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EXCITATION AND IONIZATION OF HIGHLY CHARGED IONS BY ELECTRON IMPACT

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Douglas H. Sampson

The Pennsylvania State University
University Park, Pennsylvania 16802

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Abstract

The reduced cross sections $Q_R^H(n\ell,u)$ have been calculated for ionization from the $n\ell$ = 4s, 4p, 4d and 4f sublevels and the results fitted to simple functions of the impact electron energy u in threshold units. With these values plus those obtained in our earlier work results are now available for all the sublevels 1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d and 4f. From the values for $Q_R^H(n\ell,u)$ one can readily obtain the cross section for direct ionization from any of these sublevels in any highly charged complex ion using the simple procedures given in our earlier work. The total ionization cross section with inclusion of the excitation-autoionization contribution has been obtained for Be-like and Li-like ions. The results for the Li-like ions N^{4+} and O^{5+} are in generally good agreement with recent results of Crandall and co-workers. Basic hydrogenic ion data for scaled R-matrix elements and collision strengths have been calculated for the transitions 1s-2s, 2p, 3s, 3p, 3d; 2s, 2p-3s, 3p, 3d, 4s, 4p, 4d, 4f; and 3s, 3p, 3d-4s, 4p, 4d, 4f, 5s, 5p, 5d, 5f, 5g for the eight impact electron energies in threshold units ε = 1.0, 1.2, 1.5, 1.9, 2.5, 4.0, 6.0, and 10.0. Collision strengths and radiative line strengths for the $\Delta n = 0$ transitions in He-like and Be-like ions have been calculated for additional Z values so that results are now available for He-like ions with Z = 6, 8, 10, 12, 14, 16, 18, 20, 22, 24, 26, 28, 30, 36, 42, 48, 54, 64 and 74 and for Be-like ions with the same Z values for $Z \geq 12$. All these collision strength data have been fitted to simple functions of the impact electron energy that are readily integrated over a Maxwellian to obtain collision rates. Preliminary results have been obtained for the n = 2 to n = 3 transitions in Be-like ions.

I. Introduction

The purpose in the work reported here is to obtain cross sections for excitation and ionization of very highly charged ions by electron impact for use in controlled thermonuclear fusion research, where such data are needed for diagnostic purposes and for estimating the energy losses due to the presence of highly charged impurity ions. Since a very large amount of cross section data is needed for these purposes, it is advantageous to use an approach which is rapid and yet quite accurate. The present approach satisfies these requirements for very highly charged ions.

The method used is a Coulomb-Born-Exchange method that is equivalent to use of first order time dependent perturbation theory in which the perturbation consists of the entire electrostatic interaction between the electrons plus all relativistic corrections. Hence, the zeroth order Hamiltonian H_o for scattering of an electron by an ion of nuclear charge number Z with N bound electrons is a sum of N + 1 independent non-relativistic hydrogenic-ion Hamiltonians, H_i, which can be written

$$H_i = -\frac{1}{2}\left(\nabla_i^2 + \frac{2}{r_i}\right) \tag{1}$$

$$H_o = \sum_{i=1}^{N+1} H_i, \tag{2}$$

where energy is in units of $2Z^2$ Rydbergs and distances are in units of a_o/Z. The zeroth order wave functions, which are eigenfunctions of the Hamiltonian H_o, are antisymmetric sums of products of N + 1 hydrogenic-ion wave functions. In order to represent scattering one of these must be a free coulomb function and the other N are hydrogenic bound state functions.

