PHYSICAL REVIEW A VOLUME 45, NUMBER 3 1 FEBRUARY 1992

Rapid-ionization approach based on the factorization method

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(Received 16 August 1991)

The factorization method of Bar-Shalom, Klapisch, and Oreg [Phys. Rev. A **38**, 1773 (1988)] is extended to relativistic-distorted-wave cross sections for ionization by electron impact. This leads to a very great simplification for complex ions. In particular, when mixing is confined to the states in a complex (having the same set of n values, parity, and J value), the ionization cross section takes the form of a summation over states of the product of a readily calculated quantity that depends only on target-ion properties, such as mixing coefficients and angular momenta, and a cross section having exactly the same form as a hydrogenic cross section except that the radial functions should be calculated using the appropriate potential for the ion being considered. Similar results are obtained for intermediate coupling using LS-coupling notation and for totally nonrelativistic calculations. Only slightly more complicated formulas apply when mixing is included outside a complex. It is also noted that similar expressions apply for photoionization. Sample numerical results are obtained and compared with relativistic calculations of Moores and Pindzola [Phys. Rev. A **42**, 5384 (1990)]. Quite good agreement is obtained when mixing is included among the same set of states.

PACS number(s): 34.80.Kw

I. INTRODUCTION

Recently there has been increased interest in the properties of highly charged ions with very large values for the nuclear charge number Z, partly due to the interest in developing ultrashort-wavelength lasers. Also, increasingly accurate measurements of various electron-ion scattering processes involving very highly charged ions are being made as a result of technological advances associated with ion sources, traps, and storage rings [1,2]. For such ions with $Z \gtrsim 25$ or 30, the j dependence of the radial functions for some orbitals becomes significant so that a fully relativistic approach based on the Dirac equation should be used in calculating their properties.

One of the processes of interest is ionization of highly charged ions by electron impact. Recently several fully relativistic computer programs have been obtained and applied to the calculation of cross sections for ionization of highly charged ions by electron impact [3–9]. Since relativistic ionization cross sections tend to be lengthy to compute and many are needed, it is desirable to have a very rapid method of calculation. Our purpose here is to show how such an approach can be obtained by extending the recent factorization method of Bar-Shalom, Klapisch, and Oreg [10] for excitation to ionization. For excitation this approach leads to a huge reduction in the angular part of the calculation. This is very beneficial when that part of the calculation is large in a conventional treatment. This occurs when a small number of orbital transitions contribute to a very large number of transitions, such as in the case for inner-shell excitation of Na-like ions and transitions between excited levels of Ne-like and Ni-like ions, all of which are of interest for x-ray-laser research. Also, as pointed out in Ref. [11] and used in large-scale calculations in Refs. [12–17], the factorization method is ideal for calculating cross sections for a given class of transitions simultaneously for a large part of an isoelectronic sequence by using fits of the radial part to a power series in Z. As we will show, similar benefits occur for ionization when the factorization method is used. In fact, the simplification in the appropriate formula for ionization is even somewhat greater. Moreover, similar simple formulas apply for photoionization and for semirelativistic or totally nonrelativistic calculations expressed in LS-coupling notation.

In the next lengthy section the pertinent theory is outlined. Then in Sec. III A discussion of results and comparison with other work is given. In the final section we give a brief summary and conclusions.

II. THEORY

In outlining the appropriate theory we will follow the procedure used in Ref. [18], where results for ionization were obtained by first considering excitation to a highly excited bound level. Also many of the equations of Ref. [18] apply with only slight modification because the angular part of the matrix elements of the Coulomb interaction between electrons $1/r_{ij}$ is the same in jj coupling for a relativistic treatment as for a nonrelativistic treatment. Since considerable use of these equations will be made, equation (x) of Ref. [18] will be designated equation (S,x).

First we will obtain the result for hydrogenic ions using the factorization method. There is little advantage in this for calculating hydrogenic cross sections. We do it because, in later considering complex ions by the factorization method, we will see that the result for ionization takes the form of a summation of the product of a readily calculated quantity that depends only on the ion properties and a cross section having exactly the same form as a hydrogenic cross section except that the radial functions should be calculated using the appropriate potential for the actual ion.

A. Hydrogenic ions

The nonrelativistic cross section for excitation of hydrogenic ions is expressed in *jj* coupling by Eq. (S,20). This also applies for relativistic calculations of excitation of hydrogenic ions after a few modifications are made. First the impact electron energy in Rydbergs, which occurs in the denominator of Eq. (S,20) and which we will designate ε(Ry), should be replaced by k^2, where k is the impact electron wave number. It is related to ε(Ry) by the relativistic expression

$$k^2=\varepsilon(\mathrm{Ry})\left[1+\frac{\alpha^2}{4}\varepsilon(\mathrm{Ry})\right] , \tag{1}$$

where α is the fine-structure constant $e^2/\hbar c$. Also the "direct" and "exchange" radial integrals D^λ and E^λ given by Eqs. (S,14) and (S,18) should be replaced by the relativistic expressions, Eqs. (9) and (10) of Ref. [11].

We digress for a moment to repeat these equations and other related equations for convenience and later reference

$$\begin{aligned}&D^\lambda(n_a l_a j_a \varepsilon l j;\, n_a' l_a' j_a' \varepsilon' l' j')\\ &\quad=2\int_0^\infty \int_0^\infty [P_{n_a l_a j_a}(r_1)P_{n_a' l_a' j_a'}(r_1)+Q_{n_a l_a j_a}(r_1)Q_{n_a' l_a' j_a'}(r_1)]\frac{r_<^\lambda}{r_>^{\lambda+1}}[P_{\varepsilon l j}(r_2)P_{\varepsilon' l' j'}(r_2)+Q_{\varepsilon l j}(r_2)Q_{\varepsilon' l' j'}(r_2)]dr_1 dr_2 ,\end{aligned} \tag{2}$$

and

$$\begin{aligned}&E^\lambda(n_a l_a j_a \varepsilon l j;n_a' l_a' j_a' \varepsilon' l' j')\\ &\quad=2\int_0^\infty \int_0^\infty [P_{n_a l_a j_a}(r_1)P_{\varepsilon' l' j'}(r_1)+Q_{n_a l_a j_a}(r_1)Q_{\varepsilon' l' j'}(r_1)]\frac{r_<^\lambda}{r_>^{\lambda+1}}[P_{\varepsilon l j}(r_2)P_{n_a' l_a' j_a'}(r_2)+Q_{\varepsilon l j}(r_2)Q_{n_a' l_a' j_a'}(r_2)]dr_1 dr_2 ,\end{aligned} \tag{3}$$

where $r_<(r_>)$ is the lesser (greater) of r_1 and r_2. In these equations (l_a,l) and (j_a,j) are the initial orbital and total angular momentum quantum numbers for the bound electron and the impact electron, respectively. n_a is the initial principal quantum number. Primes on symbols indicate corresponding final-state quantities. The "large" and "small" components $P_{n_a l_a j_a}\equiv P_{n_a\kappa_a}$ and $Q_{n_a l_a j_a}\equiv Q_{n_a\kappa_a}$ of the radial function satisfy the coupled Dirac equations

$$\left[\frac{d}{dr}+\frac{\kappa_a}{r}\right]P_{n_a\kappa_a}=\frac{\alpha}{2}\left[\varepsilon_{n_a\kappa_a}-V+\frac{4}{\alpha^2}\right]Q_{n_a\kappa_a} . \tag{4}$$

and

$$\left[\frac{d}{dr}-\frac{\kappa_a}{r}\right]Q_{n_a\kappa_a}=\frac{\alpha}{2}(V-\varepsilon_{n_a\kappa_a})P_{n_a\kappa_a} , \tag{5}$$

where $\varepsilon_{n_a\kappa_a}$ is the energy eigenvalue and κ_a is the relativistic quantum number satisfying

$$\kappa_a=l_a,\ j_a=l_a-\tfrac{1}{2},\ \kappa_a=-(l_a+1),\ j_a=l_a+\tfrac{1}{2} . \tag{6}$$

For the special case of hydrogenic ions, $V=-2Z/r$, where Z is the nuclear charge number. The bound-state radial functions satisfy the normalization condition

$$\int_0^\infty [P_{n_a\kappa_a}^2(r)+Q_{n_a\kappa_a}^2(r)]dr=1 . \tag{7}$$

Although the free-electron radial functions $P_{\varepsilon l j}\equiv P_{\varepsilon\kappa}$ and $Q_{\varepsilon l j}\equiv Q_{\varepsilon\kappa}$ satisfy equations analogous to Eqs. (4)–(6), the normalization condition is

$$\int_0^\infty [P_{\varepsilon'\kappa}(r)P_{\varepsilon\kappa}(r)+Q_{\varepsilon'\kappa}(r)Q_{\varepsilon\kappa}(r)]dr=\pi\delta(\varepsilon-\varepsilon') . \tag{8}$$

