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Validity of the independent-processes approximation for resonance structures in electron-ion scattering cross sections

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The total inelastic cross section for electron-ion scattering may be found in the independent-processes approximation by adding the resonant cross section to the nonresonant background cross section. We study the validity of this approximation for electron excitation of multiply charged ions. The resonant-excitation cross section is calculated independently using distorted waves for various Li-like and Na-like ions using $(N+1)$-electron atomic-structure methods previously developed for the calculation of dielectronic-recombination cross sections. To check the effects of interference between the two scattering processes, we also carry out detailed close-coupling calculations for the same atomic ions using the R-matrix method. For low ionization stages, interference effects manifest themselves sometimes as strong window features in the close-coupling cross section, which are not present in the independent-processes cross section. For higher ionization stages, however, the resonance features found in the independent-processes approximation are found to be in good agreement with the close-coupling results.

I. INTRODUCTION

Resonant processes dominate electron-ion scattering in many laboratory and astrophysical plasmas through resonant excitation,[1] the inner-shell excitation-autoionization[2] contribution to ionization, and dielectronic recombination.[3] Despite the ever-increasing energy resolution, experiments on dielectronic recombination[4–6] and on ionization[7–10] are still well described, in general, by the independent-processes approximation using distorted waves.[11–16] As the resolution increases further[17,18] and high-resolution resonant-excitation experiments[19] come on line, how well can we expect the independent-processes approximation to perform and what are the alternatives? We are particularly interested in the validity of the independent-processes approximation for excitation and ionization since it enables us to make use of general codes that were developed previously for dielectronic recombination.

Excitation resonances arise naturally in the close-coupling approximation,[20] which automatically takes into account the effect of overlapping resonances and interference with the nonresonant background. The R-matrix approach[21] is probably the most efficient implementation of the close-coupling method in that it readily lends itself to the generation of resonance structure. However, there are several drawbacks. First, radiation damping is not normally included.[22] This can be a serious omission for $\Delta n>0$ transitions for resonant excitation in highly charged ions[23,24] and particularly so for the excitation-autoionization contribution to ionization.[25,26] Furthermore, there is no dielectronic recombination without radiation damping. Second, the number of coupled channels that must be included rises rapidly[27] with the complexity of the ionic structure. The number of coupled channels is also increased on going from a nonrelativistic Hamiltonian[28] to a Breit-Pauli[29] or Dirac Hamiltonian.[30] Finally, the mapping out of resonance structures is still a major task even with the latest asymptotics.[31] The number of continuum coupled channels included explicitly can be reduced[32] or distorted waves can be used[33,34] for the scattered electron, while the resonances are still retained through the $(N+1)$-electron bound channels, but the problem soon rapidly increases in size and the resonances still have to be mapped out.[33,34]

Multichannel quantum-defect theory[35] (MCQDT) has some advantages. Interference effects are retained.[35] The scattering equations need only be solved just above the highest threshold in close-coupling or distorted-wave approximations and radiation damping can be included[36,37] for the core. The drawbacks are that MCQDT relies on extrapolation and so is unreliable or unworkable for low-lying states,[37] it is still a many-coupled-channel problem to delineate the resonance structure, and the omission of radiation damping of the Rydberg electron can be serious for low-lying resonances.[37,38] Also, intermediate-coupling effects are usually[37] taken into account through the use of recoupling or term-coupling coefficients.[39] This approach is only valid when the fine-structure splittings are much smaller than the term splittings (and the transition energy).

The independent-processes approximation using distorted waves views[40–43] resonances from the point of view of a structure problem rather than a scattering problem. Resonance features are calculated using perturbation theory, radiation damping is routinely included, and the method is easily applied to excitation, ionization, and recombination using nonrelativistic, Breit-Pauli and Dirac Hamiltonians. However, although interference effects can be included,[44,45] they greatly increase the complexity of the problem and are generally omitted.

Previous comparisons[40,27,46] between the close-coupling approximation and the independent-processes approximation using distorted waves have been made between rate coefficients for resonant excitation (i.e., integrated over all resonance structure) using different atomic structures, while comparisons[26,47] for ionization are further complicated by radiation damping. Some detailed comparisons[33,48] have been made between close-coupling and distorted-wave resonances, but mostly within the framework of multichannel quantum-defect theory. Of course, comparisons[49,50] for excitation at energies above all resonance structures have shown that the results of close-coupling and distorted-wave approximations are generally in good agreement for ions that are ionized a few times or more.

