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Rapid relativistic distorted-wave approach for calculating cross sections for ionization of highly charged ions

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The rapid relativistic distorted-wave method of Zhang, Sampson, and Mohanty [Phys. Rev. A **40**, 616 (1989)] for excitation, which uses the atomic-structure data of Sampson *et al.* [Phys. Rev. A **40**, 604 (1989)], has been extended to ionization. In this approach the same Dirac-Fock-Slater potential evaluated using a single mean configuration is used in calculating the orbitals of all electrons bound and free. Values for the cross sections Q for ionization of various ions have been calculated, and generally good agreement is obtained with other recent relativistic calculations. When results are expressed in terms of the reduced ionization cross section Q_R, which is proportional to I^2Q, they are close to the nonrelativistic Coulomb-Born-exchange values of Moores, Golden, and Sampson [J. Phys. B **13**, 385 (1980)] for hydrogenic ions except for high Z and/or high energies. This suggests that fits of the Q_R to simple functions of the impact electron energy in threshold units with coefficients that are quite slowly varying functions of an effective Z can probably be made. This would be convenient for plasma-modeling applications.

I. INTRODUCTION

Highly charged ions with very large values for the nuclear charge number Z are becoming of increased interest in the study of high-temperature plasmas, partly due to the interest in developing ultrashort-wavelength lasers. For highly charged 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 the properties of such ions. For the applications to high-temperature plasma modeling, it is also desirable to have a very rapid relativistic approach because an immense amount of atomic data is required. In Refs. 1 and 2 such an approach was developed, and in Refs. 3–6 it was applied to large-scale production of collision strengths, or equivalently excitation cross sections, and oscillator strengths. As discussed in these references, the approach appears to be accurate for

$$Z \gtrsim 2N \quad \text{or} \quad 2.5N \;, \tag{1}$$

were N is the number of bound electrons per ion.

The approach was also recently extended to give cross sections for excitation of highly charged ions to specific magnetic sublevels by a directive beam of electrons.[7] This was motivated by the need for such cross sections in the modeling and design of electron-beam ion trap (EBIT) experiments at the Lawrence Livermore National Laboratory.[8–10] For this purpose ionization cross sections are needed, as well. Of course, ionization cross sections are also needed for the modeling of high-temperature plasmas, and recently electron-impact ionization cross sections for U^{91+} and U^{90+} have been measured.[11] The purpose of the present work is to extend the approach of Refs. 1–7 to give relativistic electron-impact ionization cross sections. Since ionization is like excitation summed over many final levels, as seen by comparing Eqs. (2) and (13) below, one expects the range of accuracy for ionization to be at least as great as for excitation given by Eq. (1).

In Sec. II the theory used in the present work is described. Then in Sec. III numerical results are given for ionization from the 1*s*, 2*s*, $2p_{1/2}$, and $2p_{3/2}$ subshells of various types of ions with various values of Z, and comparison is made with other recent works.[12–16]

II. OUTLINE OF THEORY

The present relativistic distorted-wave ionization program was obtained by modification of the relativistic distorted-wave excitation program of Ref. 2. Hence we first briefly review the approach used for excitation. Then we indicate the modifications required for ionization. By combining Eqs. (1) and (3) of Ref. 2, one can write the expression for the relativistic distorted-wave cross section $Q(i-f)$ for the excitation transition $i-f$ in an N-electron ion in the form

$$Q(i-f)=\frac{8\pi a_0^2}{k^2 g_i}\sum_J (2J+1)\sum_{\kappa,\kappa'}\left|\left\langle \Psi_i \left| \sum_{\substack{q,p\\ q<p}}^{N+1} \frac{1}{r_{qp}} \right| \Psi_f \right\rangle\right|^2 . \tag{2}$$

Here a_0 is the Bohr radius, k is the relativistic wave number of the impact electron, g_i is the statistical weight of the initial level of the N-electron target ion, and κ and κ' are the initial and final relativistic angular momentum quantum numbers of the free electron. The Ψ_i and Ψ_f in Eq. (2) are the initial and final antisymmetric wave functions for the total $(N+1)$-electron system consisting of target ion plus free electron, and J is the total angular momentum quantum number for this entire system. The relation between k, the relativistic momentum p, and the kinetic energy ε of the impact electron is

$$k^2=\frac{p^2a_0^2}{\hbar^2}=\varepsilon\left[1+\frac{\alpha^2}{4}\varepsilon\right], \tag{3}$$

where α is the fine-structure constant $e^2/\hbar c$ and ε is in Rydbergs. The κ in Eq. (2) is related to the orbital and total angular momentum quantum numbers l and j for the impact electron in the usual way:

$$\kappa=l, j=l-\tfrac{1}{2};\quad \kappa=-(l+1),\quad j=l+\tfrac{1}{2}\ . \tag{4}$$

Of course, analogous relations apply between κ', l', and j' pertaining to the scattered electron.

