PHYSICAL REVIEW A VOLUME 34, NUMBER 2 AUGUST 1986

Branching ratios for excitation to highly excited levels or ionization of complex ions

Douglas H. Sampson
Department of Astronomy, The Pennsylvania State University, University Park, Pennsylvania 16802

(Received 20 December 1985; revised manuscript received 14 April 1986)

For excitation to very high levels or ionization of a complex ion there are sometimes several possible final states for the remaining core (next higher stage of ionization in the case of ionization). Then formulas, such as the widely used ionization formula of Lotz or other ionization and excitation formulas in which the cross section is expressed essentially as a product of the number of electrons in the initial subshell times a cross section having the form of a hydrogenic ion cross section, must be multiplied by an additional factor giving the relative probability or branching ratio for the particular final state of the core. This problem was considered previously by Bely and Schwartz [Astron. Astrophys. 1, 281 (1969)] for the case of ionization. They used *LS* coupling, exchange was neglected and the remaining core was assumed to contain one or two partially filled subshells. Here we have included exchange and we have obtained the branching ratios for *jj* coupling as well as *LS* coupling for the general situation that any number of filled and partially filled subshells are present. The results apply for both collisional and radiative transitions.

I. INTRODUCTION

The present paper deals with some aspects of excitation to highly excited levels and ionization of the highly charged ions that exist in high-temperature plasmas such as those occurring in fusion energy research, some areas of astrophysical research and in research to produce x-ray lasers. In modeling such high temperature, non-LTE plasmas it is generally necessary to make a detailed treatment of the lower bound energy levels of the ions in the dominant stages of ionization. However, due to the necessity of keeping the computations from being prohibitively lengthy and also because the highly excited levels are of less importance one usually makes a less detailed treatment of them. Specifically, they are simply designated by their n values, their nl values, or possibly by their nlj values in the case of ions with very large nuclear charge number Z, and not by additional quantum numbers such as J_t' the total angular momentum quantum number for the ion. In fact, since the dependence of these highly excited levels on J_t' is weak, it is generally valid to sum over J_t' values. Also it is usually assumed that the cross section for electron impact excitation to such highly excited levels or ionization is approximately equal to the number of electrons w in the lower subshell from which the excitation or ionization occurs multiplied by an approximate cross section $Q_{\rm H}^{ps}$ that has the form of a hydrogenic ion cross section

$$Q \simeq w Q_{\rm H}^{ps} , \tag{1}$$

where $Q_{\rm H}^{ps}$ may contain some factors such as an effective Z to account for effects of the inactive bound electrons. An example of this is Eqs. (5) and (8) of Ref. 1. Another is the widely used semiempirical ionization formula of Lotz,[2,3] which is essentially of the form of Eq. (1) except that it is equivalent to making the additional approximation of using an approximate reduced cross section for ionization from the 1s sublevel in treating ionization from any sublevel, as noted in Refs. 1 and 4.

In the present work we are interested in determining more precisely the conditions for which Eq. (1) is valid and in determining how it must be modified even in treating very highly charged ions for particular cases. These cases are likely to become of increased interest in the near future as plasma modeling continues to become more sophisticated and more complex ions are treated in greater detail. They can occur whenever the remaining core of more tightly bound electrons in the case of excitation, or the ion in the next higher stage of ionization in the case of ionization, has one or more partially filled subshells. The reason for this is that the final core configuration might then give rise to several possible states. Then the right-hand side of Eq. (1) should be multiplied by a factor giving the relative probability or branching ratio for the particular final state of the core. Bely and Schwartz[5] have previously considered this problem for the case of ionization and gave approximate values for the branching ratio factors obtained when *LS* coupling was used, both configuration mixing and intermediate coupling type mixing were omitted, exchange was neglected, and the remaining core had one or two partially filled subshells. Although the assumptions or approximations made in obtaining their results were stated, no details of the derivation of their results were given. Here we make similar approximations to those made by Bely and Schwartz except that we do include exchange and we obtain general results applicable for ions with any number of filled and partially filled subshells. It turns out that inclusion of exchange does not alter the expressions for the branching ratios. However, it is satisfying to be able to demonstrate this, especially since exchange does often have quite a significant effect on the cross sections near threshold, as seen for example from the results given in Tables I of Refs. 1, 6, and 7. It would have been preferable if we were also able to include mixing effects; however, this would have greatly complicated the situation and would not have allowed us to derive simple, general, analytical expressions for the branching ratios. On the other hand, we do obtain results for pure *jj* coupling, as well as *LS* coupling, and usually one or the other coupling scheme is at least a moderately good approximation.

An outline of the work done in the remaining sections of the paper is as follows. First we summarize the general equations determining the collision strengths and cross sections for highly charged ions. Then we apply them to cases of increasing complexity beginning with hydrogenic ions and then going to ions with a single active electron outside filled subshells. This is followed by consideration of excitation to a highly excited level or the continuum (the case of ionization) from a subshell initially containing any number electrons. We then consider the case that in addition a partially filled subshell of inactive or spectator electrons is present. This is followed by consideration of the case that there are three partially filled subshells of inactive electrons present. From these results one can see how to generalize to any number of inactive closed subshells and partially filled subshells in addition to the active subshell. In each case results are first obtained in *jj* coupling, then the corresponding *LS* coupling results are given. In the final section the formulas we have obtained are applied to a few specific examples to give illustrative numerical values for the branching ratios. Also we include two Appendixes. In Appendix A it is shown that our results for branching ratios apply as well for the corresponding radiative transitions. In Appendix B we discuss how the quantum numbers entering our expressions for the branching ratios must be interpreted when an alternative coupling scheme is used for obtaining intermediate angular momenta rather than the more standard scheme of coupling successively the total angular momenta of each subshell, as we assumed in the derivation of our results.

II. GENERAL EQUATIONS FOR HIGHLY CHARGED IONS

As is well known, the cross section $Q(i\text{-}f)$ for the transition $i \to f$ can be expressed in terms of the collision strength $\Omega(i\text{-}f)$ by the equation

$$\Omega(i\text{-}f)=\frac{\pi a_0^2}{g_i E(\mathrm{Ry})}\Omega(i\text{-}f) , \tag{2}$$

where g_i is the statistical weight of the initial level i and E(Ry) is the impact electron energy in rydbergs. For highly charged ions of interest here the elements of the reactance matrix $\underline{R}$ are generally small so that unitarization is not necessary. Also for such ions it is convenient to scale out the major Z dependence as in Ref. 8. Then the collision strength can be written[9]

$$Z^2\Omega(\beta_t J_t-\beta_t' J_t') =2\sum_{J}(2J+1)\sum_{\substack{l,l'\\ j,j'}} |ZR(\beta_t J_t kljJ;\beta_t' J_t' k'l'j'J)|^2 , \tag{3}$$

where ZR and $Z^2\Omega$ are slowly varying functions of the nuclear charge number Z that become independent of Z in the limit $Z \to \infty$, if relativistic effects are neglected. In Eq. (3), J_t, j, and J are the total angular momentum quantum numbers of the target ion, the impact electron, and the complete system, respectively. β_t represents all additional quantum numbers necessary to specify the initial state of the target ion, k^2 is the impact electron energy in Z^2 rydbergs and l is the orbital angular momentum quantum number of the impact electron. Primes on symbols indicate the corresponding final-state quantum numbers.

The reactance matrix has a direct and an exchange part

$$ZR=ZR^d-ZR^e , \tag{4}$$

where in detail for inelastic scattering of an electron by a target ion with N bound electrons

$$ZR^d(\beta_t J_t kljJ;\beta_t' J_t' k'l'j'J)=2\sum_{\substack{M_t,m,\\ M_t',m'}} C(J_t j M_t m;JM)C(J_t' j' M_t' m';JM) \times\int dx_1\int dx_2\cdots\int dx_{N+1}\,\Psi^*_{\beta_t J_t M_t}(x_i^{-1})u^*_{kljm}(x_i) \times\left[\sum_{q\,(\neq i)}\frac{1}{r_{qi}}\right]\Psi_{\beta_t' J_t' M_t'}(x_i^{-1})u_{k'l'j'm'}(x_i) , \tag{5}$$

and

$$ZR^e(\beta_t J_t kljJ;\beta_t' J_t' k'l'jJ) =2N\sum_{\substack{M_t,m,\\ M_t',m'}} C(J_t j M_t m;JM)C(J_t' j' M_t' m';JM) \times\int dx_1\int dx_2\cdots\int dx_{N+1}\,\Psi^*_{\beta_t J_t M_t}(x_i^{-1})u^*_{kljm}(x_i)\left[\sum_{q\,(\neq i)}\frac{1}{r_{qi}}\right]\Psi_{\beta_t' J_t' M_t'}(x_j^{-1})u_{k'l'j'm'}(x_j) ,\quad j\neq i . \tag{6}$$

Here the C's are Clebsch-Gordan coefficients written in the notation of Ref. 10; x_i stands for the coordinates, spatial and spin, of electron i; x_i^{-1} designates the coordinates of all $N+1$ electrons except electron i; $\Psi_{\beta_t J_t M_t}(x_i^{-1})$ is the initial wave function of the target ion and $u_{kljm}(x_i)$ is the impact electron wave function

$$u_{kljm}(x)=F_{kl}(r)\sum_{m_s,m_l} C(\tfrac{1}{2}lm_sm_l;jm)Y_{lm_l}(\theta,\phi)\delta(m_s\,|\,\sigma)\ . \tag{7}$$

In applying Eqs. (5) and (6) we will generally choose $i=N+1$ and $j=N$.

III. HYDROGENIC IONS

Since we intend to express the cross section for excitation to highly excited levels or ionization in terms of a cross section with the same form as a hydrogenic ion cross section Q_{H} we first consider the case of hydrogenic ions, where $N=1$. Then

$$\Psi_{\beta_tJ_tM_t}(x_{N+1}^{-1})=u_{n_al_aj_am_a}(x_1)=R_{n_al_a}(r_1)\sum_{m_{sa},m_{la}} C(\tfrac{1}{2}l_am_{sa}m_{la};j_am_a)Y_{l_am_{la}}(\theta_1,\phi_1)\delta(m_{sa}\,|\,\sigma_1)\ . \tag{8}$$

The interaction r_{12}^{-1} can be expanded in the standard form in terms of Racah tensors

$$\frac{1}{r_{12}}=\sum_{\lambda=0}^{\infty}\frac{r_<^{\lambda}}{r_>^{\lambda+1}}\underline{C}^{\lambda}(1)\cdot\underline{C}^{\lambda}(2)\ . \tag{9}$$

Then Eq. (5) applied to this case can be written in the form

$$ZR^{d}(n_al_aj_akljJ;n_a'l_a'j_a'k'l'J)=2\sum_{\lambda=0}^{\infty}D^{\lambda}(n_al_akl;n_a'l_a'k'l')\langle\tfrac{1}{2}l_aj_a\tfrac{1}{2}ljJM\,|\,\underline{C}^{\lambda}(1)\cdot\underline{C}^{\lambda}(2)\,|\,\tfrac{1}{2}l_a'J_a'\tfrac{1}{2}l'j'JM\rangle\ , \tag{10}$$

where the angular matrix element is readily evaluated using standard irreducible tensor techniques, as given for example in Ref. 10 and the Appendixes of Refs. 11 and 12,

$$\langle\tfrac{1}{2}l_aj_a\tfrac{1}{2}ljJM\,|\,\underline{C}^{\lambda}(1)\cdot\underline{C}^{\lambda}(2)\,|\,\tfrac{1}{2}l_a'j_a'\tfrac{1}{2}l'j'JM\rangle=(-1)^{J+j+j_a'}\begin{Bmatrix} j_a & \lambda & j_a' \\ j' & J & j \end{Bmatrix}\langle\tfrac{1}{2}l_aj_a||\underline{C}^{\lambda}||\tfrac{1}{2}l_a'j_a'\rangle\langle\tfrac{1}{2}lj||\underline{C}^{\lambda}||\tfrac{1}{2}l'j'\rangle\ . \tag{11}$$

Here

$$\langle\tfrac{1}{2}l_1j_1||\underline{C}^{\lambda}||\tfrac{1}{2}l_2'j_2'\rangle=(-1)^{j_1+1/2+l_2'+\lambda}[(2j_1+1)(2j_2'+1)]^{1/2}\begin{Bmatrix} l_1 & \lambda & l_2' \\ j_2' & \frac{1}{2} & j_1 \end{Bmatrix}\langle l_1||\underline{C}^{\lambda}||l_2'\rangle \tag{12}$$

and

$$\langle l_1||\underline{C}^{\lambda}||l_2'\rangle=(-1)^{l_1}[(2l_1+1)(2l_2'+1)]^{1/2}\begin{pmatrix} l_1 & \lambda & l_2' \\ 0 & 0 & 0 \end{pmatrix}\ . \tag{13}$$

The D^{λ} in Eq. (10) is the radial matrix element

$$D^{\lambda}(n_al_akl;n_a'l_a'k'l')=\int_0^{\infty}dr_1\,r_1^2\int_0^{\infty}dr_2\,r_2^2R_{n_al_a}(r_1)F_{kl}(r_2)\frac{r_<^{\lambda}}{r_>^{\lambda+1}}R_{n_a'l_a'}(r_1)F_{k'l'}(r_2)\ . \tag{14}$$

The exchange part of the reactance matrix obtained by applying Eq. (6) to the case of hydrogenic ions becomes

$$ZR^{e}(n_al_aj_akljJ;n_a'l_a'j_a'k'l'jJ)$$
$$=2\sum_{\substack{m_a,m,\\ m_a',m'}} C(j_ajm_am;JM)C(j_a'j'm_a'm';JM)\int dx_1\int dx_2\,u^{*}_{n_al_aj_am_a}(x_1)u^{*}_{kljm}(x_2)\frac{1}{r_{12}}u_{n_a'l_a'j_a'}(x_2)u_{k'l'j'm'}(x_1)\ . \tag{15}$$