The approach of this paper is to calculate resonant-excitation cross sections in the distorted-wave isolated-resonance approximation,[40] without averaging over[51] the Lorentzian profile, to add them to a nonresonant background (independent-processes approximation[40]) and compare them with the results of a close-coupling calculation that uses the same N-electron atomic structure. The only differences (at this stage) should be due to interference effects and coupling in the radial function for the continuum or Rydberg electron. We choose $\Delta n=0$ transitions for several ions from the Li-like and Na-like sequences as they are amenable to planned[19] electron-energy-loss spectroscopy measurements and one sequence (Li-like) has a simple resonance structure while the other (Na-like) is more complex. Of course, resonant-excitation cross sections have already been calculated for a number of Li-like[41,48,52] and Na-like[53,54] ions but they are not of direct relevance to the present detailed comparisons.

The layout of the paper is as follows. We outline the theory behind the calculations in Sec. II; in Sec. III we describe its application to Li-like and Na-like ions, and we present the results of our calculations in Sec. IV.

II. THEORY

A. Independent-processes approximation

In the independent-processes approximation, the total excitation cross section from an initial state i to a final state k is given by

$$\sigma_T(i;k)=\sigma_{\mathrm{NR}}(i;k)+\sigma_{\mathrm{RE}}(i;k)\ , \tag{1}$$

where $\sigma_{\mathrm{NR}}(i;k)$ is the nonresonant background cross section. The resonant-excitation cross section at an incident energy E_c is given by

$$\sigma_{\mathrm{RE}}(i;k)=\frac{(2\pi a_0 I_H)^2}{E_c}\times\sum_j \frac{\omega(j)}{2\omega(i)}\frac{\tau_0 A_a(j\to i)A_a(j\to k)L_j(E_c)}{\sum_h A(j\to h)} \tag{2}$$

where the Lorentz profile is given by

$$L_j(E_c)=\frac{(1/2\pi)\Gamma_j}{(E_c+E_i-E_j)^2+\frac{1}{4}\Gamma_j^2}\ . \tag{3}$$

The total width $\Gamma_j=\hbar\sum_h A(j\to h)$ may contain contributions from radiative A_r as well as autoionization A_a rates. Here, $\omega(j)$ is the statistical weight of the $(N+1)$-electron doubly excited state j with energy E_j, $\omega(i)$ is the statistical weight of the N-electron initial state i with energy E_i, I_H is the ionization potential energy of hydrogen and $(2\pi a_0)^2\tau_0=2.6741\times10^{-32}\ \mathrm{cm}^2\,\mathrm{s}$.

Equation (2) is very similar to that which we use[11] for dielectronic recombination, but then the Auger yield is replaced by the fluorescence yield, and the cross section is usually energy averaged[51] over an arbitrary bin width before convoluting with the required velocity distribution. Consequently, we may apply the AUTOSTRUCTURE package[55-58] in either of its nonrelativistic,[56] Breit-Pauli[56] or semirelativistic[58] forms. The sum over intermediate states is routinely taken over $n=2-1000$ and $l=0-30$. The only approximation made for high-n states is that the radial function for the Rydberg electron is approximated[57] by a suitably normalized zero-energy continuum function. Full configuration mixing and energy dependence is retained at every stage through diagonalization of the N-electron and $(N+1)$-electron Hamiltonians.

B. Close-coupling approximation

The solution of the close-coupling equations for electron excitation yields a scattering matrix that contains both background and resonant-excitation contributions, which when "squared," results in a cross section that contains the interference between the two contributions. We make use of the R-matrix method[21] to solve the close-coupling equations. In this method[21] the $(N+1)$-electron wave function is expanded in the inner region in terms of a finite set of bound-continuum and bound-bound functions, the latter being included both to satisfy the orthogonality conditions imposed on the former and, optionally, to allow for correlation. The continuum function is additionally expanded in terms of a finite set of basis functions; it is this feature that facilitates the solution of the resonant-scattering problem at many energies. The expansion coefficients are determined by the diagonalization of the $(N+1)$-electron Hamiltonian within the inner region and by the imposition of suitable boundary conditions. We make use of the nonrelativistic version of the R-matrix code developed for the Opacity Project,[31,59] since it enables us to use the same N-electron wave functions as in our distorted-wave calculations (see also Sec. III). This version[31] includes routines to solve the asymptotic coupled equations perturbatively,[60] as well as routines to "top-up" dipole collision strengths from high partial waves.[61,62]

