\rho} t} V_{\rho i} = \sum_{\alpha\beta} D_{f\alpha} (e^{-i\tilde{H}t})_{\alpha\beta} V_{\beta i} \tag{18}$$

can be obtained without diagonalizing $\tilde{H}$. The integral of the absolute value squared equals

$$\int_0^{\infty} |D_{fi}(t)|^2 dt = i \sum_{\rho\rho'} D_{f\rho} V_{\rho i} D^*_{f\rho'} V^*_{\rho' i} / (\tilde{E}^*_{\rho'} - \tilde{E}_{\rho}), \tag{19}$$

which should be compared with Eq. (14). This method allows the utilization of parallel computers in the calculation of DR rates in crossed electric and magnetic fields because $D_{fi}(t)$ can be obtained using standard time propagation techniques. This time dependent method has been tested on the simple systems above and gives very accurate results.

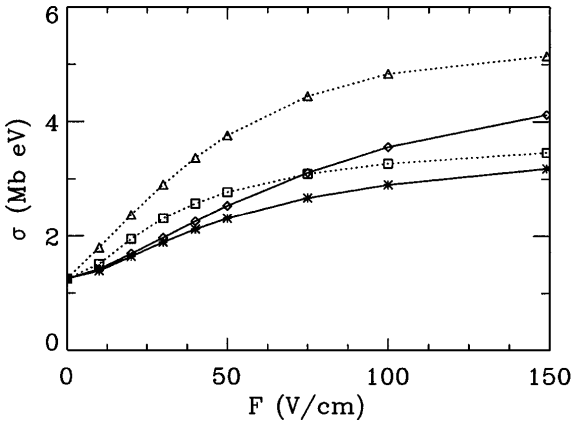


FIG. 2. Plot of the numbers in Table II. The dotted lines with squares ($B = 0$) and triangles ($B = 300$ G) are the isolated resonance approximation results, while the solid lines with asterisks ($B = 0$) and diamonds ($B = 300$ G) include the interaction through the continuum.

In conclusion, we have shown that DR cross sections in static fields are strongly affected by interactions between resonances through a common continuum. The interacting resonance effect extends over a large number of $n$ manifolds and significantly changes the total recombination rate in certain temperature and field ranges. Field enhanced DR cross section calculated in a configuration average approximation are substantially reduced when going from the real Hamiltonian formulation of isolated resonance theory to the complex Hamiltonian formulation of interacting resonance theory. We expect that future field enhanced DR cross sections in a full intermediate coupling approximation will also be affected by interactions between resonances.

This work was supported by the Department of Energy, with Rollins College and Auburn University.

[1] *Recombination of Atomic Ions*, edited by W. G. Graham *et al.*, NATO ASI, Ser. B, Vol. 296 (Plenum Press, New York, 1992).
[2] P. C. W. Davies and M. J. Seaton, J. Phys. B **2**, 757 (1969).
[3] R. H. Bell and M. J. Seaton, J. Phys. B **18**, 1589 (1985).
[4] K. J. LaGattuta, Phys. Rev. A **36**, 4662 (1987).
[5] S. L. Haan and V. L. Jacobs, Phys. Rev. A **40**, 80 (1989).
[6] M. S. Pindzola, N. R. Badnell, and D. C. Griffin, Phys. Rev. A **46**, 5725 (1992).
[7] S. N. Nahar and A. K. Pradhan, Phys. Rev. Lett. **68**, 1488 (1992).
[8] F. Robicheaux, T. W. Gorczyca, M. S. Pindzola, and N. R. Badnell, Phys. Rev. A **52**, 1319 (1995).
[9] H. L. Zhang and A. K. Pradhan, Phys. Rev. Lett. **78**, 195 (1997).
[10] T. W. Gorczyca and N. R. Badnell, Phys. Rev. Lett. **79**, 2783 (1997).
[11] A. Burgess and H. P. Summers, Astrophys. J. **157**, 1007 (1969).
[12] V. L. Jacobs, J. Davis, and P. C. Kepple, Phys. Rev. Lett. **37**, 1390 (1976).
[13] V. L. Jacobs and J. Davis, Phys. Rev. A **19**, 776 (1979).
[14] K. LaGattuta and Y. Hahn, Phys. Rev. Lett. **51**, 558 (1983).
[15] C. Bottcher, D. C. Griffin, and M. S. Pindzola, Phys. Rev. A **34**, 860 (1986).
[16] K. LaGattuta, I. Nasser, and Y. Hahn, Phys. Rev. A **33**, 2782 (1986).
[17] F. Robicheaux and M. S. Pindzola, Phys. Rev. Lett. **79**, 2237 (1997).
[18] T. Bartsch *et al.*, Phys. Rev. Lett. **79**, 2233 (1997).
[19] H. Feshbach, Ann. Phys. (N.Y.) **19**, 287 (1962).
[20] Y. Hahn, Adv. At. Mol. Phys. **21**, 123 (1985).
[21] D. C. Griffin, F. Robicheaux, and M. S. Pindzola, Phys. Rev. A (to be published).