This approach has the following advantages: (1) No orthogonality

problems arise and exchange is included in a completely consistent manner because the wave functions of all electrons, free and bound, are eigenfunctions of Hamiltonians of exactly the same form given by Eq (1), above. (2) The results for the scaled cross section Z^2Q or scaled collision strength $Z^2\Omega$ for any highly charged ion, regardless of its complexity, can be expressed in terms of the scaled non-relativistic R-matrix elements ZR_H for hydrogenic ions, even with inclusion of the first order relativistic corrections. This occurs because we include in the relativistic corrections only the dominant terms, those going as the highest power of Z, see Eq (3) below. These consist of a sum of single particle operators and hence make no direct contribution to the matrix elements determining the inelastic scattering cross sections; however, they do have the important indirect effect of introducing intermediate coupling effects, as discussed below in connection with Eq (3). The fact that the results for complex ions can be expressed in terms of the ZR_H for hydrogenic ions leads to an immense reduction in computational effort because it is the calculation of the basic transition matrix elements (R-matrix elements) that requires most of the computer time in cross section calculations. In the present approach this needs to be done only for the relatively simple case of hydrogenic ions. Then the results can be used over and over again to calculate cross sections or collision strengths for any transition in any complex ion with very little additional computational effort. (3) Configuration mixing or interaction and intermediate coupling effects can be readily included (and are being included in all of our recent and current work on excitation) through use of mixing coefficients obtained by diagonalizing the perturbation H' consisting of the electrostatic interaction between the bound electrons in

the target ion and the relativistic interactions. Specifically, when we use the same units as used in writing Eqs (1) and (2)

$$H' = \sum_{j>i}^{N} \sum_{i=1}^{N-1} \frac{1}{Zr_{ij}} + \frac{1}{2}\alpha^2 Z^2 \sum_{i=1}^{N} \left[-\frac{1}{4}\nabla_i^4 + \left(\frac{Z-\sigma_{n_i\ell_i}}{Z}\right)\frac{1}{r_i^3}\vec{\ell}_i\cdot\vec{s}_i - \frac{1}{4}\nabla_i^2\left(\frac{1}{r_i}\right)\right], \quad (3)$$

where $\sigma_{n_i\ell_i}$ represents the screening by the other bound electrons of the nuclear charge seen by electron i and all other symbols have their customary meanings. This part of the calculation is also greatly simplified by the fact that our zeroth order target ion wave functions are composed of antisymmetrical sums of products of hydrogenic-ion wave functions. We note that mixing is included only among states with a common total angular momentum quantum number J_a and belonging to the same complex, i.e. having the same set of principal quantum numbers and parity. Including mixing among states in additional configurations would correspond to including contributions of higher order in powers of $1/Z$ and α^2Z^2 and hence should not be done when working in the regime for which the present perturbation approach is valid unless all terms of the next order are included, which is very difficult to do. This may be a source of error in using more elaborate programs designed principally for neutral atoms or slightly charged ions in treating highly charged ions. (4) In fact, a fourth advantage of the present method is that it is probably generally much less prone to error than most other methods due to its simplicity, and when errors are made they are more readily detected.

We note that when all relativistic corrections are neglected the approach we are using gives exact non-relativistic results for the scaled collision strength $Z^2\Omega$ in the limit $Z \to \infty$. For this reason they have sometimes been

referred to as $Z = \infty$ results. However, since the approach can be regarded as a perturbation theory approach, as discussed above, it should be accurate whenever the perturbation is small relative to H_o. This tends to be the case when $Z >> N$ because then the interaction of each electron with the nucleus, which is included in the zeroth order Hamiltonian, greatly exceeds the electron-electron interaction included in the perturbation. However, Z should not be so large that treatment of relativistic corrections as part of the perturbation, as we do in obtaining intermediate coupling effects, becomes invalid. As indicated by the comparisons with other theoretical work and experiment made in references 1 and 2, which are attached, it appears that with possibly a few exceptions for transitions with very small collision strengths the method is accurate for excitation to within 30% when Z is in the range

$$3N \lesssim Z \lesssim 74. \tag{4}$$

In fact, for most of this range the results appear to be somewhat more accurate than this and they appear to be as reliable as those obtained with much more elaborate methods.

In the case of ionization the method appears to be accurate down to a lower value of Z than for excitation. Specifically the comparisons in references 3 and 4 and in references 5 and 6, which are attached, suggest that the approach is accurate for ionization to within $\sim$25% when

$$Z/N \geq 2. \tag{5}$$

The accuracy is expected to improve as the degree of ionization increases, i.e. as Z/N increases. The greater range of accuracy for ionization, despite the fact that we have neglected configuration mixing and intermediate coupling in treating ionization, probably arises because ionization is similar to excitation

summed over many final states so that errors tend to cancel out.