III. APPLICATION TO Li- AND Na-LIKE IONS

We consider the $2s$-$2p$ transition in C^{3+}, O^{5+}, and Ne^{7+} and the $3s$-$3p$ and $3s$-$3d$ transitions in Si^{3+}, Ar^{7+}, and Ti^{11+}, in both the close-coupling and independent-processes approximations. The same N-electron orbitals were used in both sets of calculations and were generated using a single-configuration Hartree-Fock frozen-core approximation,[63] a $1s^2$ core for the Li-like ions and a $1s^2 2s^2 2p^6$ core for the Na-like ions.

A. Independent-processes approximation

For the Li-like ions, we consider the following resonant-excitation transitions (the $1s^2$ core has been suppressed)

$$2s+e^- \rightleftarrows 3l3l' \rightarrow 2p+e^-$$

and for the Na-like ions (the $1s^2 2s^2 2p^6$ core has been suppressed)

$$\begin{array}{ccc} 3s+e^- \rightleftarrows & \left|\begin{array}{c} 3dnl \\ 4l'nl \end{array}\right| & \rightarrow \left|\begin{array}{c} 3p+e \\ 3d+e^- \end{array}\right. . \\ & \downarrow & \\ & 4l''+e^- & \end{array}$$

In the Na-like case we also looked at the effect of radiative transitions of the form

$$4l'''nl \rightarrow 3l''nl + h\nu_1$$

and

$$4l'''nl \rightarrow 4l'''n'l' + h\nu_2$$

that were stable against autoionization. It was convenient to carry out two-state close-coupling calculations to generate the nonresonant-background cross section to be added to the resonant-excitation cross section.

For the resonant-excitation cross section, we calculated the continuum orbitals and, for Na-like ions, the Rydberg ($n>4$) orbitals in a slightly different distorting potential than the Hartree-Fock frozen-core orbitals. A local frozen-core potential was generated with Slater-type-orbitals, and the subsequently generated continuum and Rydberg orbitals were then Schmidt orthogonalized to the core orbitals. The coupling present in the $(N+1)$-electron orbitals obtained from the close-coupling calculation manifests itself mainly in the position of the resonances. We can investigate this effect in the distorted-wave approximation by including extra configurations purely for mixing purposes, in the Li-like case, for example, of the form $3l4l'$. Finally, the use of a discrete energy mesh with the Lorentzian profile of Eq. (3) means that we may not hit the peak value ($E_c = E_j - E_i$) of a narrow resonance.

B. Close-coupling approximation

We carried out a five-state ($2s,2p,3s,3p,3d$) calculation for the Li-like ions and a seven-state ($3s,3p,3d,4s,4p,4d,4f$) calculation for the Na-like ions for all partial waves up to a total angular momentum of $L=10$ (Li-like) or $L=12$ (Na-like). The only $(N+1)$-electron bound configurations retained in the eigenfunction expansion were those required by orthogonality. Fifteen (Li-like) or 20 (Na-like) continuum-basis orbitals were used and the R-matrix boundary was taken such that all of the bound orbitals had decayed to less than $0.002(Z+N+1)^{1/2}$ beyond it. The resonances were mapped out using a linear mesh of 2000–3000 points. Even so, as with the distorted-wave results, narrow resonances may still not be mapped out to their maximum peak height.

IV. RESULTS

The close-coupling and independent-processes results are for the LS-coupling scheme and neglect radiation damping. The effects of intermediate coupling and radiation damping were investigated for the independent-processes approximation and were found to be negligible for the ions and transitions ($\Delta n=0$) considered here.