The initial antisymmetrized function Ψ_i in Eq. (2) can be written[17]

$$\Psi_i=\frac{1}{(N+1)^{1/2}}\sum_{k=1}^{N+1}(-1)^{N+1-k}\times\sum_{M_t,m}C(J_tjM_tm;JM)\times\Psi_{\beta_tJ_t}(x_k^{-1})u_{\varepsilon ljm}(x_k)\ , \tag{5}$$

where x_k designates the space and spin coordinates of electron k, and x_k^{-1} means the space and spin coordinates for all N electrons other than electron k. The $\Psi_{\beta_tJ_t}(x_k^{-1})$ is the initial antisymmetrized target-ion wave function constructed of Dirac spinors or orbitals as in Eq. (4) of Ref. 1. Here J_t is the quantum number corresponding to the total initial angular momentum of the target ion and β_t represents all other quantum numbers required to specify the initial state of the target ion. The $u_{\varepsilon ljm}$ in Eq. (5) is a Dirac spinor for the initial free electron (impact electron) in a central potential $V(r)$ due to the target ion. Specifically,

$$u_{\varepsilon ljm}(x)\equiv u_{\varepsilon\kappa m}(x)=\frac{1}{r}\begin{bmatrix}P_{\varepsilon\kappa}(r)\chi_{\kappa m}(\theta,\phi,\sigma)\\ iQ_{\varepsilon\kappa}(r)\chi_{-\kappa m}(\theta,\phi,\sigma)\end{bmatrix}, \tag{6}$$

where the $\chi_{\kappa m}$ are the usual spin angular momentum functions, and the large and small components of the radial functions $P_{\varepsilon\kappa}$ and $Q_{\varepsilon\kappa}$ satisfy the coupled Dirac equations

$$\left[\frac{d}{dr}+\frac{\kappa}{r}\right]P_{\varepsilon\kappa}(r)=\frac{\alpha}{2}\left[\varepsilon-V+\frac{4}{\alpha^2}\right]Q_{\varepsilon\kappa}(r)\ , \tag{7}$$

and

$$\left[\frac{d}{dr}-\frac{\kappa}{r}\right]Q_{\varepsilon\kappa}(r)=-\frac{\alpha}{2}(\varepsilon-V)P_{\varepsilon\kappa}(r)\ . \tag{8}$$

Similar to Eq. (5), the final function Ψ_f in Eq. (2) for the excitation cross sections is given by

$$\Psi_f=\frac{1}{(N+1)^{1/2}}\sum_{k=1}^{N+1}(-1)^{N+1-k}\times\sum_{M_t',m'}C(J_t'j'M_t'm';JM)\times\Psi_{\beta_t'J_t'}(x_k^{-1})u_{\varepsilon'l'j'm'}(x_k)\ , \tag{9}$$

where primed quantities pertain to the final state in the exactly analogous way that corresponding unprimed quantities in Eq. (5) pertain to the initial state.

In order to extend Eq. (2) to ionization, all that is required is the following: (1) The $\Psi_{\beta_t'J_t'}(x_k^{-1})$ in Eq. (9) must be replaced by an antisymmetrized wave function for an N-electron system corresponding to the final $(N-1)$-electron ion plus an ejected electron:

$$\Psi_{\beta_t'J_t'}(x_k^{-1})=\frac{1}{N^{1/2}}\sum_{p\neq k}^{N+1}(-1)^{N-p}\sum_{M_t'',m''}C(J_t''j''M_t''m'';J_t'M_t')\Psi_{\beta_t''J_t''}(x_p^{-1})u_{\varepsilon''l''j''m''}(x_p)\ , \tag{10}$$

