Distorted-wave calculations of dielectronic recombination cross sections in the Li isoelectronic sequence

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(Received 31 July 1984)

The dielectronic recombination cross sections associated with the $2s \rightarrow 2p$ transition in the Li-like ions B^{2+}, C^{3+}, and O^{5+} have been calculated in the distorted-wave approximation. We compare calculated cross sections to selected doubly excited configurations of the type $2pnl$ in C^{3+} in pure LS coupling, intermediate coupling, and a configuration-average approximation. The LS-coupled results are about 33% low as compared to intermediate coupling for low and intermediate values of n and l, while the configuration-average approximation agrees quite well with the intermediate-coupled results for relatively low values of n or l, but tends to overestimate the intermediate-coupled cross sections at intermediate values of n or l. All three methods should agree at high values of n or l. In addition, we calculate the total cross sections associated with the $2s \rightarrow 2p$ excitation for all three ions using the configuration-average approximation, and we compare our results to merged electron-ion beam measurements of the cross sections for B^{2+} and C^{3+}. The sensitivity of these cross sections to experimental conditions is also examined.

I. INTRODUCTION

Dielectronic recombination (DR) is the process by which a free electron collisionally excites an ion and is simultaneously captured into a doubly excited state which then stabilizes through the emission of a photon. It is of interest because it is the dominant process by which continuum electrons are captured in low-density astrophysical and laboratory plasmas. Since being invoked by Burgess[1] to account for discrepancies in measured temperatures of the solar corona, DR has received much theoretical attention. Various approaches to the theory are discussed in several review articles,[2,3] and recently a number of calculations of DR cross sections and rate coefficients have been reported.[4–7]

Direct cross-section measurements of dielectronic recombination are extremely difficult and until last year no such measurements existed. However, in the last two years two crossed-beam[8,9] and two merged-beam experiments[10,11] were successful, and for the first time we have experimental data with which the results of various theoretical methods may be compared. Accurate calculations of DR cross sections are also very difficult because of the large number of doubly excited, intermediate states which must be included. The effects of overlapping resonances, and configuration mixing and intermediate coupling in the bound states may be important. Nevertheless, the inclusion of all of these effects is impractical at the present time, and to date most cross sections have been calculated in an isolated-resonance, single-configuration approximation, employing either autoionizing and radiative rates which are averaged over all states of a given configuration (configuration-average approximation) or else calculated in pure LS coupling.

The effects of overlapping resonances in DR cross sections have been considered previously[12] and are presently under investigation by a number of workers. These effects are expected to be small, but no extensive results have yet been published. The influence of configuration mixing between the intermediate states has been studied for a limited range of states by several investigators,[7,13] but no complete multiconfiguration DR cross sections have yet been reported. Several authors have suggested that intermediate coupling is important,[3,12] but a systematic study of the effects of intermediate coupling has not yet been completed.

The influence of external electric fields, which surely exist in the beam experiments as well as in plasmas, has been of great interest, and a calculation of the effects of such fields within the electron-ion interaction region on the DR cross section of Mg^+ has been reported recently.[14] However, we feel that some of the internal effects listed above should be further investigated before we know how much of the difference between approximate theory and experiment may be due to the effects of fields.

In this paper we present the results of distorted-wave calculations of the DR cross section for the resonance states associated with the $2s \rightarrow 2p$ excitation in the Li-like ions B^{2+}, C^{3+}, and O^{5+}. We include a comparison of DR cross sections to configurations within selected Rydberg series in C^{3+} using pure LS coupling, intermediate coupling, and the configuration-average approximation. On the basis of this comparison we calculate the total cross sections for all three ions in the configuration-average approximation. Our results for the total cross sections in B^{2+} and C^{3+} are compared to the experimental values of Dittner *et al.*[11] and the previous calculations of McLaughlin and Hahn[5,6] in which pure LS coupling was assumed.

II. CALCULATIONAL METHODS

In the isolated-resonance approximation, the energy-averaged cross section for DR from a state of the initial

level i of an N-electron ion through all states of a particular doubly excited resonance level j of the $(N+1)$-electron ion to the states of all possible bound levels f of that ion can be written as a resonant-recombination cross section multiplied by a branching ratio for radiative stabilization:

$$\bar{\sigma}=\frac{8\pi^2}{\Delta\epsilon k_i^3}\frac{g_j}{2g_i}\sum_{l_i}\left|\left\langle\alpha_j J\left|\sum_{m=1}^{N}\frac{1}{r_{N+1,m}}\right|\alpha_i l_i J\right\rangle\right|^2 \times\frac{\sum_f A^r(j\to f)}{\sum_{i'}A^a(j\to i')+\sum_f A^r(j\to f)}\,. \quad (1)$$