A. Li-like ions

In Figs. 1 and 2 we present our results for the $2s$-$2p$ excitation of C^{3+} and O^{5+} in the vicinity of the $3l3l'$ resonances. The interference effects are small in general and there is good agreement between the results of the close-coupling and independent-processes approximations for the resonance structures. The main difference is in the contribution from the $3p3d\ ^1F$ and $3d^2\ ^1G$ resonances, at 24.5 eV in C^{3+}. The $3p3d\ ^1F$ resonance appears as a window in the close-coupling results for C^{3+} but this effect is substantially reduced by O^{5+}. The independent-processes calculations included the $3l4l'$ configurations (see Sec. III). They have little effect on the shape of the resonances but lower their energies by up to 1.5 eV in C^{3+}. The effect is greater for the higher-lying resonances than for the lower-lying ones and for C^{3+} than for O^{5+}. The differences between the results of the two sets of cal-

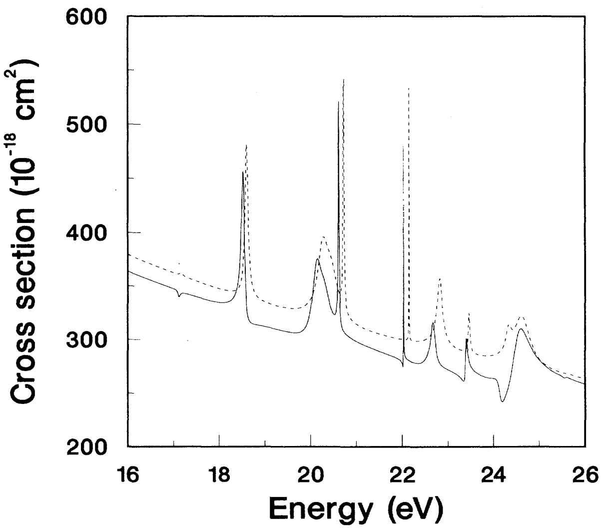

FIG. 1. Excitation cross section for the $2s$-$2p$ transition in C^{3+}. ——, five-state close coupling; — — —, distorted wave.

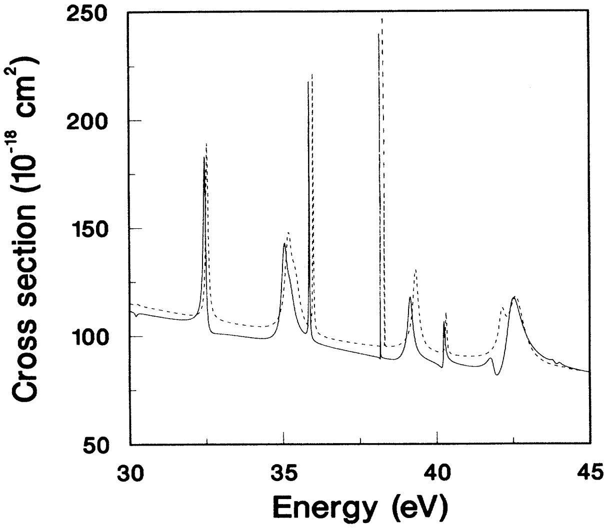

FIG. 2. Excitation cross section for the 2*s*-2*p* transition in O^{5+} ——, five-state close coupling; — — —, distorted wave.