In the following sections we will discuss the specific work done in each of the areas of ionization and excitation during the current period August 1, 1979 - August 31, 1980. However, before proceeding with this we say a word about the attachments to this progress report. They consist of the following: (a) Reprints of work reported in the previous progress report, which were published during the current period. These are the first three attachments. (b) Galley proofs of three papers which will appear in the October, 1980, issue of Ap. J. Suppl. and which were attached in preliminary form to the previous progress report. These are the next three attachments. (c) Two reprints and three preprints of work done entirely during the current period. These are the last five attachments.

II. Ionization Results

(a) Direct Ionization

The reduced cross section $Q_R^H(n\ell,u)$ for ionization from the $n\ell$ = 3p and 3d sublevels of hydrogenic ions, as well as all lower sublevels considered in our earlier work 4, 7, were calculated using the Coulomb-Born-exchange method and the results given in Ref. 5. This is the attached J. Phys. B reprint by Moores, Golden and Sampson. During the current year this work was continued and results for $Q_R^H(n\ell,u)$ for ionization from the 4s, 4p, 4d and 4f sublevels were obtained in Ref. 8. This is the attached reprint by Golden and Sampson entitled "Ionization from the 4s, 4p, 4d and 4f Sublevels of Highly Charged Ions." Thus, results for $Q_R^H(n\ell,u)$ for all the 10 sublevels 1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p, 4d and 4f are now available. This is expected to cover all cases of appreciable interest. The new results have been fitted to the same

form as that proposed in Ref 3 and used in our earlier work.[4, 5] Specifically,

$$Q_R^H(n\ell,u) = \frac{1}{u}\left\{A''(n\ell)\log_e(u) + D''(n\ell)(1-\frac{1}{u})^2 + \left[\frac{c''(n\ell)}{u}+\frac{d''(n\ell)}{u^2}\right]\left[1 - \frac{1}{u}\right]\right\}, \quad (6)$$

where u is the impact electron energy in threshold units. Eq (6) is readily integrated over a Maxwellian to obtain collision rates, e.g. Eq (11) of Ref. 3. It also goes into the correct Bethe approximation form at high energies $u >> 1$ given by Eq (9) of Ref. 7. Values for the coefficients entering Eq (6) for 3d and all lower sublevels are given in Table 2 of Ref. 5, while those for the 4s, 4p, 4d and 4f sublevels are given in Table 2 of Ref. 8.

The results for $Q_R^H(n\ell,u)$ have very wide application because from them one can obtain results for the cross section for direct ionization from sublevel $n\ell$ of any highly charged ion, which is over half ionized in accordance with Eq (5), regardless of its state of excitation. This can be done by following the simple prescriptions given in our earlier work[3,7]. Specifically, according to the prescription given in Ref. 3, the cross section for ionization from sublevel $n\ell$ of an ion in level j is

$$Q_j(n\ell,u) = \pi a_o^2 \left(\frac{n}{Z_{eff}(n\ell)}\right)^4 r_{n\ell}\, Q_R^H(n\ell,u) \quad (7)$$

Here $r_{n\ell}$ is the number of electrons in sublevel $n\ell$ and $Z_{eff}^j(n\ell)$ is an effective nuclear charge number, which can be written

$$Z_{eff}^j(n\ell) = Z - \sigma_{n\ell}(C_j), \quad (8)$$

where $\sigma_{n\ell}(C_j)$ is a screening parameter that takes into account the screening of the nuclear charge by the other bound electrons and is assumed to depend only on the configuration C_j. Values for $Z_{eff}(n\ell)$ or $\sigma_{n\ell}$ assuming all electrons

other than the active one are in the lowest states allowed by the Pauli principal have been given in Table 3 of references 5 and 7 and in Table 2 of Ref. 4. Recently in the attached Ref. 8 a general procedure was given for obtaining Z_{eff} for any sublevel of any ion in any state of excitation, see Eqs (6) - (11) and Table 3 of Ref. 8. This procedure is consistent with our earlier recommendations except for a few of those for inner shell ionization given in Ref. 7.