Now we return to a consideration of Eq. (S,20) and separate the sums over λ in the direct and exchange contributions, letting $\lambda\rightarrow\lambda'$ in the latter. Also in order to apply the factorization method, we make use of the well-known formula [19]

$$\begin{aligned}\begin{Bmatrix} j_a & \lambda' & j' \\ j_a' & J & j \end{Bmatrix} &=\sum_t(-1)^{t+\lambda'+J}(2t+1)\\ &\quad\times\begin{Bmatrix} j_a & j' & \lambda' \\ j & j_a' & t \end{Bmatrix}\begin{Bmatrix} j_a & t & j_a' \\ j' & J & j \end{Bmatrix} .\end{aligned} \tag{9}$$

Then applying all this to Eq. (S,20) and dropping the Z^2 factor because we do not assume that the principal Z dependence has been scaled out, we have the relativistic expression for the cross section for electron-impact excitation of a hydrogenic ion

$$Q_H(n_al_aj_a-n_a'l_a'j_a')=\frac{8\pi a_0^2}{(2j_a+1)k^2}\sum_H(2J+1)\sum_{\substack{l,l'\\j,j'}}\Bigg[\sum_\lambda\begin{Bmatrix}j_a & \lambda & j_a'\\ j' & J & j\end{Bmatrix}D^\lambda(n_al_aj_a\varepsilon lj;n_a'l_a'j_a'\varepsilon'l'j')\langle j_a\|C^\lambda\|j_a'\rangle\langle j\|C^\lambda\|j'\rangle$$

$$-\sum_{\lambda'}\sum_t(-1)^{2j'+\lambda'+t}(2t+1)\begin{Bmatrix}j_a & j' & \lambda'\\ j & j_a' & t\end{Bmatrix}\begin{Bmatrix}j_a & t & j_a'\\ j' & J & j\end{Bmatrix}$$

$$\times E^{\lambda'}(n_al_aj_a\varepsilon lj;n_a'l_a'j_a'\varepsilon'l'j')\langle j_a\|C^{\lambda'}\|j'\rangle\langle j\|C^{\lambda'}\|j_a'\rangle\Bigg]^2\,, \tag{10}$$

where

$$\langle j_1\|C^\lambda\|j_2\rangle=-(-1)^{j_1-1/2}[(2j_1+1)(2j_2+1)]^{1/2}\times\begin{pmatrix}j_1 & \lambda & j_2\\ \frac{1}{2} & 0 & -\frac{1}{2}\end{pmatrix}\,. \tag{11}$$

We note that the compact result given by Eq. (11) is equivalent to that given by Eqs. (S,12), (S,13), and (S,19), except for a slight change in the phase factor because we here assume l is coupled before $s=\frac{1}{2}$.

The result given by Eq. (10) can be considerably simplified by performing the summation over J using the formula [19]

$$\sum_J(2J+1)\begin{Bmatrix}j_a & \lambda & j_a'\\ j' & J & j\end{Bmatrix}\begin{Bmatrix}j_a & \lambda' & j_a'\\ j' & J & j\end{Bmatrix}=\frac{\delta_{\lambda\lambda'}}{2\lambda+1}\,. \tag{12}$$

Then, after interchanging the labeling λ' and t in the exchange contribution so that the results look more like the factorization results in Ref. [10], and using the fact that $(-1)^{2j'}=-1$ because j' is a half integer, the result can be written

$$Q_H(n_al_aj_a-n_a'l_a'j_a')=\frac{8\pi a_0^2}{(2j_a+1)k^2}\sum_\lambda Q^\lambda(n_al_aj_a,n_a'l_a'j_a')\,, \tag{13}$$

where

$$Q^\lambda(n_al_aj_a,n_a'l_a'j_a')=\sum_{\substack{l,l'\\j,j'}}P^\lambda(n_al_aj_a\varepsilon lj;n_a'l_a'j_a'\varepsilon'l'j')^2 \tag{14}$$

and

$$P^\lambda(n_al_aj_a\varepsilon lj;n_a'l_a'j_a'\varepsilon'l'j')=(2\lambda+1)^{-1/2}D^\lambda(n_al_aj_a\varepsilon lj;n_a'l_a'j_a'\varepsilon'l'j')\langle j_a\|C^\lambda\|j_a'\rangle\langle j\|C^\lambda\|j'\rangle$$

$$+\sum_t(-1)^{\lambda+t}(2\lambda+1)^{1/2}\begin{Bmatrix}j_a & j' & t\\ j & j_a' & \lambda\end{Bmatrix}E^t(n_al_aj_a\varepsilon lj;n_a'l_a'j_a'\varepsilon'l'j')\langle j_a\|C^t\|j'\rangle\langle j\|C^t\|j_a'\rangle\,. \tag{15}$$

In order to obtain the relativistic cross section for ionization from sublevel $n_al_aj_a$ in a hydrogenic ion we simply replace the final excited bound electron with an ejected electron, sum over its angular momenta, and integrate over its energy. Also the π in Eq. (13) is omitted due to the different normalization for a free-electron function, see Eq. (8). The result can be written

$$Q_H(n_al_aj_a)=\frac{8a_0^2}{(2j_a+1)k^2}\int_0^{(\varepsilon-I)/2}d\varepsilon''\sum_\lambda Q^\lambda(n_al_aj_a)\,, \tag{16}$$

where I is the ionization energy and

$$Q^\lambda(n_al_aj_a)=\sum_{\substack{l,l',l''\\j,j',j''}}P^\lambda(n_al_aj_a\varepsilon lj;\varepsilon''l''j''\varepsilon'l'j')^2 \tag{17}$$

in which P^λ is given by Eq. (15) with n_a', l_a', and j_a' everywhere replaced by ε'', l'' , and j''. This also means that the D^λ and E^λ in Eq. (15) should be given by Eqs. (2) and (3) with $P_{n_a'l_a'j_a'}$ and $Q_{n_a'l_a'j_a'}$ everywhere replaced by $P_{\varepsilon''l''j''}$ and $Q_{\varepsilon''l''j''}$. Finally we note that this procedure corresponds to using the "natural" phase approximation as defined in Ref. [5].

B. Complex ions

Now we consider complex ions and again we first obtain results for excitation to a highly excited bound level. The distorted-wave cross section for an excitation transition $\Delta_tJ_t-\Delta_t'J_t'$ can be expressed in terms of the reactance matrix R. For ions more than a few times ionized the elements of the reactance matrix are small, especially for excitation to very highly excited levels. Hence, unitarization is unnecessary. Then the cross section is given by

$$Q(\Delta_t J_t - \Delta'_t J'_t) = \frac{2\pi a_0^2}{g_t k^2} \sum_J (2J+1) \sum_{\substack{l,l' \\ j,j'}} |R(\Delta_t J_t \varepsilon l j J;\Delta'_t J'_t \varepsilon' l' j')|^2 . \tag{18}$$

Here J_t and J are the total angular momentum quantum numbers of the target ion and the total system, respectively. g_t is the statistical weight of the initial level of the target ion and Δ_t designates all quantum numbers in addition to J_t that are necessary to specify the initial level of the target ion. Other symbols have the same meanings as in Sec. II A. Primes on symbols indicate corresponding final-state quantities. In general the initial and final levels of the ion will each be mixtures of pure states having the same total angular momentum and parity. Thus

$$R(\Delta_t J_t \varepsilon l j J;\Delta'_t J'_t \varepsilon' l' j') = \sum_{\beta_t,\beta'_t} b^{J_t}(\Delta_t,\beta_t) b^{J'_t}(\Delta'_t,\beta'_t) \times R(\beta_t J_t \varepsilon l j J;\beta'_t J'_t \varepsilon' l' j') , \tag{19}$$

where β_t designates all quantum numbers in addition to J_t necessary to specify the pure state $\beta_t J_t$, which contributes to $\Delta_t J_t$ with corresponding mixing coefficient $b^{J_t}(\Delta_t,\beta_t)$. Again, primes on symbols indicate corresponding final-state quantities.

