

## Effect of the configuration interaction between resonances for dielectronic recombination and resonant transfer excitation of Na-like ions

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(Received 26 June 1996)

It is shown in the present study that configuration interaction between the  $2p^53l3l'nl''$  resonances formed by electrons incident on Na-like ions leads to a reduction in the calculated dielectronic recombination cross section by as much as a factor of 2. This explains the previous discrepancies between independent theoretical calculations and experimental measurements of dielectronic recombination [Linkemann *et al.*, Nucl. Instrum. Methods Phys. Res. Sect. B **98**, 154 (1995)] and resonant transfer plus excitation [Bernstein *et al.*, Phys. Rev. A **40**, 4085 (1989)]. New calculations are performed for  $\text{Fe}^{15+}$ ,  $\text{Se}^{23+}$ , and  $\text{Nb}^{30+}$  using the independent-processes, isolated-resonance, distorted-wave method, and comparison with experiment is made where available. [S1050-2947(96)09311-0]

PACS number(s): 34.80.Kw

### I. INTRODUCTION

When a beam of electrons is incident on an atomic ion, it is possible that energy may be transferred from one of these electrons to one of the electrons bound to the target ion. If the initial electron loses enough energy, it becomes bound as well. Subsequent radiative stabilization of this state completes the process known as dielectronic recombination (DR) [1]. A similar process, known as resonant transfer and excitation plus x-ray emission (RTEX) [2] occurs when atomic ions are made incident on neutral atoms or molecules. In the ionic rest frame, the moving atom or molecule is seen as a source of electrons with a broad momentum distribution. For high projectile energies, the impulse approximation [3] is used to relate the RTEX cross section  $\sigma_{\text{RTEX}}(E_p)$  of ions incident on atoms or molecules to the DR cross section  $\sigma_{\text{DR}}(E_e)$  of electrons incident on the same ion:

$$\sigma_{\text{RTEX}}(E_p) = \int dp_z J(p_z) \sigma_{\text{DR}}(E_e). \quad (1)$$

The distribution of the target-electron momentum  $p_z$  is given by the Compton profile

$$J(p_z) = \int \int dp_x dp_y |\Psi(p_x, p_y, p_z)|^2, \quad (2)$$

and the electron energy is related to that momentum by

$$E_e = \frac{m}{M} E_p - E_t + p_z \sqrt{2E_p/M}, \quad (3)$$

where  $m$  and  $M$  are the electron and projectile masses, respectively, and  $E_t$  is the ionization threshold of the target atom or molecule. Thus, either process ultimately depends on the DR cross section.

Most calculations of  $\sigma_{\text{DR}}(E_e)$  make use of perturbative methods, such as the independent-processes plus isolated-

resonance approximation [4–6]. Although such results usually compare favorably with experimental measurement, there are certain notable exceptions [1]. For instance, the RTEX measurements of neonlike  $\text{Nb}^{31+}$  incident on  $H_2$  by Bernstein *et al.* [7] were accurately modeled by the calculations of Hahn *et al.* [8], and independently by Badnell [9]. However, similar results for Na-like  $\text{Nb}^{30+}$  on  $H_2$  from these two independent theoretical calculations yielded a peak RTEX cross section that was roughly twice the measured value of Bernstein *et al.* [7]. This discrepancy only worsened as the charge  $q$  on the projectile ions  $\text{Nb}^{q+}$  decreased, i.e., as more electrons were added. A similar discrepancy of roughly a factor of two was observed in a recent joint theoretical-experimental study of dielectronic recombination of Na-like  $\text{Fe}^{15+}$  [10].