In Ref. 7 the alternative expression to Eq (7) given by*

$$Q_j(n\ell,u) = \pi a_o^2 \left(\frac{I_H}{I^j_{n\ell}}\right)\left(\frac{n}{Z_{eff}(n\ell)}\right)^2 r_{n\ell}\, Q_R^H(n\ell,u) \qquad (9)$$

was proposed, where $I^j_{n\ell}/I_H$ is the ionization energy in Rydbergs of sublevel $n\ell$ of the ion in level j. Either procedure has equal apriori validity because in the limit $Z \to \infty$, where the approach gives the exact non-relativistic results, $I^j_{n\ell}/I_H \to [Z_{eff}(n\ell)/n]^2 \to (Z/n)^2$. Actually the two proposals give nearly the same values in most cases. They differ most when Z is quite small. The biggest difference for ions satisfying Eq (5) occurs for Li-like carbon ions, where Eq (7) gives results about 15% lower than Eq (9). Earlier we favored Eq (7) because it appeared to give better agreement with the experimental results for ionization rates that are available for relatively low Z. However, Eq (9) appears to agree slightly better with the recent direct ionization cross section measurements of Crandall et al[9] for Li-like nitrogen and oxygen ions.

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*For the more complex ions in which more than one level is possible for the final configuration of the ion, the results given by Eqs (7) or (9) must be multiplied by an additional factor giving the relative probability for ionization to the particular final level, as done for example in considering case 4 in Sec 6 of Ref. 4.

(b) Inner Shell Excitation-Autoionization Contributions

The results discussed thus far apply only to direct ionization from any sublevel $n\ell$. Innershell excitation followed by autoionization also contributes to the total ionization cross section and appears to give quite a large contribution in some cases[9,10]. Although this probably occurs for too large a value of u to have a major effect on ionization rates in most cases, for some it is expected to be important. This is most likely for ions with a single electron outside filled shells, where the number of electrons that can contribute to innershell-excitation-autoionization is large relative to the single valence electron, which can only directly ionize.

During the current year we have been calculating the excitation-autoionization contribution using the same general method used in our other work and discussed in the Introduction. After summation over final states the results for this contribution by the present method take a very simple form expressible in terms of the scaled hydrogenic ion collision strength $Z^2\Omega_H$. In Ref. 6, which is the attached reprint of a Letter to the Editor of J. Phys. B: Atom. Molec. Phys. by Sampson and Golden, results were given for the total ionization cross section including excitation-autoionization contributions for Li-like ions. The results for C^{3+}, N^{4+} and O^{5+} were found to be in mostly very good agreement with the measurements of Crandall et al[9], especially for the more highly charged Li-like ions N^{4+} and O^{5+}. Near the end of Ref. 6, a simple physical explanation for the observed[9] increase in the relative importance of the excitation-autoionization contribution with Z for $Z \leq 8$ was given in terms of the effects of the greater screening of the nuclear charge by the other bound electrons in the case of a

2s electron than a 1s electron. It was also predicted that the importance of the excitation-autoionization contribution would moderate for higher Z. In Ref. 11, which is the attached preprint by Sampson and Golden entitled "Ionization Cross Sections with Inclusion of Excitation-Autoionization Contributions for Ions with 5 or Less Bound Electrons," we have included the effect of the branching ratio for autoionization, as opposed to radiative decay. This was done using a simple procedure suggested by Hahn[12]. In Ref. 6 this ratio was taken to be unity, which is a good approximation for low Z. However, it becomes important as Z increases. In fact, in Ref. 11 it is found that the importance of the excitation-autoionization contribution as measured by the ratio of the second peak (the excitation-autoionization peak) to the first peak in the ionization cross section reaches a maximum in Li-like ions for $Z \underset{\sim}{} 13$. It then slowly declines with Z for higher Z due to the increased importance of radiative decay from the upper autoionizing levels. For Be-like ions the excitation-autoionization contribution is generally found to be somewhat less important than for Li-like ions, as expected, due to the greater number of valence electrons that contribute to direct ionization. The contribution is still less important for the boron and higher isoelectronic sequences until the sodium sequence is reached. In our immediate future work on ionization we intend to consider Na-like and Mg-like ions, where the excitation-autoionization contribution is known to be large due to the large number of n=1 and n=2 electrons that can be innershell excited and then autoionize compared with the one or two n=3 valence electrons that can directly ionize.

