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Relativistic cross sections for excitation of highly charged ions to specific magnetic sublevels by an electron beam

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A program has been developed for making calculations of fully relativistic distorted-wave cross sections for excitation of highly charged ions to specific magnetic sublevels M_f by a beam of electrons. The approach uses the same Dirac-Fock-Slater potential for all electrons and is expected to be accurate for nuclear charge number $Z \gtrsim 2.5N$, where N is the number of bound electrons per ions. To our knowledge there is at present no other fully relativistic program available with which we could compare results for this type of cross section. However, the present results for He-like, Li-like, and Ne-like iron and for Ne-like molybdenum are compared with other partially relativistic results, and generally good agreement is obtained for these ions. It is expected that the present program will be useful for comparison with and interpretation of experimental results for very highly charged ions, such as those obtained in electron-beam ion-trap experiments at Livermore [R. E. Marrs *et al.*, Phys. Rev. Lett. **60**, 1715 (1988)].

I. INTRODUCTION

There has been considerable interest in the cross sections for excitation of very highly charged ions by electron impact for the purpose of determining the populations of the energy levels of such ions and predicting the emergent spectra from both laboratory and astrophysical high-temperature plasmas. For such purposes, at least if the electron distribution function is isotropic, it is only necessary to know the total excitation cross sections. However, for comparisons with experiment, more detailed cross sections are often required. For example, if the measurements involve the detection of the fluorescence radiation produced by ions excited by a directive electron beam, the results depend on the cross sections for excitation to the specific magnetic sublevels of the target ions.[1-3] These cross sections are also needed in studying the emission from plasmas with an anisotropic electron distribution function, as noted by Inal and Dubau.[1]

Recently several authors have made calculations of the cross sections for excitation to specific magnetic sublevels of the target ion.[1-3] Mitroy[2] and Mitroy and Norcross[3] have done so using a nonrelativistic *LS*-coupling approach. Inal and Dubau[1] have considered the more highly charged ions Fe^{23+} and Fe^{24+} and have also used nonrelativistic radial functions, but they included intermediate-coupling effects though a perturbative treatment of relativistic interactions in the atomic structure calculations. Specifically, they have made distorted-wave calculations using the well-known programs of Eissner and co-workers and Seraph[4-6] modified to give cross sections for excitation to specific magnetic sublevels. In the present work we have developed a fully relativistic distorted-wave program for calculating cross sections for excitation to specific magnetic sublevels of highly charged ions with moderate to very high values for the nuclear charge number Z. Our work was motivated by the recent electron-beam ion-trap (EBIT) experiments at Livermore.[7] In these experiments cross sections for Ba^{46+} were measured and it is anticipated that results for ions with even considerably higher values of Z will be obtained in future EBIT experiments.[8,9] For such high-Z ions a fully relativistic approach is necessary for accurate calculations of the cross sections.

To our knowledge no other fully relativistic code for calculating cross sections for excitation to the magnetic sublevels of the target ion exists with which we could compare results. However, after outlining the theory of the present approach in the next section, in Sec. III we give a sample of our results and make comparisons of them with the results for moderate values of Z by other largely nonrelativistic or semirelativistic approaches.

II. THEORY

Cross sections with any degree of detail can be determined if the scattering amplitude is given. Following Rose,[10] Carse and Walker,[11] and Walker,[12] we can define a relativistic amplitude $B^{m_{si}}_{m_{sf}}$ for scattering an electron with spin m_{si}, wave number k_i, and direction $\hat{\mathbf{k}}_i$ into direction $\hat{\mathbf{k}}_f$ with wave number k_f and final spin m_{sf} accompanied by change in the state of the target ion from $\beta_i J_i M_i$ to $\beta_f J_f M_f$,

$$B_{m_{sf}}^{m_{si}}=\frac{2\pi}{k_i}\sum_{\substack{l_i,m_{li},j_i,m_i\\ l_f,m_{lf},j_f,m_f}}(i)^{l_i-l_f+1}\exp[i(\delta_{\kappa i}+\delta_{\kappa f})]Y_{l_i}^{m_{li}*}(\hat{\mathbf{k}}_i)Y_{l_f}^{m_{lf}}(\hat{\mathbf{k}}_f)C(l_i\tfrac{1}{2}m_{li}m_{si};j_im_i)C(l_f\tfrac{1}{2}m_{lf}m_{sf};j_fm_f)T(\alpha_i,\alpha_f)\ . \tag{1}$$

Here $T(\alpha_i,\alpha_f)$ is an element of the relativistic T matrix with

$$\alpha_i=k_il_ij_im_i\beta_iJ_iM_i,\quad \alpha_f=k_fl_fj_fm_f\beta_fJ_fM_f\ , \tag{2}$$

in which β_i designates all quantum numbers required to specify the initial state of the target ion in addition to the quantum numbers J_i and M_i corresponding to the total angular momentum of the ion and its z component, respectively. The quantity β_f has similar meaning for the final state. The Y's and C's are spherical harmonics and Clebsch-Gordan coefficients, respectively. The phase factors δ_{κ_i} and δ_{κ_f}, which contain the so-called Coulomb phase factor plus the modification of it due to the departure of the potential from a pure Coulomb potential for small r, are discussed in the Appendix. The κ_i and κ_f are initial and final values for the relativistic quantum number κ, which is related to the orbital and total angular momentum quantum numbers l and j for the free electron by the well-known relations

$$\kappa=-l-1,\quad j=l+1/2\ , \tag{3}$$

$$\kappa=l,\quad j=l-1/2\ . \tag{4}$$

It is convenient to choose the z axis to be in the direction $\hat{\mathbf{k}}_i$ of the impact electron. Then $m_{li}=0$ and

$$Y_{l_i}^{m_{li}*}(\hat{\mathbf{k}}_i)\rightarrow\left[\frac{2l_i+1}{4\pi}\right]^{1/2}\ . \tag{5}$$