We have reexamined the problem of  $n=2 \rightarrow 3$  dielectronic recombination of Na-like ions in order to unveil the cause of this discrepancy. Specifically, we are concerned mostly with the dielectronic capture process followed by the autoionization or radiative decay of the following resonances:

$$e^- + 2p^63s \rightarrow 2p^53s3lnl' \rightarrow \begin{cases} 2p^63s \\ 2p^63l \\ 2p^6nl' \end{cases} + e^- \quad (4a)$$

$$\rightarrow \begin{cases} 2p^63s3l \\ 2p^63snl' \\ 2p^63lnl' \end{cases} + \hbar\omega. \quad (4b)$$

In the earlier study of Badnell [9], for instance,  $LS$  coupling was used for the Na-like ion  $\text{Nb}^{30+}$ , and only the  $2p^53s3lnl'$  configurations were included in the basis describing the resonance states. The other configurations involving a  $2p$  hole and two  $M$ -shell electrons, i.e.,  $2p^53p^2nl$ ,  $2p^53p3dnl$ , and  $2p^53d^2nl$ , were not included in

this basis, and for nontrivial reasons. First, these configurations are not directly accessible via a one-step capture process from the  $2p^63s+e^-$  continuum, since it is a three-electron transition. Second, even if configuration interaction (CI) between the directly accessible  $2p^53s3lnl'$  configuration and these others is included, a higher-order process itself, the net effect is usually just a redistribution of the DR cross section among these resonances [11], leading to no appreciable effect in the total cross section. Indeed, most studies of CI between resonances [11–13] find that the only significant effect is caused by shifts in the energy positions of the resonances, which, due to the energy dependence on the radiative rates, alters the computed DR cross section. The CI being considered here is between configurations with approximately the same energy positions, so that this shifting effect is expected to be minimal. Third, inclusion of all  $2p^53l3l'nl''$  configurations in the basis description of the resonances would have led to a prohibitively time-demanding computation a few years ago, particularly for the Mg-like and Al-like ions considered also.

Nevertheless, the increased computational power of today's computers, and the mounting evidence that the previous theoretical results are perhaps a factor of 2 too high, warrant a second look at possible CI effects. Bearing in mind the increased computational time required for calculations that include this additional CI, we have broken down investigation of these effects into various stages. In the next section, we discuss some of the qualitative aspects of the effect of the present type of CI on DR cross sections. In Sec. III, we consider a model problem in which two resonances interact, one with allowed capture and radiative rates, the other with neither. Quantitative expressions for the DR probability as a function of the CI strength are derived for this case in the low- and high-charged limits. We then consider in Sec. IV one group of resonances in the Na-like  $2 \rightarrow 3$  DR case. The important CI effects are revealed, which can be understood by analogy to the model problem. We then present the results of calculations for the full  $2 \rightarrow 3$  DR and/or RTE cross sections for  $\text{Fe}^{15+}$ ,  $\text{Se}^{23+}$ , and  $\text{Nb}^{30+}$  in Sec. V. The effects of CI and intermediate coupling are demonstrated, and comparison with experiment is made where available. A brief conclusion follows.

## II. CONFIGURATION INTERACTION (CI) EFFECTS

The effect of CI between resonances on calculated DR cross sections has been the subject of a number of previous studies [11–13], where independent methods concluded that the effect on total cross sections is not expected to exceed 3% for  $\text{Fe}^{22+}$  and  $\text{Fe}^{23+}$  [12], 5% for other Li-like ions [13], or, for general cases based on qualitative considerations of Cowan and Griffin [11], no more than 10–20%. This latter study found that the largest effects occurred when CI was included between states that differed significantly in their energy relative to final radiative-decay states, thus altering the energy-dependent radiative rates. The configurations that were allowed to interact all had radiative rates comparable to the final recombined states, however. Also mentioned in that study, but never actually considered, was the effect of CI with configurations that cannot radiatively stabilize to final recombined states. For this reason, we have reexamined the

qualitative aspects of CI with nonradiatively stabilizing configurations in the following section.