There is the problem with Eq. (15) that irreducible tensor techniques cannot be applied directly to it because they require that the electrons be ordered in the same way in the initial and final states and also coupled in the same manner. However, this is easily remedied by interchanging the order of $u_{n_a'l_a'j_a'm_a'}(x_2)$ and $u_{k'l'j'm'}(x_1)$ and then using

$$C(j_a'j'm_a'm';JM)=(-1)^{j_a'+j'-J}C(j'j_a'm'm_a';JM)\ . \tag{16}$$

Then applying Eq. (9) to (15) and using the same procedures that lead to Eqs. (10) and (11) one obtains

$$ZR^{e}(n_al_aj_akljJ,n_a'l_a'j_a'k'l'j'J)=2(-1)^{j_a'+j+2j'}\sum_{\lambda=0}^{\infty}E^{\lambda}(n_al_akl,n_a'l_a'k'l')\begin{Bmatrix} j_a & \lambda & j' \\ j_a' & J & j \end{Bmatrix}\langle j_a||\underline{C}^{\lambda}||j'\rangle\langle j||\underline{C}^{\lambda}||j_a'\rangle\ , \tag{17}$$

where

$$E^{\lambda}(n_a l_a kl, n'_a l'_a k'l') = \int_0^{\infty} dr_1\, r_1^2 \int_0^{\infty} dr_2\, r_2^2 R_{n_a l_a}(r_1) F_{kl}(r_2) \frac{r_<^{\lambda}}{r_>^{\lambda+1}} F_{k'l'}(r_1) R_{n'_a l'_a}(r_2) \tag{18}$$

and we have used the abbreviated form

$$\langle j_1 || \underline{C}^{\lambda} || j'_2 \rangle \equiv \langle \tfrac{1}{2} l_1 j_1 || \underline{C}^{\lambda} || \tfrac{1}{2} l'_2 j'_2 \rangle \,. \tag{19}$$

Now we apply Eqs. (10), (11), and (17) to Eqs. (3) and (4). Then this is applied to Eq. (2) with $g_i = 2j_a + 1$ to give for the Z-scaled hydrogenic ion cross section

$$\begin{aligned} Z^2 Q_{\mathrm{H}}(n_a l_a j_a\text{-}n'_a l'_a j'_a) &= \frac{8\pi a_0^2}{(2j_a+1)E(\mathrm{Ry})} \sum_J (2J+1) \sum_{\substack{l,l',\\ j,j'}} \Bigg[\sum_{\lambda=0}^{\infty} \Bigg\{ D^{\lambda}(n_a l_a kl; n'_a l'_a k'l') \begin{Bmatrix} j_a & \lambda & j'_a \\ j' & J & j \end{Bmatrix} \langle j_a || \underline{C}^{\lambda} || j'_a \rangle \langle j || \underline{C}^{\lambda} || j' \rangle \\ &\qquad - (-1)^{2j'-J} E^{\lambda}(n_a l_a kl; n'_a l'_a k'l') \begin{Bmatrix} j_a & \lambda & j' \\ j'_a & J & j \end{Bmatrix} \langle j_a || \underline{C}^{\lambda} || j' \rangle \langle j || \underline{C}^{\lambda} || j'_a \rangle \Bigg\} \Bigg]^2 , \end{aligned} \tag{20}$$

where we used the fact that $(-1)^{2J+2(j+j'_a)} = 1$ because both J and $j + j'_a$ are integers. Of course, only a few values of λ contribute to Eq. (20) due to the presence of the 6-j symbols there and in Eq. (12).

As noted previously, it is our intention to show that the cross section for excitation to a very high bound level or ionization of any complex ion can can be expressed in the form of Eq. (1) modified to contain a branching ratio factor (which will be unity in some cases). In order to do this with exchange included it is necessary to perform the summation over J in Eq. (20). In doing this we use the relation[10–12]

$$\sum_J (2J+1) \begin{Bmatrix} j_a & \lambda & j'_a \\ j' & J & j \end{Bmatrix} \begin{Bmatrix} j_a & \lambda' & j'_a \\ j' & J & j \end{Bmatrix} = \frac{\delta_{\lambda\lambda'}}{2\lambda+1} \tag{21}$$

in evaluating the terms proportional to $D^{\lambda} D^{\lambda'}$, a similar relation with j'_a and j' interchanged in evaluating terms proportional to $E^{\lambda} E^{\lambda'}$ and the relation

$$\sum_J (-1)^J (2J+1) \begin{Bmatrix} j_a & \lambda & j'_a \\ j' & J & j \end{Bmatrix} \begin{Bmatrix} j_a & \lambda' & j' \\ j'_a & J & j \end{Bmatrix} = (-1)^{\lambda+\lambda'} \begin{Bmatrix} j' & j & \lambda \\ j'_a & j_a & \lambda' \end{Bmatrix} \tag{22}$$

in evaluating the terms proportional to $D^{\lambda} E^{\lambda'}$. The result is

$$\begin{aligned} Z^2 Q_{\mathrm{H}}(n_a l_a j_a\text{-}n'_a l'_a j'_a) = \frac{8\pi a_0^2}{(2j_a+1)E(\mathrm{Ry})} \sum_{\substack{l,l',\\ j,j'}} \Bigg[& \sum_{\lambda=0}^{\infty} \frac{1}{2\lambda+1} [D^{\lambda}(n_a l_a kl; n'_a l'_a k'l') \langle j_a || \underline{C}^{\lambda} || j'_a \rangle \langle j || \underline{C}^{\lambda} || j' \rangle]^2 \\ & - 2 \sum_{\lambda=0}^{\infty} \sum_{\lambda'=0}^{\infty} (-1)^{2j'+\lambda+\lambda'} D^{\lambda}(n_a l_a kl; n'_a l'_a k'l') E^{\lambda'}(n_a l_a kl; n'_a l'_a k'l') \\ & \qquad \times \begin{Bmatrix} j' & j & \lambda \\ j'_a & j_a & \lambda' \end{Bmatrix} \langle j_a || \underline{C}^{\lambda} || j'_a \rangle \langle j || \underline{C}^{\lambda} || j' \rangle \langle j_a || \underline{C}^{\lambda'} || j' \rangle \langle j || \underline{C}^{\lambda'} || j'_a \rangle \\ & + \sum_{\lambda=0}^{\infty} \frac{1}{2\lambda+1} [E^{\lambda}(n_a l_a kl; n'_a l'_a k'l') \langle j_a || \underline{C}^{\lambda} || j' \rangle \langle j || \underline{C}^{\lambda} || j'_a \rangle]^2 \Bigg] \,. \end{aligned} \tag{23}$$

Often one is not interested in the value for j'_a and hence sums over j'_a. The detailed result is obtained by substituting for all the $\langle j_1 || \underline{C}^{\lambda} || j'_2 \rangle$ in Eq. (23) using Eqs. (19) and (12) and then performing the summations over j', j'_a, and j using Racah algebra very similar to that used in Sec. IV in obtaining Eq. (43). One obtains

$$\sum_{j_a'} Z^2 Q_{\mathrm{H}}(n_a l_a j_a\text{-}n_a' l_a' j_a') = Z^2 Q_{\mathrm{H}}(n_a l_a\text{-}n_a' l_a')$$

$$= \frac{16\pi a_0^2}{(2l_a+1)E(\mathrm{Ry})} \sum_{l,l'} \Bigg[\sum_{\lambda=0}^{\infty} \frac{1}{2\lambda+1} [D^{\lambda}(n_a l_a kl; n_a' l_a' k'l') \langle l_a || \underline{C}^{\lambda} || l_a' \rangle \langle l || \underline{C}^{\lambda} || l' \rangle]^2$$

$$- \sum_{\lambda=0}^{\infty} \sum_{\lambda'=0}^{\infty} (-1)^{\lambda+\lambda'} D^{\lambda}(n_a l_a kl; n_a' l_a' k'l') E^{\lambda'}(n_a l_a kl; n_a' l_a' k'l')$$

$$\times \langle l_a || \underline{C}^{\lambda} || l_a' \rangle \langle l || \underline{C}^{\lambda} || l' \rangle \langle l_a || \underline{C}^{\lambda} || l' \rangle \langle l || \underline{C}^{\lambda} || l_a' \rangle$$

$$+ \sum_{\lambda=0}^{\infty} \frac{1}{2\lambda+1} [E^{\lambda}(n_a l_a kl; n_a' l_a' k'l') \langle l_a || \underline{C}^{\lambda} || l' \rangle \langle l || \underline{C}^{\lambda} || l_a' \rangle]^2 \Bigg] . \quad (24)$$

Of course, this result for $Z^2 Q_{\mathrm{H}}(n_a l_a\text{-}n_a' l_a')$ can also be obtained with a completely *LS* coupling treatment. For example, it can be obtained by performing the summation over L values in the expressions for the collision strength or cross section given in Ref. 8 after using Eq. (55) of that reference and noting that Eq. (13) applies for the $\langle l_a || \underline{C}^{\lambda} || l_i' \rangle$'s in Eq. (24). It should be mentioned that the hydrogenic collision strengths in Ref. 8 as well as those for transitions to more highly excited levels given in Refs. 13 and 14, are defined to include the spin statistical weight factor of 2 so that in using Eq. (2) to obtain the cross section from their values for $Z^2\Omega_{\mathrm{H}}$ one should use $g_i = (2l_a+1)$.

In using the above results given by Eqs. (20), (23), and (24) in later sections we assume they have been calculated using the nonrelativistic Z scaled radial matrix elements D^{λ} and E^{λ} obtained with the assumption that both bound and free electrons see the same nuclear charge Z. Then the D^{λ}, E^{λ}, $Z^2 Q_{\mathrm{H}}$ become independent of Z.

IV. IONS WITH CLOSED SUBSHELLS IN ADDITION TO THE ACTIVE SUBSHELL

In treating complex ions, those with more than a single bound electron, we assume that the usual procedure is followed in which the wave functions for complex ions are built up of single electron orbitals of the form of Eq. (8). These and the orbitals for the free electron given by Eq. (7) are assumed to be normalized and orthogonal. Then it is easily seen that nonvanishing matrix elements will occur only when the same electrons occur initially and finally in each inactive closed subshell. Of course, there will be many terms of this kind resulting from permutations of the electrons between the different subshells, but this is exactly canceled by the normalization factors in the target ion wave function. Thus, the form of the results for inelastic scattering is completely unaffected by the presence of closed subshells of inactive electrons. Hence, hereafter we can ignore them. A consequence of this is that the form of the results given by Eqs. (20), (23), and (24) apply for ions with a single active electron outside closed subshells, as well as hydrogenic ions. Of course, the accurate radial functions and hence the D^{λ}'s and E^{λ}'s will differ from the hydrogenic ones due to the presence of the inactive electrons, but we will neglect this difference except to take it into account by dividing by the square of an effective nuclear charge number Z_{eff}. Then the cross section for a complex ion with a single valence electron is given by

$$Q(n_a l_a j_a\text{-}n_a' l_a' j_a') = \frac{1}{Z_{\mathrm{eff}}^2} [Z^2 Q_{\mathrm{H}}(n_a l_a j_a\text{-}n_a' l_a' j_a')] , \quad (25)$$

where $Z^2 Q_{\mathrm{H}}$ is given by Eq. (23). Of course, a similar result applies for $n_a l_a\text{-}n_a' l_a'$ transitions with the quantity in the braces replaced with that given by Eq. (24), or for ionization with this quantity replaced with the $Z^2 Q_{\mathrm{H}}$ for ionization. These are all examples of Eq. (1) for the case that $w=1$. We next consider the case that there are additional electrons in the active subshell and work out the results applicable when *jj* coupling is assumed.

A. Results in *jj* coupling

It is well known[10,11] that for two equivalent electrons an antisymmetrical wave function is given by

$$\Psi(n_a l_a j_a^2 J_a M_a \,|\, x_1 x_2) = \sum_{m_1, m_2} C(j_a j_a m_1 m_2; J_a M_a) \times u_{n_a l_a j_a m_1}(x_1) u_{n_a l_a j_a m_2}(x_2) . \quad (26)$$

Although this appears to have the form of an unsymmetrized function, the Clebsch-Gordan coefficients insure antisymmetry. Similarly, for three equivalent electrons an antisymmetrized wave function is given by

$$\Psi(n_a l_a j_a^3 J_a M_a \,|\, x_1 x_2 x_3) = \sum_{J_1} (j_a^2 J_1 \,|\, \} j_a^3 J_a) \sum_{M_1, m_3} C(J_1 j_a M_1 m_3; J_a M_a) \Psi(n_a l_a j_a^2 J_1 M_1 \,|\, x_1 x_2) u_{n_a l_a j_a m_3}(x_3) , \quad (27)$$

where $\Psi(n_a l_a j_a^2 J_1 M_1 \,|\, x_1 x_2)$ is given by Eq. (26) with J_1 and M_1 replacing J_a and M_a and the $(\,|\, \})$ are coefficients of fractional parentage (Cfp). Although Eq. (27) has the appearance of an unsymmetrized function, it actually is completely antisymmetric in all three electrons due to the properties of the Cfp and the Clebsch-Gordan coefficients. One can continue this procedure for any number w of equivalent electrons so the completely antisymmetrical wave function for w equivalent electrons in a subshell a can be written

$$\Psi(n_a l_a j_a^w \alpha_a J_a M_a \,|\, x_1 x_2 \cdots x_w) = \sum_{J_1,\alpha_1} (j_a^{w-1}\alpha_1 J_1 \,|\, \} j_a^w \alpha_a J_a) \sum_{M_1,m_a} C(J_1 j_a M_1 m_a; J_a M_a) \Psi(n_a l_a j_a^{w-1}\alpha_1 J_1 M_1 \,|\, x_1 x_2 \cdots x_{w-1}) u_{n_a l_a j_a m_a}(x_w) \,, \tag{28}$$

where the electrons are in the definite increasing order 1, 2, 3, . . . , w, but the Cfp and the Clebsch-Gordan coefficients maintain antisymmetry. In Eq. (28) the symbol α_1 represents any additional quantum numbers, such as the seniority number, required to completely specify a state when there are several states with the j_a^{w-1} configuration having the same J_1 value. An analogous statement applies to α_a and the j_a^w configuration. The functions in Eq. (28) are assumed to be orthogonal and normalized, which requires that the Cfp obey the relation

$$\sum_{\alpha_1,J_1} (j_a^{w-1}\alpha_1 J_1 \,|\, \} j_a^w \alpha_a J_a)(j_a^{w-1}\alpha_1 J_1 \,|\, \} j_a^w \alpha_a' J_a) = \delta_{\alpha_a \alpha_a'} \,. \tag{29}$$

