

Nature of Interacting Resonances in Electron-Ion Excitation

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The calculations of Badnell *et al.* [Phys. Rev. A **48**, R2519 (1993)] demonstrated an apparent breakdown of the isolated-resonance approximation within certain resonant contributions to the $3s^2\ ^1S \rightarrow 3s3p\ ^3P$ transition in Fe^{14+} . We have now carried out detailed analyses of selected resonant structures for this transition. Comparing calculations using the independent-processes and isolated-resonance approximation, interacting resonance theory, and the R -matrix close-coupling method, we determine the nature of the interactions between resonances and demonstrate the sensitivity of the size of the resonant contribution to the positions of the resonances.

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The ability to accurately predict the strength of certain atomic collision processes remains crucial to the understanding of a variety of astrophysical and laboratory plasmas. Especially important is the electron-impact excitation of atomic ions. Because of their influence on level populations and radiative line emissions, accurate excitation cross sections form the basis of many plasma temperature and density diagnostics. The formation of short-lived resonances can lead to significant enhancements of nondipole transitions, for which the nonresonant background cross sections are relatively weak. In order to gain a more complete understanding of the nature of such resonant structures, we compare resonant cross-section calculations based on a perturbative independent-processes, isolated-resonance (IPIR) approximation, a perturbative interacting resonance approximation, and a nonperturbative close-coupling (CC) approximation. A key finding of this Letter is that the strength of the resonant contribution to electron-impact excitation can be affected significantly by direct configuration interaction (CI) between resonances, causing it to be very sensitive to the energy separation between the resonances. On the other hand, indirect interactions through a common continuum are found to be less important.

The most widely used perturbative approach for electron-ion excitation is the IPIR approximation [1], in which both the interference between the direct and resonant contributions and the interaction between resonant states are ignored. In this approximation, the total electron-impact excitation cross section from an initial level i to a final level f is the sum of the direct excitation cross section and the cross section for resonant excitation followed by autoionization, $\sigma_{\text{REA}}(i \rightarrow f)$, which in atomic units is given by

$$\begin{aligned} \sigma_{\text{REA}}(i \rightarrow f) &= \frac{\pi}{2g_i k_i^2} \sum_{l_i} \sum_{l_f} \sum_{\alpha} \frac{g_{\alpha} A_{\alpha}(\alpha \rightarrow i, l_i) A_{\alpha}(\alpha \rightarrow f, l_f)}{(E - \epsilon_{\alpha})^2 + \Gamma_{\alpha}^2/4}. \end{aligned} \quad (1)$$

In Eq. (1), k_i is the linear momentum of the incident electron, g_i is the statistical weight of the initial level, g_{α} and ϵ_{α} are the statistical weight and energy of the resonant level α , respectively, $A_{\alpha}(\alpha \rightarrow i, l_i)$ and $A_{\alpha}(\alpha \rightarrow f, l_f)$ are the autoionizing rates to the initial and final levels plus continuum electrons with angular momenta l_i and l_f , respectively, and Γ_{α} is the total (autoionizing and radiative) width of the resonance α .

The IPIR approximation has been employed to calculate the excitation cross section, including resonant contributions, in a number of highly ionized species [1–3]. Recently, however, Badnell *et al.* [4] discovered some large differences between resonances calculated using the R -matrix close-coupling (CCR) approach [5] and the IPIR approximation for the $3s^2\ ^1S \rightarrow 3s3p\ ^3P$ transition in Fe^{14+} . Similar discrepancies have also been discovered in other Mg-like ions [6]. It is the purpose of this Letter to explain the reasons for this apparent breakdown in the IPIR approximation and to provide a better understanding of the nature of the interactions between resonances.

The two most likely sources of these discrepancies are the following: direct CI between the resonant states, which is of order V in perturbation theory, and interactions between resonances through the adjacent continua, which are of order V^2 in perturbation theory, where V is the two-electron electrostatic-interaction operator. Direct CI is included within the CC formalism in terms

of the interactions between closed channels. However, in most applications of the IPIR approximation, CI is included within the N -electron target states, but is ignored between the $(N+1)$ -electron autoionizing states, for all but the lowest Rydberg states. This practice is in the spirit of the distorted-wave approximation, which ig-

nores CI in the $(N+1)$ -electron continuum; it also avoids the diagonalization of large matrices.