Another effect that needs to be considered is that of intermediate coupling. For certain systems, one expects intermediate coupling to give rise to additional resonances or decay states. For instance, in Li-like ions, even singly charged  $\text{Be}^+$ , there is an increase in the  $\Delta n=0$  DR cross section by a factor of 3/2 due to the accessibility of L-S-forbidden capture resonances [14,15]. This factor diminishes to 1 for higher-charged systems, however. For the same Li-like systems, but for  $\Delta n > 0$  resonances, intermediate-coupling effects are only about 10% [16], on the other hand. Indeed, we find for Na-like ions that these effects cause an increase for some charge states and resonances, and a decrease for others. Consequently, we will not examine the effects of additional resonances and/or decay states within the context of a model problem, since no general rule applies for the resultant changes in the DR cross sections. Furthermore, we determined that the net effect of intermediate coupling on the present calculations is simply to redistribute the CI effects and so may be understood by considering a model CI problem.

## III. MODEL PROBLEM OF TWO INTERACTING RESONANCES

We first qualify the behavior of CI between resonances as it will apply to Na-like systems, by means of the following model problem. Consider two autoionizing resonance states which, neglecting the interaction with any accessible continua, are described by the single-configuration wave functions  $\Psi_1^r$  and  $\Psi_2^r$ . Let  $\Psi_i^c$  be the initial continuum wave function and assume that, using perturbation theory [17], the first resonance has a capture (autoionization) rate given by

$$A = 2\pi |\langle \Psi_i^c | V | \Psi_1^r \rangle|^2, \quad (5)$$

where  $V$  is the interelectron potential. We next assume that the second resonance is inaccessible from this initial continuum, but can autoionize, with a rate comparable to the first resonance, to a second continuum described by the wave function  $\Psi_f^c$ , i.e.,

$$2\pi |\langle \Psi_i^c | V | \Psi_2^r \rangle|^2 = 0, \quad (6)$$

$$2\pi |\langle \Psi_f^c | V | \Psi_2^r \rangle|^2 = A. \quad (7)$$

Furthermore, let us assume that the first resonance can also autoionize with a comparable rate to the second continuum, viz,

$$2\pi |\langle \Psi_f^c | V | \Psi_1^r \rangle|^2 = A. \quad (8)$$

We also assume that the first resonance can radiatively stabilize with rate  $R$  to a bound state with wave function  $\Psi^b$ , whereas the second cannot:

$$\frac{4\omega^3}{3c^3} |\langle \Psi_1^r | D | \Psi^b \rangle|^2 = R, \quad (9)$$

$$\frac{4\omega^3}{3c^3} |\langle \Psi_2^r | D | \Psi^b \rangle|^2 = 0. \quad (10)$$

Here,  $\omega$  is the photon energy and  $D$  is the dipole operator. This model was chosen because it resembles cases we will encounter in the DR of Na-like ions in the next section. By allowing CI between the two resonances, we have two resonances described by mixed wave functions:

$$\bar{\Psi}_1^r = c_1 \Psi_1^r + c_2 \Psi_2^r, \quad (11)$$

$$\bar{\Psi}_2^r = c_2 \Psi_1^r - c_1 \Psi_2^r. \quad (12)$$

The mixing coefficients satisfy the orthonormality relation  $c_1^2 + c_2^2 = 1$ . The energy-averaged DR cross section for each resonance takes the general form [17]

$$P_r = \frac{A_{r1} \sum_j R_{rj}}{\sum_i A_{ri} + \sum_k R_{rk}}, \quad (13)$$

where  $A_{ri}$  denotes the autoionization rate from the resonance  $r$  to the  $i$ th accessible continuum ( $i=1$  is the initial continuum),  $R_{rk}$  is the radiative rate from the resonance  $r$  to any lower recombined state  $k$ , and the sum over  $j$  includes only bound recombined states. In the single-configuration approximation, the probability of capture followed by decay only involves the first resonance and is given by

$$P_{NOCI} = A \frac{R}{2A + R}. \quad (14)$$

However, including CI results in contributions from both resonances giving

$$P_{CI} = c_1^2 A \frac{c_1^2 R}{2c_1^2 A + 2c_2^2 A + c_1^2 R} + c_2^2 A \frac{c_2^2 R}{2c_2^2 A + 2c_1^2 A + c_2^2 R}. \quad (15)$$