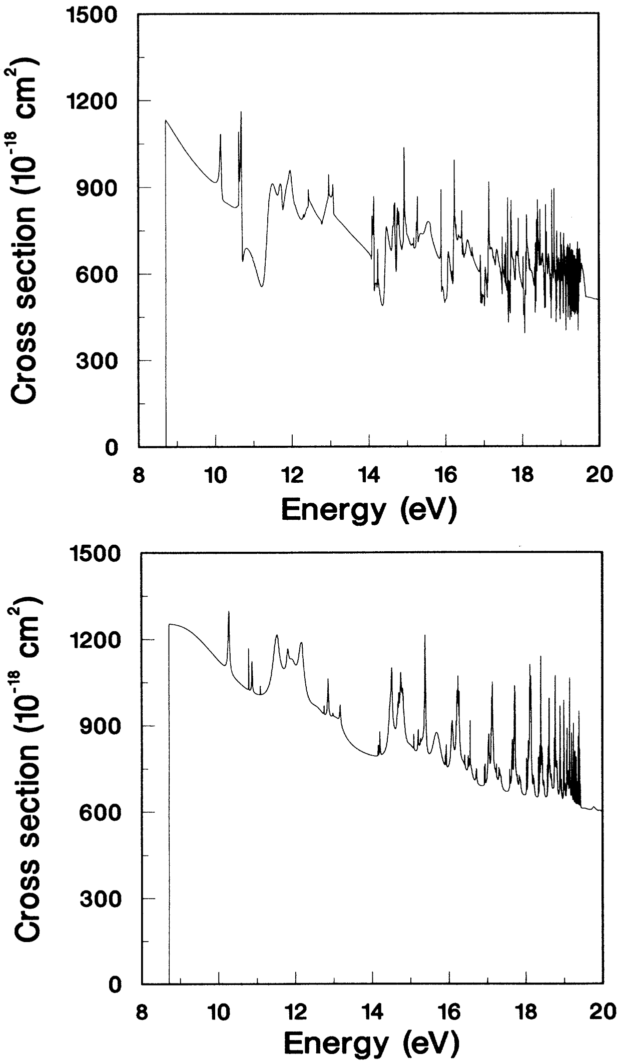

FIG. 3. Excitation cross section for the 3*s*-3*p* transition in Si^{3+}. Upper, seven-state close coupling; lower, distorted wave.

culations off-resonance is due to the difference between the five-state close-coupling and two-state close-coupling cross sections and is $\leq 10\%$ even for C^{3+}. Our results for Ne^{7+} (not shown) are similar to those for O^{5+} and show a further small improvement in the agreement between the close-coupling and independent-processes approximations.

B. Na-like ions

In Figs. 3–8 we present our results for the 3*s*-3*p* and 3*s*-3*d* excitations of Si^{3+}, Ar^{7+}, and Ti^{11+}. Since the resonance energies from the close-coupling and independent-processes approximations are slightly different, caution must be exercised in making peak-to-peak comparisons of narrow resonances as they may be mapped-out to different fractions of their maximum peak height. Generally, we may say that interference effects

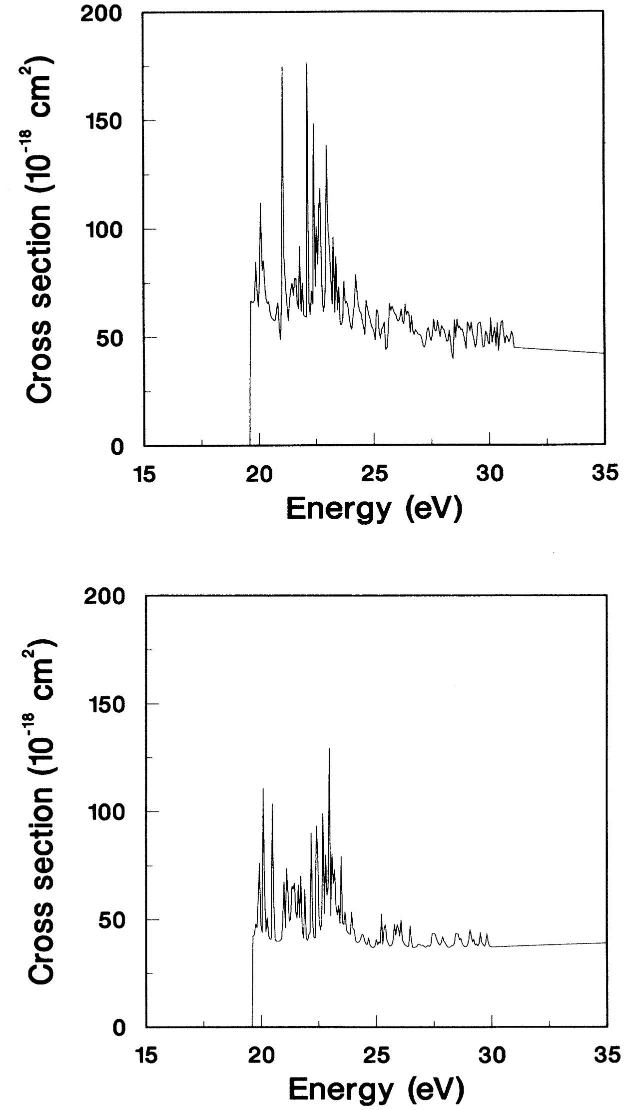

FIG. 4. Excitation cross section for the 3*s*-3*d* transition in Si^{3+}. Upper, seven-state close coupling; lower, distorted wave.