Interactions between resonances through a common continuum can be incorporated within a perturbative formalism by applying Feshbach resonance theory [7]. The resonant-excitation-autoionization contribution is then

$$\sigma_{\text{REA}}(i \rightarrow f) = \frac{16\pi}{2g_i k_i^3 k_f} \sum_{l_i} \sum_{l_f} \left| \sum_{\alpha} \sum_{\beta} g_{\beta}^{1/2} \langle \Psi_f | V | \phi_{\alpha} \rangle \Omega_{\alpha, \beta}^{-1} \langle \phi_{\beta} | V | \Psi_i \rangle \right|^2. \quad (2)$$

In Eq. (2), Ψ_i and Ψ_f are the initial- and final-state wave functions, including the continuum electron, respectively; ϕ_{α} and ϕ_{β} are the wave functions for the $(N+1)$ -electron resonant levels α and β , respectively; and the elements of the matrix Ω are given by

$$\Omega_{\alpha\beta} = \delta_{\alpha\beta}(E - \epsilon_{\alpha} + i\Gamma_{\alpha}/2) - (1 - \delta_{\alpha\beta})\Lambda_{\alpha\beta}. \quad (3)$$

In the pole approximation, the elements of the matrix Λ are given by

$$\Lambda_{\alpha\beta} = -2i \sum_j \sum_{l_j} \frac{1}{k_j} \langle \phi_{\alpha} | V | \Psi_j \rangle \langle \Psi_j | V | \phi_{\beta} \rangle - i\pi \sum_m \langle \phi_{\alpha} | D | \Phi_m \rangle \langle \Phi_m | D | \phi_{\beta} \rangle. \quad (4)$$

In Eq. (4), Φ_m is an $(N+1)$ -bound-electron wave function, D is the dipole-radiation field operator, and continuum normalization is chosen as 1 times a sine function. If one ignores the interaction between resonances [$\Omega_{\alpha\beta} = \delta_{\alpha\beta}(E - \epsilon_{\alpha} + i\Gamma_{\alpha}/2)$] and assumes that the resonances do not overlap, Eq. (2) reduces to the IPIR approximation [Eq. (1)].

The calculations of the resonant contributions for the $3s^2 1S \rightarrow 3s3p^3 P$ excitation in Fe^{14+} , discussed here, were carried out in LS coupling using a CI expansion described in Ref. [4]. The CCR calculations were performed using modified versions of the Opacity project R -matrix codes [8] and the orbitals for the CCR calculations were generated using the multiconfiguration Hartree-Fock programs of Fischer [9]. The perturbation-theory calculations were carried out in the distorted-wave approximation using bound-state orbitals, distorted waves, and matrix elements generated with Cowan's atomic structure codes [10]. Care was taken to assure that the slightly different bound-state orbitals for the two sets of calculations would not cause any significant differences in results. The effects of the radiative interaction were not included within the perturbation-theory calculations, since they were not part of the CCR calculations.

We have investigated the effects of interacting resonances for several of the resonant structures within the $3s^2 1S \rightarrow 3s3p^3 P$ transition. However, for this Letter, we focus on the structure due to resonances of the form $3s3d(^3D)7l$ and $3s3p(^1P)14l$. The discrepancies between the CCR and the IPIR calculations occur for most of the $LS\Pi$ symmetries within this resonant structure; for illustrative purposes, we consider the interactions between the lower energy $3s3d(^3D)7f^2 H^{\circ}$,

$3s3d(^3D)7h^2 H^{\circ}$ resonant pair and the slightly higher energy $3s3p(^1P)14g^2 H^{\circ}$, $3s3p(^1P)14i^2 H^{\circ}$ resonant pair. The interactions within each pair are negligibly small.

A comparison of the calculated $^2 H^{\circ}$ partial cross sections for this resonance structure, with and without CI between the pairs of resonances, is shown in Fig. 1. We notice from Fig. 1(a) that the resonances, without the inclusion of CI, are small. Furthermore, by comparing the partial cross section calculated from the IPIR approximation [Eq. (1)] with that calculated from interacting resonance theory [Eq. (2)], we see that interactions between the resonant pairs through the continuum are small. However, from Fig. 1(b), we see that direct CI has a very large effect on the size of the resonant structure; and that when CI is included, the effects of interactions through the continua are negligible. It is also interest-