The final antisymmetrized wave function for the case of excitation of one of the equivalent electrons in the $n_a l_a j_a^w$ configuration to an excited state $n_a' l_a' j_a'$ is also of the form of Eq. (28) with the following exceptions: (1) the Cfp and summation over J_1 and α_1 is omitted, (2) an orbital $u_{n_a' l_a' j_a' m_a'}$ replaces $u_{n_a l_a j_a m_a}$, (3) one must include an antisymmetrized sum over all the possible states with any of the w electrons being in the excited level, (4) and then in order to have a normalized function one must multiply by the factor $(w)^{-1/2}$. Thus, the final state wave function can be written

$$\Psi(n_a l_a j_a^{w-1}\alpha_a'' J_a'' n_a' l_a' j_a' J_a' M_a' \,|\, x_1 x_2 \cdots x_w) = \frac{1}{\sqrt{w}} \sum_{p=1}^{w} (-1)^{w-p} \sum_{M_a'',m_a'} C(J_a'' j_a' M_a''; J_a' M_a') \Psi(n_a l_a j_a^{w-1}\alpha_a'' J_a'' M_a'' \,|\, x_1 x_2 \cdots x_{p-1}, x_{p+1} \cdots x_w) u_{n_a' l_a' j_a' m_a'}(x_p) \,, \tag{30}$$

where the $w-1$ electrons in $\Psi(n_a l_a j_a^{w-1}\alpha_a'' j_a'' M_a'' \,|\, x_1 x_2 \cdots x_{p-1}, x_{p+1} \cdots x_w)$ are in the definite increasing order 1, 2, 3, . . . , w with, of course, the value p omitted. Since, as noted previously, additional filled subshells of inactive electrons make no contribution, we can apply Eqs. (28) and (30) as the initial and final target ion wave functions to Eq. (5) with $N = w$ and $i = w+1$,

$$\begin{aligned} ZR^d(n_a l_a j_a^w \alpha_a J_a k l j J; n_a l_a j_a^{w-1}\alpha_a'' J_a'' n_a' l_a' j_a' J_a' k' l' j' J) &= \frac{2}{\sqrt{w}} \sum_{J_1,\alpha_1} (j_a^{w-1}\alpha_1 J_1 \,|\, \} j_a^w \alpha_a J_a) \sum_{\substack{M_a,m,\\ M_a',m'}} C(J_a j M_a m; JM) C(J_a' j' M_a' m'; JM) \\ &\quad \times \sum_{\substack{M_1,m_a,\\ M_a'',m_a'}} C(J_1 j_a M_1 m_a; J_a M_a) C(J_a'' j_a' M_a'' m_a'; J_a' M_a') \int dx_1 \int dx_2 \cdots \int dx_{w+1} \\ &\quad \times \Psi^*(n_a l_a j_a^{w-1}\alpha_1 J_1 M_1 \,|\, x_1 x_2 \cdots x_{w-1}) u^*_{n_a l_a j_a m_a}(x_w) u^*_{kljm}(x_{w+1}) \left[\sum_{q=1}^{w} \frac{1}{r_{qw+1}} \right] \\ &\quad \times \sum_{p=1}^{w} (-1)^{w-p} \Psi(n_a l_a j_a^{w-1}\alpha_a'' J_a'' M_a'' \,|\, x_1 x_2 \cdots x_{p-1}, x_{p+1} \cdots x_w) u_{n_a' l_a' j_a' m_a'}(x_p) u_{k'l'j'm'}(x_{w+1}) \,. \end{aligned} \tag{31}$$

Due to the orthogonality of the u functions one sees that only terms with $q = p$ can contribute. Although the initial target ion function given by Eq. (28) has all the electrons in the definite increasing order 1, 2, . . . , w, it is actually an antisymmetric function due to the properties of the Cfp, as noted previously. Thus in evaluating Eq. (31) we can permute the coordinates in the initial target ion wave function so they are in the same positions as they are in the final target ion wave function in determining the contribution of each term in the summation over p. This introduces a phase factor $(-1)^{w-p}$ that exactly cancels the effect of the similar phase factor in Eq. (31). Then the sum over p gives w contributions all with the same value and the total value for ZR^d is equal to the right-hand side of Eq. (31) with the sums over p and q removed, the phase factor omitted, both p and q set equal to w and the result multiplied by w. Also, since both the initial and final total system functions have the electrons in the same order 1, 2, 3, . . . , $w+1$ and the same type of coupling, we can use irreducible tensor techniques to evaluate this result for ZR^d. After again using Eq. (9) with w and $w+1$ replacing 1 and 2, respectively, we have

$$ZR^{d}(n_a l_a j_a^{w}\alpha_a J_a klj J;n_a l_a j_a^{w-1}\alpha_a'' J_a'' n_a' l_a' j_a' J_a' k'l'j'J)$$
$$=2\sqrt{w}\sum_{J_1,\alpha_1}(j_a^{w-1}\alpha_1^{w-1}\alpha_1 J_1\,|\,\}j_a^{w}\alpha_a J_a)\sum_{\lambda=0}^{\infty}D^{\lambda}(n_a l_a kl,n_a' l_a' k'l')$$
$$\times\langle j_a^{w-1}\alpha_1 J_1 j_a J_a jJM\,|\,\underline{C}^{\lambda}(w)\cdot\underline{C}^{\lambda}(w+1)\,|\,j_a^{w-1}\alpha_a'' J_a'' j_a' J_a' j'JM\rangle\ , \quad (32)$$

where D^{λ} is given by Eq. (14). Now using standard formulas as given in Ref. 10 or the Appendixes of Refs. 11 and 12, one has

$$\langle j_a^{w-1}\alpha_1 J_1 j_a J_a jJM\,|\,\underline{C}^{\lambda}(w)\cdot\underline{C}^{\lambda}(w+1)\,|\,j_a^{w-1}\alpha_a'' J_a'' j_a' J_a' j'JM\rangle$$
$$=(-1)^{J+j+J_a'}\begin{Bmatrix} J_a & \lambda & J_a' \\ j' & J & j \end{Bmatrix}\langle j_a^{w-1}\alpha_1 J_1 j_a J_a||\underline{C}^{\lambda}(w)||j_a^{w-1}\alpha_a'' J_a'' j_a' J_a'\rangle\langle j||\underline{C}^{\lambda}||j'\rangle \quad (33)$$

in which

$$\langle j_a^{w-1}\alpha_1 J_1 j_a J_a||\underline{C}^{\lambda}(w)||j_a^{w-1}\alpha_a'' J_a'' j_a' J_a'\rangle=\delta_{\alpha_1\alpha_a''}\delta_{J_1 J_a''}(-1)^{J_a+J_a''+j_a'+\lambda}[(2J_a+1)(2J_a'+1)]^{1/2}\begin{Bmatrix} j_a & \lambda & j_a' \\ J_a' & J_a'' & J_a \end{Bmatrix}\langle j_a||\underline{C}^{\lambda}||j_a'\rangle\ , \quad (34)$$

and the $\langle j_1||\underline{C}^{\lambda}||j_2'\rangle$ are given by Eqs. (19), (12), and (13). Thus

$$ZR^{d}(n_a l_a j_a^{w}\alpha_a J_a klj J;n_a l_a j_a^{w-1}\alpha_a'' J_a'' n_a' l_a' j_a' J_a' k'l'j'J)$$
$$=2\sqrt{w}\,(j_a^{w-1}\alpha_a'' J_a''\,|\,\}j_a^{w}\alpha_a J_a)\sum_{\lambda=0}^{\infty}D^{\lambda}(n_a l_a kl,n_a' l_a' k'l')(-1)^{J+J_a+J_a'+j+j_a'+J_a''+\lambda}$$
$$\times[(2J_a+1)(2J_a'+1)]^{1/2}\begin{Bmatrix} J_a & \lambda & J_a' \\ j' & J & j \end{Bmatrix}\begin{Bmatrix} j_a & \lambda & j_a' \\ J_a' & J_a'' & J_a \end{Bmatrix}\langle j_a||\underline{C}^{\lambda}||j_a'\rangle\langle j||\underline{C}^{\lambda}||j'\rangle\ . \quad (35)$$

In applying Eq. (6) to obtain ZR^{e} for this situation we again let $N=w$ and choose $i=w+1$, $j=w$. Then only the term $q=w$ contributes and we get a result of the form of Eq. (32) except that E^{λ} given by Eq. (18) replaces D^{λ} and in the final state wave function it is state j_a' that is a function of particle $w+1$ and state j' that is a function of w, while in order to apply irreducible tensor techniques the electrons in the final state must be in the same order $1, 2, \ldots, w, w+1$ that they are in the initial state. Thus we must recouple in order that we have both the same coupling scheme and the same order for the electrons in initial and final states. This is accomplished by using the standard recoupling formula[10–12]

$$|j_a^{w-1}\alpha_a'' J_a'' j_a' J_a' j'JM\rangle=\sum_{J_2}(-1)^{j'+j_a'+J_a'+J_2}[(2J_2+1)(2J_a'+1)]^{1/2}\begin{Bmatrix} J_a'' & j' & J_2 \\ J & j_a' & J_a' \end{Bmatrix}|j_a^{w-1}\alpha_a'' J_a'' j' J_2 j_a' JM\rangle\ . \quad (36)$$

Then proceeding in an exactly analogous way as in obtaining Eq. (35) we obtain

$$ZR^{e}(n_a l_a j_a^{w}\alpha_a J_a klj J;n_a l_a j_a^{w-1}\alpha_a'' J_a'' n_a' l_a' j_a' J_a' k'l'j'J)$$
$$=2\sqrt{w}\,(j_a^{w-1}\alpha_a'' J_a''\,|\,\}j_a^{w}\alpha_a J_a)\sum_{\lambda=0}^{\infty}E^{\lambda}(n_a l_a kl;n_a' l_a' k'l')$$
$$\times\sum_{J_2}(-1)^{J_a''+2J_2+J_a'+2j'+j+j_a'+J+J_a+\lambda}(2J_2+1)[(2J_a+1)(2J_a'+1)]^{1/2}$$
$$\times\begin{Bmatrix} J_a'' & j' & J_2 \\ J & j_a' & J_a' \end{Bmatrix}\begin{Bmatrix} J_a & \lambda & J_2 \\ j_a' & J & j \end{Bmatrix}\begin{Bmatrix} j_a & \lambda & j' \\ J_2 & J_a'' & J_a \end{Bmatrix}\langle j_a||\underline{C}^{\lambda}||j'\rangle\langle j||\underline{C}^{\lambda}||j_a'\rangle\ . \quad (37)$$

The summation over J_2 can be performed and the product of three 6-j symbols expressed as a 9-j symbol by slightly rearranging them and using the formula[11]

$$\sum_{J_2}(-1)^{2J_2}(2J_2+1)\begin{Bmatrix} J_a'' & j_a & J_a' \\ J & j' & J_2 \end{Bmatrix}\begin{Bmatrix} J_a & j & J \\ j_a' & J_2 & \lambda \end{Bmatrix}\begin{Bmatrix} j_a & \lambda & j' \\ J_2 & J_a'' & J_a \end{Bmatrix}=\begin{Bmatrix} J_a'' & J_a & j_a \\ j_a' & j & \lambda \\ J_a' & J & j' \end{Bmatrix}\ . \quad (38)$$

Now we apply this to Eq. (37) and then substitute that as well as Eq. (35) for ZR^d into Eqs. (4) and (3). Then we sum over J_a' since, as noted in Sec. I, one is generally not interested in results for specific final total angular momentum of the target ion in the case of excitation to a very highly excited level. In evaluating the contribution proportional to $D^\lambda D^{\lambda'}$ that arises in squaring the reactance matrix elements we first perform the summation over J and then the summations over λ' and J_a' using the standard relations[11]

$$\sum_J (2J+1) \begin{Bmatrix} J_a & \lambda & J_a' \\ j' & J & j \end{Bmatrix} \begin{Bmatrix} J_a & \lambda' & J_a' \\ j' & J & j \end{Bmatrix} = \frac{\delta_{\lambda\lambda'}}{2\lambda+1} \tag{39}$$

and

$$\sum_{J_a'} (2J_a'+1) \begin{Bmatrix} j_a & \lambda & j_a' \\ J_a' & J_a'' & J_a \end{Bmatrix}^2 = \frac{1}{2j_a+1} \; . \tag{40}$$

In evaluating the part proportional to $E^\lambda E^{\lambda'}$ we use the orthogonality relation for 9-j symbols

$$\sum_{J,J_a'} (2J_a'+1)(2J+1) \begin{Bmatrix} J_a'' & J_a & j_a \\ j_a' & j & \lambda \\ J_a' & J & j' \end{Bmatrix} \begin{Bmatrix} J_a'' & J_a & j_a \\ j_a' & j & \lambda' \\ J_a' & J & j' \end{Bmatrix} = \frac{\delta_{\lambda\lambda'}}{(2\lambda+1)(2j_a+1)} \; , \tag{41}$$

while in evaluating the terms proportional to $D^\lambda E^{\lambda'}$ we rearrange the first 6-j in Eq. (35) and the 9-j in Eq. (38) and then use the relation[11]

$$\sum_J (2J+1) \begin{Bmatrix} J_a & j & J \\ j' & J_a' & \lambda \end{Bmatrix} \begin{Bmatrix} j_a & J_a'' & J_a \\ \lambda' & j_a' & j \\ j' & J_a' & J \end{Bmatrix} = (-1)^{2\lambda} \begin{Bmatrix} j_a & \lambda' & j' \\ j & \lambda & j_a' \end{Bmatrix} \begin{Bmatrix} J_a'' & j_a' & J_a' \\ \lambda & J_a & j_a \end{Bmatrix} , \tag{42}$$

where the phase factor can be ignored because λ is an integer. With slight rearrangement the second of these 6-j symbols is seen to be the same as the second 6-j in Eq. (35). Thus, we can again perform the summation over J_a' using Eq. (40) in evaluating these terms. It should be mentioned that in performing the summations leading to Eqs. (39)–(42) we could ignore the phase factors because it is quite easily seen that after use of Eq. (38) the phase factors in Eqs. (35) and (37) differ only by $2j'$ and are both integers. Thus collecting results we have

$$\begin{aligned} &\sum_{J_a'} Z^2 \Omega(n_a l_a j_a^w \alpha_a J_a\text{-}n_a l_a j_a^{w-1} \alpha_a'' J_a'' n_a' l_a' j_a' J_a') \\ &= \frac{8(2J_a+1)}{(2j_a+1)} w[(j_a^{w-1}\alpha_a'' J_a'' \,|\, \} j_a^w \alpha_a J_a)]^2 \\ &\quad \times \sum_{\substack{l,l',\\ j,j'}} \Bigg\{ \sum_{\lambda=0}^{\infty} \frac{1}{2\lambda+1} [D^\lambda(n_a l_a k l; n_a' l_a' k' l') \langle j_a || \underline{C}^\lambda || j_a' \rangle \langle j || \underline{C}^\lambda || j' \rangle]^2 \\ &\qquad - 2 \sum_{\lambda=0}^{\infty} \sum_{\lambda'=0}^{\infty} (-1)^{2j'+\lambda+\lambda'} D^\lambda(n_a l_a k l; n_a' l_a' k' l') E^{\lambda'}(n_a l_a k l; n_a' l_a' k' l') \begin{Bmatrix} j_a & \lambda' & j' \\ j & \lambda & j_a' \end{Bmatrix} \\ &\qquad \times \langle j_a || \underline{C}^\lambda || j_a' \rangle \langle j || \underline{C}^\lambda || j' \rangle \langle j_a || \underline{C}^{\lambda'} || j' \rangle \langle j || \underline{C}^{\lambda'} || j_a' \rangle \\ &\qquad + \sum_{\lambda=0} \frac{1}{2\lambda+1} [E^\lambda(n_a l_a k l; n_a' l_a' k' l') \langle j_a || C^\lambda || j' \rangle \langle j || C^\lambda || j_a' \rangle]^2 \Bigg\} \; . \end{aligned} \tag{43}$$