We note that for O^{4+} the experimental results of Crandall et al[10] exceed those in Ref. 11 by about 15 to 25% at and above the peak of the ionization

cross section. In contrast to the implications of the discussion on page three of Ref. 10, this is the only case that their experimental results are available for Be-like ions satisfying Eq (5). This is about equal to the magnitude of the discrepancy between experiment and our results[6] for the analogous case of Li-like carbon, where Z/ N also is 2. We expect improvement in our results for Be-like ions with increase in Z similar to that found for the Li-like ions N^{4+} and O^{5+} in Ref. 6.

III. Excitation Results

(a) General Remarks

Our excitation results are expressed in terms of the collision strength Ω. The well known relationship between the cross section $Q(i\to k)$ and the collision strengths $\Omega(i-k)$ for a transition $i\to k$ is

$$Q(i\to k) = \frac{\pi a_o^2}{\omega_i} \left(\frac{I_H}{E}\right) \Omega(i-k) , \tag{10}$$

where ω_i is the statistical weight of the initial state i and (E/I_H) is the impact electron energy in Rydbergs. In our approach the quantity directly calculated is the scaled collision strength $Z^2\Omega(i-k)$. Similar to the case of ionization, we use the approximate relation

$$\Omega(i-k) = \frac{1}{Z_{eff}^{\,2}} \left[Z^2\Omega(i-k)\right]_{cal}, \tag{11}$$

where the quantity in the braces is our directly calculated value for $Z^2\Omega(i-k)$ and Z_{eff} is an effective nuclear charge number that takes into account approximately the screening of the nuclear charge by the inactive bound electrons. For $\Delta n \neq 0$ transitions, i.e. transitions involving a change in radial quantum number n, we use the same value for Z_{eff} as used for ionization from the same

lower level, while for the $\Delta n = 0$ transitions we use an average of the Z_{eff} for ionization from the initial and final levels of the transition.

(b) Hydrogenic Ion Results

As mentioned in the Introduction, the basic data in our approach are the scaled hydrogenic ion R-matrix elements ZR_H because the $[Z^2\Omega]_{cal}$ that we calculate with our approach can always be expressed in terms of the ZR_H, regardless of the complexity of the ion being considered. A considerable amount of this basic ZR_H data is available from the earlier work in References 13 and 14. However, it was decided that it would be desirable to have data out to higher impact electron energies than are usually covered in References 13 and 14 and for additional transitions. In Ref. 15, which is the attached preprint by Golden, Clark, Goett and Sampson entitled "Scaled Collision Strengths for Hydrogenic Ions", results have been calculated for all the 46 transitions 1s-2s, 2p, 3s, 3p, 3d; 2s, 2p-3s, 3p, 3d, 4s, 4p, 4d, 4f; and 3s, 3p, 3d-4s, 4p, 4d, 4f, 5s, 5p, 5d, 5f, 5g for the eight impact electron energies in threshold units ϵ = 1.0, 1.2, 1.5, 1.9, 2.5, 4.0, 6.0 and 10.0. Some of these transitions were considered for the lower energies in the earlier work[13,14], but were redone in Ref. 15 because the calculations for low energies require very little computer time with the present efficient program and because the present program is also believed to be more accurate. It was obtained by modifying the efficient ionization program of Ref. 5 to do excitation. Actually it is too lengthy to publish the extensive hydrogenic R-matrix data obtained, which has been put on tape and punched on cards. Thus, in Ref. 15 we simply give the results for the scaled hydrogenic collision strengths $Z^2\Omega_H$ and