The reactance matrix has a direct and an exchange part

$$R = R^d - R^e . \tag{20}$$

In obtaining detailed results for the pure or unmixed expressions for R^d and R^e we first consider the case where there are only filled, or closed, subshells in addition to the active one, which we label a. Again the results of Ref. [18] apply with singlet modifications. Specifically, Eqs. (S,32)–(S,38) are applicable after modifications analogous to those of Sec. II A are made. In particular, in order to use the factorization method, the 9-j in Eq. (S,38) should be reexpressed using the formula [19]

$$\begin{Bmatrix} J''_a & J_a & j_a \\ j'_a & j & \lambda \\ J'_a & J & j' \end{Bmatrix} = \sum_t (-1)^{2t}(2t+1) \begin{Bmatrix} J_a & t & J'_a \\ j' & J & j \end{Bmatrix} \begin{Bmatrix} j_a & t & j'_a \\ J'_a & J''_a & J_a \end{Bmatrix} \begin{Bmatrix} j_a & j' & \lambda \\ j & j'_a & t \end{Bmatrix} , \tag{21}$$

where the factor $(-1)^{2t}$ can be omitted because here t is an integer. Then applying the resulting expressions for R^d and R^e to Eq. (20), the result can be written

$$\begin{aligned} R(\beta_t J_t \varepsilon l j J;\beta'_t J'_t \varepsilon' l' j') &= R(n_a l_a j_a^{\omega} \alpha_a J_a \varepsilon l j J; n_a l_a j_a^{\omega-1} \alpha''_a J''_a n'_a l'_a j'_a J'_a \varepsilon' l' j' J) \\ &= 2\sqrt{\omega}(j_a^{\omega-1}\alpha''_a J''_a |\} j_a^{\omega} \alpha_a J_a)[(2J_t+1)(2J'_t+1)]^{1/2}(-1)^{J'_t+J''_t+j'_a+J_t+j+J} \\ &\quad \times \Bigg[\sum_\lambda (-1)^\lambda \begin{Bmatrix} J_t & \lambda & J'_t \\ j' & J & j \end{Bmatrix} \begin{Bmatrix} j_a & \lambda & j'_a \\ J'_t & J''_t & J_t \end{Bmatrix} D^\lambda(n_a l_a j_a \varepsilon l j; n'_a l'_a j'_a \varepsilon' l' j') \langle j_a \| C^\lambda \| j'_a \rangle \langle j \| C^\lambda \| j' \rangle \\ &\quad + \sum_{\lambda'} \sum_t (-1)^{\lambda'}(2t+1) \begin{Bmatrix} J_t & t & J'_t \\ j' & J & j \end{Bmatrix} \begin{Bmatrix} j_a & t & j'_a \\ J'_t & J''_t & J_t \end{Bmatrix} \begin{Bmatrix} j_a & j' & \lambda' \\ j & j'_a & t \end{Bmatrix} \\ &\quad \times E^{\lambda'}(n_a l_a j_a \varepsilon l j; n'_a l'_a j'_a \varepsilon' l' j') \langle j_a \| C^{\lambda'} \| j' \rangle \langle j \| C^{\lambda'} \| j'_a \rangle \Bigg] . \end{aligned} \tag{22}$$

In giving the exchange contribution in Eq. (22) we used the fact that since j' is an integer $(-1)^{2j'} = -1$. In writing Eq. (22) all symbols used previously have retained the same meanings and D^λ, and E^λ are given by Eqs. (2) and (3). However, now the potentials used in Eqs. (4) and (5) determining $P_{n_a \kappa_a}$ and $Q_{n_a \kappa_a}$ and in the analogous equations determining $P_{\varepsilon\kappa}$ and $Q_{\varepsilon\kappa}$ should be those appropriate for the complex ion being considered. Here J_a is the initial total angular momentum of the active subshell a with occupation ω, while J''_a is the final total angular momentum of this subshell with occupation $\omega - 1$. The $(|\})$ is a coefficient of fractional parentage. The α_a stands for any additional quantum numbers, such as the seniority number, required to completely specify the state when there are several states with the j_a^{ω} configuration having the same J_a value. An analogous statement applies to α''_a, J''_a, and the $j_a^{\omega-1}$ configuration.

In giving the final detailed form of the right-hand side of Eq. (22) we have largely replaced the subscript a with the subscript t as compared with Eq. (21) and Eqs. (S,32)–(S,38), which lead to Eq. (22). Our reasons for doing this should be explained. Of course, in the present case, where any spectator electrons are in closed subshells, $J_a = J_t$, the total angular momentum of the ion, and $J_a'' = J_t''$, the total angular momentum of the remaining core after one electron has been removed and put in the excited final level $n_a' l_a' j_a'$. Also J_a', which is formed by coupling j_a' to J_a'', is equal to the final total angular momentum of the ion J_t'. Thus it was valid to replace J_a, J_a'', and J_a' with J_t, J_t'', and J_t'. The reason for doing so is that when we go to more complex cases with spectator electrons in particularly filled subshells, the factors where these replacements have been made remain unchanged and we only need add additional factors to account for the presence of the spectator electrons.

These additional factors all come from the fact that in order to use irreducible tensor techniques to evaluate the matrix elements, as done, for example, in Eqs. (S,32)–(S,37), the coupling must be of the same type for the initial and final states. This was considered in Ref. [18] and leads to Eqs. (S,52) and (S,58). Here as in Ref. [18] it will be assumed that the final excited level $n_a' l_a' j_a'$ is always higher than any partially filled spectator subshells because our intention is eventually to replace $n_a' l_a' j_a'$ by a free-electron state in order that we may have ionization.

By the same arguments that lead to Eq. (S,53) one finds that, if there are only lower partially filled subshells than the active subshell a and these have total angular momentum J_b, then the extra factor that should multiply the right-hand side of Eq. (22) is

$$(-1)^{J_b + j_a + J_a'' + J_t}[(2J_t''+1)(2J_a+1)]^{1/2} \begin{Bmatrix} j_a & J_a'' & J_a \\ J_b & J_t & J_t'' \end{Bmatrix} . \tag{23}$$

In this case the initial total angular momentum of the ion J_t equals J_{ba}, where J_{ba} is formed by coupling J_b to J_a. Similarly the final total angular momentum of the core J_t'' equals J_{ba}'', which is formed by coupling J_b to J_a''. We note that Eq. (23) also applies for the case where there are no partially filled lower subshells than subshell a, but there is a single partially filled inactive higher subshell with total angular momentum J_b, provided the phase factor is replaced with $(-1)^{J_b + j_a + J_a + J_t''}$. Of course, according to standard practice one would then couple J_a first in the coupling of J_a to J_b so J_t and J_t'' would equal J_{ab} and J_{ab}'', respectively.

If there are partially filled lower subshells than subshell a having total angular momentum J_b and also a single partially filled higher subshell having total angular momentum J_c, then the extra factor multiplying the right-hand side of Eq. (22) should be

$$(-1)^{J_b + J_c + 2j_a + 2J_{ba} + J_a'' + J_t''}[(2J_{ba}''+1)(2J_a+1)(2J_t''+1)(2J_{ba}+1)]^{1/2} \begin{Bmatrix} j_a & J_a'' & J_a \\ J_b & J_{ba} & J_{ba}'' \end{Bmatrix} \begin{Bmatrix} j_a & J_{ba}'' & J_{ba} \\ J_c & J_t & J_t'' \end{Bmatrix} . \tag{24}$$

In this case, the initial total angular momentum of the ion J_t equals J_{bac}, which is formed by coupling J_{ba} to J_c, and the final total angular momentum of the core J_t'' equals J_{bac}'', which is formed by coupling J_{ba}'' to J_c. If, in addition to the situation for which Eq. (24) applies, there were yet another still higher partially filled subshell with total angular momentum J_d, then the extra factor multiplying the right-hand side of Eq. (22) would be

$$(-1)^{J_b + J_c + J_d + 3j_a + 2J_{ba} + J_{bac} + J_a'' + J_{bac}'' + J_t''}[(2J_{ba}''+1)(2J_a+1)(2J_{bac}''+1)(2J_{ba}+1)(2J_t''+1)(2J_{bac}+1)]^{1/2}$$
$$\times \begin{Bmatrix} j_a & J_a'' & J_a \\ J_b & J_{ba} & J_{ba}'' \end{Bmatrix} \begin{Bmatrix} j_a & J_{ba}'' & J_{ba} \\ J_c & J_{bac} & J_{bac}'' \end{Bmatrix} \begin{Bmatrix} j_a & J_{bac}'' & J_{bac} \\ J_d & J_t & J_t'' \end{Bmatrix} , \tag{25}$$

in which J_t'' and J_t would equal J_{bacd}'' and J_{bacd}, respectively. This pattern can be continued for any number of partially filled inactive subshells. For example, if in addition to the situation for which Eq. (25) applies there were still one other higher partially filled subshell with total angular momentum J_e, the extra factor multiplying Eq. (22) could be obtained by replacing J_t and J_t'' in Eq. (25) with J_{bacd} and J_{bacd}'' and then multiplying the result by the factor

$$(-1)^{J_e + j_a + J_{bacd} + J_t''}[(2J_t''+1)(2J_{bacd}+1)]^{1/2}$$
$$\times \begin{Bmatrix} j_a & J_{bacd}'' & J_{bacd} \\ J_e & J_t & J_t'' \end{Bmatrix} , \tag{26}$$

where J_t'' and J_t here equal J_{bacde}'' and J_{bacde}, respectively.