Comparing this with Eq. (23) we see that after slight rearrangement of the 6-j in Eq. (43), the parts being summed over l, l', j, and j' are of exactly the same form. However, the D^λ and E^λ actually differ from those pertaining to hydrogenic ions due to the screening of the nuclear charge by the inactive electrons. As in the case of Eq. (25), we take this into account approximately by dividing by a Z_{eff}^2 in obtaining Ω. Then substituting this into Eq. (2) with $g_i = 2J_a+1$ one sees that

$$\sum_{J_a'} Q(n_a l_a j_a^w \alpha_a J_a\text{-}n_a l_a j_a^{w-1} \alpha_a'' J_a'' n_a' l_a' j_a' J_a') = w[(j_a^{w-1} \alpha_a'' J_a'' \,|\, \} j_a^w \alpha_a J_a)]^2 \frac{1}{Z_{\text{eff}}^2} [Z^2 Q_{\text{H}}(n_a l_a j_a\text{-}n_a' l_a' j_a')] \; . \tag{44}$$

Of course, if one is not interested in the particular value for j_a' and sums over it, Eq. (24) applies so that $Z^2Q_{\mathrm{H}}(n_al_a\text{-}n_a'l_a')$ should be used for the Z^2Q_{H} in Eq. (44). Similarly, since ionization is like excitation summed over J_a', j_a', and l_a' plus a range of n_a' values, the same form given by Eq. (44) applies for ionization with Z^2Q_{H} for ionization used on the right-hand side. One sees that the branching ratio factor is simply the Cfp squared in these cases. In fact, Eq. (25) can be regarded as a special case of Eq. (44) in which both the Cfp and w are unity. Other cases where the Cfp is unity and hence the results reduce to the form of Eq. (1) are when $w=2$ and when w is the value required to fill the subshell. If one were not interested in the particular final state of the core and hence summed over α_a'' and J_a'' one sees from Eq. (29) that Eq. (1) would always result.

B. *LS* coupling results

We now consider the situation in which *LS* coupling rather than *jj* coupling is used for the target ion. In this case, where the spins of all bound electrons are coupled together to form total spin S_a, the l_a's are coupled together to form total orbital angular momentum L_a and then S_a and L_a are coupled to form J_a, the equation replacing Eq. (28) for the initial state with w equivalent electrons is

$$\begin{aligned}
\Psi(n_al_a^w\alpha_aS_aL_aJ_aM_a\,|\,x_1x_2\cdots x_w)
&= \sum_{S_1,L_1,\alpha_1}(l_a^{w-1}\alpha_1S_1L_1\,|\,\}l_a^w\alpha_aS_aL_a)\sum_{M_{Sa},M_{La}}C(S_aL_aM_{Sa}M_{La};J_aM_a)\\
&\qquad\times\sum_{\substack{M_{S1},m_{sa},\\ M_{L1},m_{la}}}C(S_1\tfrac{1}{2}M_{S1}m_{sa};S_aM_{Sa})C(L_1l_aM_{L1}m_{la};L_aM_{La})\\
&\qquad\times\Psi(n_al_a^{w-1}\alpha_1S_1L_1M_{S1}M_{L1}\,|\,x_1x_2\cdots x_{w-1})u_{n_al_am_{la}m_{sa}}(x_w)\\
&\equiv\sum_{S_1,L_1,\alpha_1}(l_a^{w-1}\alpha_1S_1L_1\,|\,\}l_a^w\alpha_aS_aL_a)\,|\,n_al_a^{w-1}\alpha_1S_1L_1n_al_a\alpha_aS_aL_aJ_aM_a\rangle\;. \qquad (45)
\end{aligned}$$

Again as in Eq. (28) the electrons are in the definite increasing order 1, 2, 3, . . . , w, but the function is nevertheless antisymmetrical due to the properties of the Cfp and the Clebsch-Gordan coefficients. The function $u_{n_al_am_{la}m_{sa}}(x)$ in Eq. (45) is given by Eq. (8) with the Clebsch-Gordan coefficient and the summation over m_{sa} and m_{la} omitted. For the final state for excitation to a very highly excited level we will want to couple the spin and orbital angular momentum for this excited orbital to form j_a', that is we use $u_{n_a'l_a'j_a'm_a'}$ in place of $u_{n_a'l_a'm_{la}'m_{sa}'}$. Thus, the final target ion wave function is

$$\begin{aligned}
\Psi(n_al_a^{w-1}\alpha_a''S_a''L_a''J_a''n_a'l_a'j_a'J_aM_a\,|\,x_1x_2\cdots x_w)
&=\sum_{M_a'',m_a'}C(J_a''j_a'M_a''m_a';J_a'M_a')\sum_{M_{Sa}'',M_{La}''}C(S_a''L_a''M_{Sa}''M_{La}'';J_a''M_a'')\\
&\qquad\times\frac{1}{\sqrt{w}}\sum_{p=1}^{w}(-1)^{w-p}\Psi(n_al_a^{w-1}\alpha_a''S_a''L_a''M_{Sa}''M_{La}''\,|\,x_1x_2\cdots x_{p-1},x_{p+1}\cdots x_w)\\
&\qquad\times u_{n_a'l_a'j_a'm_a'}(x_p)\;, \qquad (46)
\end{aligned}$$

where, as in the analogous Eq. (30), the $w-1$ equivalent electrons are in the definite increasing order $1,2,\ldots,p-1,p+1,\ldots,w$. However, the coupling in Eq. (46) is different than in Eq. (45) so that to use the techniques of irreducible tensors we must transform Eq. (45) so that it is coupled in the same manner as Eq. (46). Thus, using the standard recoupling formula[11]

$$\begin{aligned}
|\,n_al_a^{w-1}\alpha_1S_1L_1n_al_aS_aL_aJ_aM_a\rangle &= \sum_{J_1,j_a}[(2S_a+1)(2L_a+1)(2J_1+1)(2j_a+1)]^{1/2}\begin{Bmatrix} S_1 & L_1 & J_1\\ \frac{1}{2} & l_a & j_a\\ S_a & L_a & J_a\end{Bmatrix}\\
&\qquad\times|\,n_al_a^{w-1}\alpha_1S_1L_1J_1n_al_aj_aJ_aM_a\rangle \qquad (47)
\end{aligned}$$

we have

$$\begin{aligned}
\Psi(n_a l_a^w \alpha_a S_a L_a J_a M_a \,|\, x_1 x_2 \cdots x_w)
&= \sum_{S_1,L_1,\alpha_1} (l_a^{w-1}\alpha_1 S_1 L_1 \,|\,\}\, l_a^w \alpha_a S_a L_a) \\
&\quad \times \sum_{J_1,j_a} [(2S_a+1)(2L_a+1)(2J_1+1)(2j_a+1)]^{1/2} \begin{Bmatrix} S_1 & L_1 & J_1 \\ \frac{1}{2} & l_a & j_a \\ S_a & L_a & J_a \end{Bmatrix} \\
&\quad \times \sum_{M_1,m_a} C(J_1 j_a M_1 m_a; J_a M_a) \\
&\quad \times \sum_{M_{S1},M_{L1}} C(S_1 L_1 M_{S1} M_{L1}; J_1 M_1)\Psi(n_a l_a^{w-1}\alpha_1 S_1 L_1 M_{S1} M_{L1} \,|\, x_1 x_2 \cdots x_{w-1}) u_{n_a l_a j_a m_a}(x_w) ,
\end{aligned} \tag{48}$$

where the electrons remain in the definite order 1, 2, 3, . . . , w. We can then proceed as in the jj coupling case. In fact the arithmetic is essentially identical because it is only the inactive electrons that are now coupled in a different manner. Thus, the only differences are that we have the extra recoupling factor of Eq. (47), we have the additional Kronecker deltas $\delta_{S_1 S_a''}\delta_{L_1 L_a''}$ in the analog of Eq. (34) and we have the additional summations over S_1, L_1 and over j_a. When we square the matrix elements, the latter results in Eq. (40) being replaced with

$$\sum_{J_a'} (2J_a'+1) \begin{Bmatrix} j_a & \lambda & j_a' \\ J_a' & J_a'' & J_a \end{Bmatrix} \begin{Bmatrix} j_{a1} & \lambda & j_a' \\ J_a' & J_a'' & J_a \end{Bmatrix} = \frac{\delta_{j_a j_{a1}}}{(2j_a+1)} . \tag{49}$$

Also in one of the 9-j symbols of Eq. (41) the j_a should be replaced with j_{a1}, which leads to a factor $\delta_{j_a j_{a1}}$ on the right-hand side. This and the similar factor in Eq. (49) are then removed by the summation over j_{a1}. Thus the result obtained in place of Eq. (44) is

$$\begin{aligned}
&\sum_{J_a'} Q(n_a l_a^w \alpha_a S_a L_a J_a\text{-}n_a l_a^{w-1}\alpha_a'' S_a'' L_a'' J_a'' n_a' l_a' j_a' J_a') \\
&\quad = w[(l_a^{w-1}\alpha_a'' S_a'' L_a'' \,|\,\}\, l_a^w \alpha_a S_a L_a)]^2 \\
&\quad\quad \times \sum_{j_a} (2S_a+1)(2L_a+1)(2J_a''+1)(2j_a+1) \begin{Bmatrix} S_a'' & L_a'' & J_a'' \\ \frac{1}{2} & l_a & j_a \\ S_a & L_a & J_a \end{Bmatrix}^2 \frac{1}{Z_{\text{eff}}^2} [Z^2 Q_{\text{H}}(n_a l_a j_a\text{-}n_a' l_a' j_a')] .
\end{aligned} \tag{50}$$

If we are not interested in the value for j_a', as would probably usually be the case, we sum over j_a'. Then, as in Eq. (44), $Z^2 Q_{\text{H}}(n_a l_a\text{-}n_a' l_a')$ replaces $Z^2 Q_{\text{H}}(n_a l_a j_a\text{-}n_a' l_a' j_a')$. Also for the case of LS coupling one might not be interested in the value for J_a'', the total angular momentum of the remaining core. Thus, if one sums over J_a'' after summing over j_a', one sees from the analog of Eq. (41) that the summation over J_a'' and j_a remove the 9-j factor in Eq. (50) so the result reduces to a form similar to Eq. (44),

$$\begin{aligned}
\sum_{J_a', j_a', J_a''} Q(n_a l_a^w \alpha_a S_a L_a J_a\text{-}n_a l_a^{w-1}\alpha_a'' S_a'' L_a'' J_a'' n_a' l_a' j_a' J_a') &= Q(n_a l_a^w \alpha_a S_a L_a\text{-}n_a l_a^{w-1}\alpha_a'' S_a'' L_a'' n_a' l_a') \\
&= w[(l_a^{w-1}\alpha_a'' S_a'' L_a'' \,|\,\}\, l_a^w \alpha_a S_a L_a)]^2 \frac{1}{Z_{\text{eff}}^2} [Z^2 Q_{\text{H}}(n_a l_a\text{-}n_a' l_a')].
\end{aligned} \tag{51}$$

Of course, as in the case of Eq. (44), the results given by Eqs. (50) and (51) also apply for ionization when the $Z^2 Q_{\text{H}}$ for ionization is used on the right-hand sides. It is interesting to note that the results for ionization agree with the corresponding formulas of Bely and Schwartz,[5] their Eqs. (16) and (15), except that they do not explicitly utilize a Z_{eff}, as we do.

V. EFFECTS OF A PARTIALLY FILLED INACTIVE SUBSHELL

We next consider the case that an additional partially filled subshell of inactive or spectator electrons is present. We call this subshell b and assume it contains m electrons with a total angular momentum J_b. The initial total angular momentum J_a of the active subshell a containing w electrons is coupled to J_b to form initial total angular momentum J_{ba} for the target ion. In the final state of the target ion the highly excited electron in state $n_a'l_a'j_a'$ has its angular momentum j_a' coupled last so we couple J_a'', the total angular momentum of the remaining w-1 electrons in subshell a, to J_b to form J_{ba}'' and then couple j_a' to this to form a total angular momentum J_a' for the final state of the target ion. Perhaps this could more appropriately be called J_{ba}', but we will continue to use J_a' to indicate the total angular momentum of the target ion in the final state in all cases. In order to use irreducible tensor techniques the coupling must be of the same type for initial and final states so we transform the coupling of the initial state using the standard recoupling formula[11]

$$| J_b(J_1 j_a J_a)J_{ba}M_{ba}\rangle=\sum_{J_{b1}}(-1)^{J_b+J_1+j_a+J_{ba}}[(2J_{b1}+1)(2J_a+1)]^{1/2}\begin{Bmatrix} j_a & J_1 & J_a \\ J_b & J_{ba} & J_{b1}\end{Bmatrix}| J_b J_1 J_{b1} j_a J_{ba} M_{ba}\rangle\ , \tag{52}$$

where J_{b1} is formed by coupling J_1 to J_b and J_1 has the same meaning as in Eq. (28). Then the arithmetic proceeds as before in obtaining Eqs. (43) and (44) except for the presence of the extra recoupling term in Eq. (52) and the fact that in the analogs of Eqs. (32), (33), and (34) the inactive parts $j_a^{w-1}\alpha_1 J_1$ and $j_a^{w-1}\alpha_a''J_a''$ of the initial and final wave functions are replaced with $(j_b^m\alpha_b J_b)(j_a^{w-1}\alpha_1 J_1)J_{b1}$ and $(j_b^m\alpha_b J_b)(j_a^{w-1}\alpha_a''J_a'')J_{ba}''$, respectively. This leads to the extra Kronecker delta $\delta_{J_{b1}J_{ba}''}$ in the analog of Eq. (34). In addition, J_{ba} and J_{ba}'' play the roles of J_a and J_a'' in the Racah algebra that leads to the analog of Eq. (44). We should also mention that if we had not assumed the same $\alpha_b J_b$ for the inactive subshell b in the initial and final states, this would have been insured in the analog of Eq. (34) by an extra factor $\delta_{\alpha_b\alpha_b'}, \delta_{J_bJ_b'}$. Thus, carrying out the Racah algebra, which is the same as previously, one obtains in place of Eq. (44)

$$\sum_{J_a'}Q((n_bl_bj_b^m\alpha_bJ_b)(n_al_aj_a^w\alpha_aJ_a)J_{ba}\text{-}(n_bl_bj_b^m\alpha_bJ_b)(n_al_aj_a^{w-1}\alpha_a''J_a'')J_{ba}''n_a'l_a'j_a'J_a')$$
$$=w[(j_a^{w-1}\alpha_a''J_a''\,|\,\}j_a^w\alpha_aJ_a)]^2(2J_{ba}''+1)(2J_a+1)\begin{Bmatrix} j_a & J_a'' & J_a \\ J_b & J_{ba} & J_{ba}''\end{Bmatrix}^2\frac{1}{Z_{\text{eff}}^2}[Z^2Q_{\text{H}}(n_al_aj_a\text{-}n_a'l_a'j_a')]\ . \tag{53}$$

As usual, if we sum over j_a', then $Z^2Q_{\text{H}}(n_al_a\text{-}n_a'l_a')$ replaces $Z^2Q_{\text{H}}(n_al_aj_a\text{-}n_a'l_a'j_a')$. Also, if this is replaced by Z^2Q_H for ionization the result applies for the ionization cross section for the case that the remaining next higher stage of ionization is in the same state as the core in Eq. (53). If one sums over the total angular momentum J_{ba}'' of the core, the extra recoupling factor in Eq. (53) as compared with Eq. (44) is seen to be removed by using an equation analogous to Eq. (40).