Hartree atomic units are employed and the continuum normalization is chosen as one times a sine function. In the above expression k_i is the linear momentum and l_i is the angular momentum of the continuum electron; $\Delta\epsilon$ is an energy bin width larger than the largest resonance width; J is the total angular momentum of the $(N+1)$-electron system; g_i and g_j are the statistical weights of the initial level of the N-electron ion and the resonance level of the $(N+1)$-electron ion, respectively; α_i is used to designate the initial level in intermediate coupling; and α_j is used to designate all quantum numbers other than J needed to specify the resonance level in intermediate coupling. The radiative rate from a state of the resonance level j to all states of a particular bound level f in atomic units is given by

$$A^r(j\to f)=\frac{4\omega^3}{3c^3}\frac{1}{g_j}\left|\left\langle\alpha_f J_f\left|\left|\sum_{m=1}^{N+1}\mathbf{r}_m\right|\right|\alpha_j J\right\rangle\right|^2, \quad (2)$$

where ω is the transition frequency, c is the speed of light, and we have chosen the dipole length form of the electromagnetic field interaction. The autoionization rate from a state within the level j of the $(N+1)$-electron ion to all states within the level i' of the N-electron ion is given by

$$A^a(j\to i')=\frac{4}{k_{i'}}\sum_{l_{i'}}\left|\left\langle\alpha_{i'}l_{i'}J\left|\sum_{m=1}^{N}\frac{1}{r_{N+1,m}}\right|\alpha_j J\right\rangle\right|^2. \quad (3)$$

The above rates can be converted to $\sec^{-1}$ by dividing by $\hbar=2.4189\times10^{-17}$ hartree sec. From Eqs. (3) and (1) we see that the cross section may be written as

$$\bar{\sigma}=\frac{2\pi^2}{\Delta\epsilon k_i^2}\frac{g_j}{2g_i}\frac{A^a(j\to i)\sum_f A^r(j\to f)}{\sum_{i'}A^a(j\to i')+\sum_f A^r(j\to f)}\,. \quad (4)$$

We have not included in the sums over radiative rates the transitions from the resonance level j to other autoionizing levels. Such final levels will either emit an Auger electron or decay to a bound level or another autoionizing level with the emission of a photon. Since the autoionizing rate will dominate for lower autoionizing levels, as discussed by McLaughlin and Hahn,[7] this cascade effect can be approximated by including transitions to autoionizing levels in the sum over radiative rates in the denominator, but not in the sum in the numerator. This correction appears to have a small effect in low stages of ionization[7] and we have not included it here.

The general cross-section expression of Eq. (4), and the corresponding transition rates, may be evaluated for any explicit, pure coupling scheme. In general, however, one should evaluate these cross sections in intermediate coupling, and this can be done using the atomic-structure program developed by Cowan.[15] However, it is extremely tedious to carry out the calculation of the total cross section or rate coefficient in intermediate coupling because of the very large number of intermediate levels involved. Thus when performing survey calculations for a variety of atomic ions, it is useful to develop a method which dramatically reduces the number of individual rates which must be calculated.

First we determine the average cross section from a state in the initial configuration of the N-electron ion to all states within a particular doubly excited configuration of the $(N+1)$-electron ion (see Merts *et al.*, Appendix B[16]):

$$\bar{\sigma}=\frac{2\pi^2}{\Delta\epsilon k_i^2}\frac{1}{2G_i}\sum_j g_j\frac{\sum_i A^a(j\to i)\sum_f A^r(j\to f)}{\sum_{i'}A^a(j\to i')+\sum_f A^r(j\to f)}\,, \quad (5)$$

where we have assumed that the energy spread within each configuration is small so that $\frac{1}{2}k_i^2$ is the average energy difference between configurations, and G_i is the total statistical weight of the initial configuration. For doubly excited configurations, such as those considered here for which there are no possible autoionizing transitions other than to the initial configuration of the N-electron ion, Eq. (5) can be greatly simplified in two limiting cases.[15,16] For configurations in which $\sum_i A^a(j\to i) \gg \sum_f A^r(j\to f)$ for all levels j, Eq. (5) becomes

$$\bar{\sigma}=\frac{2\pi^2}{\Delta\epsilon k_i^2}\frac{G_j}{2G_i}\bar{A}^r, \quad (6)$$

where G_j is the total statistical weight of the doubly excited configuration and $\bar{A}^r$ is the configuration-average radiative rate

$$\bar{A}^r=\frac{1}{G_j}\sum_j g_j\sum_f A^r(j\to f)\,, \quad (7)$$

where the sum over f includes all states of the bound configurations for which radiative transitions are possible. This limiting case will be valid for doubly excited configurations for which the Rydberg electron has relatively low values of n and l and the coupling is not so pure that selection rules will render the autoionization rate unusually small for certain levels.