Now we apply Eq. (22), with the appropriate modifications just discussed for more complex cases, to Eqs. (19) and (18). In doing this we can omit the phase factor $(-1)^{J_t + j + J}$ because J is formed from coupling J_t and j so $J_t + j + J$ is an integer. Also we will again interchange the labels t and λ' in the exchange part in order that the result be more like that obtained in Sec. II A. The summation over J can be performed immediately using the formula [19]

$$\sum_J (2J+1) \begin{Bmatrix} J_t & C & J_t' \\ j' & J & j \end{Bmatrix} \begin{Bmatrix} J_t & C' & J_t' \\ j' & J & j \end{Bmatrix} = \frac{\delta_{CC'}}{2C+1} . \tag{27}$$

Then the result for the cross section can be written in the factorized form

$$Q(U-U')=\frac{8\pi a_0^2}{(2J_t+1)k^2}\sum_{\substack{S,S'\\S_1,S_2'}}\sum_{\lambda}B^{\lambda}(U,SS_1;U',S'S_1')Q^{\lambda}((n_al_aj_a,n_a'l_a'j_a';n_{a1}l_{a1}j_{a1},n_{a1}'l_{a1}'j_{a1}')\ , \tag{28}$$

where we used $g_t=(2J_t+1)$. In order to simplify the notation we used $U=\Delta_tJ_t$ and $U'=\Delta_t'J_t'$ for the initial and final levels. Also, we let $S=\beta_tJ_t$ and $S_1=\beta_{t1}J_t$ indicate pure states contributing to U, while $S'=\beta_t'J_t'$ and $S_1'=\beta_{t1}'J_t'$ indicate pure states contributing to U'. Thus,

$$U=\sum_S b(U,S)|S\rangle,\quad U'=\sum_{S'}b(U',S')|S'\rangle\ , \tag{29}$$

while the b's in Eq. (29) are the mixing coefficients formally written $b^{J_t}(\Delta_t,\beta_t)$ and $b^{J_t'}(\Delta_t',\beta_t')$. Similar to Eq. (14), except that now due to mixing, nondiagonal terms contribute,

$$\begin{aligned}Q^{\lambda}&(n_al_aj_a,n_a'l_a'j_a';n_{a1}l_{a1}j_{a1},n_{a1}'l_{a1}'j_{a1}')\\&=\sum_{\substack{l,l'\\j,j'}}P^{\lambda}(n_al_aj_a\varepsilon lj;n_a'l_a'j'_a,\varepsilon'l'j')\\&\quad\times P^{\lambda}(n_{a1}l_{a1}j_{a1}\varepsilon lj;n_{a1}'l_{a1}'j_{a1}'\varepsilon'l'j')\end{aligned} \tag{30}$$

where the P^{λ} are given by Eq. (15), but, of course, the radial functions entering Eqs. (2) and (3) should now be calculated using the appropriate potentials for the actual complex ion being considered. The B^{λ} in Eq. (28) are readily calculated quantities depending only on the properties of the ion. In particular, we can write

$$B^{\lambda}(U,SS_1;U',S'S_1')=F^{\lambda}(US,U'S')F^{\lambda}(US_1,U'S_1')\ , \tag{31}$$

where

$$F^{\lambda}(US,U'S')=b(U,S)f^{\lambda}(S,S')b(U',S')\ . \tag{32}$$

For the case that Eq. (22) directly applies

$$\begin{aligned}f^{\lambda}(S,S')&=[(2J_t+1)(2J_t'+1)]^{1/2}(-1)^{J_t'+J_t''+j_a'}\\&\quad\times\sqrt{\omega}(j_a^{\omega-1}\alpha_a''J_a''|\}j_a^{\omega}\alpha_aJ_a)\\&\quad\times\begin{Bmatrix}j_a&\lambda&j_a'\\J_t'&J_t''&J_t\end{Bmatrix}\ ,\end{aligned} \tag{33}$$

and in this special case J_t, J_t', and J_t'', equal J_a, J_a' and J_a'', respectively. For more complex cases all that is required is that the right-hand side of Eq. (38) be multiplied by the appropriate one of Eqs. (23)–(25), or in the most complex case discussed, by Eq. (25) modified as discussed in connection with Eq. (26).

As in Sec. II A, in order to obtain results for ionization by electron impact we simply replace the final excited bound electron with a free ejected electron having energy ε'' and orbital and total angular momenta l'' and j''. Then we sum over J_t', l'', and j'', integrate over ejected electron energy and divide by π to account for the different normalization for a free electron [see Eq. (8)]. Since now J_t'' is the total angular momentum of the final ion with one less bound electron and is a good quantum number, the phase factor in Eq. (33) with j_a' replaced by j'' will not contribute to the cross section because J_t' is formed from J_t'' and j'' so $J_t'+J_t''+j''$ is an integer. Also the summation over J_t' can be performed using the analog of Eq. (27)

$$\sum_{J_t'}(2J_t'+1)\begin{Bmatrix}j_a&\lambda&j''\\J_t'&J_t''&J_t\end{Bmatrix}\begin{Bmatrix}j_{a1}&\lambda&j''\\J_t'&J_t''&J_t\end{Bmatrix}=\frac{\delta_{j_aj_{a1}}}{2j_a+1}\ . \tag{34}$$

Generally only states with the same parity can mix. In order that this be satisfied for both the initial and final levels of the ion, while Eq. (34) is also satisfied, it is necessary that $l_{a1}=l_a$. Moreover, it is usually valid for highly charged ions to include mixing only among states in a complex, that is, with the same set of n values, as well as parity and J value. In addition, for ionization both $n_a'l_a'j_a'\rightarrow\varepsilon''l''j''$ and $n_{a1}'l_{a1}'j_{a1}'\rightarrow\varepsilon''l''j''$. Hence, it is apparent that only diagonal terms contribute to Eq. (30) in this case. Thus, collecting results, the relativistic cross section for ionization from initial ion level U to final ion level U'' with one less bound electron can be expressed in the very simple form

$$Q(U-U'')=\sum_{\substack{S,S''\\S_1,S_1''}}B(U,SS_1;U'',S''S_1'')Q_H^{ps}(n_al_aj_a)\ , \tag{35}$$

where Q_H^{ps} is given by Eqs. (15), (16), and (17), except that now the I in Eq. (16) is the actual ionization energy of the complex ion, and the radial functions entering the expressions for D^{λ} and E^{λ} are those calculated using the appropriate potential for the complex ion being considered. Here, similar to Eq. (31),

$$B(U,SS_1;U'',S''S_1'')=F(US,U''S'')F(US_1,U''S_1'')\ , \tag{36}$$

where

$$F(US,U''S'')=b(U,S)f(S,S'')b(U'',S'')\ . \tag{37}$$

As before, S, and S_1 are states contributing to the initial target-ion level U. Similarly S'' and S_1'' are states with total angular momentum J_t'' contributing to final ion level U'' with corresponding mixing coefficients $b(U'',S'')$ and $b(U'',S_1'')$. For the simple case where there are only filled subshells in addition to the active subshell a the factor $f(S,S'')$ is given by

$$f(S,S'')=\sqrt{\omega}(j_a^{\omega-1}\alpha_a''J_a''|\}j_a^{\omega}\alpha_aJ_a)\ . \tag{38}$$

Again for more complex cases all that is required is that the right-hand side of Eq. (38) be multiplied by the appropriate one of Eqs. (23)–(25), or for the most complex case considered, by Eq. (25) modified as discussed in connection with Eq. (26).

One might have thought that the summation over S_1 in Eq. (35) would not be necessary due to the $\delta_{j_a j_{a1}}$ in Eq. (34); however, the same orbital transition can occur from different states contributing to the initial ion level. For example, in oxygenlike ions, ionization from the $2p_{3/2}$ subshell can occur from any of the states $(2s_{1/2}^2 2p_{1/2}^2 2p_{3/2}^2)_0$, $(2s_{1/2}^2 2p_{3/2}^4)_0$, and $(2p_{1/2}^2 2p_{3/2}^4)_0$, which all contribute to each of the even-parity levels with $J_t=0$. Also, ionization from $2p_{1/2}$ can occur from the first and last of these three states.

By procedures like that given in the Appendix of Ref. [18], one finds that Eq. (35) also applies for photoionization if the collisional ionization cross sections on both sides of the equation are replaced with corresponding photoionization cross sections. Of course, Eq. (35) applies as well when nonrelativistic calculations have been made and expressed in *jj* coupling notation. The only difference would be that the radial integrals D^λ and E^λ in Eq. (15) would be calculated nonrelativistically. Also in that case the Q_H^{ps} in Eq. (35) becomes independent of j_a and one would usually want results expressed in *LS*-coupling notation. Both of these matters will be discussed in Sec. II C.