Now we consider this situation when LS coupling is used for the target ion. In the final state the spins of the $w-1$ remaining electrons in subshell a are coupled together to form total spin for the subshell S_a''. Those of the m electrons in an inactive subshell b are coupled to form total spin S_b for that subshell. Then S_b and S_a'' are coupled to form S_{ba}''. Similarly, the orbital angular momenta are coupled to form total orbital angular momenta L_a'' and L_b for subshells a and b, which are then coupled to form L_{ba}''. Then S_{ba}'' and L_{ba}'' are coupled to form total angular momentum J_{ba}'' for the core. Finally this is coupled to j_a' to form the final total angular momentum J_a' for the target ion. For the initial state the coupling is similar except that subshell a has w electrons with total spin S_a and orbital angular momentum L_a, which are coupled to S_b and L_b of subshell b to form S_{ba} and L_{ba}. Finally these are coupled together to form initial total angular momentum J_{ba} for the target ion. In order that the coupling be of the same type for the initial state as the final state it is necessary to use the analog of the recoupling formula used in Eq. (52) for both spins and orbital angular momenta. Specifically,

$$| S_b(S_1\tfrac{1}{2}S_a)S_{ba},L_b(L_1l_aL_a)L_{ba}J_{ba}M_{ba}\rangle$$
$$=\sum_{S_{b1},L_{b1}}(-1)^{S_b+S_1+1/2+S_{ba}+L_b+L_1+l_a+L_{ba}}$$
$$\times[(2S_{b1}+1)(2S_a+1)(2L_{b1}+1)(2L_a+1)]^{1/2}\begin{Bmatrix} \tfrac{1}{2} & S_1 & S_a \\ S_b & S_{ba} & S_{b1}\end{Bmatrix}\begin{Bmatrix} l_a & L_1 & L_a \\ L_b & L_{ba} & L_{b1}\end{Bmatrix}$$
$$\times| S_bS_1S_{b1}\tfrac{1}{2}S_{ba},L_bL_1L_{b1}l_aL_{ba}J_{ba}M_{ba}\rangle\ , \tag{54}$$

where S_{b1} and L_{b1} are formed by coupling S_1 to S_b and I_1 to L_b, respectively, and S_1 and L_1 have the same meaning as in Eq. (45). In addition, we must still use the analog of the recoupling in Eq. (47) so that the spin $\frac{1}{2}$ and l_a are coupled to form j_a, while S_{b1} and L_{b1} are coupled to form J_{b1}, which is then coupled to j_a to form J_{ba}. That is we must use

$$\begin{aligned} | S_b S_1 S_{b1} \tfrac{1}{2} S_{ba}, L_b L_1 L_{b1} l_a L_{ba} J_{ba} M_{ba} \rangle = \sum_{J_{b1}, j_a} & [(2S_{ba}+1)(2L_{ba}+1)(2J_{b1}+1)(2j_a+1)]^{1/2} \\ & \times \begin{Bmatrix} S_{b1} & L_{b1} & J_{b1} \\ \frac{1}{2} & l_a & j_a \\ S_{ba} & L_{ba} & J_{ba} \end{Bmatrix} | S_b S_1 S_{b1} L_b L_1 L_{b1} J_{b1} \tfrac{1}{2} l_a j_a J_{ba} M_{ba} \rangle \; . \end{aligned} \tag{55}$$

Then proceeding as previously, except that in analogy to the discussion leading to Eq. (53) we have a larger inactive part which leads to additional factors $\delta_{S_{b1}S''_{ba}}$, $\delta_{L_{b1}L''_{ba}}$ and $\delta_{J_{b1}J''_{ba}}$, we obtain in place of Eq. (50):

$$\begin{aligned} \sum_{J'_a} Q((n_b l_b^m \alpha_b S_b L_b)(n_a l_a^w \alpha_a S_a L_a) S_{ba} L_{ba} J_{ba} \text{-} (n_b l_b^m \alpha_b S_b L_b)(n_a l_a^{w-1} \alpha''_a S''_a L''_a) S''_{ba} L''_{ba} J''_{ba} n'_a l'_a j'_a J'_a) \\ = w[(l_a^{w-1} \alpha''_a S''_a L''_a \,|\, \} l_a^w \alpha_a S_a L_a)]^2 \\ \times \sum_{j_a} (2S''_{ba}+1)(2S_a+1)(2L''_{ba}+1)(2L_a+1)(2S_{ba}+1)(2L_{ba}+1)(2J''_{ba}+1)(2j_a+1) \\ \times \begin{Bmatrix} \frac{1}{2} & S''_a & S_a \\ S_b & S_{ba} & S''_{ba} \end{Bmatrix}^2 \begin{Bmatrix} l_a & L''_a & L_a \\ L_b & L_{ba} & L''_{ba} \end{Bmatrix}^2 \begin{Bmatrix} S''_{ba} & L''_{ba} & J''_{ba} \\ \frac{1}{2} & l_a & j_a \\ S_{ba} & L_{ba} & J_{ba} \end{Bmatrix}^2 \frac{1}{Z_{\text{eff}}^2} [Z^2 Q_{\text{H}}(n_a l_a j_a \text{-} n'_a l'_a j'_a)] \; . \end{aligned} \tag{56}$$

Of course, if we sum over j'_a, as will usually be desired, $Z^2 Q_{\text{H}}(n_a l_a \text{-} n'_a l'_a)$ will replace $Z^2 Q_{\text{H}}(n_a l_a j_a \text{-} n'_a l'_a j'_a)$. Also if we do not care about the value for the final total angular momentum of the core J''_{ba}, as will often be the case when LS coupling is used, then the summations over j_a and J''_{ba} remove the 9-j symbol and give

$$\begin{aligned} Q((n_b l_b^m \alpha_b S_b L_b)(n_a l_a^w \alpha_a S_a L_a) S_{ba} L_{ba} \text{-} (n_b l_b^m \alpha_b S_b L_b)(n_a l_a^{w-1} S''_a L''_a) S''_{ba} L''_{ba} n'_a l'_a) \\ = w[(l_a^{w-1} \alpha''_a S''_a L''_a \,|\, \} l_a^w \alpha_a S_a L_a)]^2 (2S''_{ba}+1)(2S_a+1)(2L''_{ba}+1)(2L_a+1) \\ \times \begin{Bmatrix} \frac{1}{2} & S''_a & S_a \\ S_b & S_{ba} & S''_{ba} \end{Bmatrix}^2 \begin{Bmatrix} l_a & L''_a & L_a \\ L_b & L_{ba} & L''_{ba} \end{Bmatrix}^2 \frac{1}{Z_{\text{eff}}^2} [Z^2 Q_{\text{H}}(n_a l_a \text{-} n'_a l'_a)] \; . \end{aligned} \tag{57}$$

If we also summed over S''_{ba} and L''_{ba} the result would reduce to that given by Eq. (51). Also the results given by Eqs. (56) and (57) apply for ionization if $Z^2 Q_{\text{H}}$ for ionization is used on the right-hand side. In this case the results agree with the results given by Eqs. (18) and (17) of Bely and Schwartz for the corresponding transitions.

It should be noted that the results given by Eqs. (53), (56), and (57) apply whether subshell b is a lower subshell than a so its angular momenta are coupled first to form S_{ba}, L_{ba}, J_{ba}, etc., as we have assumed, or subshell b is a higher subshell so that according to standard practice its angular momenta are coupled second. The only effect is a phase factor that vanishes after squaring the matrix elements. However, in the latter case one would probably write J_{ab} instead of J_{ba}, etc.

VI. EFFECTS OF SEVERAL PARTIALLY FILLED INACTIVE SUBSHELLS

It is easily seen that the results of the previous section, i.e., Eqs. (53), (56), and (57) are still applicable for any number of partially filled subshells in addition to the active subshell a, if these are all lower subshells than subshell a so their angular momenta are coupled together first. The only difference is that then J_b, S_b, and L_b must represent the total angular momentum, the total spin angular momentum, and the total orbital angular momentum, respectively, of all of the electrons in these lower partially filled subshells, not just those in subshell b. However, Eqs. (53), (56), and (57) are not general enough to apply when when there are partially filled inactive subshells that are both higher and lower than subshell a, or if there are not lower ones, but two or more higher ones. Thus we now consider these cases and as usual we first treat the problem assuming jj coupling.

Specifically we assume that in addition to a lower partially filled subshell b with m electrons, there are two partially filled subshells c and d with r and p electrons, respectively, that are higher than the active subshell. That is, they have higher values of nl or j. The total angular momenta of subshells b, c, and d are J_b, J_c, and J_d. We assume that the initial total angular momentum J_a of the active subshell a containing w electrons is first coupled to J_b to form J_{ba}. Then J_c is coupled to this to form J_{bac} and finally J_d is coupled to this to form initial total angular momentum J_{bacd} for the ion. In the final state the total angular momentum J_a'' of the remaining $w-1$ electrons in subshell a is coupled to J_b to form J_{ba}''. Then J_c is coupled to this to form J_{bac}''. Then J_d is coupled to this to form total final angular momentum J_{bacd}'' for the core. Finally j_a', the final angular momentum of the active electron, is coupled to this to form total final angular momentum J_a' for the ion. As usual, in order to use irreducible tensor techniques we must recouple the initial state so it is coupled in the same manner as the final state. That is, one of the electrons in subshell a must be coupled last of all. This requires an initial recoupling as in Eq. (52) followed by two additional recouplings to push j_a beyond both J_c and J_d so it is coupled last. The result is

$$
\begin{aligned}
&|\,J_b(J_1 j_a J_a)J_{ba}J_cJ_{bac}J_dJ_{bacd}M_{bacd}\rangle \\
&\quad=\sum_{J_{b1},J_{b1c},J_{b1cd}} (-1)^{J_b+J_c+J_d+3j_a+2J_{ba}+J_{bac}+J_1+J_{b1c}+J_{b1cd}} \\
&\qquad\times[(2J_{b1}+1)(2J_a+1)(2J_{b1c}+1)(2J_{ba}+1)(2J_{b1cd}+1)(2J_{bac}+1)]^{1/2} \\
&\qquad\times\begin{Bmatrix} j_a & J_1 & J_a \\ J_b & J_{ba} & J_{b1}\end{Bmatrix}\begin{Bmatrix} j_a & J_{b1} & J_{ba} \\ J_c & J_{bac} & J_{b1c}\end{Bmatrix}\begin{Bmatrix} j_a & J_{b1c} & J_{bac} \\ J_d & J_{bacd} & J_{b1cd}\end{Bmatrix}|\,J_bJ_1J_{b1}J_cJ_{b1c}J_dJ_{b1cd}j_aJ_{bacd}M_{bacd}\rangle\ . \qquad (58)
\end{aligned}
$$

Here J_1 has the same meaning as in Eq. (28) and J_{b1} is formed by coupling J_1 to J_b. Then J_{b1c} is formed by coupling J_c to J_{b1}, while J_{b1cd} is formed by coupling J_d to J_{b1c}. Finally J_{bacd} is formed by coupling j_a to J_{b1cd}. Thus, the coupling is in the same manner as for the final state so that irreducible tensor techniques can be used. One might be concerned that a great many terms should arise in taking the matrix elements leading to the cross section due to permutations of the electrons between the partially filled subshells done in such a way that the electrons are in the same positions in the initial and final states, as required in order that the matrix elements not vanish. However, as in the case of closed subshells discussed at the beginning of Sec. IV, the effect of this is exactly canceled by the normalization factors in the target ion wave functions so it can be ignored. Then the arithmetic is the same as it was in obtaining Eqs. (43) and (44) except for the extra recoupling terms in Eq. (58) and the fact that in the analogs of Eqs. (32), (33), and (34) the inactive parts $j_a^{w-1}\alpha_1 J_1$ and $j_a^{w-1}\alpha_a''J_a''$ are replaced with the much larger inactive parts

$$(j_b^m\alpha_bJ_b)(j_a^{w-1}\alpha_1J_1)J_{b1}(j_c^r\alpha_cJ_c)J_{b1c}(j_d^p\alpha_dJ_d)J_{b1cd}$$

and

$$(j_b^m\alpha_bJ_b)(j_a^{w-1}\alpha_a''J_a'')J_{ba}''(j_c^r\alpha_aJ_c)J_{bac}''(j_d^p\alpha_dJ_d)J_{bacd}''\ ,$$

respectively. This leads to the extra Kronecker deltas $\delta_{J_{b1}J_{ba}''}\delta_{J_{b1c}J_{bac}''}\delta_{J_{b1cd}J_{bacd}''}$ in the analog of Eq. (34). Also, J_{bacd} and J_{bacd}'' play the roles of J_a and J_a'' in the Racah algebra that leads to the analog of Eq. (44). We note that if the states of the inactive subshells had not been assumed to be the same in the initial and final target ion functions this would have been insured by additional Kronecker deltas in the analog of Eq. (34). The extra phase factors from Eq. (58) drop out in squaring the matrix elements to obtain the cross section and the result one obtains in place of Eq. (44) is

$$
\begin{aligned}
&\sum_{J_a'}Q((n_bl_bj_b^m\alpha_bJ_b)(n_al_aj_a^w\alpha_aJ_a)J_{ba}(n_cl_cj_c^r\alpha_cJ_c)J_{bac}(n_dl_dj_d^p\alpha_dJ_d)J_{bacd}\text{-}(n_bl_bj_b^m\alpha_bJ_b)(n_al_aj_a^{w-1}\alpha_a''J_a'')J_{ba}''(n_cl_cj_c^r\alpha_cJ_c) \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\times J_{bac}''(n_dl_dj_d^p\alpha_dJ_d)J_{bacd}''n_a'l_a'j_a'J_a') \\
&\quad=w[(j_a^{w-1}\alpha_a''J_a''\,|\,\}j_a^w\alpha_aJ_a)]^2(2J_{ba}''+1)(2J_a+1)(2J_{bac}''+1)(2J_{ba}+1)(2J_{bacd}''+1)(2J_{bac}+1) \\
&\quad\times\begin{Bmatrix} j_a & J_a'' & J_a \\ J_b & J_{ba} & J_{ba}''\end{Bmatrix}^2\begin{Bmatrix} j_a & J_{ba}'' & J_{ba} \\ J_c & J_{bac} & J_{bac}''\end{Bmatrix}^2\begin{Bmatrix} j_a & J_{bac}'' & J_{bac} \\ J_d & J_{bacd} & J_{bacd}''\end{Bmatrix}^2\frac{1}{Z_{\text{eff}}^2}[Z^2Q_{\text{H}}(n_al_aj_a\text{-}n_a'l_a'j_a')]\ . \qquad (59)
\end{aligned}
$$