For configurations in which $\sum_i A^a(j\to i) \ll \sum_f A^r(j\to f)$ for all j, Eq. (5) becomes

$$\bar{\sigma}=\frac{2\pi^2}{\Delta\epsilon k_i^2}\frac{G_j}{2G_i}\bar{A}^a, \quad (8)$$

where the configuration-average autoionizing rate is given by

$$\bar{A}^a=\frac{1}{G_j}\sum_j g_j\sum_i A^a(j\to i)\,. \quad (9)$$

This limiting case will be valid for doubly excited config-

urations for which the Rydberg electron has relatively high values of n or l and selection rules do not make the radiative rate unusually small for certain levels. The configuration-average approximation for the DR cross section is an interpolation between these two limiting cases:

$$\bar{\sigma}_{\rm CA}=\frac{2\pi^2}{\Delta\epsilon k_i^2}\frac{G_j}{2G_i}\frac{\bar{A}^a\bar{A}^r}{\bar{A}^a+\bar{A}^r}\ . \tag{10}$$

For configurations such that $\sum_i A^a(j\rightarrow i)$ and $\sum_f A^r(j\rightarrow f)$ are comparable, this approximation will tend to overestimate the cross section;[12] however, this is only true for a limited range of n and l and, as we shall see, Eq. (10) may yield a total cross section in good agreement with that calculated using Eq. (5) and intermediate coupling eigenvectors. $\bar{A}^a$ and $\bar{A}^r$ are independent of the coupling scheme and therefore can be evaluated in any convenient representation. For simplicity we have chosen to determine expressions for these rates, and thereby the cross section, using the uncoupled representation.

As noted previously by Gau and Hahn,[17] when considering the autoionizing rate, one must distinguish two cases depending on how many electronic subshells are involved in the transition. The first one is written as

$$(n_1l_1)^{q_1}(n_2l_2)^{q_2}(n_3l_3)^{q_3}\rightarrow(n_1l_1)^{q_1+1}(n_2l_2)^{q_2-1}(n_3l_3)^{q_3-1}k_il_i\ . \tag{11}$$

For this case the configuration-average autoionization rate is given by

$$\bar{A}^a_1=\frac{2}{k_i}(4l_1+2-q_1)q_2q_3\times\sum_{l_i}(2l_i+1)\left[\sum_\lambda a(l_1,l_2,l_3,l_i,\lambda)[R^\lambda(n_1l_1,k_il_i;n_2l_2,n_3l_3)]^2+\sum_{\lambda'}b(l_1,l_2,l_3,l_i,\lambda')[R^{\lambda'}(k_il_i,n_1l_1;n_2l_2,n_3l_3)]^2-\sum_\lambda\sum_{\lambda'}c(l_1,l_2,l_3,l_i,\lambda,\lambda')R^\lambda(n_1l_1,k_il_i;n_2l_2,n_3l_3)R^{\lambda'}(k_il_i,n_1l_1;n_2l_2,n_3l_3)\right]\ . \tag{12}$$

In Eq. (12), $R^\lambda(ij;rt)$ is the usual Slater radial integral for the Coulomb interaction between electrons, and the angular coefficients in terms of the standard 3-j and 6-j symbols are given by

$$a(l_1,l_2,l_3,l_i,\lambda)=\begin{pmatrix}l_1&\lambda&l_2\\0&0&0\end{pmatrix}^2\begin{pmatrix}l_i&\lambda&l_3\\0&0&0\end{pmatrix}^2\Big/(2\lambda+1)\ , \tag{13}$$

$$b(l_1,l_2,l_3,l_i,\lambda')=\begin{pmatrix}l_1&\lambda'&l_3\\0&0&0\end{pmatrix}^2\begin{pmatrix}l_i&\lambda'&l_2\\0&0&0\end{pmatrix}^2\Big/(2\lambda'+1)\ , \tag{14}$$

$$c(l_1,l_2,l_3,l_i,\lambda,\lambda')=\begin{Bmatrix}l_1&l_2&\lambda\\l_i&l_3&\lambda'\end{Bmatrix}[(2\lambda+1)(2\lambda'+1)a(l_1,l_2,l_3,l_i,\lambda)b(l_1,l_2,l_3,l_i,\lambda')]^{1/2}\ . \tag{15}$$

The second case is written as

$$(n_1l_1)^{q_1}(n_2l_2)^{q_2}\rightarrow(n_1l_1)^{q_1+1}(n_2l_2)^{q_2-2}k_il_i\ . \tag{16}$$