In the limit  $A \gg R$ , which is the usual case for lower-charged low- $n$  resonances, we see that

$$\frac{P_{CI}}{P_{NOCI}} \Big|_{A \gg R} \rightarrow c_1^4 + c_2^4, \quad (16)$$

which varies between 1.0 and 0.5 depending on the degree of mixing. Thus, for the case of strong mixing ( $c_1 \sim c_2 \sim 1/\sqrt{2}$ ) the effect of CI is to halve the calculated DR cross section. Note, however, that in the limit  $R \gg A$  this ratio is instead

$$\frac{P_{CI}}{P_{NOCI}} \Big|_{R \gg A} \rightarrow c_1^2 + c_2^2 = 1. \quad (17)$$

This indicates that as the nuclear charge  $Z$  is increased along an isoelectronic series, and therefore the ratio of the radiative to autoionization rates  $R/A$  is increased, the effect of CI for a given resonance will lessen irrespective of the strength of the CI.

#### IV. ANALYSIS OF THE $2p^5 3s 3d 4p$ RESONANCES

We quantify the previous qualitative reduction by considering an actual calculation for the DR cross section. In order to simplify the analysis, we assume that L-S coupling is valid and we focus on a single group of resonances, namely,

$3lnl' = 3d4p$ . In the absence of CI between resonances, i.e., the isolated resonance approximation, the processes necessary to consider are the following:

$$e^- + 2p^6 3s \rightarrow 2p^5 3s 3d 4p \rightarrow \left\{ \begin{array}{l} 2p^6 3s \\ 2p^6 3d \\ 2p^6 4p \end{array} \right\} + e^- \quad (18a)$$

$$\rightarrow \left\{ \begin{array}{l} 2p^6 3s 4p \\ 2p^6 3d 4p \end{array} \right\} + \hbar \omega. \quad (18b)$$

Not included above are radiative decays to autoionizing states (such as  $2p^5 3s 3d^2$ ), which usually are weaker radiative transitions and also have a lower probability of cascading to recombined states.

If CI is included within the  $3l3l'$  complex, then the intermediate configurations  $2p^5 3s 3d 4p$  in Eq. (18a) will mix with the following:  $\{2p^5 3s^2 4p, 2p^5 3p^2 4p, 2p^5 3d^2 4p\}$ . The first of these is directly accessible from the  $2p^6 3s + e^-$  continuum, and is therefore routinely included in calculations anyway. The third of these does not mix strongly with the  $2p^5 3s 3d 4p$  configuration, on the one hand, and also has a strong radiative rate to the  $2p^6 3d 4p$  configuration due to the  $3d \rightarrow 2p$  decay, on the other hand. Thus CI's with these configurations are not expected to be too important [11]. The  $2p^5 3p^2 4p$  configurations are quite different, however. First, they are not directly accessible from the  $2p^6 3s + e^-$  continuum, since this involves a three-electron transition. Second, there is strong CI between the  $2p^5 3s 3d 4p$  and  $2p^5 3p^2 4p$  configurations due to the  $3s 3d + 3p^2 \ ^1D$  dipole core mixing. Third, these configurations cannot radiate to any bound state, since only odd-parity orbitals are occupied, and the decay to the final  $2p$  orbital can only be from an even-parity orbital. This intermediate configuration can therefore only autoionize or radiatively decay to autoionizing states; in either case, it does not lead to dielectronic recombination. The most probable process due to the effect of the above CI can be shown schematically as

$$e^- + 2p^6 3s \rightarrow 2p^5 3s 3d 4p \xrightarrow{CI} 2p^5 3p^2 4p \rightarrow 2p^6 3p + e^-. \quad (19)$$

The above considerations can be shown to dramatically alter the full calculated cross sections. In Fig. 1, we show a comparison of CI versus no-CI calculations for the DR cross section of  $\text{Fe}^{15+}$  in the vicinity of the  $2p^5 3s 3d 4p$  resonances. Both calculations included all three continua  $2p^6 3l$ ,  $l=(0,1,2)$ , the  $2p^5 3s 3d 4p$  resonance configurations, and the  $2p^6 3s 4p$  and  $2p^6 3d 4p$  bound states. The CI calculation also included the  $2p^5 3p^2 4p$  configuration interaction. The effect of CI is to reduce the three prominent resonances by nearly a factor of 2. We point out that this mixing gives rise to three other resonances, which are more  $2p^5 3p^2 4p$  in character and appear at lower energies, but these do not contribute significantly to the total DR cross section.