where $\Psi_{\beta_t''J_t''}$ is the antisymmetrized wave function corresponding to the final $(N-1)$-electron ion with total angular momentum J_t'', and $u_{\varepsilon''l''j''m''}(x_p)$ is a Dirac spinor for the ejected electron analogous to the Dirac spinor $u_{\varepsilon ljm}$ given by Eqs. (6)–(8) for the impact electron. A consequence of this is that then $P_{n_\alpha'l_\alpha'j_\alpha'}$ and $Q_{n_\alpha'l_\alpha'j_\alpha'}$ in the direct and exchange radial-scattering matrix elements given by Eqs. (9) and (10) of Ref. 2 are replaced with $P_{\varepsilon''l''j''}$ and $Q_{\varepsilon''l''j''}$. (2) Equation (2) must be summed over the total final angular momentum J_t' for the system consisting of the $(N-1)$-electron final ion with total angular momentum J_t'' plus the ejected electron with total angular momentum j''. (3) Equation (2) must also be summed over κ'' or, equivalently, j'' and l'' for the ejected electron. (4) Equation (2) must be integrated over the range 0 to $(\varepsilon-I)/2$ for the energy ε'' of the ejected electron, where I is the ionization energy. (5) Finally, one must divide by a factor of π to account for the fact that a final bound electron function with normalization

$$\int_0^\infty[P_{n_\alpha'\kappa_\alpha'}^2(r)+Q_{n_\alpha'\kappa_\alpha'}^2(r)]dr=1 \tag{11}$$

has been replaced with a free ejected electron function with normalization

$$\int_0^\infty[P_{\varepsilon''\kappa''}(r)P_{\varepsilon'''\kappa''}(r)+Q_{\varepsilon''\kappa''}(r)Q_{\varepsilon'''\kappa''}(r)]dr=\pi\delta(\varepsilon''-\varepsilon''')\ . \tag{12}$$

In summary, the relativistic distorted-wave ionization cross section is given by

$$Q=\frac{8a_0^2}{k^2g_i}\sum_J(2J+1)\sum_{J_t'}\sum_{\kappa,\kappa',\kappa''}\int_0^{(\varepsilon-I)/2}d\varepsilon''\left|\left\langle\Psi_i\left|\sum_{\substack{q,p\\q<p}}^{N+1}\frac{1}{r_{qp}}\right|\Psi_f\right\rangle\right|^2, \tag{13}$$

with Eq. (10) applied to Eq. (9) for Ψ_f.

All the orbitals bound and free entering Eq. (13) are Dirac spinors of the form given by Eq. (6) with the radial functions satisfying equations of the form of Eqs. (7) and (8). In fact, in the present approach the same central potential $V(r)$ is used for all electrons bound and free, and so the orbitals are all automatically orthogonal. This potential is the relativistic Hartree-Fock-Slater potential or so-called Dirac-Fock-Slater potential given in rydbergs by

$$V(r)=-\frac{2Z}{r}+V_c(r)-\left[\frac{24}{\pi}\rho\right]^{1/3} , \tag{14}$$

where

$$V_c(r)=\sum_{n'\kappa'} w_{n'\kappa'}\int_0^\infty \frac{2}{r_>}[P^2_{n'\kappa'}(r_2)+Q^2_{n'\kappa'}(r_2)]dr_2 , \tag{15}$$

and

$$\rho(r)=\frac{1}{4\pi r^2}\sum_{n'\kappa'} w_{n'\kappa'}[P^2_{n'\kappa'}(r)+Q^2_{n'\kappa'}(r)] . \tag{16}$$

Here $w_{n'\kappa'}$ 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 subscript a used in Eq. (11) to distinguish bound orbitals from free ones has been dropped here for convenience.

In the application to excitation in Refs. 3–6, the potential given by Eqs. (14)–(16) was evaluated using a single mean configuration with fractional occupation numbers in which the occupation for the active electron was approximately split between initial and final shells. In obtaining the ionization results given in Sec. III, we mostly used the initial configuration of the target ion in determining the potential with Eqs. (14)–(16). For example, in considering either inner-shell ionization or ionization of the valence electron of Li-like ions in the ground level, the configuration $1s^22s$ was used, while for ionization of a $2p_{1/2}$ electron in a Li-like ion the configuration $1s^22p_{1/2}$ was used. This is a simple, straightforward procedure. However, one that would more nearly correspond to the procedure used successfully for excitation in Refs. 3–7 would be to reduce the occupation number of the initial subshell of the active electron by 0.5 and put an occupation number of 0.5 in a very high subshell to mock up the effect of the ejected electron. Thus a few test cases, for which results in Sec. III are indicated by asterisks as superscripts, were done this way. Specifically, test cases were done using the mean configurations