are much stronger for the $3s$-$3p$ transition than for the $3s$-$3d$. For Si^{3+} there are some significant differences between the results of the close-coupling and independent-processes approximations, particularly for the $3s$-$3p$ transition. For example, there is a large window resonance at 11 eV due to the $^3G^e$ partial wave which is repeated at higher energies (14 eV, 16 eV, . . .). It is not always easy to designate a particular term to a given resonance arising from a close-coupling calculation. However, our independent-processes calculation places the $3d4d\ ^3G$ resonance at about 11 eV, the others ($3d4d$ and $4p4f$) are either too high or too low in energy. The smooth drop from the $3s$-$3p$ threshold is deceptive; there are in fact two broad resonances centered around 9 eV arising from the $3d4p\ ^1F$ and ^1P terms which contribute about 20% of the cross section. Turning to the $3s$-$3d$ transition, there is a marked drop in the resonance strength above 23 eV; this is the position of the $4s$ limit, above which the $4lnl'$ resonances preferentially autoionize to the $4s$ continuum rather than the $3d$ one. As we move to Ar^{7+} and Ti^{11+}, we see that the interference effects are greatly reduced for the $3s$-$3p$ transition but even more so for the $3s$-$3d$ transition. This might be expected from z-scaling arguments[64] similar to those applied to the Beutler-Fano profile for window resonances in photoionization. Overall, there is much better agreement between the results of the close-coupling and independent-processes approximations for those two ions.

We looked at the gross differences between the results of the two approximations by convoluting them with a broad Gaussian. We found that the differences were about 25% for Si^{3+} but less than 10% for Ar^{7+} and Ti^{11+}, for both transitions. We deduced that most of this difference was due to the nonresonant background as fol-

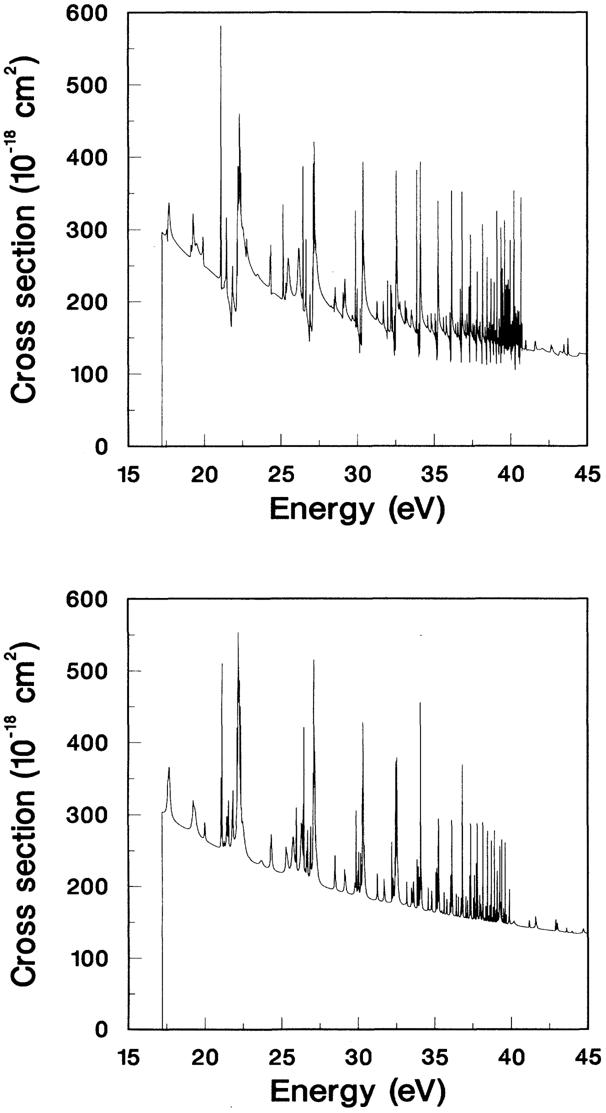

FIG. 5. Excitation cross section for the $3s$-$3p$ transition in Ar^{7+}. Upper, seven-state close coupling; lower, distorted wave.