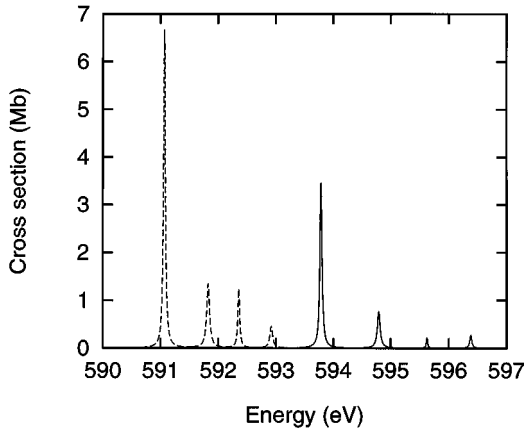


FIG. 1. Partial DR cross section for the  $2p^5 3s 3d 4p$  resonances in  $\text{Fe}^{15+}$ . Dashed line, single-configuration approximation for the resonances; solid line, configuration interaction with the  $2p^5 3p^2 4p$  configuration included.

## V. RESULTS

In the following subsections, we present the results for electrons incident on various Na-like ions. We ran two separate cases in each instance. The first included only the *KMM* resonances. Since these resonances are expected to show the greatest degree of interaction, we included all configurations within the  $n=3$  complex. All the configurations used for the initial continua, the intermediate resonance states, and the final bound states are listed in Table I, where  $kl$  denotes a continuum distorted-wave orbital. For higher-energy resonances, we used instead the slightly reduced configuration description shown in Table II. Here  $nl'$ , the valence orbital, is varied from  $4 \leq n \leq 100$  and  $0 \leq l' \leq 5$ . It was verified on smaller runs that only the inclusion of the  $2p^5 3p^2 nl'$  configuration gave a significant change in the total cross section, while mixing with other configurations, such as  $2p^5 3p 3dnl'$ , was unimportant. Also found to be unimportant was the inclusion of  $2p^5 3l 3l' kl''$  continuum configurations, at least for the highly-charged ions considered here. The results for all Na-like ions were obtained from calculations using this basis, and partial waves of total angular momenta  $L=0-4$  were included. The results of both RTE and DR calculations for each ion are described in the following subsections. All calculations used the program AUTOSTRUCTURE [18].

TABLE I. Configuration basis used for *LMM* DR of Na-like ions. *a*: configurations which were included in [9]. *b*: configurations which were not included in [9].

Continua <i>a</i>	Resonances		Bound states	
	<i>a</i>	<i>b</i>	<i>a</i>	<i>b</i>
$2p^6 3skl$	$2p^5 3s^2 3p$	$2p^5 3p^3$	$2p^6 3s^2$	$2p^6 3p^2$
$2p^6 3pkl$	$2p^5 3s^2 3d$	$2p^5 3p^2 3d$	$2p^6 3s 3p$	$2p^6 3p 3d$
$2p^6 3dkl$	$2p^5 3s 3p^2$	$2p^5 3p 3d^2$	$2p^6 3s 3d$	$2p^6 3d^2$
	$2p^5 3s 3p 3d$	$2p^5 3d^3$		
	$2s 2p^6 3s^2 3p$	$2s 2p^6 3p^3$		
	$2s 2p^6 3s^2 3d$	$2s 2p^6 3p^2 3d$		
	$2s 2p^6 3s 3p^2$	$2s 2p^6 3p 3d^3$		