Also we express the T matrix in terms of the reactance matrix R,

$$T=\frac{-2iR}{1-iR}\simeq-2iR\ , \tag{6}$$

where the final approximation, which we use, gives ununitarized cross sections. As is well known, this is a very good approximation in treating highly charged ions, for which the elements of the R matrix are much less than unity. In addition, we use the reactance matrix elements $R(\gamma_i,\gamma_f)$ in the totally coupled representation because we want to use the values calculated with the relativistic distorted-wave program of Zhang, Sampson, and Mohanty,[13] which uses the completely coupled representation. The relation between these is

$$R(\alpha_i,\alpha_f)=\sum_{J,M}C(J_ij_iM_im_i;JM)C(J_fj_fM_fm_f;JM)\times R(\gamma_i,\gamma_f)\ , \tag{7}$$

where

$$\gamma_i=k_il_ij_i\beta_iJ_iJM,\quad \gamma_f=k_fl_fj_f\beta_fJ_fJM\ , \tag{8}$$

in which J and M are the quantum numbers corresponding to the total angular momentum of the complete system, target ion plus free electron, and its z component, respectively. It turns out that the $R(\gamma_i,\gamma_f)$ are independent of M. Now applying all this to Eq. (1) we obtain

$$B_{m_{sf}}^{m_{si}}=\frac{2\pi^{1/2}}{k_i}\sum_{\substack{l_i,j_i,m_i\\ l_f,m_{lf},j_f,m_f}}\sum_{J,M}(i)^{l_i-l_f}(2l_i+1)^{1/2}\exp[i(\delta_{\kappa_i}+\delta_{\kappa_f})]Y_{l_f}^{m_{lf}}(\hat{\mathbf{k}}_f)C(l_i\tfrac{1}{2}0m_{si};j_im_i)$$
$$\times C(l_f\tfrac{1}{2}m_{lf}m_{sf};j_fm_f)C(J_ij_iM_im_i;JM)C(J_fj_fM_fm_f;JM)R(\gamma_i,\gamma_f)\ , \tag{9}$$

where, of course, m_i must equal m_{si} because $m_{li}=0$.

For unpolarized electrons, for which one can average over initial spins and sum over final spins, the differential cross section is given by

$$\frac{dQ}{d\hat{k}_f}=\tfrac{1}{2}\sum_{m_{si},m_{sf}}|B_{m_{sf}}^{m_{si}}|^2 \tag{10}$$

and the total cross section for the transition $\alpha_iJ_iM_i\rightarrow\alpha_fJ_fM_f$ is given by

$$Q(\beta_iJ_iM_i\rightarrow\beta_fJ_fM_f)=\tfrac{1}{2}\sum_{m_{si},m_{sf}}\int|B_{m_{sf}}^{m_{si}}|^2d\hat{\mathbf{k}}_f\ . \tag{11}$$

When Eq. (9) is substituted into Eq. (11) some simplification occurs because

$$\int Y_{l'_f}^{m_{l'f}*}(\hat{\mathbf{k}}_f)Y_{l_f}^{m_{lf}}(\hat{\mathbf{k}}_f)d\hat{\mathbf{k}}_f=\delta_{m_{l'f}m_{lf}}\delta_{l'_fl_f}\ . \tag{12}$$

Then after performing the summation over $m_{l'f}$ and l'_f one can use

$$\sum_{m_{sf},m_{lf}} C(l_f\tfrac{1}{2}m_{lf}m_{sf};j_f'm_f')C(l_f\tfrac{1}{2}m_{lf}m_{sf};j_fm_f)=\delta_{j_f'j_f}\delta_{m_f'm_f} \tag{13}$$

so the dependence of Eq. (11) on the final phase factor δ_{κ_f} drops out. The detailed result is

$$\begin{aligned} Q(\beta_iJ_iM_i\to\beta_fJ_fM_f)=\frac{2\pi}{k_i^2}\sum_{\substack{l_i,l_i',j_i,j_i'\\ m_{si},l_f,j_f,m_f}}\ \sum_{J,J'M}&(i)^{l_i-l_i'}[(2l_i+1)(2l_i'+1)]^{1/2}\exp[i(\delta_{\kappa_i}-\delta_{\kappa_i'})]\\ &\times C(l_i\tfrac{1}{2}0m_{si};j_im_i)C(l_i'\tfrac{1}{2}0m_{si};j_i'm_i)C(J_ij_iM_im_i;JM)\\ &\times C(J_ij_i'M_im_i;J'M)C(J_fj_fM_fm_f;JM)C(J_fj_fM_fm_f;J'M)\\ &\times R(\gamma_i,\gamma_f)R(\gamma_i',\gamma_f')\ , \end{aligned} \tag{14}$$

where γ'_f differs from γ_f only in that J' replaces J, and γ_i' differs from γ_i only in that J', l_i' and j_i' replace J, l_i, and j_i, respectively.