The configuration-average autoionization rate for this case is given by

$$\bar{A}^a_2=\frac{2}{k_i}\frac{(4l_1+2-q_1)q_2(q_2-1)(4l_2+2)}{4l_2+1}\sum_{l_i}(2l_i+1)\times\left[\sum_\lambda a(l_1,l_2,l_2,l_i,\lambda)[R^\lambda(n_1l_1,k_il_i;n_2l_2,n_2l_2)]^2-\tfrac{1}{2}\sum_\lambda\sum_{\lambda'}c(l_1,l_2,l_2,l_i,\lambda,\lambda')R^\lambda(n_1l_1,k_il_i;n_2l_2,n_2l_2)\times R^{\lambda'}(n_1l_1,k_il_i;n_2l_2,n_2l_2)\right]\ . \tag{17}$$

For either case the radiative transition can be written as

$$(n_1l_1)^{q_1-1}(n_2l_2)^{q_2}\rightarrow(n_1l_1)^{q_1}(n_2l_2)^{q_2-1}\ , \tag{18}$$

and the configuration-average radiative rate between any two configurations is given by[15]

$$\bar{A}^r=\frac{4\omega^3}{3c^3}\frac{q_2(4l_1+3-q_1)2l_>}{(4l_1+2)(4l_2+2)}\times\left[\int_0^\infty P_{n_2l_2}(r)rP_{n_1l_1}(r)dr\right]^2\ , \tag{19}$$

where $l_> = \max(l_1, l_2)$. For the first case, using the notation of Eq. (11), the configuration-average cross section is given by

$$\bar{\sigma}^1_{\rm CA} = \frac{2\pi^2}{\Delta\epsilon k_i^2} \frac{(q_1+1)(4l_2+3-q_2)(4l_3+3-q_3)}{2q_2q_3(4l_1+2-q_1)} \frac{\bar{A}^a_1 \bar{A}^r}{\bar{A}^a_1 + \bar{A}^r} , \tag{20}$$

and for case 2, using the notation of Eq. (16),

$$\bar{\sigma}^2_{\rm CA} = \frac{2\pi^2}{\Delta\epsilon k_i^2} \frac{(q_1+1)(4l_2+3-q_2)(4l_2+4-q_2)}{2q_2(q_2-1)(4l_1+2-q_1)} \frac{\bar{A}^a_2 \bar{A}^r}{\bar{A}^a_2 + \bar{A}^r} . \tag{21}$$

A new program named DRACULA, for dielectronic recombination average configuration using local approximation, has been developed which generates configuration-average cross sections for an atomic ion in a semiautomatic way using the above expressions. The bound-state energies and the atomic orbitals for the many configurations needed to evaluate the DR cross section are generated using the radial wave-function code developed by Cowan.[15] These radial wave functions are solutions to the Hartree-Fock equations with relativistic modifications,[18] which include the mass-velocity and Darwin corrections within modified differential equations. The continuum orbitals needed to evaluate the Coulomb matrix elements were calculated in a local distorting potential constructed in a semiclassical exchange approximation.[19] This exchange term simplifies the solution of the differential equations and gives results in close agreement with results obtained from a full nonlocal Hartree-Fock continuum program.

It is, of course, impractical to generate Hartree-Fock orbitals for all the configurations needed in the calculation of a total DR cross section. For a given Rydberg series of doubly excited configurations, $\bar{A}^a$ goes approximately as $1/n^3$, while for high values of n, $\bar{A}^r$ is nearly a constant. Thus, we extrapolated the autoionizing rates to high values of n by fitting the calculated values of $n^3\bar{A}^a$ to the formula $a+b/n^2+c/n^4$. There is no simple extrapolation formula for $\bar{A}^a$ as a function of l which is of sufficient accuracy. Therefore, we calculated the autoionizing rates for lower members of the Rydberg series corresponding to $l=9$–15 using hydrogenic wave functions. $\bar{A}^r$ does not present a problem since it is again nearly constant for high values of l.

For the calculations reported here we used a value of the energy bin width $\Delta\epsilon=0.005$ hartrees, which is identical to the value employed by McLaughlin and Hahn.[5,6] It should be noted that when calculating the total energy-averaged cross section, one must sum over the values of $\bar{\sigma}$ for all resonant states within a given energy width.