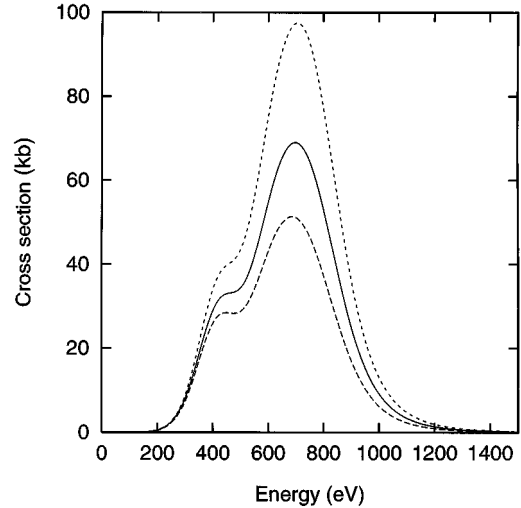


FIG. 2. RTE cross section for  $\text{Fe}^{15+} + \text{H}_2$ : short-dashed line, L-S results with no CI; long-dashed line, L-S results with  $2p^5 3p^2 nl$  mixing; solid line, IC results with  $2p^5 3p^2 nl$  mixing.

### A. $\text{Fe}^{15+}$

The RTE cross sections for  $\text{Fe}^{15+}$  are shown in Fig. 2 for three different levels of approximation. First we performed LS calculations with the basis set used in the previous study [9]. The resulting RTE cross section shows a peak of about 100 Kb. When additional CI is included, however (configurations listed under *b* in Tables I and II), the cross sections peak at about 50 Kb instead. This is consistent with the previous model problems covered earlier, where inclusion of CI in L-S calculations reduced the cross section by as much as a factor of 2. We also show the results from an intermediate-coupling calculation that included this additional CI. For this case, intermediate-coupling effects increase the cross section compared to the L-S CI calculations, but the peak is still only about 70 Kb. It should also be pointed out that the intermediate-coupled no-CI results were almost identical to the L-S no-CI ones, indicating that only when CI was included did intermediate-coupling have any effect. For the present case, intermediate coupling just changes the degree of CI mixing and, therefore, according to the considerations of Sec. III, the overall reduction of the cross section. It does not give rise to any additional autoionization channels, however, another way in which intermediate coupling can affect the computed cross section.

TABLE II. Configuration basis used for *LMn* ( $n > 3$ ) DR of Na-like ions. *a*: configurations which were included in [9]. *b*: configurations which were not included in [9].

Continua <i>a</i>	Resonances		Bound states	
	<i>a</i>	<i>b</i>	<i>a</i>	<i>b</i>
$2p^6 3skl$	$2p^5 3s^2 nl'$	$2p^5 3p^2 nl'$	$2p^6 3s^2$	$2p^6 3p^2$
$2p^6 3pkl$	$2p^5 3s 3p nl'$		$2p^6 3s 3p$	
$2p^6 3dkl$	$2p^5 3s 3d nl'$		$2p^6 3s 3d$	
$2p^6 nl' kl$			$2p^6 3s nl'$	
			$2p^6 3p nl'$	
			$2p^6 3d nl'$	

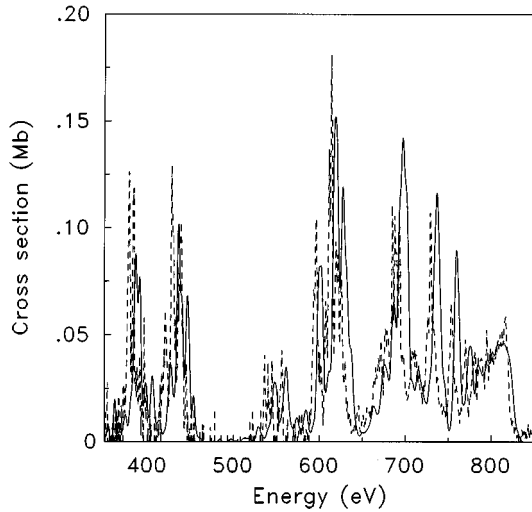


FIG. 3. DR cross section for  $\text{Fe}^{15+}$ . Solid line, present IC results with  $2p^33p^2nl$  mixing, convoluted with the experimental energy distribution function; dashed line, experimental results (Ref. [10]).