$Z^2\Omega_H^e$. However, as summarized in Ref. 15, it has been shown in references 16 and 17 that, even with such effects as intermediate coupling and configuration mixing included, the $[Z^2\Omega]_{cal}$ to be used in Eq (11) for many transitions of interest in He-like and Li-like ions can be expressed in terms of $Z^2\Omega_H$ and $Z^2\Omega_H^e$ multiplied by factors involving the mixing coefficients. We note that Ref. 17 is the attached J. Phys. B reprint by Sampson, Clark and Parks. Of course, the results for $Z^2\Omega_H$ also apply directly for hydrogenic ions satisfying Eq (4), i.e. with $Z \gtrsim 3$.

In our future work we plan to calculate results for additional transitions in hydrogenic ions including transitions between sublevels with the same principal quantum number n for n = 3, 4 and 5, i.e. for transitions such as 3s-3p, 3p-3d etc. Recently considerable interest has been expressed in such transitions in H-like and He-like ions.[18]

(c) Intermediate Coupling Results for $\Delta n = 0$ Transitions in Complex Ions Including Fits to the Data

We consider now the work on excitation of complex ions and discuss first the transitions involving no change in principal quantum number n. In treating these so-called $\Delta n = 0$ transitions special problems arise. The theory for this was developed very thoroughly in Ref. 1 and applied to He-like and Be-like ions in references 1, 2 and 19. These papers are the three papers for which the galley proofs are attached. During the current year results were calculated for this type of transitions for considerably more Z values so that we now have intermediate coupling results for Z = 6, 8, 10, 12, 14, 16, 18, 20, 22, 24, 26, 28, 30, 36, 42, 48, 54, 64, and 74 for He-like ions. For Be-like ions we have results for the same Z values except that we begin with Z = 12.

Fits to the new data plus the data given in references 1, 2 and 19 have also been made. The results are given in Ref 20. The general form used for the fits is

$$[Z^2\Omega]^{fit}_{cal} = c_o + \frac{c_1}{(a+\varepsilon)} + \frac{c_2}{(a+\varepsilon)^2} + (5/3)Z^2S \log_e(\varepsilon). \qquad (12)$$

Here ε is the impact electron energy in threshold units; c_o, c_1, c_2 and a are adjustable parameters determined with a rapid program that uses least squares fit procedures; and Z^2S is the scaled radiative line strength. In this connection we digress for a moment to note that the comparisons with other calculations and experiment made in references 1 and 2 indicate that results by the present method for electric dipole line strengths are essentially as accurate as those by more elaborate methods for Z in the range satisfying Eq (4). Since they are also needed in application of the Coulomb-Bethe approximation to obtain the large ℓ contribution to the collision strengths for allowed transitions, we now regularly calculate Z^2S for all transitions for which it is non-vanishing.

Returning to the discussion of Eq (12), we note that for very high energies the correct asymptotic form for $Z^2\Omega$ is $(4/3)Z^2S \log_e(\varepsilon)$. However, it appears that this form is not reached for $\Delta n = 0$ transitions until ε is extremely high. For the range of energies covered by our data, which is expected to include the entire range of appreciable interest in plasma applications, the form given by Eq (12) gives extremely good fits, usually to within a fraction of a percent for the transitions in which Z^2S is not zero or very small, and the accuracy is usually only slightly less for the other types of transitions. On the other hand, for $\Delta n \neq 0$ transitions it appears that the best fits are

obtained with $(4/3)Z^2S$ replacing $(5/3)Z^2S$ in the final term of Eq (12). This is indicated by the fact that very good fits to the data for $Z^2\Omega_H$ were obtained in Ref. 15 using the form given by Eq (12), but with c_o and $5/3Z^2S$ replaced with the Bethe coefficients D' and A', where A' = 4/3 Z^2S.