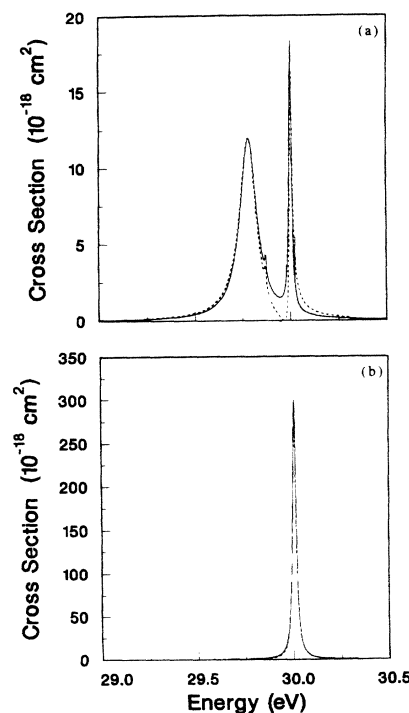


FIG. 1. Partial cross section for the resonant contributions of $3s3d(^3D)7l^2 H^{\circ}$ and $3s3p(^1P)14l^2 H^{\circ}$ to the $3s^2 1S \rightarrow 3s3p^3 P$ transition. Solid curve, IPIR approximation; dashed curve, interacting resonance theory. (a) No CI between resonant pairs; (b) with CI between resonant pairs.

ing to note that the area under the resonance curve in Fig. 1(b) is more than 4 times that of Fig. 1(a). This large increase in the resonance contribution can be understood by examining the Auger rates. Without CI, it is found that the $3s3d(^3D)7l^2H^0$ resonances have a small probability of formation but a large probability of autoionizing to $3s3p^3P$, while the reverse is true of the $3s3p(^1P)14l^2H^0$ resonances. When CI between the resonant pairs is included, the probability of formation of the $3s3d(^3D)7l^2H^0$ decreases further, but the probability of autoionization from the $3s3p(^1P)14l^2H^0$ resonances to $3s3p^3P$ increases dramatically, accounting for the large increase in the strength of the higher energy resonant structure.

We have also performed a four-state ($3s^2^1S$, $3s3p^3P$,

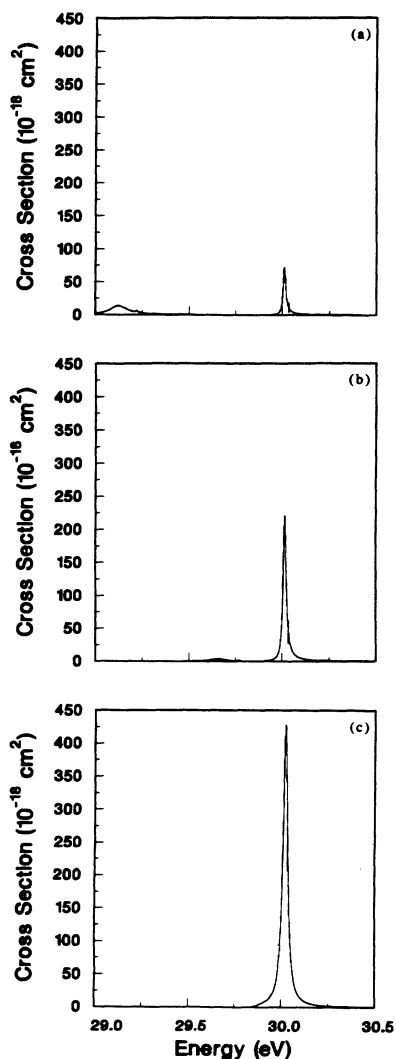


FIG. 2. $^2H^0$ partial cross section for the $3s^2^1S \rightarrow 3s3p^3P$ transition, from a four-state CCR calculation, showing the resonant contributions as a function of separation between resonances. (a) 4.0 times, (b) 1.5 times, and (c) 0.5 times the energy separation between resonances employed in Fig. 1.

$3s3p^1P$, $3s3d^3D$) CCR calculation for the $^2H^0$ symmetry in this energy region and the resonant structure at 30 eV is nearly identical to that shown in Fig. 1(b). Thus, the IPIR approximation agrees very well with the CC approximation, but only when CI between the $(N+1)$ -electron resonance states is included.