For initially randomly orientated target ions, the case of interest here, one can average over initial magnetic sublevels M_i of the target ion and obtain the result for the cross section for excitation to a specific final magnetic sublevel M_f,

$$Q(\beta_iJ_i\to\beta_fJ_fM_f)=\frac{1}{2J_i+1}\sum_{M_i}Q(\alpha_iJ_iM_i\to\alpha_fJ_fM_f)\ , \tag{15}$$

where the cross section on the right-hand side is given by Eq. (14). As a partial check on Eq. (14) one can see if it leads to the correct total cross section $Q(\beta_iJ_i\to\beta_fJ_f)$ obtained by summing Eq. (15) over M_f. When this is done the summation over M_f and m_f eliminates the last two Clebsch-Gordan coefficients in Eq. (14) by the analog of Eq. (13). Next one can remove the middle two by performing the sum over M_i and M, and finally one can eliminate the first two by performing the summation over $m_{si}=m_i$. The result obtained is indeed the correct well-known expression

$$\begin{aligned} &Q(\beta_iJ_i\to\beta_fJ_f)\\ &\quad=\frac{2\pi}{(2J_i+1)k_i^2}\sum_{\substack{l_i,l_f\\ j_i,j_f}}\sum_J(2J+1)|R(\gamma_i,\gamma_f)|^2\ . \end{aligned} \tag{16}$$

Before proceeding to give some sample numerical results and to compare them with other work, we say a few words about the method used to calculate the relativistic reactance matrix elements $R(\gamma_i,\gamma_f)$. As noted previously, this is done using the approach and code of Zhang, Sampson, and Mohanty,[13] which uses the atomic structure data of Sampson, Zhang, Mohanty, and Clark.[14] Specifically, the $R(\gamma_i,\gamma_f)$ are equal to 2 times the matrix element in Eq. (3) of Ref. 13, which is calculated using the wave functions given by Eqs. (5) and (6) of Ref. 13. These are constructed from orbitals for both the bound and free electrons that are solutions of the Dirac equation for the same central potential. Hence, all orbitals, bound and free, are automatically orthogonal. Specifically, this potential is the relativistic Hartree-Fock-Slater, or so-called Dirac-Fock-Slater potential given in rydbergs by

$$V(r)=-\frac{2Z}{r}+V_c(r)-\left[\frac{24}{\pi}\rho(r)\right]^{1/3}\ , \tag{17}$$

where the term $(-2Z/r)$ is the contribution due to the nuclear charge. The $V_c(r)$ term is the spherically averaged classical potential due to the bound electrons

$$V_c(r)=\sum_{n'\kappa'}w_{n'\kappa'}\int_0^\infty\frac{2}{r_>}[P_{n'\kappa'}^2(r_2)+Q_{n'\kappa'}^2(r_2)]dr_2\ , \tag{18}$$

in which $w_{n'\kappa'}$ is the occupation number of subshell $n'\kappa'=n'l'j'$, the summation is over all occupied subshells, $r_>$ is the greater of r and r_2, and $P_{n'\kappa'}$ and $Q_{n'\kappa'}$ are the so-called large and small components of the radial function of an electron in the $n'\kappa'$ subshell. The final term in Eq. (17) is the exchange energy of an electron in a free-electron gas of density $\rho(r)$ averaged over all possible momenta of the electron and with the Kohn-Sham[15] value for the numerical coefficient. Following Slater[16] we use for $\rho(r)$ the number density of the bound electrons at distance r from the nucleus. The spherically averaged value for this is

$$\rho(r)=\frac{1}{4\pi r^2}\sum_{n'\kappa'}w_{n'\kappa'}[P_{n'\kappa'}^2(r)+Q_{n'\kappa'}^2(r)]\ . \tag{19}$$

We note that in applying Eqs. (17)–(19) to determine the radial function for the bound electrons in a particular subshell $n\kappa$ the potential given by the first two terms on the right-hand side of Eq. (17) would be the relativistic Hartree potential, if in Eq. (18) $w_{n'\kappa'}$ were replaced with $w_{n'\kappa'}-1$ when $n'\kappa'=n\kappa$. The undesirable feature that $V_c(r)$ given by Eq. (18) contains self-interaction is at least partially canceled out by the fact that with the use of Eq. (19) self-exchange energy is also included in Eq. (17).

In determining the potential with Eqs. (17)–(19) we used a single mean configuration with noninteger occupation numbers for some subshells. For example, in the calculations of excitation from the ground levels of He- and Li-like ions to the levels of the $1s2p$ and $1s2s2p$ configurations, for which numerical results are given in the next section, we used the mean configurations

$$1s^{1.5}2p_{1/2}^{0.25}2p_{3/2}^{0.25} \tag{20}$$

and

$$1s^{1.5}2s^{1.0}2p_{1/2}^{0.25}2p_{3/2}^{0.25}\ , \tag{21}$$

respectively, in determining the potential with Eqs. (17)–(19). Similarly in calculating the results for the optically allowed transitions from the ground level to the $n=3$ levels in neonlike ions also given in the next section we used the mean configuration

$$1s_{1/2}^{2}2s_{1/2}^{1.9}2p_{1/2}^{1.9}2p_{3/2}^{3.7}3s_{1/2}^{0.1}3p_{1/2}^{0.1}3p_{3/2}^{0.1}3d_{3/2}^{0.1}3d_{5/2}^{0.1}\ . \tag{22}$$

In each of these cases the choice can be regarded as equal splitting of the occupation of the active electron between initial and final shells. Actually test cases[13,14] have indicated that slight changes in the mean configuration used in determining the potential have little effect on results.

It should be noted that the mean configuration is used solely in determining the potential with Eqs. (17)–(19). Generally we include at least all the mixing among the states in a complex, i.e., having the same set of n values, parity, and J value. The results given in the next section include only the complete mixing among the states in each complex.