As previously mentioned, the joint theoretical-experimental study of DR of  $\text{Fe}^{15+}$  found the theory to be much higher than experiment for many of the prominent resonances [10]. The present theoretical results, including additional CI and spin-orbit effects, are shown in Fig. 3 compared to experiment [10]. The theoretical cross section has been convoluted with the experimental energy distribution function using the parameters  $T_{\parallel}=2.4$  meV and  $T_{\perp}=0.1$  eV [10]. It is clearly seen that the additional CI has brought theory and experiment into much better agreement. The remaining discrepancy we attribute to a lack of convergence of our CI basis, leading to somewhat inaccurate resonance positions and widths. Nonetheless, we feel that, due to the above considerations, the most important configurations have been included in our expansion.

#### B. $\text{Cu}^{18+}$

We simply mention that for resonant transfer excitation of  $\text{Cu}^{18+} + \text{H}_2$ , a similar factor of 2 reduction resulted from the inclusion of additional CI. These latest results will be compared to the experimental values in a forthcoming paper [19].

#### C. $\text{Se}^{23+}$

The RTE cross sections for  $\text{Se}^{23+}$  are shown in Fig. 4. For this charge state, the *LMM* resonances are sufficiently separated from the *LMn* ( $n>3$ ) complex that, even with the broad Compton profile, two peaks can be distinguished. For the *LMM* resonances, the L-S CI results are lower than the L-S no-CI results, and the intermediate-coupled CI results are even lower. For the *LMn* resonances, on the other hand, the intermediate-coupled CI results are higher than the L-S CI results, though still lower than the L-S no-CI results. This is a perfect example of why it is difficult to estimate the effects of intermediate coupling—for certain cases the effect is an increase in the RTE cross section, for other cases the effect is a decrease. We also show the DR cross section for this system, in Fig. 5, in anticipation of ongoing experimental work [20].

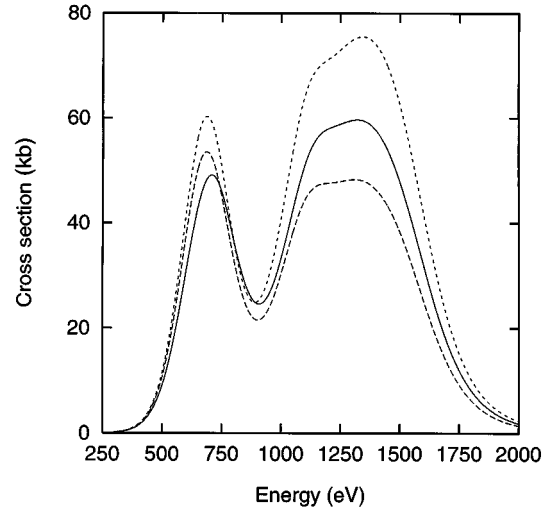


FIG. 4. RTE cross section for  $\text{Se}^{23+} + \text{H}_2$ . Short-dashed line, L-S results with no CI; long-dashed line, L-S results with  $2p^53p^2nl$  mixing; solid line, IC results with  $2p^53p^2nl$  mixing.

#### D. $\text{Nb}^{30+}$

The experimental [7] and theoretical [8,9] studies of RTE of niobium ions first yielded the large discrepancies for RTE of Na-like ions. We therefore concentrate only on the RTE cross section for this system. These results are shown in Fig. 6. It is evident that the additional CI reduces the theoretical cross section considerably, bringing it into better agreement with the experimental data points. Thus, the previous discrepancy between theory and experiment can be attributed to a lack of this additional CI in the earlier calculations. We note that there was no large disagreement between theory and experiment for  $\text{Nb}^{31+}$ , however. For this system, the  $\Delta n=1$  resonant capture process is given by