It is also interesting to study the interactions between these resonances as a function of separation between pairs. This was accomplished by repeating the four-state CCR calculations, mentioned above, at various energies of the $3s3d^3D$ threshold. In this way, it is possible to move the $3s3d(^3D)7l^2H^0$ resonances with respect to the $3s3p(^1P)14l^2H^0$ resonances. The results for 4.0 times, 1.5 times, and 0.5 times the energy separation between resonant pairs employed in Fig. 1 (approximately 0.22 eV) are shown in Fig. 2. From Fig. 2(a), we see that even when the separation is increased by a factor of 4, the resonant structure at 30 eV is still approximately 4 times higher than that obtained from the IPIR approximation with no CI. We see from Figs. 2(b) and 2(c) that as the resonances get closer, the lower energy resonant structure begins to disappear and the higher energy one continues to increase in magnitude.

One might expect this effect to continue as the resonances are forced even closer. However, when the resonances are overlapping, interactions through the continua become important, and offset some of the enhancement due to direct CI. In Fig. 3, we demonstrate this by comparing IPIR calculations, which include direct CI (solid curve), with perturbative calculations which include both direct CI and interference through the continuum (dotted curve) at an energy separation of approximately one-fourth that of Fig. 1. At this separation, destructive

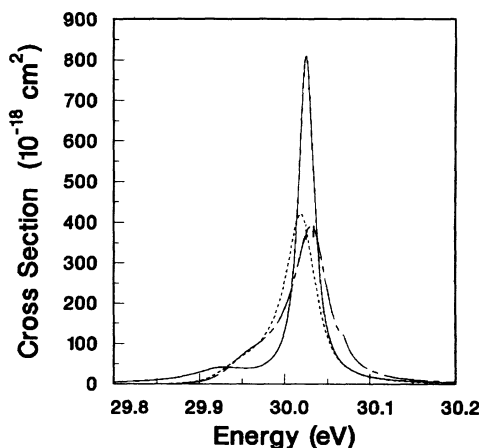


FIG. 3. $^2H^0$ partial cross section for the $3s^2^1S \rightarrow 3s3p^3P$ transition showing the resonant contributions for an energy separation between resonant pairs equal to approximately 0.25 times that employed in Fig. 1. Solid curve, IPIR approximation with direct CI; dotted curve, interacting resonance theory with direct CI; dash-dotted curve, four-state CCR calculation.

interference between resonances through the continua decreases the height of the resonant structure by about a factor of 2. By comparing this with the results of a four-state CCR calculation at the same separation (dash-dotted curve), we see that the interacting resonance theory [Eq. (2)] gives a fairly accurate representation of this additional interaction. As an independent check of the results shown in Figs. 2 and 3, we have also performed four-state CCR calculations at various resonance separations using a completely different R -matrix program [11], and obtained nearly identical results. With this code, we also turned the direct CI between resonances on and off and thereby confirmed the importance of CI on the size of the resonant structure.

It is also worth noting that in the case of the interaction between the $3s3d(^3D)7l$ pair and the $3s3p(^1P)14l$ pair for the ^{21}Ie symmetry, the resonances are completely overlapping, and all the effects discussed above are present, but much more pronounced. Direct CI increases the area under the resonance curve by approximately 200; however, interaction through the continuum reduces this enhancement by a factor of about 3, so that the overall enhancement of the resonance structure is approximately 64. Again, the agreement between the interacting resonance theory calculation and the CCR calculation for this symmetry is excellent [6].

In conclusion, we have shown that the resonant contribution to electron-impact excitation can be affected significantly by interactions between resonances, and that the primary mechanism for such interactions is direct CI, rather than interactions through the continuum. In order for such interactions to have an appreciable effect, they must be relatively close; however, CI can be significant when the resonances are far from overlapping, which is not true of interactions through the continua. For overlapping resonances, both types of interactions should be included within a perturbative calculation. It is interesting to contrast this with dielectronic recombination, which appears to be far less sensitive to the interactions between resonances [12].

We have also demonstrated the extreme sensitivity of the resonance structure to the positions of the individual resonances. This may make accurate perturbative or nonperturbative calculations of the resonance contribution to excitation difficult for complex structures, for which there are often a large number of closely spaced

resonances. However, additional efforts will be required to establish how important these effects will be on the determination of the rate coefficients needed for plasma diagnostics.

In highly charged ions, the effects of the radiative interaction on the resonant contribution to excitation can become important. Although radiative damping is easily included within a perturbative approach, a general treatment within a nonperturbative CC formalism has yet to be developed. In addition, in complex ionic systems, perturbative approaches often have advantages over CC methods because of the sheer number of atomic states involved. With this new understanding of the nature of the interactions between resonances, it may be possible to develop efficient numerical techniques to incorporate the important resonant interactions, within a perturbative formalism.

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