III. EFFECTS OF INTERMEDIATE COUPLING

In the Li isoelectronic sequence, the DR transitions associated with the $2s \rightarrow 2p$ excitation are initiated with the recombination transitions of the form

$$k_i l_i + X^{+q}(2s) \rightarrow X^{+(q-1)}(2pnl) \tag{22}$$

followed by the radiative transitions of the form

$$X^{+(q-1)}(2pnl) \rightarrow X^{+(q-1)}(2snl) + h\nu \tag{23}$$

or

$$X^{+(q-1)}(2pnl) \rightarrow X^{+(q-1)}(2pn'l') + h\nu' , \tag{24}$$

where the configurations $2pn'l'$ are bound. While for low values of n and l radiative decays of the type represented by Eq. (24) may be quite important, for high values of n or l they are either forbidden or have small rates for the lower stages of ionization considered here. The only competing autoionizing process is that corresponding to the reverse of Eq. (22).

From Eq. (22) we see that in order to conserve parity and orbital angular momentum, $l_i = l \pm 1$, when $l \neq 0$. Thus in pure LS coupling, the $4(2l+1)$ states of $2pnl$, for which the total orbital angular momentum $L=l$, cannot be populated by the recombination process of Eq. (22). Since there are a total of $12(2l+1)$ states in this configuration, this amounts to one-third of the possible states. Furthermore, it is easily shown that the radiative rates associated with the transitions of the type given by Eq. (23) are the same for each of the LS terms, and therefore are equal to $\bar{A}^r$. Thus for configurations in which $\bar{A}^a \gg \bar{A}^r$, and for which decays of the type given in Eq. (24) have negligible rates, we would expect the DR cross section in pure LS coupling to be given by

$$\bar{\sigma}_{\rm LS} = \frac{2\pi^2}{\Delta\epsilon k_i^2} \frac{\frac{2}{3}G_j}{2G_i} \bar{A}^r = \tfrac{2}{3}\bar{\sigma}_{\rm CA} \tag{25}$$

[see Eqs. (5) and (6)]. This factor of $\frac{2}{3}$ for $s \rightarrow p$ dielectronic transitions in LS coupling was first pointed out by Trefftz.[12]

Now let us consider the situation in intermediate coupling. For those doubly excited configurations $2pnl$ with relatively low values of n and l, the electrostatic interaction will be much larger than the spin-orbit interactions, and the states will be fairly pure in LS coupling. Nevertheless, for these same configurations, the autoionizing rates to the allowed LS states will typically be 10^3–10^5 times the radiative rates from these states, and any slight amount of mixing of the states for which $L=l$ with the states for which $L=l\pm1$, will cause the condition $\sum_i A^a(j \rightarrow i) \gg \sum_f A^r(j \rightarrow f)$ to hold for all intermediate-coupled states.[12] Thus Eq. (6) should be valid in intermediate coupling and $\bar{\sigma}_{\rm IC} \cong \bar{\sigma}_{\rm CA}$. As n or l increases the electrostatic interaction will decrease, while the spin-orbit interaction of the $2p$ electron will remain essentially the same. Thus as the ratio of $\sum_i A^a(j \rightarrow i)$ to $\sum_f A^r(j \rightarrow f)$ decreases, the mixing of the LS states will increase and, for example, in the configuration $2p10h$ the states are more pure in j-j coupling than they are in LS coupling. The agreement between the DR cross section in intermediate coupling and that calculated using the configuration-average approximation should then persist until the smaller values of $\sum_i A^a(j \rightarrow i)$ are no longer much larger than $\sum_f A^r(j \rightarrow f)$ at which point the CA approximation will begin to overestimate the cross section. At the other extreme, for high values of n or l,

TABLE I. Dielectronic recombination cross sections for selected transitions of the type $k_i l_i + C^{3+}(2s) \rightarrow C^{2+}(2pnl)$, calculated using Cowan's atomic-structure program (Ref. 15).