$$e^- + 2p^6 \rightarrow 2p^5 3lnl', \quad (20)$$

so that all possible configurations are routinely included in

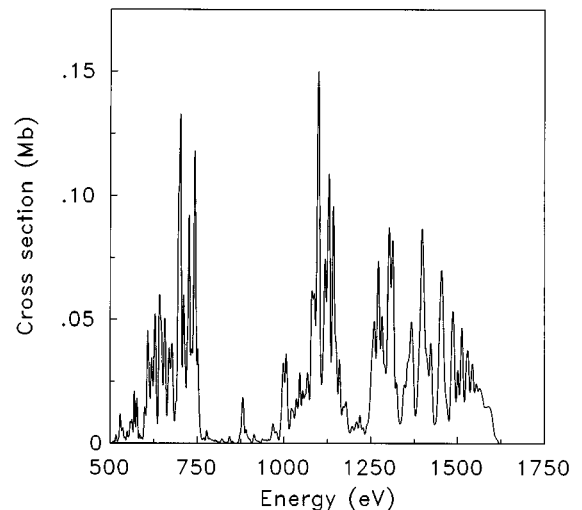


FIG. 5. Theoretical DR cross section for  $\text{Se}^{23+}$ . Solid line, present IC results with  $2p^53p^2nl$  mixing, convoluted with the experimental energy distribution function.

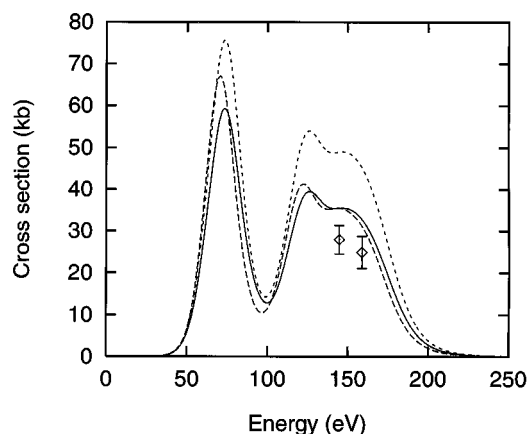


FIG. 6. RTE cross section for  $\text{Nb}^{30+} + \text{H}_2$ . Short-dashed line, L-S results with no CI; long-dashed line, L-S results with  $2p^5 3p^2 nl$  mixing; solid line, IC results with  $2p^5 3p^2 nl$  mixing; diamonds, experimental data points (Ref. [7]).

the basis for the resonances [9]. On the other hand, for  $\text{Nb}^{29+}$ , the  $\Delta n = 1$  resonant capture process is

$$e^- + 2p^6 3s^2 \rightarrow 2p^5 3s^2 3lnl'. \quad (21)$$

Similar to the present case of  $\text{Nb}^{30+}$ , strong CI effects with additional, previously omitted configurations, such as  $2p^5 3p^2 3lnl'$ , for instance, are to be expected. This explains

why the discrepancy between theory and experiment persisted for all  $\text{Nb}^{q+}$  ions with  $q < 31$ . The proper inclusion of the required additional CI for systems with  $q < 30$  would lead to even more time demanding computations than the present ones, however, so that we will leave those calculations for a future study.

## VI. CONCLUSION

We have demonstrated that additional CI with configurations that are neither accessible from the initial continuum nor radiate to the final recombined states of the electron-ion system has a significant effect on the total DR or RTE cross section. For the present case of electrons incident on Na-like ions, the cross section was reduced by as much as a factor of 2. This has resolved previous discrepancies between theoretical calculations and experimental measurements for both the  $\text{Fe}^{15+}$  and  $\text{Nb}^{30+}$  systems. This reduction is consistent with the considerations presented for a simplified problem of the interaction between two resonances, one which is not accessible from the initial continuum or final recombined states. It was also shown that intermediate coupling effects tended to increase the cross section somewhat due to the resultant change in CI strength between resonances.

## ACKNOWLEDGMENTS

N.R.B. was supported in part by NATO Contract No. CRG 940134 with the University of Strathclyde.

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