Finally we note that comparisons made in Ref. 13 and 14 indicate that for such things as oscillator strengths and total collision strengths results by the present approach are essentially as accurate as those by the most elaborate relativistic programs now available when $Z \gtrsim 2.5N$, where N is the number of bound electrons per ion.

III. NUMERICAL RESULTS AND DISCUSSION

To our knowledge there are no other fully relativistic results, i.e., results based on the Dirac equation, available for excitation to specific magnetic sublevels with which we can make comparison. However, we can make comparison with the results of Inal and Dubau[1] for excitation from the ground levels of He- and Li-like iron to the levels of the $1s2p$ and $1s2s2p$ configurations. This is done in Tables I and II. Also we could include comparison with the results obtained with the program of Clark *et al.*,[17] which is based on the distorted-wave method of Mann.[18] This uses the atomic structure data generated with the program of Abdallah, Clark, and Cowan,[19] which in turn is based on Cowan's Hartree-Fock approach.[20] The physics involved in their method is similar to that of Inal and Dubau[1] (briefly discussed in Sec. I) except that the Hartree-Fock potential is used in place of a scaled Thomas-Fermi-Dirac potential and the relativistic mass-velocity and Darwin terms are included in the Hamiltonian determining the bound orbitals. Then the only relativistic interaction they treat perturbatively is the spin-orbit interaction.

TABLE I. Comparison of results for the collision strengths for excitation from the ground level to the magnetic sublevels M_f of various $1s2p$ levels in He-like iron. In each case upper entries are present fully relativistic values, second entries are from the code of Ref. 17, and third entries are from Ref. 1. Numbers in the square brackets are powers of 10 by which adjacent entries should be multiplied. All transition energies ΔE were approximated by the same value 493 Ry in Ref. 1. Also, as is discussed in the text, for most transitions the present results were calculated for slightly different values for the impact electron energy E_t(Ry) than those listed.

Excited level	M_f	ΔE (Ry)			E_t (Ry)		
			550	700	900	1200	2000
$1s2p\ ^1P_1$	0	493.2	1.69[−3]	2.37[−3]	3.09[−3]	3.85[−3]	4.99[−3]
or		493.0	1.69[−3]	2.39[−3]	3.07[−3]	3.76[−3]	4.68[−3]
$(1s_{1/2}2p_{3/2})_1$			1.69[−3]	2.38[−3]	3.06[−3]	3.76[−3]	4.69[−3]
	1	493.2	4.19[−4]	6.12[−4]	8.84[−4]	1.30[−3]	2.32[−3]
		493.0	4.18[−4]	6.20[−4]	8.98[−4]	1.31[−3]	2.30[−3]
			4.06[−4]	5.84[−4]	8.87[−4]	1.35[−3]	2.39[−3]
$1s2p\ ^3P_1$	0	490.7	2.08[−4]	2.42[−4]	2.85[−4]	3.37[−4]	4.20[−4]
or		490.6	2.19[−4]	2.55[−4]	2.99[−4]	3.47[−4]	4.16[−4]
$(1s_{1/2}2p_{1/2})_1$							
	1	490.7	2.65[−4]	2.09[−4]	1.76[−4]	1.69[−4]	2.16[−4]
		490.6	2.66[−4]	2.09[−4]	1.78[−4]	1.72[−4]	2.20[−4]
$1s2p\ ^3P_2$	0	491.9	2.91[−4]	1.98[−4]	1.27[−4]	7.35[−5]	2.50[−5]
or		491.7	3.08[−4]	2.10[−4]	1.35[−4]	7.76[−5]	2.63[−5]
$(1s_{1/2}2p_{3/2})_2$							
	1	491.9	2.37[−4]	1.61[−4]	1.04[−4]	6.04[−5]	2.12[−5]
		491.7	2.50[−4]	1.70[−4]	1.10[−4]	6.36[−5]	2.23[−5]
			2.45[−4]	1.65[−4]	1.05[−4]	6.05[−5]	2.10[−5]
	2	491.9	7.46[−5]	5.00[−5]	3.32[−5]	2.11[−5]	9.70[−6]
		491.7	7.63[−5]	5.13[−5]	3.42[−5]	2.19[−5]	1.02[−5]
			7.55[−5]	4.96[−5]	3.28[−5]	2.09[−5]	9.74[−6]

TABLE II. Comparison of results for the collision strengths for inner-shell excitation from the ground level to the magnetic sublevels M_f of various levels of the $1s2s2p$ configuration in Li-like iron. In each case upper entries are present fully relativistic results, second entries are from the code of Ref. 17, and third entires are from Ref. 1. Numbers in the square brackets designate powers of 10 by which adjacent entries should be multiplied. The transition energy ΔE was approximated by 493 Ry in Ref. 1. Also, as discussed in the text, for most transitions the present results were calculated for slightly different values for the impact electron energy E_i(Ry) than those listed.