nl	k_i^2	σ_{LS}[a] (10^{-20} cm^2)	σ_{IC}[b] (10^{-20} cm^2)	σ_{CA}[c] (10^{-20} cm^2)	$\frac{\sigma_{LS}}{\sigma_{IC}}$	$\frac{\sigma_{CA}}{\sigma_{IC}}$
$4d$	0.018 82	341.2	662.8	671.2	0.52	1.01
$10d$	0.5016	2.126	3.552	3.552	0.60	1.00
$15d$	0.5521	1.5050	2.354	2.354	0.64	1.00
$20d$	0.5697	1.3592	2.078	2.078	0.65	1.00
$4f$	0.0294	164.8	259.6	266.8	0.63	1.03
$10f$	0.5022	2.260	3.428	3.434	0.66	1.00
$15f$	0.5523	1.897	2.868	2.882	0.66	1.01
$20f$	0.5698	1.789	2.710	2.740	0.66	1.01
$5g$	0.2323	5.704	8.480	8.526	0.67	1.01
$10g$	0.5023	2.626	3.934	3.942	0.67	1.00
$15g$	0.5523	2.382	3.568	3.586	0.67	1.01
$20g$	0.5698	2.296	3.434	3.472	0.67	1.01
$10h$	0.5023	3.196	4.774	4.818	0.67	1.01
$15h$	0.5523	2.886	4.276	4.376	0.67	1.02
$20h$	0.5698	2.752	4.030	4.234	0.68	1.05
$10i$	0.5023	3.654	5.332	5.680	0.69	1.07
$15i$	0.5523	3.194	4.558	5.150	0.70	1.13
$20i$	0.5698	2.902	3.920	4.958	0.74	1.26
$10k$	0.5023	3.334	4.602	6.446	0.73	1.40
$15k$	0.5523	2.854	3.932	5.784	0.73	1.47
$20k$	0.5698	2.526	3.484	5.436	0.73	1.56
$10l$	0.5023	2.618	3.560	5.864	0.74	1.65
$15l$	0.5523	2.418	3.286	5.418	0.74	1.65
$20l$	0.5698	2.174	2.866	4.586	0.76	1.60

[a]Equation (5) assuming pure LS states.
[b]Equation (5) using intermediate-coupled eigenvectors from Cowan's code.
[c]Equation (10) using average radiative and autoionizing rates from Cowan's code. These results agree very well with results from DRACULA.

$\sum_f A^r(j \rightarrow f) \gg \sum_i A^a(j \rightarrow i)$ and the DR cross section will become independent of coupling, and $\bar{\sigma}_{IC} \cong \bar{\sigma}_{LS} \cong \bar{\sigma}_{CA}$.

The above general observations are confirmed by the results of calculations (using Cowan's atomic-structure program[15]) shown in Table I. We see that the agreement between the intermediate-coupled results and those calculated using the CA approximation are in excellent agreement for $l \leq 5$ and that the LS-coupled results are low by a factor of about $\frac{2}{3}$ as expected. For higher values of l, the discrepancy between the IC results and the CA cross sections increases, while the LS and IC values grow closer. However, the cross sections for $l > 8$ decrease very rapidly and the discrepancy between the IC results and those obtained using the CA approximation for high values of l should not have a major effect on the total cross section.

For values of n above 35 or so, the smaller values of $\sum_i A^a(j \rightarrow i)$ will begin to come close enough to $\sum_f A^r(j \rightarrow f)$ that the CA method will again overestimate the cross section. This difficulty will persist until n is high enough that $\sum_f A^r(j \rightarrow f) \gg \sum_i A^a(j \rightarrow i)$. However, in the electron-ion beam experiments, high Rydberg states should be ionized by the field of the analyzer used to separate the final charged species. Thus we might expect that the CA approximation should provide results in better agreement with experiment for cases in which the analyzing fields are large enough to ionize Rydberg states beginning with those values of n for which the above difficulty begins.

IV. TOTAL DIELECTRONIC RECOMBINATION CROSS SECTIONS

Based on the comparison of calculational methods presented in the last section, we have calculated total dielectronic recombination cross sections for the Li-like ions B^{2+}, C^{3+}, and O^{5+} using the configuration-average approximation. Our results along with data from the recent merged electron-ion beam experiments[11,20] are presented in Figs. 1 and 2 for B^{2+} and C^{3+}. The smooth theoretical curves were obtained by convoluting the spectrum of narrow resonance peaks generated by DRACULA with a Gaussian energy distribution with a full width at half maximum equal to 3.0 eV. This particular energy width was found experimentally[11] to best represent the distribution of relative electron-ion energies in the merged beams.

In the merged-beam experiment the recombined ions in high Rydberg states will be field ionized as they move at high velocities through the field of the analyzing magnet. Thus in order to compare our theoretical results with experiment, we included in our calculations only those Rydberg states up to a maximum principal quantum number

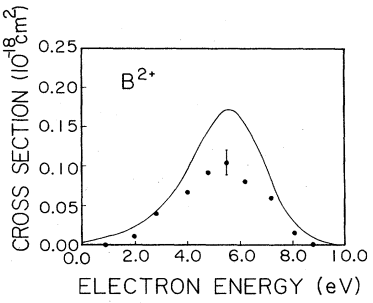

FIG. 1. Dielectronic recombination cross section for B^{2+}. The solid curve is a configuration-average result convoluted with a 3.0-eV full width at half maximum (FWHM) Gaussian over all resonances with $n \leq 22$. The circles are experimental measurements (Ref. 11).