C. Modifications for near-neutral atoms or ions

Although our interest here is principally in relativistic results for highly charged ions, the convenient expressions obtained in Sec. II B also apply with slight modification for distorted-wave ionization calculations in general. In particular, we consider here the modifications that may be needed in treating near-neutral atoms and ions of either high or low Z. For such cases there are two kinds of modifications that might be required. One of these is that one might not want to restrict the mixing to states in the same complex. This is especially true if Z is quite large, so that even ionization from the ground level involves ionization from shells with large n for which states with neighboring n values have quite nearly the same energy. The other is that one might want results expressed using *LS*-coupling notation, which is far more familiar to most workers, rather than *jj* coupling notation, which is natural for relativistic calculations.

First we consider inclusion of mixing outside the states in a complex. In this case, Eq. (34) and the argument following it regarding parity still apply, so $j_{a1}=j_a$ and $l_{a1}=l_a$. Thus, the angular part of the calculation is unchanged and Eq. (35) still applies, except that in performing the summation over states in Eq. (35) there will be additional contributions. These are terms in which $Q_H^{ps}(n_a l_a j_a)$ is replaced by $Q_H^{ps}(n_a n_{a1} l_a j_a)$, where the latter is also given by Eqs. (16) and (17), except that $Q^\lambda(n_a l_a j_a)$ is replaced with

$$Q^\lambda(n_a n_{a1} l_a j_a)=\sum_{\substack{l,l',l''\\ j,j',j''}} P^\lambda(n_a l_a j_a \varepsilon l j;\varepsilon'' l'' j'' \varepsilon' l' j') \times P^\lambda(n_{a1} l_a j_a \varepsilon l j;\varepsilon'' l'' j'' \varepsilon' l' j') \ . \tag{39}$$

Now we consider the modifications to Eq. (35) that are required if *LS*-coupling notation is used in place of *jj* coupling. Similar considerations were made in Sec. IV B of Ref. [18] and again we can make use of some of the equations in that reference. Of course, in using *LS* coupling one couples the orbital angular momenta of all electrons in each subshell nl to get a total orbital angular momentum for each subshell. Then these are coupled together successively, working outward from lower to higher subshells until a total orbital angular momentum L_t for the atom or ion is obtained. Similarly, spins are coupled in an analogous manner until total spin S_t is obtained. Then L_t and S_t are coupled to give total angular momentum for the ion J_t. However, for the final state of the ion we use this procedure only for the core, which corresponds to one less electron in the active subshell a. For the final excited electron in the subshell a' we couple l_a' and spin $s_a'=\frac{1}{2}$ to form j_a', as for *jj* coupling, because we will eventually go to the limit that this becomes a free (ejected) electron to give ionization. Then in order to use irreducible tensor techniques to evaluate the reactance matrix, one must recouple the initial ion wave function so that it is coupled in the same way. For the case where there are only filled subshells in addition to the active subshell a, the appropriate equations are given by Eqs. (S,45)–(S,48). Evaluation of the pure or unmixed reactance matrix elements then proceeds as in the *jj* coupling case because it is only the inactive electrons that are *LS* coupled. The final result for the cross section when one proceeds to ionization is given by an equation like Eq. (35)

$$Q(U-U'')=\sum_{j_a} \sum_{\substack{S,S''\\ S_1,S_1''}} B(U,SS_1;U'',S''S_1'')Q_H^{ps}(n_a l_a j_a) \ , \tag{40}$$

where again Eqs. (36) and (37) apply. However, the states S (or S_1) and S'' (or S_1'') contributing to the initial and final ion levels are now pure *LS*-coupled states. Hence, the mixing coefficients now entering Eq. (37) will differ from those in the *jj* coupling case, but the numerical values obtained for $Q(U-U'')$ will be the same if the same physical approximations have been made in the calculations.

Also in the case where *LS* coupling is used, the $f(S,S'')$ in Eq. (37) must be given by

$$f(S,S'')=[(2L_t+1)(2S_t+1)(2J_t''+1)(2j_a+1)]^{1/2} \times\sqrt{\omega}(l_a^{\omega-1}\alpha_a'' L_a'' S_a'' | \} l_a^{\omega}\alpha_a L_a S_a) \times\begin{Bmatrix} L_t'' & l_a & L_t \\ S_t'' & 1/2 & S_t \\ J_t'' & j_a & J_t \end{Bmatrix} , \tag{41}$$

in place of Eq. (38). In Eq. (41) the *LS*-coupling coefficients of fractional parentage (| }) will generally differ from the *jj* coupling ones in Eq. (38). In addition, the initial occupation ω of the active subshell a will usually differ (be larger) for *LS* coupling because the subshell is indicated by $n_a l_a$ instead of $n_a l_a j_a$.

The extra factor in Eq. (41) as compared with Eq. (38) arises from the recoupling of the initial target-ion wave function discussed above Eq. (40) [see Eq. (S,48)]. However, it is important to note that the 9-j in Eq. (41) differs by a phase factor from that in Eq. (S,50) because here we have assumed L is coupled before S, rather than S before L as in Ref. [18].

Of course, Eq. (41) directly applies only when there are filled or empty subshells in addition to the active one. For that case we have used the fact that $L_a = L_t$, $S_a = S_t$, $J_a = J_t$, $L_a'' = L_t''$, $S_a'' = S_t''$, and $J_a'' = J_t''$ in writing the recoupling factor. This was done because this factor then remains unchanged when one considers more complicated cases in which there are partially filled subshells in addition to the active subshell. In such cases additional recoupling of the initial target-ion wave function is necessary in order to use irreducible tensor techniques in determining matrix elements, as considered in Ref. [18] in connection with Eq. (S,54). This results in the right-hand side of Eq. (41) being multiplied by extra factors.

These extra factors are factors like those given by Eqs. (23)–(26) for the similar situation when jj coupling is used, except that for each factor in the jj coupling case there are two factors. These are each exactly like the jj factor except that in one of them spins everywhere replace corresponding total angular momenta and in the other, orbital angular momenta replace corresponding total angular momenta. For example, we consider the case that there are no partially filled higher subshells, but there are lower subshells with total spin S_b and total orbital angular momentum L_b. Then, analogous to Eq. (23) for the similar jj coupling case the extra factor multiplying the right-hand side of Eq. (41) is

$$(-1)^{L_b + l_a + L_a'' + L_t}[(2L_t''+1)(2L_a+1)]^{1/2}\begin{Bmatrix} l_a & L_a'' & L_a \\ L_b & L_t & L_t'' \end{Bmatrix}(-1)^{S_b + 1/2 + S_a'' + S_t}[(2S_t''+1)(2S_a+1)]^{1/2}\begin{Bmatrix} \frac{1}{2} & S_a'' & S_a \\ S_b & S_t & S_t'' \end{Bmatrix} . \tag{42}$$

In this case the initial total orbital and spin angular momenta of the target ion are $L_t = L_{ba}$ and $S_t = S_{ba}$, while the total orbital and spin angular momenta of the final ion are $L_t'' = L_{ba}''$ and $S_t'' = S_{ba}''$. Of course, L_{ba}'' is obtained by coupling L_b to L_a'', and S_{ba}'' is obtained by coupling S_b to S_a''. As is the case of Eq. (35), if mixing is included among states outside the complex, then there will be contributions to Eq. (40) from additional terms in which $Q_H^{ps}(n_a l_a j_a)$ is replaced with $Q_H^{ps}(n_a n_{a1} l_a j_a)$, determined as discussed in connection with Eq. (39).

From comparison of Eqs. (41) and (42) with the analogous Eqs. (38) and (23), it appears that $f(S,S'')$ is considerably more complex when LS coupling is used than when jj coupling is used in writing the basis states. However, there are many more subshells when they are labeled by n, l, and j values, as in jj coupling, than when they are labeled by n and l, as in LS coupling.

When LS-coupling notation is strictly appropriate, the radial functions are calculated nonrelativistically, as in the well-known University College London program, "superstructure" [20], or semirelativistically as in Cowan's well-known program [21]. Then intermediate coupling effects are calculated perturbatively. In either case the radial functions depend only on n and l, rather than on n, l, and j, as in a fully relativistic treatment based on use of the Dirac equation. When the radial functions are independent of j values, the same is true of the Q_H^{ps} or Q_H given by Eqs. (16) and (17). This is considered in the Appendix and leads to Eq. (A10), or when mixing is included among states outside the complex, to Eq. (A10) modified by Eqs. (A13)–(A15).