Excited level	M_f	ΔE (Ry)	E_i (Ry) 550	700	900	1200	2000
$(1s2p\,^3P)2s\,^4P_{3/2}$	1/2	487.1	1.36[−4]	1.20[−4]	1.15[−4]	1.19[−4]	1.38[−4]
or		487.0	1.40[−4]	1.25[−4]	1.22[−4]	1.25[−4]	1.42[−4]
$[(1s_{1/2}2s_{1/2})_1 2p_{1/2}]_{3/2}$							
	3/2	487.1	2.84[−4]	2.04[−4]	1.47[−4]	1.11[−4]	9.78[−5]
		487.0	2.88[−4]	2.06[−4]	1.49[−4]	1.13[−4]	1.01[−4]
$(1s2p\,^1P)2s\,^2P_{3/2}$	1/2	490.4	1.27[−3]	1.82[−3]	2.40[−3]	3.07[−3]	4.20[−3]
or		490.2	1.29[−3]	1.83[−3]	2.39[−3]	3.01[−3]	3.97[−3]
$[(1s_{1/2}2s_{1/2})_1 2p_{3/2}]_{3/2}$			1.29[−3]	1.77[−3]	2.28[−3]	2.87[−3]	3.84[−3]
	3/2	490.4	4.14[−4]	6.16[−4]	8.99[−4]	1.33[−3]	2.38[−3]
		490.2	4.16[−4]	6.21[−4]	9.08[−4]	1.34[−3]	2.35[−3]
			3.99[−4]	5.85[−4]	8.47[−4]	1.25[−3]	2.19[−3]
$(1s2p\,^3P)2s\,^2P_{3/2}$	1/2	491.7	2.99[−4]	2.13[−4]	1.50[−4]	1.05[−4]	6.94[−5]
or		491.4	3.19[−4]	2.27[−4]	1.59[−4]	1.10[−4]	7.12[−5]
$[(1s_{1/2}2s_{1/2})_0 2p_{3/2}]_{3/2}$							
	3/2	491.7	7.88[−5]	5.62[−5]	4.23[−5]	3.48[−5]	3.49[−5]
		491.4	8.16[−5]	5.85[−5]	4.45[−5]	3.71[−5]	3.70[−5]

The comparisons are made between results for the collision strengths Ω rather than the cross section Q because Inal and Dubau[1] gave their results in terms of Ω. The relationship between these is

$$Q=\frac{\pi a_0^2}{k_i^2 g_i}\Omega \ , \tag{23}$$

where a_0 is the Bohr radius and g_i is the statistical weight of the initial level, which is $2J_i+1$ in the present case. The relativistic value for the square of the wave number k_i to be used in Eq. (23) is

$$k_i^2=\frac{a_0^2 p_i^2}{\hbar^2}=E_i(\mathrm{Ry})\left[1+\frac{\alpha^2}{4}E_i(\mathrm{Ry})\right] \ , \tag{24}$$

where E_i(Ry) is the kinetic energy of the impact electron in rydbergs and α is the fine-structure constant $e^2/(\hbar c)$. These units for k_i differ from those in Eq. (14) by the a_0 factor in Eq. (24). Thus, if the k_i^2 in Eq. (14) were expressed in these units πa_0^2 would replace the π in Eq. (14). Hence, from Eqs. (14), (15), and (23) one sees that our expression for $\Omega(\beta_i J_i \rightarrow \beta_f J_f M_f)$ is given by 2 times the summation part of Eq. (14) after it has also been summed over M_i. In the approaches of Refs. 1 and 17 Eq. (23) also applies, but of course, their partially relativistic matrix elements replace our fully relativistic ones in Ω and in place of Eq. (24) $k_i^2=E_i(\mathrm{Ry})$. For the energies considered here the latter has little effect.

One sees from inspection of Tables I and II that the three sets of results are in very good agreement. This should be expected because the relativistic effects on the radial functions and phase factors δ_κ are small for $Z=26$ and the differences in treatment of the potential due to the electrons has small effect because the nuclear potential dominates.

It should be mentioned that the results by the program of Clark *et al.*[17] were calculated using the values of E_i listed in the tables and the corresponding values of E_f determined with the equation

$$E_i=E_f+\Delta E \tag{25}$$

and the transition energies ΔE given in the tables. However, Inal and Dubau[1] used the approximation that the same transition energy $\Delta E=493$ Ry was used for all transitions. Hence, except for excitation to the $1s2p\,^1P_1$ level in He-like iron, the values they used for the final electron energy E_f determined with Eq. (25) are too small. On the other hand, as discussed in Sec. II C of Ref. 13, in order to obtain improved efficiency in treating groups of transitions in a given kind of ion, our program calculates results for all the transitions in a group for the same fixed set of final electron energies. In considering He-like iron this set was chosen so that it led to the values for E_i listed in Table I in the case of the $1s^2\,^1S_0-1s2p\,^1P_1$ transitions, but then this corresponds to slightly lower values for E_i for the other transitions, which have smaller ΔE. For Li-like iron, the set of E_f used led to the exact values for E_i listed in Table II only for the $1s^22s\,^2S_{1/2}-(1s2p\,^1P_1)2s\,^2P_{3/2}$ transitions. Since there is little difference in the transition energies, neither this procedure nor the approximation of Inal and Dubau[1] of using the same value for ΔE for all transitions has significant effect on the results for the collision strengths.

We have also compared present results with those obtained with the program of Ref. 17 for excitation from the ground level to the excited, odd-parity levels with $n=3$ and $J_f=1$ in neonlike iron and molybdenum in Tables III and IV, respectively. In doing this we have used the following abbreviations in indicating the *LS*-coupled or *jj*-coupled state making the dominant contribution to each of the excited energy levels:

$$2p3l_a\,{}^{2S+1}L_{J_f}=1s^2 2s^2 2p^5 3l_a\,{}^{2S+1}L_{J_f}\,, \qquad (26)$$

$$2s3l_a\,{}^{2S+1}L_{J_f}=1s^2 2s 2p^6 3l_a\,{}^{2S+1}L_{J_f}\,, \qquad (27)$$

$$(2p_{3/2}3l_{aj_a})_{J_f}=(1s^2_{1/2}2s^2_{1/2}2p^2_{1/2}2p^3_{3/2}3l_{aj_a})_{J_f}\,, \qquad (28)$$

$$(2p_{1/2}3l_{aj_a})_{J_f}=(1s^2_{1/2}2s^2_{1/2}2p_{1/2}2p^4_{3/2}3l_{aj_a})_{J_f}\,, \qquad (29)$$

and

$$(2s_{1/2}3l_{aj_a})_{J_f}=(1s^2_{1/2}2s_{1/2}2p^2_{1/2}2p^4_{3/2}3l_{aj_a})_{J_f}\,. \qquad (30)$$