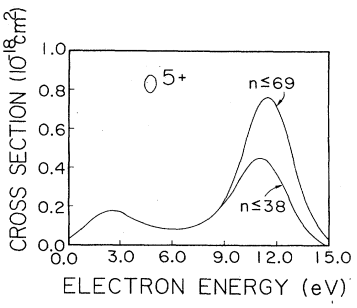

FIG. 3 Dielectronic recombination cross section for O^{5+}. The solid curves are configuration-average results convoluted with a 3.0-eV FWHM Gaussian. All resonances included are less than or equal to the n value given on the curve.

n_{max} determined from the following semiclassical field-ionization formula:

$$n_{max}=(6.2\times10^{10}q^3/v_iB)^{1/4}\ , \tag{26}$$

where q is the charge of the ion before recombination, v_i is the ion velocity in m/s, and B is the magnetic field in tesla.[11,21] This equation is based on a comparison of quantum-mechanical tunneling with radiative decay, but does not include the deviations from a purely hydrogenic system nor the variation of rate with Stark quantum numbers. The value of n_{max} can also be calculated using a classical formula in which field ionization is assumed to occur when the unperturbed energy is above the local maximum in the combined potential of the screened nucleus and the external electric field.[21] In this case the form of Eq. (26) remains the same but the coefficient 6.2×10^{10} becomes 3.2×10^{10}. The results of several experimental studies of field ionization from selected Rydberg states in the alkali-metal atoms[22,23] indicate that the general form of the equation for n_{max} may be valid, but that a better coefficient may be somewhere in between the two values given above. Nevertheless, a proper treatment of field ionization for nonhydrogenic systems is quite complex and, in the absence of something better, Eq. (26) seems most appropriate.

For B^{2+} the value of n_{max} was found to be 22, and the resulting configuration-average results shown in Fig. 1 are a factor of 1.5 higher than experiment. For C^{3+} in Fig. 2, the two sets of data correspond to measurements performed with different analyzing fields. In the case of the experiment reported on earlier in Ref. 11, the calculated value of n_{max} is 26, and the theory and the experiment agree quite well at the cross-section peak near 7.0 eV. The theoretical peak near 0.5 eV is due to contributions from the $2p4d$ and $2p4f$ configurations, which have large radiative rates of the type given in Eq. (24). Although some of the $2p4d$ levels may lie below the ionization limit for C^{3+}, the remaining levels of $2p4d$ together with those of the $2p4f$ configuration should give rise to some sort of low-energy peak. However, in a merged-beam apparatus there are known experimental problems[20] associated with the measurement of cross-section peaks at such low relative energies.

The latest measurements on C^{3+} were performed with a much lower analyzing field corresponding to a value of n_{max} equal to 44.[20] In this case the discrepancy between theory and experiment is larger with the peak in the experimental cross section about 20% higher in magnitude and appearing about 1 eV lower than the corresponding

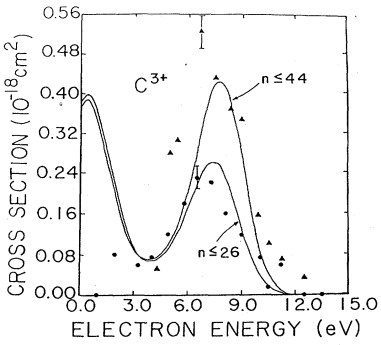

FIG. 2. Dielectronic recombination cross section for C^{3+}. The solid curves are configuration-average results convoluted with a 3.0-eV FWHM Gaussian over all resonances with $n \leq 26$ and $n \leq 44$, respectively. The circles are experimental measurements for which the analyzing field should field-ionize states with $n > 26$ (Ref. 11). The triangles are preliminary measurements for which the analyzing field should field-ionize states with $n > 44$ (Ref. 20).

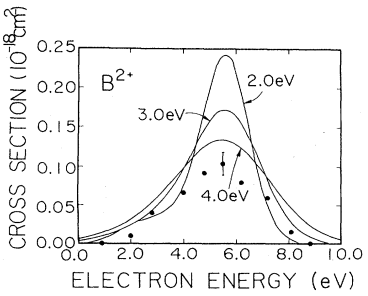

FIG. 4. Sensitivity of the dielectronic recombination cross section for B^{2+} to the choice of beam energy width. Each solid curve is a configuration-average result convoluted with the FWHM Gaussian given on the curve over all resonances $n \leq 22$. Experimental measurements are from Ref. 11.