For very low Z atoms and ions it is well known that pure LS coupling becomes a good approximation. That is, intermediate coupling effects become negligible and the energies of the initial and final ions become independent of J_t and J_t''. Then the only dependence on j_a, J_t'', and J_t is in the f factor given by Eq. (41). Also L_t, S_t, L_t'', and S_t'' are good quantum numbers in this case. Then one can sum Eq. (40) over j_a and J_t'' using [19]

$$\sum_{J_t'', j_a} (2J_t''+1)(2j_a+1)\begin{Bmatrix} L_t'' & l_a & L_t \\ S_t'' & \frac{1}{2} & S_t \\ J_t'' & j_a & J_t \end{Bmatrix}^2 = \frac{1}{(2L_t+1)(2S_t+1)} . \tag{43}$$

This leads to a result for pure LS coupling that has a form like Eq. (35)

$$Q(U-U'') = \sum_{\substack{S,S'' \\ S_1, S_1''}} B(U,SS_1;U'',S''S_1'')Q_H^{ps}(n_a l_a) , \tag{44}$$

where $Q_H^{ps}(n_a l_a)$ is given by Eq. (A10) with, of course, the nonrelativistic radial integrals $D^\lambda(n_a l_a \varepsilon l;\varepsilon'' l'' \varepsilon' l')$ and $E^\lambda(n_a l_a \varepsilon l;\varepsilon'' l'' \varepsilon' l')$ determined using the appropriate potentials for the ion being considered. Also the B in Eq. (44) has the same form as given by Eq. (37), and, if there are only filled subshells in addition to the active one,

$$f(S,S'') = \sqrt{\omega}(l_a^{\omega-1}\alpha_a'' L_a'' S_a'' | \} l_a^{\omega}\alpha_a L_a S_a), \tag{45}$$

which has an appearance like Eq. (38). For more complicated cases this should be multiplied by the appropriate factor discussed in the paragraph containing Eq. (42). If mixing outside a complex is included, similar to the discussion of Eqs. (35) and (40) for this situation, the summation over states in Eq. (44) will include contributions from terms in which $Q_H^{ps}(n_a l_a)$ is replaced with $Q_H^{ps}(n_a n_{a1} l_a)$ given by Eq. (A10) modified by Eqs. (A13)–(A15).

On another topic we note that in applying Eq. (35) to ionization by electron impact in complex cases, where several transitions involve ionization from the same subshell $n_a l_a j_a$, considerable computing time can be saved if for each impact electron energy the $Q_H^{ps}(n_a l_a j_a)$ [and $Q_H^{ps}(n_a n_{a1} l_a j_a)$ if mixing outside a complex is included] are calculated using three values for the transition energy spanning the range of actual transition energies. Then the results for the exact energy of each ionization transition are obtained by Lagrangian interpolation. Our tests indicate that this is accurate to better than 1%. Analogous statements apply to Eqs. (40) and (44).

III. ILLUSTRATIVE RESULTS AND DISCUSSION

With the use of Eq. (35) we have calculated relativistic cross sections for ionization of carbonlike and nitrogenlike uranium and for inner-shell ionization of neonlike xenon initially in an excited level. Results are given in Tables I–III, where comparison is made with corresponding relativistic calculations of Moores and Pindzola [8], made using the multiconfiguration Dirac-Fock (MCDF) approximation [22,23].

The present results were obtained using the more approximate Dirac-Fock-Slater atomic structure program of Ref. [24], but modified, as discussed in Ref. [16], to include the generalized Breit interaction and other QED corrections. In this program the potential V used in Eqs. (4) and (5) determining the radial functions is the Dirac-Fock-Slater potential given by Eqs. (4)–(6) of Ref. [16]. In considering a given class of transitions this potential is determined using a single mean configuration with fractional occupation numbers for some subshells corresponding to approximately splitting the occupation of the active electron between initial and final subshells. For ionization we assume an occupation number of 0.5 for a very high subshell to mock up the effect of the ejected electron. The same potential is used for all electrons, bound and free. Hence, all orbitals are automatically orthogonal and exchange is treated in a consistent manner, which can be important near threshold for some transitions.

The mean configuration used in determining the potential in the present calculations was

$$1s^2 2s^2 2\bar{p}^{\,0.5} 2p^{1.0} 8f^{0.5} \tag{46}$$

for ionization of C-like uranium,

$$1s^2 2s^2 2\bar{p}^{\,0.83} 2p^{1.67} 8f^{0.5} \tag{47}$$

for ionization of N-like uranium, and

$$1s^2 2s^{1.6} 2\bar{p}^{\,1.6} 2p^{3.3} 3s^{0.2} 3\bar{p}^{\,0.2} 3p^{0.2} 3\bar{d}^{\,0.2} 3d^{0.2} 8f^{0.5} \tag{48}$$

for inner-shell ionization of excited Ne-like xenon. Here and in the tables we have used $n\bar{l}$ and nl to indicate nlj with $j=1-\frac{1}{2}$ and $j=l+\frac{1}{2}$, respectively, as done in Ref. [8]. We note that results are insensitive to how a given total occupation is distributed among the subshells of a given shell. Also, they are insensitive to the precise high subshell used to mock up the effect of the ejected electron. For example, replacement of $8f^{0.5}$ with $6f^{0.5}$ or $10f^{0.5}$ had no effect on the results given in the tables.

Ordinarily in considering excitation, as in Refs. [12–17] the same mean configuration is used in determining the potential for the orbitals entering the radial scattering integrals given by Eqs. (2) and (3) and for the bound orbitals entering the analogous integrals that occur in diagonalizing the ion Hamiltonian to determine the energy levels. However, for determining ionization energies we used a different appropriate mean configuration for each ion. For N-like, C-like, and B-like uranium considered in Tables I and II this was $1s^2 2s^2 2\bar{p} 2p^2$, $1s^2 2s^2 2\bar{p}^{\,0.66} 2p^{1.34}$, and $1s^2 2s^2 2\bar{p}^{\,0.34} 2p^{0.66}$, respectively. For excited neonlike xenon considered in Table III, it was

$$1s^2 2s^{1.75} 2\bar{p}^{\,1.75} 2p^{3.5} 3s^{0.2} 3\bar{p}^{\,0.2} 3p^{0.2} 3\bar{d}^{\,0.2} 3d^{0.2} \ ,$$

and for the final F-like ion it was the same except the occupations of the $2s$, $2\bar{p}$, and $2p$ subshells were reduced by 0.25, 0.25, and 0.5, respectively.

TABLE I. Comparison of ionization cross sections for U^{86+}. Present results are labeled SZ. Those of Moores and Pindzola (Ref. [8]) are labeled MP.

	Threshold energy (keV)		Cross section (10^{-24} cm^2) at 2 th.u[a]	
Transition	SZ	MP	SZ	MP
$2\bar{p}^2(0)^{\text{b}} \rightarrow 2\bar{p}(1/2)$	31.06	31.06	43.5	45.2
$2\bar{p}2p(1) \rightarrow 2\bar{p}(1/2)$	27.08	27.08	29.3	31.6
$2\bar{p}2p(2) \rightarrow 2\bar{p}(1/2)$	27.06	27.06	29.3	31.6
$2\bar{p}2p(1) \rightarrow 2p(3/2)$	31.17	31.17	21.7	23.3
$2\bar{p}2p(2) \rightarrow 2p(3/2)$	31.15	31.15	21.7	23.3
$2p^2(2) \rightarrow 2p(3/2)$	27.11	27.11	58.4	62.0
$2p^2(0) \rightarrow 2p(3/2)$	27.02	27.02	58.6	62.0

[a] th.u. stands for threshold units, the incident energy divided by the threshold energy.

[b] Here $n\bar{l}$ and nl mean nlj with $j=l-\frac{1}{2}$ and $j=l+\frac{1}{2}$, respectively. The quantity in parentheses is the total angular momentum of the ion.

TABLE II. Comparison of ionization cross sections for U^{85+}. Notation as in Table I.

	Threshold energy (keV)		Cross section (10^{-24} cm^2) at 2 th.u	
Transition	SZ	MP	SZ	MP
$2\bar{p}^2 2p(3/2)\rightarrow 2\bar{p}^2(0)$	26.59	26.59	30.2	31.4
$2\bar{p}^2 2p(3/2)\rightarrow 2\bar{p}2p(1)$	30.57	30.57	16.8	17.4
$2\bar{p}^2 2p(3/2)\rightarrow 2\bar{p}2p(2)$	30.59	30.59	28.0	29.1
$2\bar{p}2p^2(3/2)\rightarrow 2\bar{p}2p(1)$	26.63	26.63	45.3	47.0
$2\bar{p}2p^2(3/2)\rightarrow 2\bar{p}2p(2)$	26.65	26.65	15.1	15.7
$2\bar{p}2p^2(5/2)\rightarrow 2\bar{p}2p(1)$	26.61	26.61	7.6	7.8
$2\bar{p}2p^2(5/2)\rightarrow 2\bar{p}2p(2)$	26.63	26.63	52.8	54.8
$2\bar{p}2p^2(1/2)\rightarrow 2\bar{p}2p(1)$	26.53	26.53	22.7	23.5
$2\bar{p}2p^2(1/2)\rightarrow 2\bar{p}2p(2)$	26.55	26.55	37.9	39.1
$2\bar{p}2p^2(3/2)\rightarrow 2p^2(2)$	30.69	30.69	22.3	23.2
$2\bar{p}2p^2(5/2)\rightarrow 2p^2(2)$	30.67	30.67	22.3	23.2
$2\bar{p}2p^2(1/2)\rightarrow 2p^2(0)$	30.68	30.68	22.3	23.2
$2p^3(3/2)\rightarrow 2p^2(2)$	26.63	26.63	75.5	78.0
$2p^3(3/2)\rightarrow 2p^2(0)$	26.72	26.72	15.1	15.6