We note that the presence of the coefficient a in Eq (12) leads to considerable improvement in accuracy over earlier fits with a = 0 and the corresponding collision rate still involves only the first and second exponential integrals. Specifically, assuming Maxwellian electrons the collisional excitation rate per ion in the lower level corresponding to use of Eq (1) is

$$C = \frac{\pi a_o^2}{\omega_i Z_{eff}^2} N_e \left(\frac{8kT}{\pi m}\right)^{1/2} \left(\frac{I_H}{kT}\right)\left\{c_o e^{-y}+\frac{5}{3}Z^2 S E_1(y)+ye^{ay}\left[c_1 E_1(ay+y)+\frac{c_2}{a+1}E_2(ay+y)\right]\right\} \quad (13)$$

where N_e and T are the electron density and temperature.

In the immediate future we also plan to calculate results for $\Delta n = 0$ transitions between the doubly excited states belonging to configurations of the kind $2\ell_a\ 2\ell_b$ in He-like ions, which we have recently learned are of interest for plasma diagnostic purposes[21]. This can be done very readily because they are like those considered in Ref. 2 for Be-like ions except that different mixing coefficients apply due to the absence of the $1s^2$ core in treating He-like ions.

(d) Intermediate Coupling Results for $\Delta n \neq 0$ Transitions In Complex Ions

In Ref. 16 and in references 17 and 22 of which reprints are attached, we obtained intermediate coupling collision strengths for various transitions in He-like ions involving a change in n value and for innershell excitation

of Li-like ions. We have also obtained intermediate coupling results for transitions between the n = 2 and n = 3 states in Be-like ions, i.e. transitions between states of the $1s^2 2\ell_a 2\ell_b$ and $1s^2 2\ell_a 3\ell_b'$ configurations. However, the latter results have not been published yet. First they were delayed because they were obtained with the screening parameter $\sigma_{n_i \ell_i}$ in Eq (3) omitted. In Ref. 2, where the $\Delta n = 0$ transitions in Be-like ions were studied, it was found that intermediate coupling results for some of the spin change transitions at moderate or fairly low Z are very sensitive to the strength of the spin-orbit interaction. Considerable improvement was obtained when the physically more reasonable choice of including $\sigma_{n_i \ell_i}$ in Eq (3) was made. Thus, we planned to redo the n = 2 to n = 3 transitions in Be-like ions using Eq (3) in obtaining the mixing coefficients. However, in the meantime we decided to calculate the basic hydrogenic ion data out to higher energies, as discussed in subsection III (b). Thus, we delayed all calculations of $\Delta n \neq 0$ transitions in complex ions until the new hydrogenic ion data was completed. It should be mentioned the results are needed to higher energies than we originally expected because the work in Ref. 23 and more recently in Ref. 24 indicate that in many cases of interest for fusion the ratio of ionization energy to kT for which a particular stage of ionization is important is often quite small $\lesssim 1$, rather than somewhat greater than 1, as in most astrophysical problems. Thus, in order to determine collision rates accurately it is sometimes necessary to have cross sections for higher energies than we originally expected. Moreover, in applications to complex ions all the Bethe coefficients are usually not available so that it is difficult to estimate the cross sections for moderately high energies unless direct calculations have been made. Recently we have

been redoing the n = 2 to n = 3 calculations in Be-like ions, but we delayed publication again because we found an inconsistency between the collision strengths and line strengths for a few transitions in applying the Coulomb-Bethe approximation for various ℓ values. This is a consistency check we generally make, as discussed below Eq (62) of the attached Ref. 1, and it has been helpful in finding inconsistencies in other work, as well as our own preliminary results. In the case of the n = 2 to n = 3 transitions it turned out that the inconsistency arose because a phase factor had been omitted in the line strength calculations. The results for these transitions in Be-like ions are expected to be ready for publication very soon.

In the very near future we also expect to proceed with calculations for additional innershell excitation transitions in Li-like ions and with calculations for both $\Delta n = 0$ and $\Delta n = 1$ transitions in boron-like ions.

Finally we note that all our recent calculations are being made using jj coupled basis states as well as the more familiar LS coupled basis states. Although this requires more work, it has several advantages, as discussed in References 1 and 2. For example, it serves as a check against numerical errors and helps in understanding the behavior of results for a given transition as Z is changed.

IV. References

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