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Breakdown of the isolated-resonance approximation for the electron-impact excitation of positive ions

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We have carried out a series of calculations, the results of which demonstrate the breakdown of the isolated-resonance approximation for the electron-impact excitation of positive ions. The specific results presented here, namely for the $3s^2\,{}^1S \rightarrow 3s3p\,{}^3P$ transition in Fe^{14+}, are not unique. All of the Mg-like ions that we have investigated so far exhibit the same breakdown. There is no reason to believe either that the Mg-like sequence is unique. This has important implications for the description of resonant processes that are strongly radiation damped, for which the isolated-resonance approximation is widely used and the standard formulation of the close-coupling approximation is not applicable.

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Resonant processes frequently dominate low-energy electron-ion scattering cross sections and, via the tail of the Maxwellian distribution function, influence the population levels of ions over a wide range of temperatures and densities, which are of interest to the study of laboratory and astrophysical plasmas. Regarding their physical description, resonances arise automatically on solving the close-coupling equations using, say, the R-matrix method [1] (denoted hereafter as the CCR approximation). However, the limited treatment of radiation damping currently implemented within the CCR approximation (the Gailitis average [2,3] for excitation or the weak-field approximation [4,1] for photoionization) limits its application to ions of "sufficiently" low-residual charge, always assuming sufficient computational resources exist to solve the close-coupling equations required. Consequently, an alternative (perturbative) approach has been pursued for highly charged (and not so highly charged) ions, namely, the independent-process and isolated-resonance approximation using distorted waves (denoted the IPIRDW approximation). It is straightforward to allow for all types of radiation damping transitions within the IPIRDW approximation [5]. It has long been known that distorted waves are generally a good approximation for an electron scattering-off of an ion that is several times ionized [6]. More recently, we have shown that interference effects between the resonant and nonresonant contributions to electron-impact excitation diminish rapidly as the charge state increases [7]. In the case of electron-ion recombination we have shown that these effects are almost always negligible [8].

One can always assess the error in the CCR approximation due to the neglect of radiation damping by turning it on and off within the IPIRDW approximation. Thus it remains to assess the importance of overlapping (i.e., interacting) resonances for electron-impact excitation and, by implication, the indirect process of dielectronic-capture double autoionization (dielectronic ionization), which contributes to ionization. That is the purpose of this paper. We have already carried out a study of interacting resonance effects in electron-ion recombination and there we found that the resonances had to be physically overlapping to obtain a significant departure from the isolated resonance results, but few examples have been noted so far [8]. However, the study reported on here indicates that overlapping resonance effects are large and commonplace for electron-impact excitation. This is probably due to the greater strength of the background and resonance cross sections, enabling the resonances to interact more strongly, i.e., over a wider energy separation, than in the case of recombination.

Now, we demonstrate by specific example the breakdown of the isolated-resonance approximation. The sequence studied is the Mg-like one, which we had begun to study in connection with ongoing experiments at Oak Ridge National Laboratory, and Fe^{14+} in particular. We used the same nonrelativistic N-electron atomic structure in both our IPIRDW and CCR calculations, details of which were given previously for the case of Ar^{6+} [9]. Briefly, we generated the 13-term configuration-interaction target expansion arising from the $3s^2$, $3s3p$, $3s3d$, $3p^2$, $3p3d$, and $3d^2$ configurations using the multiconfiguration Hartree-Fock programs of Froese Fischer [10], the orbitals for which are generated from a single-configuration Hartree-Fock approximation. We then adjusted the resulting term energies to the $(2J+1)$-weighted-average of the observed energies [11], for both sets of collision calculations. The CCR calculations were carried out using the Opacity Project version of the R-matrix codes [3]. Here, the $(N+1)$-electron bound orbit-

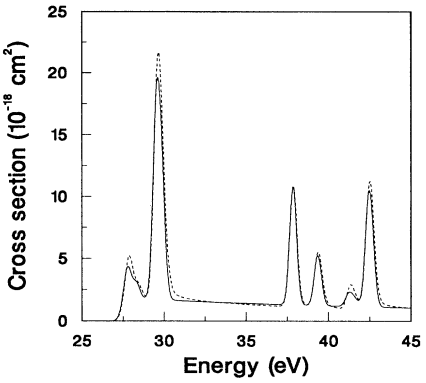

FIG. 1. Electron-impact excitation cross sections for the $3s^2\,{}^1S \rightarrow 3s3p\,{}^3P$ transition in Fe^{14+}, convoluted with a 0.5-eV full width at half maximum Gaussian function. Three-state calculations including the $3s3d\,{}^3D$ term: ——, IPIRDW approximation; — — —, CCR approximation; both this work.

al configurations are included both for orthogonality and correlation purposes. We found that including configurations beyond those required by orthogonality had a negligible effect on the collision results. The IPIRDW calculations were carried out using the AUTOSTRUCTURE code [12,13] where Schmidt orthogonalizes the continuum and Rydberg orbitals to the target/core orbitals and neglects the effects of the $3l3l'3l''$ configurations on the remaining collision problem. We found that the IPIRDW threshold partial collision strengths for $3s^2\,{}^1S \rightarrow 3s3d\,{}^{1,3}D$ and $3s3p\,{}^3P \rightarrow 3s3d\,{}^{1,3}D$ transitions differed by 1–10 % from those of the CCR calculation, the largest differences arising on the smallest partial-wave contributions. All of the calculations were carried out in the *LS* coupling scheme.