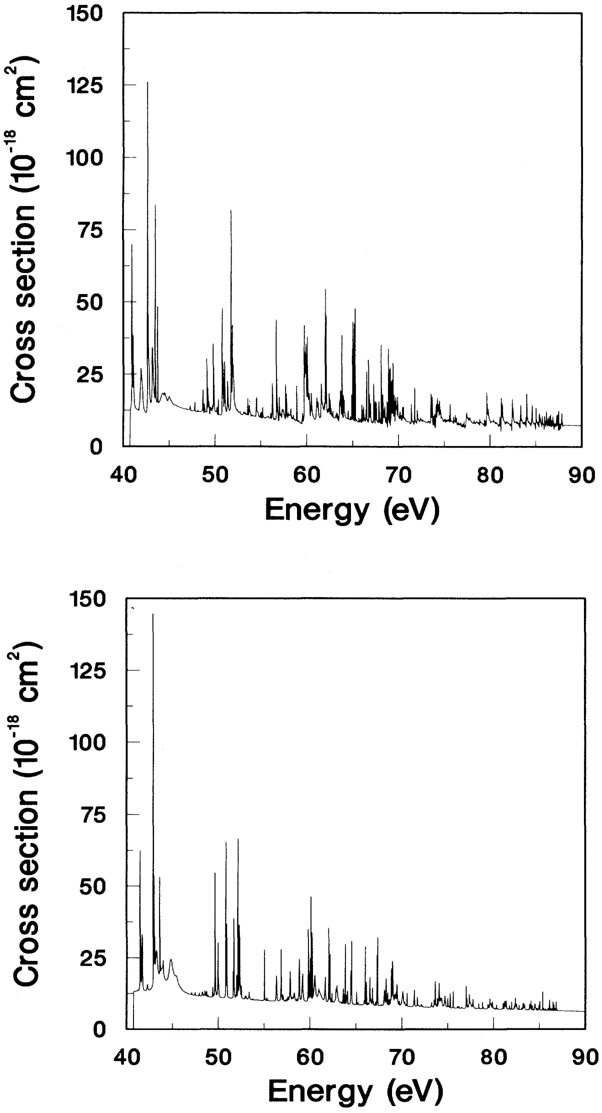

FIG. 6. Excitation cross section for the $3s$-$3d$ transition in Ar^{7+}. Upper, seven-state close coupling; lower, distorted wave.

lows. In the independent-processes approximation we found that the resonances contributed no more than 20% of the total cross section and we assumed that a similar result held for close coupling. We then compared the two-state close-coupling cross section with the seven-state, off-resonance cross section, estimated the difference, and found it to be comparable with the differences quoted above.

Finally, as we noted in the Li-like case, the additional $(N+1)$-electron-configuration mixing present in the close-coupling approximation can also produce small changes in the position and shape of the resonance features. We can test out this sensitivity in the distorted-wave approximation by varying the amount of configuration mixing present for the $(N+1)$-electron states. The same basic seven-state N-electron core is retained in each case (see Sec. III). We may then sum over each nl separately (for $n>4$) as we did for the results presented in Figs. 3–8. We may also include configuration interaction for all l states explicitly for a given n; a separate sum over each n is then required to obtain the total cross section. This was the approach that we took for the dielectronic recombination of H-like ions.[12] We can also examine n mixing if the problem[65] is dominated by low n. Model calculations that we have done show that even for Ti^{11+} some of the resonance features were still sensitive to the degree of $(N+1)$-electron-configuration mixing included in the calculation. It is an advantage of the close-coupling approximation that all of these configuration-mixing effects are automatically included.

V. CONCLUSION

We have made a detailed comparison of resonance structures calculated in the close-coupling approximation