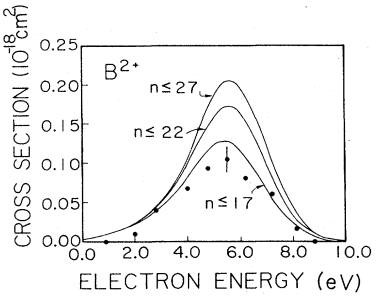

FIG. 5. Sensitivity of the dielectronic recombination cross section for B^{2+} to field ionization. Each solid curve is a configuration-average result convoluted with a 3.0-eV FWHM Gaussian over all resonances less than or equal to the n value given on the curve. Experimental measurements are from Ref. 11.

theoretical peak. The direction of the discrepancy in magnitude is somewhat surprising when one recalls that the CA approximation might be expected to overestimate the cross section when these higher values of n are included in the calculation. This may be an indication of enhancement due to field mixing in the interaction region which should increase with n. However, in all these comparisons one must recall that the uncertainty in the absolute value of the experimental cross section is about 30%.[11]

Our configuration-average results for B^{2+} and C^{3+} are between 50% and 60% higher than the LS-coupled results reported previously.[5,6] This difference is in agreement with the discussion in Sec. III and seems to indicate that a full intermediate-coupling calculation for these ions is closely represented by the configuration-average approximation.

In Fig. 3 we present configuration-average results for the dielectronic recombination cross section for O^{5+}. An energy width of 3.0 eV and the field-ionization cutoff numbers indicated on the curves are in accordance with merged-beam experiments for this ion now under way. The low-energy peak at 2.5 eV is due to contributions from the $2p6l$ configurations, the dominant member being $2p6d$.

In view of the difficulty associated with an accurate determination of the width of the energy distribution in the merged beams and the uncertainty associated with the effects of field ionization, we investigated the sensitivity of our calculated cross sections to these factors in B^{2+}. The results are shown in Figs. 4 and 5. As can be seen, a change of 1.0 eV in energy width or a change of 5 in $n_{\max}$ has a significant effect on the magnitude of the cross section. It appears that for energy widths in the range of 3.0 eV, cases such as B^{2+} are as sensitive to field-ionization effects as they are to the atomic structure of the autoionizing levels.

V. CONCLUSIONS

The results of our calculations of DR cross sections for selected transitions associated with $2s \rightarrow 2p$ excitation in C^{3+} indicate that intermediate-coupling effects may be important, and cross sections calculated in pure LS coupling will tend to underestimate the cross section. In the case of the Li isoelectronic sequence, the discrepancy occurs in low and intermediate values of n and l, since the LS selection rules which cause the difference are associated with the autoionizing transitions rather than the radiative transitions. In more complex cases involving more than one open-core subshell, there may be radiative selection rules other than $\Delta J = \pm 1,0$, which do not allow certain radiative transitions to occur in pure LS coupling; this may cause discrepancies between intermediate-coupled and LS-coupled results for high n or l, where the radiative rates are much larger than the autoionizing rates. The extent of such discrepancies will depend on the purity of the core-electron states in LS coupling.

The configuration-average approximation, on the other hand, will tend to overestimate the DR cross section calculated in intermediate coupling. However, the agreement between IC results and the CA results will be quite good for the limiting cases discussed in Sec. II [Eqs. (6) and (8)] and the major discrepancies will tend to occur for values of n and l, where the autoionizing rates and radiative rates are close in magnitude.

It is obvious that DR cross sections should be calculated in intermediate coupling, but it would be very time consuming to determine intermediate-coupling eigenvectors for all the configurations involved in a calculation of a total cross section. It would be useful to develop an approximate method to include the important effects of intermediate coupling without the necessity of doing a full structure calculation on each configuration, a problem on which we are currently working. In the interim, it may be better to use the CA approximation to estimate the total DR cross section. It provides a semiautomatic way of performing survey calculations of DR, which in a number of cases will yield cross sections in closer agreement to intermediate-coupled results than those calculated in any pure coupling scheme. In any case, the CA approximation should provide an upper limit to the total DR cross section in the absence of any field effects.

As we have seen, the DR cross section is quite sensitive to the effects of field ionization. Thus, in some cases, it may be difficult to test the accuracy of various methods of calculating the enhancement of dielectronic recombination due to fields in the electron-ion interaction region by comparing theoretical and experimental cross sections as a function of energy until a more reliable method of determining field ionization in the analyzer is incorporated in the analysis.

ACKNOWLEDGMENTS

We wish to thank R. D. Cowan for making his atomic-structure program available to us, Y. Hahn for providing us with his calculated dielectronic recombination cross sections for several transitions in C^{3+}, and Lee Collins for some helpful discussions. Finally, we wish to thank P. F. Dittner and S. Datz for providing us with their preliminary low-field C^{3+} data prior to publication. This research was supported by the Office of Fusion Energy, U.S. Department of Energy, under Contract No. DE-AC05-840R21400 with Martin Marietta Energy Systems, Inc.

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