We now present the results of a series of IPIRDW and CCR calculations for the electron-impact excitation of the $3s^2\,{}^1S \rightarrow 3s3p\,{}^3P$ transition in Fe^{14+}. The three-state results show resonances from a single Rydberg series, while the four-state results show two overlapping Rydberg series. Care was taken to ensure that the CCR resonances were sufficiently energy resolved so as to give a converged result when convoluted with a 0.5-eV full width at half maximum Gaussian function. The IPIRDW resonances were energy averaged analytically

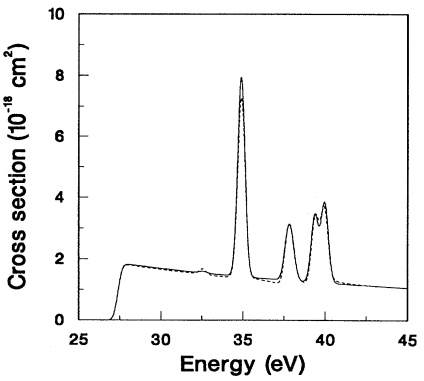

FIG. 2. As in Fig. 1, except for the $3s3d\,{}^1D$ term.

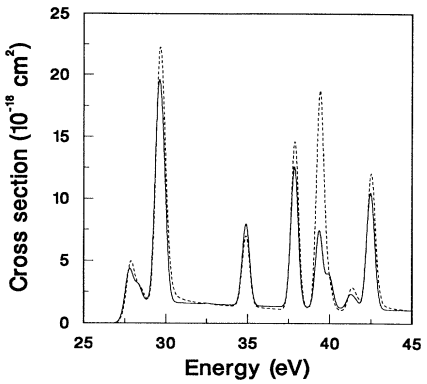

FIG. 3. As in Fig. 1, except for the four-state calculations, including the $3s3d\,{}^1D$ and ^3D terms.

before convolution and so there is no resolution problem in this approximation. In Fig. 1 we present our results for the leading resonances of the $3s3d\,{}^3Dnl$ Rydberg series. We see that the IPIRDW and CCR results are almost identical. The small differences that remain can be attributed to small energy differences between the positions of the resonances resulting from the two approximations, as well as to a residual error from not fully resolving some of the very narrow resonances in the CCR calculation. Similarly, we present IPIRDW and CCR results for the leading resonances of the $3s3d\,{}^1Dnl$ Rydberg series in Fig. 2; again we find excellent agreement between the two sets of results. As expected from our earlier work [7], interference effects between the resonant and nonresonant contributions are barely discernible. In Fig. 3 we present the results of the four-state calculations, which include simultaneously results for the $3s3d\,{}^3Dnl$ and $3s3d\,{}^1Dnl$ Rydberg series. The IPIRDW results are merely the superposition of the results shown in Figs. 1 and 2. However, the CCR results allow for the interaction of the two series of resonances. We see that there is a factor of 3 difference between the two sets of results for the peak lying at about 39 eV, which is due to the overlap of the $3s3d\,{}^3D8l$ and $3s3d\,{}^1D7l$ resonances.

We can continue in a similar fashion for series attached to other terms. In Fig. 4 we present our results for the $3s3p\,{}^1Pnl$ series. Again we find close agreement between the IPIRDW and CCR results. The small differences

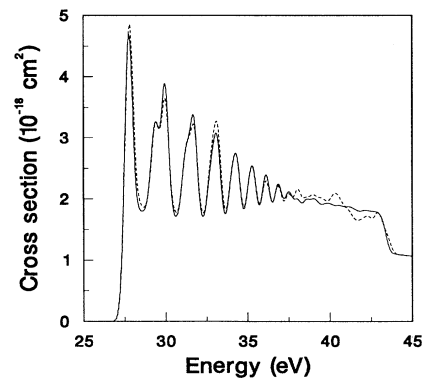

FIG. 4. As in Fig. 1, except for the $3s3p\,{}^1P$ term.

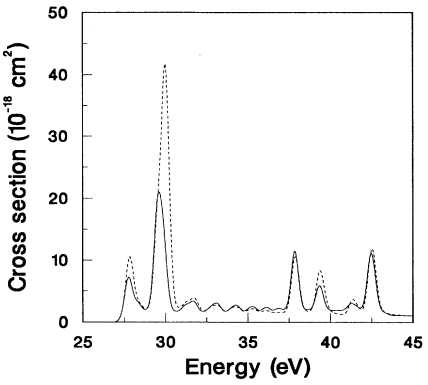

FIG. 5. As in Fig. 1, except for the four-state calculations, including the $3s3p\ ^1P$ and $3s3d\ ^3D$ terms.