It should be emphasized that the mean configurations are used solely in determining the potentials to be used in calculating the radial functions with Eqs. (3) and (4) or the analogs for free electrons, and that basically the calculations are multiconfiguration calculations. Usually we include all the mixing among the states in a complex. This was done in making the present calculations, but for comparison purposes calculations were also made with the more limited amount of mixing included by Moores and Pindzola [8]. Hence, our values given in Tables I and II and the SZ2 entries in Table III were calculated the latter way. For ionization of C-like and N-like uranium, as noted in Ref. [8], configuration mixing has very little effect, and we found the cross sections to be changed by less than 1%, usually much less, when mixing among all states in a complex was included. However, this is not true for the more complex case of inner-shell ionization of excited neonlike xenon for which results are given in Table III. The MP and SZ2 values in the table were obtained including only the mixing of the $2s^2 2\bar{p}^2 2p^3 3s$ and $2s^2 2\bar{p}2p^4 3s$ states with $J_t=1$ for the initial ion and the $2s^2 2\bar{p}^2 2p^2 3s$, $2s^2 2\bar{p}2p^3 3s$, and $2s^2 2p^4 3s$ states with $J_t''=\frac{1}{2}$ for the final ion. Actually as given in Table I of Ref. [24] and Ref. [16] there are seven states contributing to the initial levels and 15 contributing to the final levels of these transitions when all mixing within a complex is included. This was done in obtaining the SZ1 entries and one sees by comparison SZ1 and SZ2 entries that this has a significant effect on ionization cross sections for some transitions.

For the MP and SZ2 entries in Tables I and II, where mixing was allowed among the same sets of states in both sets of calculations, the differences in physical approximations made in the two sets of calculations are of two kinds. These are that (i) different potentials were used in calculating the radial functions with Eqs. (3) and (4) and their analogs for free electrons in the two sets of calculations, and (ii) the Breit interaction was included in calculating the scattering matrix elements in the MP calculations, while it was not in the present calculations. As found in Refs. [5] and [8], the effect of (ii) is generally small for ionization unless very high impact electron energies ($\gtrsim 250$ keV) are considered. Of course, this effect is most likely to be important for high Z. It may be the principal reason for the differences in Tables I and II between SZ and MP entries, which are rather small. For ionization of Xe^{44+} considered in Table III the agreement between MP and SZ2 entries is also quite good, but worse than the agreement for U^{86+} and U^{85+}. In the case Xe^{44+}, with a lower Z and larger number of bound electrons, the differences are probably mostly due to the effect of (i).

TABLE III. Comparison of ionization cross sections for Xe^{44+}. Notation as in Table I except that SZ1 and SZ2 designate present results obtained with inclusion of all mixing in a complex and with the more limited amount of mixing included by MP, respectively.

				Cross section (10^{-24} cm^2)					
	Threshold energy (keV)			1.25 th.u			1.50 th.u		
Transition	SZ1	SZ2	MP	SZ1	SZ2	MP	SZ1	SZ2	MP
$2\bar{p}^2 2p^3 3s(1)\rightarrow 2\bar{p}^2 2p^2 3s(1/2)$	7.81	7.81	7.81	92	92	75	132	133	140
$2\bar{p}^2 2p^3 3s(1)\rightarrow 2\bar{p}2p^3 3s(1/2)$	8.11	8.11	8.12	111	112	120	160	162	160
$2\bar{p}^2 2p^3 3s(1)\rightarrow 2p^4 3s(1/2)$	8.47	8.47	8.48	0.17	0.24	0.31	0.24	0.35	0.44
$2\bar{p}2p^4 3s(1)\rightarrow 2\bar{p}^2 2p^2 3s(1/2)$	7.48	7.48	7.48	0.38	0.51	0.48	0.55	0.73	0.69
$2\bar{p}2p^4 3s(1)\rightarrow 2\bar{p}2p^3 3s(1/2)$	7.78	7.78	7.78	99	124	130	142	178	180
$2\bar{p}2p^4 3s(1)\rightarrow 2p^4 3s(1/2)$	8.14	8.14	8.15	91	168	170	131	241	250

Finally, we note that a program for computing cross sections for ionization to specific magnetic sublevels of the final ion has been written [26]. This was also used to calculate numerical results for the total ionization cross sections for the transitions considered in the tables. Agreement with the results calculated with Eq. (35) was obtained to four or five significant figures. Since the same physical approximations are used, but the angular parts of calculations are done in completely different ways, this is a good check that no errors were made in either computer program.

IV. SUMMARY AND CONCLUSIONS

The factorization method of Bar-Shalom, Klapisch, and Oreg [10] for excitation has been extended to ionization by electron impact. This leads to a very large simplification for complex ions. If the mixing is confined to that among states in a complex, as is usually valid for highly charged ions, the ionization cross section reduces to a very simple form. This is Eq. (35) for *jj* coupling notation, as appropriate for relativistic calculations, Eq. (40) for *LS*-coupling notation, and Eq. (44) for pure *LS* coupling, in which intermediate coupling effects are negligible. In these equations the *B* factors, which depend only on target-ion properties such as mixing coefficients and angular momenta, are very readily calculated. The $Q_H^{ps}(n_a l_a j_a)$ or $Q_H^{ps}(n_a l_a)$ are ionization cross sections of exactly the same form as those for hydrogenic ions given by Eqs. (16) and (17) or Eq. (A10), except that the radial integrals D^λ and E^t should be evaluated using radial functions calculated with potentials appropriate for the particular ion being considered.

If mixing is included with states outside the complex, the results are nearly as simple. The only difference is there will be additional contributions in the summation over states in Eqs. (35), (40), or (44) that involve terms with $Q_H^{ps}(n_a l_a j_a)$ or $Q_H^{ps}(n_a l_a)$ replaced with $Q_H^{ps}(n_a n_{a1} l_a j_a)$ or $Q_H^{ps}(n_a n_{a1} l_1)$, which are determined as described in the discussion regarding Eq. (39) or Eqs. (A13)–(A15).

It is of interest to point out that these results apply, as well, to photoionization, if collision cross sections are everywhere replaced with corresponding photoionization cross sections. We also note that it was shown in the Appendix of Ref. [26] that a result like Eq. (35) applies in special cases, but it was not realized that it applies in general when mixing is confined to the states in a complex.

In addition to the fact that Eqs. (35), (40), and (44) are well suited for rapid calculations of ionization cross sections, they have the additional advantage that, when the Q_H^{ps} are expressed in terms of "reduced cross sections," it appears that simple fits convenient for plasma modeling calculations can be made. In particular, as discussed in Ref. [9], it appears that the "reduced cross section" can be fitted to simple functions of the impact electron energy in threshold units, like those made to nonrelativistic Coulomb-Born-exchange results in Ref. [27], but with coefficients that are slowly varying functions of *Z* and *N* or an effective *Z*.

Results with the program based on Eq. (35) were compared in Tables I–III with recent relativistic distorted-wave calculations of Moores and Pindzola [8]. The agreement was found to be quite good when the same degree of mixing was allowed. The fairly small differences in results for these cases could be attributed to the fact that different potentials were used in calculating the radial functions and that the Breit interaction was included in calculating the scattering matrix elements in Ref. [8], while it was not in the present calculations.

As an additional check on Eq. (35), another relativistic distorted-wave ionization program [25], which is based on the very different and more lengthy formation of the angular part of the calculation needed for calculating ionization to specific magnetic sublevels, was also used to calculate ionization cross sections for the cases considered in the tables. The two methods, which use the same physical approximations, gave exactly (to within 4 or 5 significant figures) the same numerical results.

ACKNOWLEDGMENTS

We wish to thank Robert E. H. Clark for discussions regarding needs for near neutral atoms and ions, including *LS*-coupling results and results when mixing outside a complex is included. This work was supported in part by the Innovative Science and Technology Office of the Strategic Defense Initiative Organization and by the U.S. Department of Energy under Grant No. DE-FG02-90ER54104 and a Lawrence Livermore National Laboratory Subcontract.