One sees that the agreement between the two sets of re-

TABLE III. Comparison of results for the collision strengths for excitation from the ground level to the magnetic sublevels M_f of the excited odd-parity levels with $n=3$ and $J_f=1$ in neonlike iron. In each case upper entries are the present fully relativistic results and the second entries are from the code of Ref. 17. Numbers in square brackets designate powers of 10 by which adjacent entries should be multiplied. Here results are given as a function of final or scattered electron energy E_f(Ry).

Excited level	M_f	ΔE (Ry)	E_f (Ry) 3	 15	 60	 150	 3000
$2p3s\,{}^1P_1$ or $(2p_{3/2}3s_{1/2})_1$	0	53.49	9.50[−4]	1.31[−3]	2.59[−3]	4.21[−3]	5.55[−3]
		53.41	1.09[−3]	1.52[−3]	2.97[−3]	4.75[−3]	6.09[−3]
	1	53.49	3.68[−4]	4.14[−4]	6.87[−4]	1.43[−3]	2.59[−3]
		53.41	3.96[−4]	4.61[−4]	7.93[−4]	1.64[−3]	2.95[−3]
$2p3s\,{}^3P_1$ or $(2p_{1/2}3s_{1/2})_1$	0	54.37	8.11[−4]	1.10[−3]	2.13[−3]	3.47[−3]	4.60[−3]
		54.30	9.35[−4]	1.29[−3]	2.48[−3]	3.96[−3]	5.10[−3]
	1	54.37	3.59[−4]	3.88[−4]	5.90[−4]	1.18[−3]	2.12[−3]
		54.30	3.91[−4]	4.37[−4]	6.88[−4]	1.36[−3]	2.45[−3]
$2p3d\,{}^3P_1$ or $(2p_{3/2}3d_{3/2})_1$	0	59.02	1.10[−3]	9.54[−4]	7.17[−4]	6.43[−4]	6.47[−4]
		58.98	1.16[−3]	9.96[−4]	7.35[−4]	6.44[−4]	6.35[−4]
	1	59.02	2.55[−3]	2.05[−3]	1.09[−3]	5.68[−4]	4.49[−4]
		58.98	2.74[−3]	2.19[−3]	1.15[−3]	5.88[−4]	4.58[−4]
$2p3d\,{}^3D_1$ or $(2p_{3/2}3d_{5/2})_1$	0	59.78	1.22[−2]	1.46[−2]	2.15[−2]	2.92[−2]	3.48[−2]
		59.70	1.33[−2]	1.58[−2]	2.32[−2]	3.11[−2]	3.66[−2]
	1	59.78	5.58[−3]	6.10[−3]	8.28[−3]	1.28[−2]	1.96[−2]
		59.70	6.04[−3]	6.63[−3]	9.03[−3]	1.41[−2]	2.14[−2]
$2p3d\,{}^1P_1$ or $(2p_{1/2}3d_{3/2})_1$	0	60.82	4.65[−2]	5.66[−2]	8.64[−2]	1.19[−1]	1.42[−1]
		60.72	4.69[−2]	5.71[−2]	8.66[−2]	1.18[−1]	1.39[−1]
	1	60.82	2.14[−2]	2.39[−2]	3.30[−2]	5.16[−2]	7.90[−2]
		60.72	2.15[−2]	2.40[−2]	3.34[−2]	5.26[−2]	8.06[−2]
$2s3p\,{}^3P_1$ or $(2s_{1/2}3p_{1/2})_1$	0	65.77	2.09[−4]	2.80[−4]	5.56[−4]	9.56[−4]	1.32[−3]
		65.79	2.22[−4]	2.93[−4]	5.71[−4]	9.70[−4]	1.31[−3]
	1	65.77	3.61[−4]	3.23[−4]	2.69[−4]	3.30[−4]	5.38[−4]
		65.79	3.70[−4]	3.31[−4]	2.75[−4]	3.38[−4]	5.53[−4]
$2s3p\,{}^1P_1$ or $(2s_{1/2}3p_{3/2})_1$	0	66.08	1.24[−3]	1.84[−3]	4.03[−3]	7.27[−3]	1.03[−2]
		66.08	1.53[−3]	2.19[−3]	4.62[−3]	8.04[−3]	1.10[−2]
	1	66.08	3.32[−4]	4.28[−4]	8.96[−4]	2.05[−3]	3.99[−3]
		66.08	3.96[−4]	5.15[−4]	1.04[−3]	2.33[−3]	4.48[−3]

sults for neonlike ions is generally good, but is slightly worse than for He- and Li-like iron. We think this is principally due to the different treatments of the electron contribution to the central potential used in calculating the orbitals, which is more significant in the case of neonlike ions. This affects the values for the mixing coefficients, as well as the radial functions. Also for neonlike molybdenum, $Z=42$ is sufficiently large that relativistic effects on the radial functions and phase factors are probably contributing significantly to the differences in the two sets of results.