Comparing this with results for the analogous simpler cases given by Eqs. (44) and (53) one sees readily how to generalize to any number of additional partially filled subshells. As noted previously, additional lower partially filled subshells have no effect if J_b represents the total angular momentum of all of them. For each higher partially filled subshell an extra recoupling factor enters. For example if a still higher partially filled inactive subshell e with angular momentum J_e were present the result would be given by the right-hand side of Eq. (59) with the extra recoupling factor

$$(2J''_{bacde}+1)(2J_{bacd}+1)\begin{Bmatrix} j_a & J''_{bacd} & J_{bacd} \\ J_e & J_{bacde} & J''_{bacde} \end{Bmatrix}^2 \tag{60}$$

included. Also, if no partially filled subshells lower than the active one were present one would simply omit the first recoupling factor in Eq. (59), i.e., the one common to Eq. (53) and then drop the subscript b on the J's in the other recoupling factors, or one could omit the last recoupling factor and let b and c represent the two higher subshells.

Also from Eq. (59) and the comparison between Eqs. (53) and (56) one sees how to generalize the results for LS coupling given by Eq. (56) to the case of any number of partially filled inactive subshells being present. All that is required are two kinds of modification. One of these is that the recoupling factor involving a 9-j symbol, which comes from the necessity to recouple the initial spin and l_a value for the active electron to form j_a, must involve the angular momenta for the entire core and initial ion. For example, for the case of two additional partially filled, higher inactive subshells c and d one should make the replacement

$$(2S_{ba}+1)(2L_{ba}+1)(2J''_{ba}+1)(2j_a+1)\begin{Bmatrix} S''_{ba} & L''_{ba} & J''_{ba} \\ \frac{1}{2} & l_a & J_a \\ S_{ba} & L_{ba} & J_{ba} \end{Bmatrix}^2$$

$$\rightarrow(2S_{bacd}+1)(2L_{bacd}+1)(2J''_{bacd}+1)(2j_a+1)\begin{Bmatrix} S''_{bacd} & L''_{bacd} & J''_{bacd} \\ \frac{1}{2} & l_a & j_a \\ S_{bacd} & L_{bacd} & J_{bacd} \end{Bmatrix}^2 . \tag{61}$$

The other required modification is that for each additional higher, partially filled subshell of inactive electrons one adds two recoupling factors of exactly the same form as the corresponding one entering Eq. (59) for jj coupling except that the total angular momentum quantum numbers are replaced by corresponding spin quantum numbers in the one case and orbital angular momentum quantum numbers in the other case. Of course, for LS coupling there are generally considerably fewer subshells than for jj coupling because they are defined by only nl values instead of nlj values. Hence, it is much less likely that one will need to go beyond use of Eq. (56) than that one will need to go beyond Eq. (53) to formulas such as Eq. (59).

As in all the simpler cases considered in previous sections, Eq. (59) and the even more general formulas for jj and LS coupling just discussed apply as well when one sums over j'_a except that $Q_{\mathrm{H}}(n_a l_a\text{-}n'_a l'_a)$ then replaces $Q_{\mathrm{H}}(n_a l_a j_a\text{-}n'_a l'_a j'_a)$. Also the formulas apply for ionization if the Q_{H} for ionization is used for Q_{H} on the right-hand side. Also, as in the simpler cases, the formulas simplify if one sums over quantum numbers of the final core (next higher stage of ionization in the case of ionization). In fact, if one sums over all of them down to and including J''_a in the jj case or L''_a and S''_a in the LS case Eq. (1) results. Of course, in order that one can perform such summations, it is necessary that the hydrogenlike cross section on the right-hand side be independent of the final core state. In general, this is only approximately true. For example, both the ionization formula of Lotz[2,3] and that given in Refs. 1, 4, 6, and 7 depend on the ionization energy, which differs slightly for the different core states.

VII. NUMERICAL EXAMPLES AND FINAL COMMENTS

All of our principal results given by Eqs. (44), (50), (51), (53), (56), (57), and (59) have been expressed in the form

$$Q=w(\mathscr{R})\frac{1}{Z_{\mathrm{eff}}^2}(Z^2Q_{\mathrm{H}}) \tag{62}$$

where $\mathscr{R}$ is the branching ratio. From our recent work in Ref. 15 and in references given there, it appears to work quite well for excitation to low levels to express the cross sections or collision strengths in terms of Z scaled hydrogenic results and effective Z's when $Z/N \gtrsim 2$. For ionization[1,16] it appears that this can be done for even slightly smaller Z/N and this might also be true for excitation to very highly excited levels, which together with ionization are our concerns here. However, we should point out that all that is really required for our results for the branching ratios to be valid is that the cross section used on the right-hand side of our formulas have the form of a hydrogenic cross section. Thus, the $Z_{\mathrm{eff}}^{-2}(Z^2Q_{\mathrm{H}})$ could be replaced with a cross section Q_{H}^{ps} in which the radial matrix elements, the D^{λ} and E^{λ} given by Eqs. (14) and (18), that enter the expression for the cross section were obtained by a much more sophisticated approach such as use of the distorted-wave method for the free-particle wave functions and the Hartree-Fock method for the bound-state functions. In fact, both bound and free radial functions could also include relativistic effects. On the other hand, our formulas were derived specifically for "direct" excitation or ionization. That is, indirect processes such as inner-shell excitation followed by autoionization were not considered. These indirect processes can make very significant contributions in some cases, such as ionization of Na-, Cu-, and Zn-like ions[16–20] which contain one or two electrons outside large filled shells that can contribute to inner-shell excitation followed by autoionization. Of course, this contribution should then be included, but in these examples the final ion is in such a simple configuration that only one state is possible so the branching ratio in the sense used here is unity.

Now we apply the formulas obtained for the branching ratios ($\mathscr{R}$) to a few specific cases. In doing this we choose cases in which the 6-j symbols and 9-j symbol simplify somewhat so a computer is not required to evaluate them. First we consider the set of transitions

$$(3p^{5\,2}P)(3d^{2\,3}P)\,^2S_{1/2}\\ -(3p^{4\;2S_a''+1}L_a'')(3d^{2\,3}P)\,^{2S_{ba}''+1}L_{ba\,J_{ba}''}''\,n_a'l_a' \tag{63}$$

and give the results for each of the possibilities for the quantum numbers of the final core. Then we will see that the sum of the values for the $\mathscr{R}$ for all of these cases equals unity, as expected. In the present case involving LS coupling and two partially filled subshells Eq. (56) applies. In (63) the inactive subshell is higher than the active one; however, as noted previously, Eq. (56) applies no matter which of the subshells is the higher one. Since $L_{ba}=0$, the 9-j symbol in Eq. (56) collapses to a 6-j symbol

$$\begin{Bmatrix} S_{ba}'' & L_{ba}'' & J_{ba}'' \\ \frac{1}{2} & l_a & j_a \\ S_{ba} & 0 & J_{ba} \end{Bmatrix}^2 = \frac{\delta_{L_{ba}''l_a}\delta_{S_{ba}J_{ba}}}{(2L_{ba}''+1)(2S_{ba}+1)} \begin{Bmatrix} J_{ba}'' & S_{ba}'' & L_{ba}'' \\ \frac{1}{2} & j_a & J_{ba} \end{Bmatrix}^2 . \tag{64}$$

We have implicitly assumed that Eq. (56) has been summed over j_a' in writing Eq. (63). Hence $Q_{\rm H}(n_al_a\text{-}n_a'l_a')$ has replaced $Q_{\rm H}(n_al_aj_a\text{-}n_a'l_a'j_a')$. Thus we can perform the summation over j_a, which removes the 6-j symbol in Eq. (64) by the analog of Eq. (40). Also since $L_{ba}=0$, we have

$$\begin{Bmatrix} l_a & L_a'' & L_a \\ L_b & 0 & L_{ba}'' \end{Bmatrix}^2 = \frac{\delta_{L_{ba}''l_a}\delta_{L_aL_b}}{(2l_a+1)(2L_a+1)} . \tag{65}$$

Thus collecting results and using the fact that $l_a=L_a=1$, $S_a=S_{ba}=\frac{1}{2}$, and $S_b=1$ we obtain for the branching ratio

$$\mathscr{R}=(\mathscr{C})^2\tfrac{2}{3}(2J_{ba}''+1)\begin{Bmatrix} \frac{1}{2} & S_a'' & \frac{1}{2} \\ 1 & \frac{1}{2} & S_{ba}'' \end{Bmatrix}^2 \delta_{L_{ba}''1} , \tag{66}$$

where $\mathscr{C}$ is the coefficient of fractional parentage. It is well known that the three possible sets of values for S_a'' and L_a'' for the p^4 configuration are (1,1), (0,2), and (0,0) with corresponding $(\mathscr{C})^2$ equal to $\frac{9}{15}$, $\frac{5}{15}$, and $\frac{1}{15}$. For the latter two cases with $S_a''=0$ one sees that the 6-j symbol squared in Eq. (66) reduces to $\delta_{S_{ba}''1}/6$ by using the analog of Eq. (65). For the case that $S_a''=L_a''=1$, the 6-j symbol limits S_{ba}'' to the values 0 or 1. In the former case the 6-j squared again reduces to $\frac{1}{6}$ and in the latter case it has the value $\frac{1}{9}$. Thus applying these values to Eq. (66) we obtain for the four possible kinds of transitions

$$\begin{aligned}(3p^{5\,2}P)(3d^{2\,3}P)\,^2S_{1/2}&-(3p^{4\,3}P)(3d^{2\,3}P)\,^1P_{J_{ba}''}n_a'l_a'\\ &-(3p^{4\,3}P)(3d^{2\,3}P)\,^3P_{J_{ba}''}n_a'l_a'\\ &-(3p^{4\,1}D)(3d^{2\,3}P)\,^3P_{J_{ba}''}n_a'l_a'\\ &-(3p^{4\,1}S)(3d^{2\,3}P)\,^3P_{J_{ba}''}n_a'l_a'\end{aligned} \tag{67}$$

the values $\mathscr{R}=(2J_{ba}''+1)/15$, $2(2J_{ba}''+1)/45$, $(2J_{ba}''+1)/27$, and $(2J_{ba}''+1)/[5(27)]$, respectively. If we sum each of these over the possible J_{ba}'' values to get results corresponding to the four possible energy terms of the final core, we get $\mathscr{R}=\frac{3}{15}$, $\frac{6}{15}$, $\frac{5}{15}$, and $\frac{1}{15}$, which do add to unity, as expected. In this case the value of w in Eq. (62) is 5.

Next we consider an application of Eq. (59). In doing this we will use the notation

$$(\{[(n_bl_bj_b)^m_{J_b}(n_al_aj_a)^w_{J_a}]_{J_{ba}}(n_cl_cj_c)^r_{J_c}\}_{J_{bac}}(n_dl_dj_d)^p_{J_d})_{J_{bacd}} \tag{68}$$

for the initial state and similar notation for the final state. We consider specifically the set of transitions

$$(\{[(3p\tfrac{1}{2})_{1/2}(3p\tfrac{3}{2})^3_{3/2}]_1(3d\tfrac{3}{2})^2_2\}_2(3d\tfrac{5}{2})^2_2)_0-(\{[(3p\tfrac{1}{2})_{1/2}(3p\tfrac{3}{2})^2_{J_a''}]_{J_{ba}''}(3d\tfrac{3}{2})^2_2\}_{J_{bac}''}(3d\tfrac{5}{2})^2_2)_{J_{bacd}''}n_a'l_a'j_a' . \tag{69}$$

Due to the fact that $J_{bacd}=0$, the last 6-j symbol in Eq. (59) collapses. Thus applying the analog of Eq. (65) and inserting the given numerical values for the unprimed quantum numbers, we get for the branching ratio in this case

$$\mathscr{R}=12(2J_{ba}''+1)(2J_{bac}''+1)\begin{Bmatrix} \frac{3}{2} & J_a'' & \frac{3}{2} \\ \frac{1}{2} & 1 & J_{ba}'' \end{Bmatrix}^2 \begin{Bmatrix} \frac{3}{2} & J_{ba}'' & 1 \\ 2 & 2 & J_{bac}'' \end{Bmatrix}^2 \delta_{\frac{3}{2},J_{bacd}''}[\mathscr{C}]^2 . \tag{70}$$

Although only the value $\frac{3}{2}$ is allowed for the total angular momentum of the core in this case there are several possible values for the other core quantum numbers allowed by the 6-j symbols. For each of these possibilities the corresponding branching ratio given by Eq. (70) is quite readily obtained using the 6-j formulas for the special cases that one entry has the value 1 or $\frac{1}{2}$ and also using the tabulated values for the $\mathscr{C}$ given, for example, on pp. 520 and 540 of Ref. 11. We group the results in three categories:

(i) $J_a''=0$, $J_{ba}''=\frac{1}{2}$, $J_{bac}''=\frac{3}{2}$ and $\frac{5}{2}$ for which the corresponding branching ratios are

$$\mathscr{R}=\frac{1}{20} \text{ and } \frac{7}{60} \; ; \tag{71}$$

(ii) $J_a''=2$, $J_{ba}''=\frac{3}{2}$, $J_{bac}''=\frac{1}{2}, \frac{3}{2}, \frac{5}{2}$, and $\frac{7}{2}$ for which the corresponding branching ratios are

$$\mathscr{R}=\frac{9}{50}\,,\ \frac{8}{50}\,,\ \frac{1}{3\times 50}\,, \text{ and } \frac{16}{50} \; ; \tag{72}$$

and

(iii) $J_a''=2$, $J_{ba}''=\frac{5}{2}$, $J_{bac}''=\frac{1}{2}, \frac{3}{2}\ \frac{5}{2}$, and $\frac{7}{2}$ for which the corresponding branching ratios are

$$\mathscr{R}=\frac{1}{6\times 50}\,,\ \frac{7}{6\times 50}\,,\ \frac{3}{50}\,, \text{ and } \frac{4}{50} \; . \tag{73}$$

If one sums up all of these values for the branching ratios corresponding to all the possibilities for the final core quantum numbers, the value unity is obtained, as expected. In this case the value of w in Eq. (62) is 3.