APPENDIX

Here we outline the demonstration that the $Q_H(n_a l_a j_a)$ given by Eqs. (16) and (17) becomes independent of the *j* value when the radial functions are independent of the *j* value, as one would expect to be true. Of course, in this case the radial integrals are independent of the *j* value,

$$D^\lambda(n_a l_a j_a \varepsilon l j;\varepsilon'' l'' j'' \varepsilon' l' j') \rightarrow D^\lambda(n_a l_a \varepsilon l;\varepsilon'' l'' \varepsilon' l') , \tag{A1}$$

$$E^\lambda(n_a l_a j_a \varepsilon l j;\varepsilon'' l'' j'' \varepsilon' l' j') \rightarrow E^\lambda(n_a l_a \varepsilon l;\varepsilon'' l'' \varepsilon' l') . \tag{A2}$$

Then one needs to show that when this is true the angular part of Eq. (16) also becomes independent of *j* values. In doing this, instead of using Eq. (11), one uses the more lengthy form [19]

$$\begin{aligned}\langle j_1 \| C^\lambda \| j_2 \rangle &= \langle l_1 \tfrac{1}{2} j_1 \| C^\lambda \| l_2 \tfrac{1}{2} j_2 \rangle \\ &= (-1)^{j_2+l_1+1/2+\lambda}[(2j_1+1)(2j_2+1)]^{1/2} \\ &\quad \times \begin{Bmatrix} l_1 & \lambda & l_2 \\ j_2 & \frac{1}{2} & j_1 \end{Bmatrix} \langle l_1 \| C^\lambda \| l_2 \rangle \end{aligned} \tag{A3}$$

for the angular factors in the application of Eq. (15) with $n_a' l_a' j_a' \rightarrow \varepsilon'' l'' j''$ to Eq. (17) for ionization. Also we write

$$\sum_{\lambda} Q^{\lambda} = \sum_{\lambda} Q_d^{\lambda} + \sum_{\lambda} Q_{\rm int}^{\lambda} + \sum_{\lambda} Q_{\rm ex}^{\lambda} \ , \tag{A4}$$

where the first part comes from the square of the part of P^{λ} [see Eq. (15)] proportional to D^{λ}, the second part is the interference part due to cross terms proportional to $D^{\lambda}E^{t}$, and the last part is the pure exchange part involving terms proportional to $E^{t}E^{t'}$. We consider the latter first and use [19]

$$\sum_{\lambda}(2\lambda+1)\begin{Bmatrix} j_a & j' & t \\ j & j'' & \lambda \end{Bmatrix}\begin{Bmatrix} j_a & j' & t' \\ j & j'' & \lambda \end{Bmatrix} = \frac{\delta_{tt'}}{2t+1} \ , \tag{A5}$$

$$\sum_{j'}(2j'+1)\begin{Bmatrix} l_a & t & l' \\ j' & \frac{1}{2} & j_a \end{Bmatrix}^2 = \frac{1}{2l_a+1} \ ;$$

$$\sum_{j''}(2j''+1)\begin{Bmatrix} l & t & l'' \\ j'' & \frac{1}{2} & j \end{Bmatrix}^2 = \frac{1}{2l+1} \ , \tag{A6}$$

and

$$\sum_{j}(2j+1) = 2(2l+1) \ . \tag{A7}$$

This leads to

$$\sum_{\lambda} Q_{\rm ex}^{\lambda} = \frac{2(2j_a+1)}{(2l_a+1)} \sum_{t} \sum_{l,l',l''} \frac{1}{2t+1} \times [E^{t}(n_a l_a \varepsilon l; \varepsilon'' l'' \varepsilon' l') \times \langle l_a \| C^{t} \| l' \rangle \langle l \| C^{t} \| l'' \rangle]^2 \ . \tag{A8}$$

A very similar result is obtained for the "direct" part, the first part of Eq. (A4), by summing over j' and j'' using equations analogous to Eqs. (A6) and then using Eq. (A7). The interference terms, which involve a product of five 6-j's is most difficult to evaluate. By introducing a factor $(-1)(-1)^{2j'}$, which equals unity because j' is a half integer, one can perform the summation over j' and express the product of three of the 6-j's as a 9-j in analogy to Eq. (S,38). Then the product of this and one of the remaining 6-j's can be summed over j to lead to a product of two 6-j's in analogy to Eq. (S,42). One of these equals the remaining of the original 6-j's. These two are then eliminated by summing over j''. Specifically,

$$\sum_{j''}(2j''+1)\begin{Bmatrix} l_a & \lambda & l'' \\ j'' & \frac{1}{2} & j_a \end{Bmatrix}^2 = \frac{1}{2l_a+1} \ . \tag{A9}$$

Finally, applying all these to Eq. (16) one finds that, when the radial functions are independent of j values, it reduces to

$$\begin{aligned} &Q_H(n_a l_a j_a - n_a' l_a' j_a') \rightarrow Q_H(n_a l_a) \\ &= \frac{16 a_0^2}{(2l_a+1)k^2} \int_0^{(\varepsilon - I)/2} d\varepsilon'' \sum_{l,l',l''} \Bigg[\sum_{\lambda} \frac{1}{2\lambda+1} D^{\lambda}(n_a l_a \varepsilon l; \varepsilon'' l'' \varepsilon' l')^2 [\langle l_a \| C^{\lambda} \| l'' \rangle \langle l \| C^{\lambda} \| l' \rangle]^2 \\ &\qquad - \sum_{\lambda} \sum_{t} (-1)^{\lambda+t} D^{\lambda}(n_a l_a \varepsilon l; \varepsilon'' l'' \varepsilon' l') E^{t}(n_a l_a \varepsilon l; \varepsilon'' l'' \varepsilon' l') \\ &\qquad \times \begin{Bmatrix} l' & l & \lambda \\ l'' & l_a & t \end{Bmatrix} \langle l_a \| C^{\lambda} \| l'' \rangle \langle l \| C^{\lambda} \| l' \rangle \langle l_a \| C^{t} \| l' \rangle \langle l \| C^{t} \| l'' \rangle \\ &\qquad + \sum_{t} \frac{1}{2t+1} E^{t}(n_a l_a \varepsilon l; \varepsilon'' l'' \varepsilon' l')^2 [\langle l_a \| C^{t} \| l' \rangle \langle l \| C^{t} \| l'' \rangle]^2 \Bigg] \ , \end{aligned} \tag{A10}$$

where

$$\langle l_1 \| C^{\lambda} \| l_2 \rangle = (-1)^{l_1} [(2l_1+1)(2l_2+1)]^{1/2} \begin{pmatrix} l_1 & \lambda & l_2 \\ 0 & 0 & 0 \end{pmatrix} \ . \tag{A11}$$

We note that Eq. (A10) is consistent with Eq. (S,24) for excitation to a high level $n_a' l_a'$, except that in the interference part of Eq. (S,24) the factor $\langle l_a \| C^{\lambda} \| l' \rangle \langle l \| C^{\lambda} \| l_a' \rangle$ should have been replaced with

$$\begin{Bmatrix} l' & l & \lambda \\ l_a' & l_a & \lambda' \end{Bmatrix} \langle l_a \| C^{\lambda'} \| l' \rangle \langle l \| C^{\lambda'} \| l_a' \rangle \ . \tag{A12}$$

Of course, if mixing is included with states outside a complex, similar to the discussion connected with Eq. (39), there will be additional contributions to the summation over states in Eq. (40). These are terms in which $Q_H^{ps}(n_a l_a j_a)$ is replaced with $Q_H^{ps}(n_{a1} l_a j_a)$, but, if the radial functions do not depend on the j value, this reduces to $Q_H^{ps}(n_a n_{a1} l_a)$ given by Eq. (A10) with the replacements

$$D^{\lambda}(n_a l_a \varepsilon l; \varepsilon'' l'' \varepsilon' l')^2 \rightarrow D^{\lambda}(n_a l_a \varepsilon l; \varepsilon'' l'' \varepsilon' l') D^{\lambda}(n_{a1} l_a \varepsilon l' \varepsilon'' l'' \varepsilon' l') \ , \tag{A13}$$

$$\begin{aligned} &D^{\lambda}(n_a l_a \varepsilon l;\varepsilon'' l'' \varepsilon' l')E^{t}(n_a l_a \varepsilon l;\varepsilon'' l'' \varepsilon' l') \\ &\quad \rightarrow \tfrac{1}{2}[D^{\lambda}(n_a l_a \varepsilon l;\varepsilon'' l'' \varepsilon' l')E^{t}(n_{a1} l_a \varepsilon l;\varepsilon'' l'' \varepsilon' l')+D^{\lambda}(n_{a1} l_a \varepsilon l;\varepsilon'' l'' \varepsilon' l')E^{t}(n_a l_a \varepsilon l j;\varepsilon'' l'' j'' \varepsilon' l' j')]\ , \end{aligned} \tag{A14}$$

and

$$E^{t}(n_a l_a \varepsilon l;\varepsilon'' l'' \varepsilon' l')^2 \rightarrow E^{t}(n_a l_a \varepsilon l;\varepsilon'' l'' \varepsilon' l')E^{t}(n_{a1} l_a \varepsilon l;\varepsilon'' l'' \varepsilon' l')\ . \tag{A15}$$

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