In summary we have developed a fully relativistic program for calculating the cross sections for excitation to specific magnetic sublevels M_f of very highly charged ions. The results agree well with those of partially relativistic programs for moderate values of Z. It is expected that the present program gives accurate results for any value of Z satisfying $Z \gtrsim 2.5N$, where N is the number of bound electrons per ion, and that it will be useful for comparison with and interpretation of experimental results for very highly charged ions, such as the EBIT results obtained by Marrs and co-workers.[7–9]

TABLE IV. Comparison of results for the collision strengths for excitation from the ground level to the magnetic sublevels M_f of the excited odd-parity levels with $n=3$ and $J_f=1$ in neonlike molybdenum. In each case upper entries are the present fully relativistic results and the second entries are from the code of Ref. 17. Numbers in square brackets designate powers of 10 by which adjacent entries should be multiplied. Here results are given as a function of scattered electron energy E_f(Ry). Note that in LS-coupling notation the fourth and fifth energy levels are nearly equal mixtures of $2p3d\,^1P_1$ and $2p3d\,^3D_1$. In fact, according to the codes of Refs. 17–20 the LS-coupling labeling of these levels should be interchanged.

Excited level	M_f	ΔE (Ry)			E_f (Ry)		
			10	50	200	500	1000
$2p3s\,^1P_1$ or $(2p_{3/2}3s_{1/2})_1$	0	175.0	3.43[−4]	4.65[−4]	8.99[−4]	1.48[−3]	2.00[−3]
		175.0	3.47[−4]	4.80[−4]	9.20[−4]	1.46[−3]	1.87[−3]
	1	175.0	1.11[−4]	1.28[−4]	2.30[−4]	4.85[−4]	8.85[−4]
		175.0	1.08[−4]	1.29[−4]	2.36[−4]	5.03[−4]	9.13[−4]
$2p3s\,^3P_1$ or $(2p_{1/2}3s_{1/2})_1$	0	182.9	2.36[−4]	3.06[−4]	5.61[−4]	9.17[−4]	1.24[−3]
		183.1	2.67[−4]	3.56[−4]	6.60[−4]	1.05[−3]	1.36[−3]
	1	182.9	1.19[−4]	1.23[−4]	1.65[−4]	3.00[−4]	5.31[−4]
		183.1	1.23[−4]	1.32[−4]	1.89[−4]	3.56[−4]	6.32[−4]
$2p3d\,^3P_1$ or $(2p_{3/2}3d_{3/2})_1$	0	187.5	2.14[−4]	1.76[−4]	1.08[−4]	6.90[−5]	5.25[−5]
		187.6	2.06[−4]	1.67[−4]	9.86[−5]	5.77[−5]	3.81[−5]
	1	187.5	7.94[−4]	6.30[−4]	3.13[−4]	1.25[−4]	5.72[−5]
		187.6	8.03[−4]	6.35[−4]	3.11[−4]	1.19[−4]	4.93[−5]
$2p3d\,^1P_1$ or $(2p_{3/2}3d_{5/2})_1$	0	189.7	1.36[−2]	1.61[−2]	2.33[−2]	3.11[−2]	3.75[−2]
		189.7	1.37[−2]	1.62[−2]	2.31[−2]	2.99[−2]	3.43[−2]
	1	189.7	6.03[−3]	6.61[−3]	8.95[−3]	1.37[−2]	2.06[−2]
		189.7	5.91[−3]	6.50[−3]	8.84[−3]	1.37[−2]	2.06[−2]
$2p3d\,^3D_1$ or $(2p_{1/2}3d_{3/2})_1$	0	196.9	1.15[−2]	1.36[−2]	1.97[−2]	2.65[−2]	3.22[−2]
		197.0	1.18[−2]	1.39[−2]	1.99[−2]	2.62[−2]	3.03[−2]
	1	196.9	5.00[−3]	5.49[−3]	7.44[−3]	1.14[−2]	1.73[−2]
		197.0	4.97[−3]	5.46[−3]	7.44[−3]	1.16[−2]	1.76[−2]
$2s3p\,^3P_1$ or $(2s_{1/2}3P_{1/2})_1$	0	204.2	2.50[−4]	3.37[−4]	6.45[−4]	1.08[−3]	1.48[−3]
		204.4	2.22[−4]	3.01[−4]	5.79[−4]	9.47[−4]	1.26[−3]
	1	204.2	1.56[−4]	1.57[−4]	1.93[−4]	3.31[−4]	5.82[−4]
		204.4	1.46[−4]	1.44[−4]	1.73[−4]	3.00[−4]	5.35[−4]
$2p3p\,^1P_1$ or $(2s_{1/2}3p_{3/2})_1$	0	206.4	6.30[−4]	8.78[−4]	1.74[−3]	2.97[−3]	4.13[−3]
		206.6	7.75[−4]	1.05[−3]	2.00[−3]	3.25[−3]	4.30[−3]
	1	206.4	1.93[−4]	2.33[−4]	4.17[−4]	8.59[−4]	1.58[−3]
		206.6	2.32[−4]	2.80[−4]	4.89[−4]	9.97[−4]	1.82[−3]