Finally we note that two Appendixes have been included. In Appendix A it is shown that the results we have obtained apply as well if collision cross sections are replaced with corresponding radiative cross sections on both sides of the equations. In other words all our results for the branching ratios apply for radiative transitions as well as collisional transitions. In Appendix B it is shown how to apply our formulas for branching ratios when an alternative coupling scheme, such as that of Hagelstein,[21,22] is used in determining the intermediate angular momenta.

ACKNOWLEDGMENTS

This work was supported by the U.S. Department of Energy under Lawrence Livermore National Laboratory Subcontract No. 6181405 and Grant No. DE-FG02-85ER53208. The author wishes to thank Dr. Andrew Hazi for suggesting this work.

APPENDIX A

Here we demonstrate that the branching ratios obtained for collisional excitation to high levels and ionization also apply for photoexcitation to highly excited levels and photoionization.

Analogously to the case of collisional transitions we will consider specifically photoexcitation to a highly excited level, but it will be seen that the branching ratios obtained apply as well for photoionization in which the final state of the ion is the same as the final state of the core in the case of excitation.

It is well known that the photoexcitation cross section for a transition i-j is proportional to the radiative oscillator strength $f(i\text{-}j)$ and that this in turn is related to the radiative line strength $S(i\text{-}j)$ by the formula

$$f(i\text{-}j)=\frac{\Delta E}{3g_i}S(i\text{-}j)\;, \tag{A1}$$

where the transition energy ΔE is in rydbergs. In particular for the transition $\beta_t J_t$-$\beta_t' J_t'$ in an ion with N bound electrons, where β_t and J_t have the same meaning as previously in Eqs. (3)—(7), the line strength is given by

$$S(\beta_t J_t\text{-}\beta_t' J_t')=\sum_{M_t,M_t'}\left|\int dx_1\int dx_2\cdots\int dx_N\,\psi_{\beta_t J_t M_t}(x_1x_2\cdots x_N)\left[\sum_{q=1}^{N}\underline{r}_q\right]\psi_{\beta_t' J_t' M_t'}(x_1x_2\cdots x_N)\right|^2\;. \tag{A2}$$

It is convenient in evaluating this equation to express the position vector $\underline{r}_q$ for the qth electron in terms of the spherical Racah tensor of order 1

$$\underline{r}_q=r_q\underline{C}^{(1)}(q)\;. \tag{A3}$$

Then

$$S(\beta_t J_t\text{-}\beta_t' J_t')=\sum_{M_t,M_t,k}\left|\int dx_1\int dx_2\cdots\int dx_N\psi^*_{\beta_t J_t M_t}(x_1x_2\cdots x_N)\left[\sum_{q=1}^{N}r_qC_k^{(1)}(q)\right]\psi_{\beta_t' J_t' M_t'}(x_1x_2\cdots x_N)\right|^2\;. \tag{A4}$$

First we consider the hydrogenic ion case, where $N=1$ and Eq. (8) applies. Then Eq. (A4) reduces to

$$\begin{aligned} &S_{\mathrm{H}}(n_a l_a j_a\text{-}n_a' l_a' j_a')\\ &\quad=\langle n_a l_a\,|\,r\,|\,n_a' l_a'\rangle^2\\ &\qquad\times\sum_{m_a,m_a',k}|\langle\tfrac{1}{2}l_a j_a m_a\,|\,C_k^{(1)}\,|\,\tfrac{1}{2}l_a' j_a' m_a'\rangle|^2\;, \end{aligned} \tag{A5}$$

where

$$\langle n_a l_a\,|\,r\,|\,n_a' l_a'\rangle=\int_0^\infty dr\,r^3R_{n_a l_a}(r)R_{n_a' l_a'}(r)\;. \tag{A6}$$

Use of the Wigner-Eckart theorem[12] gives

$$\begin{aligned} &\langle\tfrac{1}{2}l_a j_a m_a\,|\,C_k^{(1)}\,|\,\tfrac{1}{2}l_a' j_a' m_a'\rangle\\ &\qquad=(-1)^{j_a-m_a}\begin{bmatrix} j_a & l & j_a' \\ -m_a & k & m_a' \end{bmatrix}\langle j_a||\underline{C}^{(1)}||j_a'\rangle\;, \end{aligned} \tag{A7}$$

where $\langle j_a \| C^{(1)} \| j'_a \rangle$ is given by Eq. (19) with $\lambda = 1$. After Eq. (A7) is substituted into Eq. (A5) one can factor out the 3-j and use the formula[12]

$$\sum_{m_a, m'_a, k} \begin{bmatrix} j_a & 1 & j'_a \\ -m_a & k & m'_a \end{bmatrix}^2 = 1 \,. \tag{A8}$$

Then Eq. (5) reduces to

$$S_{\mathrm{H}}(n_a l_a j_a \text{-} n'_a l'_a j'_a) = (\langle n_a l_a \,|\, r \,|\, n'_a l'_a \rangle \langle j_a \| \underline{C}^{(1)} \| j'_a \rangle)^2 \,. \tag{A9}$$

Applying this to Eq. (A1) with $g_i = 2j_a + 1$ we have

$$f_{\mathrm{H}}(n_a l_a j_a \text{-} n'_a l'_a j'_a) = \frac{\Delta E}{3(2j_a+1)} (\langle n_a l_a \,|\, r \,|\, n'_a l'_a \rangle \langle j_a \| \underline{C}^{(1)} \| j'_a \rangle)^2 \,. \tag{A10}$$

If one neglects the slight dependence of ΔE on j'_a, this equation can be summed over j'_a to obtain $f_{\mathrm{H}}(n_a l_a \text{-} n'_a l'_a)$. In doing this we use Eqs. (19) and (12) with $\lambda = 1$ and then make use of the equation[11]

$$\sum_{j_a} (2j'_a + 1) \begin{Bmatrix} l_a & 1 & l'_a \\ j'_a & \frac{1}{2} & j_a \end{Bmatrix}^2 = \frac{1}{2l_a+1} \tag{A11}$$

to obtain

$$\sum_{j'_a} f_{\mathrm{H}}(n_a l_a j_a \text{-} n'_a l'_a j'_a) = f_{\mathrm{H}}(n_a l_a \text{-} n'_a l'_a) = \frac{\Delta E}{3(2l_a+1)} (\langle n_a l_a \,|\, r \,|\, n'_a l'_a \rangle \langle l_a \| \underline{C}^{(1)} \| l'_a \rangle)^2 \,, \tag{A12}$$

where $\langle l_a \| \underline{C}^{(1)} \| l'_a \rangle$ is given by Eq. (13) with $\lambda = 1$.

Next we consider the case of photoexcitation from a subshell a containing w electrons. For the same reasons as discussed at the beginning of Sec. IV the presence of additional closed subshells has no effect on the form of the results obtained. In this case the initial and final wave functions of the ion are given by Eqs. (28) and (30) so the matrix element entering Eq. (A4) becomes

$$\begin{aligned}
&\int dx_1 \int dx_2 \cdots \int dx_N \, \psi_{\beta_t J_t M_t}(x_1 x_2 \cdots x_N) \left[\sum_{q=1}^{N} r_q C_k^{(1)}(q) \right] \psi_{\beta'_t J'_t M'_t}(x_1 x_2 \cdots x_N) \\
&\quad = \frac{1}{\sqrt{w}} \sum_{\alpha_1, J_1} (j_a^{w-1} \alpha_1 J_1 \,|\, \} j_a^w \alpha_a J_a) \\
&\qquad \times \sum_{\substack{M_1, m_a, \\ M''_a, m'_a}} C(J_1 j_a M_1 m_a ; J_a M_a) C(J''_a j'_a M''_a m'_a ; J'_a M'_a) \\
&\qquad\quad \times \int dx_1 \int dx_2 \cdots \int dx_w \, \psi^*(n_a l_a j_a^{w-1} \alpha_1 J_1 M_1 \,|\, x_1 x_2 \cdots x_{w-1}) u_{n_a l_a j_a m_a}(x_w) \left[\sum_{q=1}^{w} r_q C_k^{(1)}(q) \right] \\
&\qquad\qquad \times \sum_{p=1}^{w} (-1)^{w-p} \psi(n_a l_a j_a^{w-1} \alpha''_a J''_a M''_a \,|\, x_1 x_2 \cdots x_{p-1}, x_{p+1} \cdots x_w) \\
&\qquad\qquad\quad \times u_{n'_a l'_a j'_a m'_a}(x_p) \,.
\end{aligned} \tag{A13}$$

By the same arguments as given beneath Eq. (31) one sees that this matrix element is given by the right-hand side with $p = q = w$, the summation over p and q omitted, the phase factor omitted, and the result multiplied by w. Then since the electrons are in the same increasing order 1, 2, . . . , w in both the initial and final states and are coupled in the same manner irreducible tensor techniques can be used to evaluate the result. Now substituting this into Eq. (A4) with $M_t = M_a, M'_t = M'_a$ we have

$$\begin{aligned}
&S(n_a l_a j_a^w \alpha_a J_a \text{-} n_a l_a j_a^{w-1} \alpha''_a J''_a n'_a l'_a j'_a J'_a) \\
&\quad = w \langle n_a l_a \,|\, r \,|\, n'_a l'_a \rangle^2 \sum_{M_a, M'_a, k} \left| \sum_{\alpha_1, J_1} (j_a^{w-1} \alpha_1 J_1 \,|\, \} j_a^w \alpha_a J_a) \langle j_a^{w-1} \alpha_1 J_1 j_a J_a M_a \,|\, \underline{C}_k^{(1)}(w) \,|\, j_a^{w-1} \alpha''_a J''_a j'_a J'_a M'_a \rangle \right|^2 .
\end{aligned} \tag{A14}$$

Again we use the Wigner-Eckart theorem[12]

$$\begin{aligned}
&\langle j_a^{w-1} \alpha_1 J_1 j_a J_a M_a \,|\, C_k^{(1)}(w) \,|\, j_a^{w-1} \alpha''_a J''_a j'_a J'_a M'_a \rangle \\
&\quad = (-1)^{J_a - M_a} \begin{bmatrix} J_a & 1 & J'_a \\ -M_a & k & M'_a \end{bmatrix} \langle j_a^{w-1} \alpha_1 J_1 j_a J_a \| \underline{C}^{(1)}(w) \| j_a^{w-1} \alpha''_a J''_a j'_a J'_a \rangle \,,
\end{aligned} \tag{A15}$$

where the matrix element on the right-hand side is given by Eq. (34) with $\lambda = 1$. Thus applying all this to Eq. (A14), factoring out the 3-j symbol and then using the analog of Eq. (A8) we have

$$S(n_a l_a j_a^w \alpha_a J_a\text{-}n_a l_a j_a^{w-1} \alpha_a'' J_a'' n_a' l_a' j_a' J_a')$$
$$= w[(j_a^{w-1} l_a'' J_a'' \,|\, \} j_a^w \alpha_a J_a)]^2 (2J_a+1)(2J_a'+1) \begin{Bmatrix} j_a & 1 & j_a' \\ J_a' & J_a'' & J_a \end{Bmatrix}^2 (\langle n_a l_a \,|\, r \,|\, n_a' l_a' \rangle \langle j_a \| \underline{C}^{(1)} \| j_a' \rangle)^2 \,. \quad \text{(A16)}$$

If we sum this over J_a', as generally desired for excitation to very highly excited states, the 6-j symbol is removed by use of Eq. (40) and applying the result to Eq. (A1) with $g_i = 2J_a + 1$ we obtain

$$\sum_{J_a'} f(n_a l_a j_a^w \alpha_a J_a\text{-}n_a l_a j_a^{w-1} \alpha_a'' J_a'' n_a' l_a' j_a' J_a') = \frac{\Delta E}{3(2j_a+1)} w[(j_a^{w-1} \alpha_a'' J_a'' \,|\, \} j_a^w \alpha_a J_a)]^2 (\langle n_a l_a \,|\, r \,|\, n_a' l_a' \rangle \langle j_a \| \underline{C}^{(1)} \| j_a' \rangle)^2$$
$$= w[(j_a^{w-1} \alpha_a'' J_a'' \,|\, \} j_a^w \alpha_a J_a)]^2 f_{\mathrm{H}}^{ps}(n_a l_a j_a\text{-}n_a' l_a' j_a') \,, \quad \text{(A17)}$$

where f_{H}^{ps} is a pseudo hydrogenic ion oscillator strength given by the same form as Eq. (A10). However, the ΔE used in f_{H}^{ps} is the actual transition energy, not the hydrogenic ion one, and the radial matrix element used in determining f_{H}^{ps} also generally differs from the hydrogenic ion one. This occurs because the radial functions in Eq. (A6) will in this case be different due to the screening effect of the other bound electrons. In analogy to the collision case we could scale out the major Z dependence in evaluating the radial matrix elements and utilize an effective Z so that f_{H}^{ps} is given by

$$f_{\mathrm{H}}^{ps}(n_a l_a j_a\text{-}n_a' l_a' j_a')$$
$$\simeq \frac{\Delta E}{3(2j_a+1)} \frac{1}{Z_{\mathrm{eff}}^2} [Z^2 S_{\mathrm{H}}(n_a l_a j_a\text{-}n_a' l_a' j_a')] \quad \text{(A18)}$$

where $Z^2 S_{\mathrm{H}}$ is given by Eq. (A9) with Z-scaled hydrogenic radial functions used in evaluating the matrix element given by Eq. (A6) and is independent of Z. However, as discussed for the collisional case beneath Eq. (62), this is not necessary and a more sophisticated approach such as use of Hartree-Fock functions can instead be used in evaluating the $\langle n_a l_a \,|\, r \,|\, n_a' l_a' \rangle$.