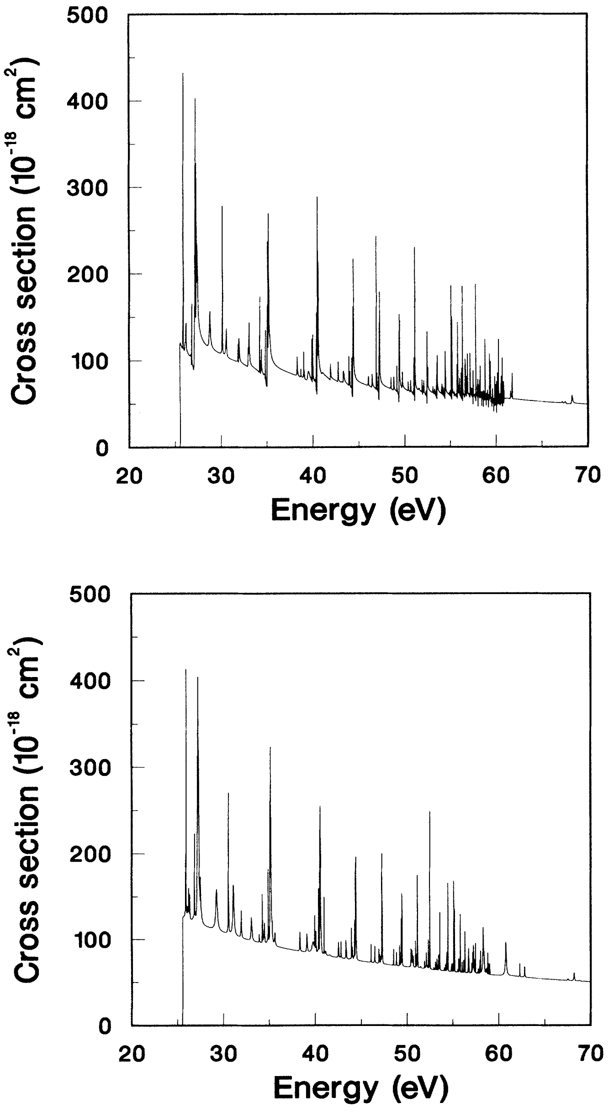

FIG. 7. Excitation cross section for the 3s-3p transition in Ti^{11+}. Upper, seven-state close coupling; lower, distorted wave.

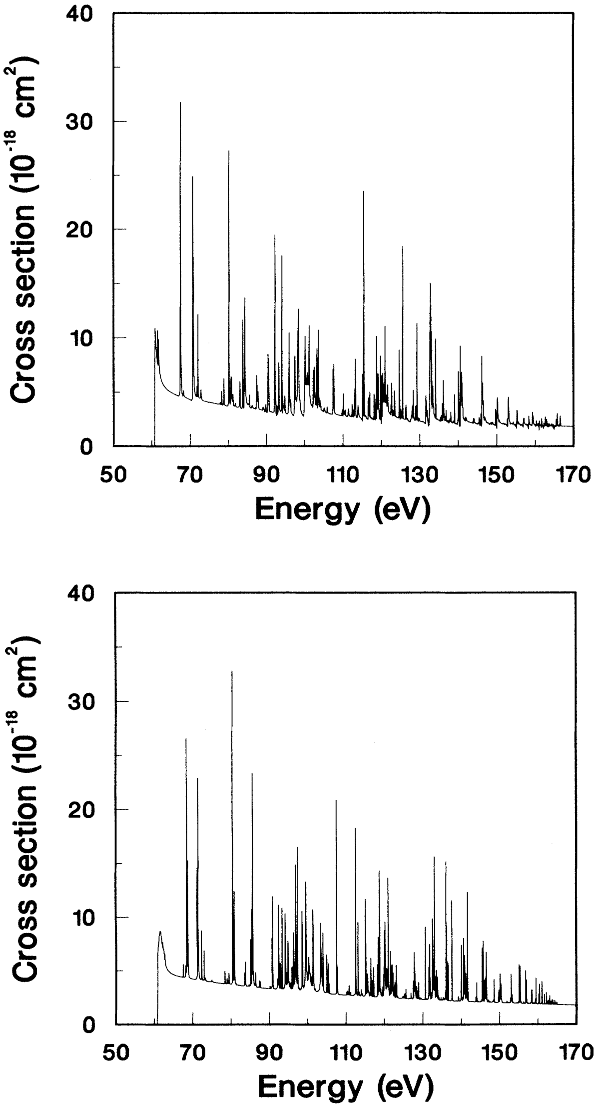

FIG. 8. Excitation cross section for the 3s-3d transition in Ti^{11+}. Upper, seven-state close coupling; lower, distorted wave.

and independent-processes approximation using distorted waves. We find that the interference effects and configuration mixing automatically included in the close-coupling approximation, but neglected by our independent-processes approximation, are small in general for ions ionized a few times and upwards. This lends support for the general use of the independent-processes approximation, using distorted-waves, for calculating the contribution from indirect processes to electron-ion scattering cross sections. This approach is particularly useful for problems involving a complex ionic structure or strong intermediate coupling or radiation damping, where the application of the close-coupling approximation is currently laborious or impractical.

Note added in proof. The 3*s*-3*p* cross section for Si^{3+} has recently been measured near threshold by Wåhlin *et al.* (Ref. 19), and it is in very good agreement with the seven-state close-coupling results of Fig. 3.

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