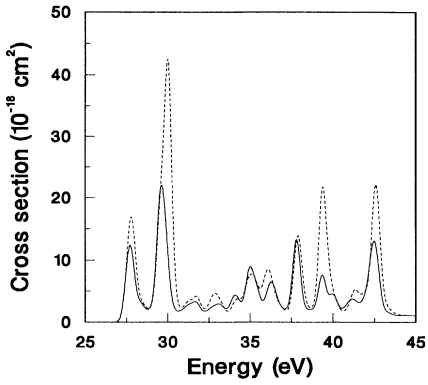

FIG. 7. As in Fig. 1, except for the eight-state calculations, including the $3s^2\ ^1S$, $3s3p\ ^{1,3}P$, $3s3d\ ^{1,3}D$, and $3p^2\ ^1S$, ^3P, and ^1D terms.

over the energy range 37–42 eV are due to the use of a finite-energy mesh in evaluating the CCR results converging on the Rydberg limit. In Fig. 5 we compare our four-state results for the $3s3p\ ^1Pnl$ and $3s3d\ ^3Dnl$ series. We now find a near factor of 2 difference between the IPIRDW and CCR results for the peak just below 30 eV, which is due to the overlap of the $3s3d\ ^3D7l$ and $3s3p\ ^1P14l$ resonances. In Fig. 6 we present the results of five-state calculations that include the resonances attached to the $3p^2\ ^1S$, ^3P, and ^1D terms. The agreement between the IPIRDW and CCR results indicates that there is little interaction between these Rydberg series. However, they do have some interaction with the $3s3d\ ^3Dnl$ series (not shown). Finally, In Fig. 7 we show the net result of all of the interacting resonances in a comparison of eight-state ($3s^2\ ^1S$, $3s3p\ ^{1,3}P$, $3s3d\ ^{1,3}D$, and $3p^2\ ^1S, ^3P, ^1D$) IPIRDW and CCR results. We observe widespread differences over the entire energy range shown. There is little of interest to see above 45 eV because the $3s3p\ ^1P$ channel opens up at $\sim$43 eV and suppresses resonances in the $3s3p\ ^3P$ channel.

Although we have demonstrated the importance of allowing for interacting resonances, as yet, we do not know the accuracy of our description of them. For example, the results presented here are for the nonrelativistic *LS* coupling problem. We need to carry out similar calculations in intermediate coupling using the Breit-Pauli Hamiltonian. This may well change the quantitative nature of the results, but the qualitative effects of interacting resonances should still be seen. In light of this, it would be highly desirable to have some experimental results so as to be able to benchmark theory. It is hoped that the electron-energy-loss spectroscopy experiment at Oak Ridge National Laboratory will be able to do just that, if not for Fe^{14+}, then at least for Ar^{6+} so as to benchmark the nonrelativistic theory.

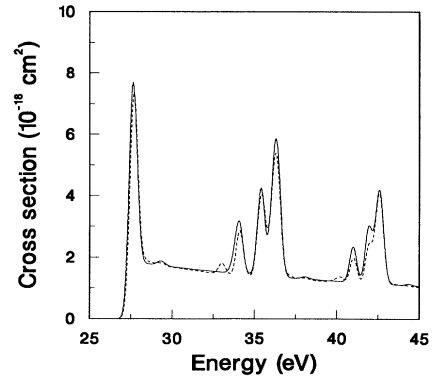

FIG. 6. As in Fig. 1, except for the five-state calculations, including the $3p^2\ ^1S$, ^3P, and ^1D terms.

In conclusion, we have demonstrated the breakdown of the isolated-resonance approximation for electron-impact excitation, specifically for the case of the $3s^2\ ^1S \rightarrow 3s3p\ ^3P$ transition in Fe^{14+}. However, this is not due to a single accidental energy degeneracy; witness Fig. 7. Nor is it specific to Fe^{14+}. We have begun to examine the same process in other Mg-like ions, and have found similar results there. It would appear that the breakdown of the isolated-resonance approximation for electron-ion excitation (and thus dielectronic ionization) is widespread. This does not mean that we can simply use the *R*-matrix method all of the time instead. Radiation damping can be an important effect in highly charged ions. The example that we looked at in this paper was for a $\delta n = 0$ core excitation, for which radiation damping is only important near the series limit, and this can be taken into account in the *R*-matrix method by Gailitis averaging [2,3]. However, $\delta n > 0$ core excitations are more strongly radiation damped, and this affects outer-shell contributions to excitation and inner-shell contributions to ionization. Indeed, radiation damping reduces the excitation-autoionization contribution by about 40% in the case of Fe^{15+} [14] and the dielectronic ionization contribution by a factor of 3 for the case of Fe^{23+} [15]. The proposal [16] to use a complex Hamiltonian to take account of radiation damping in the *R*-matrix method is only a partial solution since this deals only with radiation due to the core electron. Outer electron radiation can be just as important, or even more so, following $\delta n > 0$ core excitations. A perturbative approach to overlapping resonances (including radiation damping) is an alternative

strategy, which should be pursued also, and it is the one that we pursued before for electron-ion recombination [8].

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