Similar to Eq. (62), where we could have used Q_{H}^{ps} in place of $Z_{\mathrm{eff}}^{-2}(Z^2 Q_{\mathrm{H}})$, we can in general write for radiative transitions to highly excited levels

$$f = w(\mathscr{R}) f_{\mathrm{H}}^{ps} \quad \text{(A19)}$$

where, as in the case of Eq. (62), the final total angular momentum J_a' for the ion has always been summed over. One sees that for the case represented by Eq. (A17) the $\mathscr{R}$ is simply the square of the $\mathscr{C}$, which is the same as for the analogous collisional transition represented by Eq. (44). In fact, as we will now discuss the branching ratios for radiative transitions always have the same values as for the corresponding collisional transitions regardless of the complexity of the transition. This occurs because all the extra factors in the more complicated collisional transitions represented by Eqs. (50), (53), (56), (57), and (59) are recoupling factors that entered because it was necessary to recouple the initial ion wave function so that it is coupled in the same manner as the final ion wave function in order that irreducible tensor techniques could be used. The same is true for the radiative transitions where the same atomic wave functions apply and one must evaluate the generalization of Eqs. (A13)–(A17). In evaluating these, where the analog or generalization of Eq. (34) with $\lambda = 1$ applies, essentially the identical discussion is applicable as that leading to Eqs. (50), (53), and (59). Thus, for example, for the case that one additional lower partially filled subshell and two higher partially filled subshells of inactive or spectator electrons are present the right-hand side of the generalization of Eq. (A16) is given by the right-hand side of Eq. (59) with the replacement

$$Z_{\mathrm{eff}}^{-2}(Z^2 Q_{\mathrm{H}})$$
$$\rightarrow (2J_{bacd}+1)(2J_a'+1) \begin{Bmatrix} j_a & 1 & j_a' \\ J_a' & J_{bacd}'' & J_{bacd} \end{Bmatrix}^2$$
$$\times (\langle n_a l_a \,|\, r \,|\, n_a' l_a' \rangle \langle j_a \| C^{(1)} \| j_a' \rangle)^2 \,. \quad \text{(A20)}$$

Then when one sums over J_a' using the analog of Eq. (40) the 6-j symbol is removed, and applying the result to Eq. (A1) with $g_i = (2J_{bacd}+1)$ one obtains Eq. (A17) except that in place of the $\mathscr{C}$ squared the branching ratio has the same, much more complicated value as in Eq. (59) for the analogous collision transition. Of course, if one sums over j_a' as will often be desired, $f_{\mathrm{H}}^{ps}(n_a l_a\text{-}n_a' l_a')$ which has the form given by Eq. (A10), replaces $f_{\mathrm{H}}^{ps}(n_a l_a j_a\text{-}n_a' l_a' j_a')$. Also, since photoionization cross sections are continuous across the bound-free threshold with photoionization cross sections and the latter are like the former summed over many l_a' values, it is apparent that a relationship like that given by Eq. (A19) applies as well with photoionization cross sections replacing f values on both sides of the equation.

APPENDIX B

It is well known that for very complex ions there are many possible ways to couple the angular momenta to form intermediate angular momenta before obtaining the total angular momenta in either LS- or jj-coupling schemes. In the most common or standard approach for LS coupling[10] one first obtains total L and total S for each subshell. Then one couples the subshell L's together successively, one at a time, until the total L for the atom is obtained. A similar procedure is used for the S's and finally total L and S are coupled to form total J for the atom. Similarly for jj coupling one forms total J for each subshell and then couples these together successively, one at a time, until the total J for the atom is obtained. This standard scheme is the one followed, for example, in the widely used set of programs of Grant and co-workers.[23] It is probably most common because it is the easiest scheme to use in writing a completely general set of programs. It is this standard scheme for both LS and jj coupling that we assumed in deriving our branching ratio formulas. However, a more physical scheme is to couple all the angular momenta of the subshells of a shell together and then couple these together to get the total angular momenta for the atom. It is essentially this scheme that has been used recently by Hagelstein[21,22] and it appears to have quite wide usage, especially at the U.S. National Laboratories. Hence, we consider in this appendix how the quantum numbers in our branching rates formulas must be reinterpreted when Hagelstein's coupling scheme is followed. This will have the added benefit that one can then see how to interpret the quantum numbers in our formulas in applications to essentially any other coupling scheme as well.

In Hagelstein's scheme, in which jj coupling is used, two "excited orbitals" or subshells are allowed with total angular momenta J_{X1} and J_{X2}. These are coupled together to form J_X. This is then coupled to the total angular momentum of the "core," J_{core}, to form the total angular momentum of the atom, J_{atom}. In his earlier work the core consisted of the K and L shells (those with $n=1$ and 2), as shown in Fig. 1 of Ref. 21. More recently this has been expanded to include the K, L, and M shells, as shown in Fig. 1 of Ref. 22. It is important to note that the use of the word core here is Hagelstein's usage and this differs from our usage in the main body of the present paper, where we used core to refer to all but the active electron. In Hagelstein's core the total angular momentum J_{nlj} for each of the subshells nlj with the same nl value are coupled together to form J_{nl}. Then all of these with the same n value are coupled together starting with the highest l value to form J_n. Finally the J_n are coupled together starting with the lowest n to form J_{core}. This is depicted in Fig. 1, which is like Fig. 1 of Ref. 22. Actually, spectroscopic notation is used so that the J_n are represented by J_K, J_L, and J_M for $n=1$, 2, and 3, respectively, and, for example, J_{nlj} is represented by $J_{3d\,3/2}$ when $n=3$, $l=2$, and $j=\frac{3}{2}$. It is of interest to note that Hagelstein's scheme is a better scheme than the standard scheme in the sense that mixing effects are probably smaller in most cases so that use of our formulas, in which mixing effects were neglected, is probably more accurate. Of course, when mixing effects are included results for cross sections are independent of the coupling scheme used.

We now indicate how our formulas for branching ratios can be applied to Hagelstein's coupling scheme. In doing this we first note that the details of how the angular momenta J_b, J_c, and J_d in recoupling formulas such as Eq. (58) were obtained does not matter in the derivation of our branching ratio formulas. All that counts are the values for the angular momenta with which j_a must be recoupled in order that it be coupled last like the j_a' in the final state. Thus instead of corresponding to the total angular momenta of subshells b, c, and d, as we assumed, J_b, J_c, and J_d could each be the result of coupling the angular momenta of several subshells together, as will frequently be the case when our formulas are applied to an alternative coupling scheme such as Hagelstein's. Indeed, as noted at the beginning of Sec. VI, even for the "standard" coupling scheme we used in deriving our formulas, J_b should be the total angular momentum of all the subshells for which the angular momenta have been coupled before that of subshell a (in the usual procedure this would be all lower subshells than a). Thus, keeping this in mind it is really quite easy to see what the J values in our branching ratio formulas should represent when these formulas are applied to any particular coupling scheme. We now illustrate this by applying our formulas to the various specific possibilities when Hagelstein's coupling scheme given in Fig. 1 is used.

First we consider excitation or ionization of a $1s_{1/2}$ electron. This is the only subshell in the K shell and its total angular momentum is J_K. Thus J_K plays the role of J_a in Eq. (59), which is directly applicable in this case.

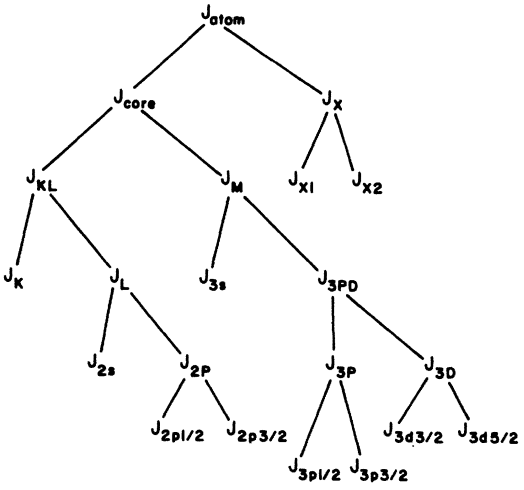

FIG. 1. Angular momentum coupling scheme used by Hagelstein in Ref. 22. The $1s_{1/2}$ orbital is described by J_K, and the L-shell orbitals or subshells have J values $J_{2s\,1/2}$, $J_{2p\,1/2}$, and $J_{2p\,3/2}$. The two $2p$ orbitals are coupled together to form J_{2P}, which is coupled with the $2s$ orbital to form J_L. The K- and L-shell momenta are coupled to form an intermediate momentum J_{KL}. The M-shell orbitals, which have angular momenta J_{3s}, $J_{3p\,1/2}$, $J_{3p\,3/2}$, $J_{3d\,3/2}$, and $J_{3d\,5/2}$, are coupled together as shown in the figure, with intermediate momenta J_{3p}, J_{3D}, J_{3PD}, and J_M. The K- and L-shell coupled momentum J_{KL} is coupled with J_M to form the core momenta J_{core}. Two excited-state orbitals are included (J_{X1} and J_{X2}) and are coupled to form J_X. The core electrons and the excited electrons are coupled to form the total atom angular momentum J_{atom}. Note that the usage of "core" here is Hagelstein's, which differs from that used in the main body of the present paper.

Since J_L is the first angular momentum coupled to J_K, it plays the role of J_b and J_{KL} plays the role of J_{ba}. The next angular momentum coupled to this is J_M so it plays the role of J_c and J_{core} plays the role of J_{bac}. Finally, since J_X is coupled to this, it plays the role of J_d and J_{atom} plays the role of J_{bacd}. Of course, for the final state corresponding identifications apply between our double primed J's and Hagelstein's quantum numbers.

Excitation or ionization of a $3s_{1/2}$ electron is very similar. The total angular momentum for this subshell is J_{3s}, which then plays the role of J_a. This is first coupled to J_{3PD} to form J_M so J_{3PD} plays the role of J_b and J_M plays the role of J_{ba}. Then J_M is coupled to J_{KL} to form J_{core} so J_{KL} plays the role of J_c and J_{core} again plays the role of J_{bac}. Finally J_X again plays the role of J_d and J_{atom} plays the role of J_{bacd}.

Excitation or ionization of one of Hagelstein's "excited orbitals" is a somewhat simpler case. If the active electron is one initially in the $X1$ subshell, then, of course J_{X1} plays the role of J_a. Since it is first coupled to J_{X2} to form J_X, one sees that J_{X2} plays the role of J_b and J_X plays the role of J_{ba}. Since J_X is coupled to J_{core} to form J_{atom}, one sees that J_{core} plays the role of J_c and J_{atom} plays the role of J_{bac}. There is no additional angular momentum playing the role of J_d so the factor

$$(2J''_{bacd}+1)(2J_{bac}+1)\begin{Bmatrix} j_a & J''_{bac} & J_{bac} \\ J_d & J_{bacd} & J''_{bacd} \end{Bmatrix}^2 \tag{B1}$$

in Eq. (59) should be omitted in this case. Of course, if it is an electron in orbital $X2$ that is active, the roles of J_{X1} and J_{X2} are reversed.

Excitation or ionization of a $2s_{1/2}$ electron is more complicated. In this case the generalization of Eq. (59) given by the discussion surrounding Eq. (60) applies. Of course, J_{2s} plays the role of J_a, and since it is first coupled to J_{2P} to form J_L, one sees that J_{2P} plays the role of J_b and J_L that of J_{ba}. Since this is then coupled to J_K to form J_{KL}, one sees that J_K and J_{KL} play the roles of J_c and J_{bac}. The next coupling is with J_M to form J_{core} so that J_M plays the role of J_d and J_{core} that of J_{bacd}. Finally J_{core} is coupled to J_X to form J_{atom} so J_X and J_{atom} play the roles of J_e and J_{bacde}.

Excitation or ionization of a $2p_{1/2}$, $2p_{3/2}$, $3p_{1/2}$, $3p_{3/2}$, $3d_{3/2}$, or $3d_{5/2}$ is still more complicated because in addition to the factor given by Eq. (60), one must expand Eq. (59) to include a factor

$$(2J''_{bacdef}+1)(2J_{bacde}+1)\begin{Bmatrix} j_a & J''_{bacde} & J_{bacde} \\ J_f & J_{bacdef} & J''_{bacdef} \end{Bmatrix}^2 . \tag{B2}$$

First we assume that the active electron is a $2p_{1/2}$ electron. Then by analogous reasoning to that used in the previous examples $J_{2p\,1/2}$, $J_{2p\,3/2}$, J_{2P}, J_{2s}, J_L, J_K, J_{KL}, J_M, J_{core}, J_X, and J_{atom} play the roles of J_a, J_b, J_{ba}, J_c, J_{bac}, J_d, J_{bacd}, J_e, J_{bacde}, J_f, and J_{bacdef}, respectively. When instead a $2p_{3/2}$ electron is active the roles of $J_{2p\,1/2}$ and $J_{2p\,3/2}$ are reversed. For excitation or ionization of a $3p_{1/2}$ electron $J_{3p\,1/2}$, $J_{3p\,3/2}$, J_{3P}, J_{3D}, J_{3PD}, J_{3s}, J_M, J_{KL}, J_{core}, J_X, and J_{atom} play the roles of J_a, J_b, J_{ba}, J_c, J_{bac}, J_d, J_{bacd}, J_e, J_{bacde}, J_f, and J_{bacdef}. Of course, if instead a $3p_{3/2}$ electron is active, the roles of $J_{3p\,1/2}$ and $J_{3p\,3/2}$ are reversed. Finally for excitation or ionization of a $3d_{3/2}$ electron $J_{3d\,3/2}$, $J_{3d\,5/2}$, J_{3D}, J_{3P}, J_{3PD}, J_{3s}, J_M, J_{KL}, J_{core}, J_X, and J_{atom} play the roles of J_a, J_b, J_{ba}, J_c, J_{bac}, J_d, J_{bacd}, J_e, J_{bacde}, J_f, and J_{bacdef}, respectively, and, if a $3d_{5/2}$ is active instead, the roles of $J_{3d\,3/2}$ and $J_{3d\,5/2}$ are reversed.

Actually in most cases these formulas will greatly simplify because some subshells or shells will be completely filled or empty so that the corresponding J value is zero. Then the corresponding recoupling factors, which have the form of Eq. (60), (B1) or (B2), will drop out. This is expected physically and is seen from the property of the 6-j symbol,

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ 0 & j_4 & j_5 \end{Bmatrix}^2 = \frac{\delta_{j_2 j_5}\delta_{j_3 j_4}}{(2j_2+1)(2j_3+1)} . \tag{B3}$$

Finally we note that the branching ratio formulas we obtained for LS coupling are very similar to those for jj coupling, but more lengthy because one has a set of recoupling factors for both L's and S's like those for the J's in jj coupling (also there is an extra 9-j factor, but this does not involve the intermediate angular momenta). Thus, one can apply essentially the same reasoning as done above for jj coupling to reinterpret the quantum numbers in our LS-coupling formulas when an alternative LS-coupling scheme is used in obtaining intermediate quantum numbers.

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