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APPENDIX

It is our purpose in this appendix to give the appropriate expressions for determining the phase factor δ_κ entering Eqs. (1), (9), and (14). One can write

$$\delta_\kappa=\delta_{\kappa c}+\Delta\delta_\kappa\ , \tag{A1}$$

where $\delta_{\kappa c}$ is the so-called relativistic Coulomb phase factor and $\Delta\delta_\kappa$ is the correction to this due to the fact that the potential at small r is not a pure Coulomb potential. First we consider $\delta_{\kappa c}$. It is given by Eq. (5.103) of Rose,[10] which we repeat for convenience,

$$\delta_{\kappa c}=\eta-\arg\Gamma(\gamma+iy)-\frac{\pi}{2}\gamma+\frac{\pi}{2}(l+1)\ , \tag{A2}$$

where

$$\gamma=[\kappa^2-(\alpha z)^2]^{1/2}\ , \tag{A3}$$

$$y=\left[1+\frac{\alpha^2}{2}E(\mathrm{Ry})\right]\frac{z}{k}\ , \tag{A4}$$

and

$$z=Z-N\ . \tag{A5}$$

Here k and $E(\mathrm{Ry})$ are the wave number and kinetic energy (in rydbergs) of the free electron. They are related by Eq. (24). Apart from a $y\ln(2kr)$ term, see Eq. (A14) below, $\delta_{\kappa c}$ is actually the difference between the phase factor for a pure Coulomb field and that for a zero field. The quantity η in Eq. (A2) is given by Eq. (5.71′) of Rose.[10] Specifically,

$$e^{2i\eta}=\frac{-(\kappa-iy/w)}{\gamma+iy}\ , \tag{A6}$$

where

$$w=\left[1+\frac{\alpha^2}{2}E(\mathrm{Ry})\right]\ . \tag{A7}$$

This leads to

$$\tan(2\eta)=\frac{-y(\kappa+\gamma/w)}{\kappa\gamma-y^2/w}\ . \tag{A8}$$

Using

$$\tan(A\pm B)=\frac{\tan A\pm\tan B}{1\mp\tan A\,\tan B} \tag{A9}$$

with $A=\arctan[y/(|\kappa|w)]$ and $B=\arctan(y/\gamma)$ one finds that for $\kappa<0$ Eq. (A8) leads to

$$\eta=\frac{1}{2}\left[\arctan\left[\frac{y}{|\kappa|w}\right]-\arctan\left[\frac{y}{\gamma}\right]\right],\quad \kappa<0\ . \tag{A10}$$

As a check on this we consider the nonrelativistic limit $\alpha\rightarrow0$. In this limit one sees that Eqs. (A3), (A4), and (A7) lead to $w\rightarrow1$, $y\rightarrow z/k$, and $\gamma\rightarrow|\kappa|=l+1$, where use was also made of Eq. (3). Thus, in this limit $\eta\rightarrow0$ and Eq. (A2) gives

$$\begin{aligned}\lim_{\alpha\rightarrow0}\delta_{\kappa c}&=\delta_{lc}=-\arg\Gamma(l+1+iz/k)\\&=\arg\Gamma(l+1-iz/k)\ ,\end{aligned} \tag{A11}$$

which agrees with the well-known nonrelativistic expression, e.g., Eq. (20) of Ref. 21 or the paragraph containing Eq. (1) of Ref. 1. The last form of Eq. (A11) follows from the fact[22] that $\Gamma(q^*)=\Gamma(q)^*$.

For the case that $\kappa>0$ one can use similar arithmetic to find that Eq. (A8) leads to

$$\eta=-\frac{1}{2}\left[\arctan\left[\frac{y}{\kappa w}\right]+\arctan\left[\frac{y}{\gamma}\right]+\pi\right],\quad \kappa>0 \tag{A12}$$

except that a factor $-\pi/2$ has been added to the right-hand side. This is necessary in order that Eq. (A12) also reduce to the correct result given by Eq. (A11) in the nonrelativistic limit. That it does is readily verified using the relation[22]

$$\arg\Gamma(l+iz/k)+\arctan\left[\frac{z}{lk}\right]=\arg\Gamma(l+1+iz/k)\ . \tag{A13}$$

One can add the factor $-\pi/2$ into Eq. (A12) because Eq. (8) determines η only to within a multiple of $\pi/2$. We note that Eqs. (A10) and (A12) agree with Walker's[12] Eqs. (11) except that his analog of Eq. (A12) has the wrong sign for the $\arctan(y/\gamma)$ term and hence is not consistent with Eq. (A8) and does not lead to Eq. (A11). It should be mentioned that he later[23] corrected his Eq. (10) by adding a term $\pi(l+1)/2$, which then gives Eq. (A2).

Now we consider the factor $\Delta\delta_\kappa$ in Eq. (A1). It is well known that for very large r the large and small components of the radial function of the free electron can be written in the form

$$P_{E\kappa}(r)=C_P(E)\sin[kr+y\ln(2kr)+\delta'_\kappa] \tag{A14}$$

and

$$Q_{E\kappa}(r)=C_Q(E)\cos[kr+y\ln(2kr)+\delta'_\kappa]\ . \tag{A15}$$

The factor $\Delta\delta_\kappa$, which corrects for the fact that the actual potential is not a pure Coulomb potential, is given by

$$\Delta\delta_\kappa=\delta'_\kappa-\delta'_{\kappa c}\ , \tag{A16}$$

where δ'_κ is the phase in Eqs. (A14) and (A15) when the radial functions are determined for the actual potential due to the ion [assumed to be the Dirac-Fock-Slater potential given by Eqs. (17)–(19) in our calculations] and $\delta'_{\kappa c}$ is the phase when the radial functions are determined using the pure Coulomb potential $-2z/r$ for all r. The value for δ'_κ is determined numerically by using

$$\delta'_\kappa = -kr_0 - y\ln(2kr_0)\ , \tag{A17}$$

where r_0 is the value of r at which the last node occurs as $P_{E\kappa}(r)$ is passing from a negative to a positive value prior to the final integration point determined as described in Sec. II B of Ref. 13. $\delta'_{\kappa c}$ is determined numerically by the same procedure except that the Dirac-Fock-Slater potential is replaced with the pure Coulomb potential $-2z/r$ in solving the differential equation for the radial functions.

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