$$1s^{1.5}2s^{1}6d^{0.5}_{5/2} , \tag{17}$$

$$1s^22s^{0.5}6d^{0.5}_{5/2} , \tag{18}$$

$$1s^22p^{0.5}_{1/2}6d^{0.5}_{5/2} , \tag{19}$$

and

$$1s^22s^22p^{1.5}_{1/2}2p^4_{3/2}6d^{0.5}_{5/2} , \tag{20}$$

in determining the potential with Eqs. (14)–(16) for inner-shell ionization of Li-like ions in the ground configuration, ionization of the valence electron in Li-like ions initially in the $1s^22s$ and $1s^22p_{1/2}$ configurations, and ionization of a $2p_{1/2}$ electron in neonlike ions in the ground configuration, respectively. These altered potentials affect results appreciably only for relatively low Z, where the electron-electron contribution to the potential is most significant.

Although we expect eventually to write a more general program, at present the computer program only calculates ionization cross sections with the form of hydrogenic cross sections except that the orbitals are calculated using the potential of Eqs. (14)–(16). Thus, in this case, $J_t''=0$ and $J_t'=j''$, and so the summation over J_t' is omitted. The present program can obviously be applied to ionization of the valence electron in Li-like, Na-like, and Cu-like ions. However, as shown in the Appendix of Ref. 18, a program such as the present one has much wider applications. In particular, it applies whenever both the initial and final states are pure states, such as is the case for ionization of He-like, Ne-like, and Ni-like ions in their ground levels, and it also applies if only either the initial or final level is a pure state. Hence it is applicable for ionization of F-like and Co-like ions as well as inner-shell ionization of Li-like, Na-like, and Cu-like ions. In order to make application to these more complex cases, one must multiply by the initial occupation number $w_{n\kappa}$ of the active subshell $n\kappa$, and if more than one state for the final ion is possible, one must multiply by a branching ratio factor R considered, for example, in Ref. 19. Also, if mixing occurs in the initial or final level, one must multiply by the square of the mixing coefficient and sum over the mixed states. It is also convenient to express results in terms of a reduced cross section Q_R by factoring out a $\pi a_0^2/I^2$ factor, where I is the ionization energy in rydbergs. Then, if both initial and final states are pure ones, the cross section for ionization from subshell $n\kappa$ is given by

$$Q=\frac{\pi a_0^2}{I^2}w_{n\kappa}RQ_R , \tag{21}$$

while, if either the initial or final state is a mixed one, Eq. (21) should be multiplied by the square of the mixing coefficient and summed over the mixed states, as mentioned previously.

Finally, we note that it is well known that the relative phase of the two final free electrons is unknown when the central field approximation has been made in determining their orbitals. The choice of phase used in our approach is what is sometimes called the "natural"-phase approximation [see Eq. (10) of Ref. 14]. This is the correct choice in the special case of a nonrelativistic treatment as $Z\rightarrow\infty$. Thus one might expect it to be a good approximation for highly charged ions.

III. NUMERICAL RESULTS AND DISCUSSION

Ionization cross sections by the present method are compared with relativistic results available by other methods in Table I. The entries labeled Ref. 16 are results calculated with the relativistic distorted-wave program used in the calculations of the direct ionization contribution, as compared with the indirect excitation-autoionization contribution, in Ref. 15 dealing with ionization of Na-like Au ($Z=79$). That program also uses the so-called natural-phase approximation [Eq. (10) of Ref. 14]. Thus it differs from the present program in the physics used only in that the bound, incident, scattered, and ejected electron functions are calculated in the Dirac-Fock potential[20] rather than the more approximate Dirac-Fock-Slater potential used here. This is seen to have little effect in the cases considered in Table I, especially for the more highly charged ions, where the nuclear potential more completely dominates. The results in Refs. 12 and 13 were obtained in a similar way to those of Ref. 16 except that the "maximum-interference"-phase approximation [see Eq. (11) of Ref. 14] was used. Of course, this gives smaller cross sections than the natural-phase approximation, but the difference is usually small. One sees that the present results are also close to those of Refs. 12 and 13, but are always larger, as expected. Finally, the results of Ref. 14 differ from the others in that they include the full lowest-order QED interaction between the electrons rather than simply the Coulomb interaction $1/r_{ij}$ in calculating the scattering amplitudes. In other words, they include the so-called generalized Breit interaction. However, they omit the exchange and interference terms, which they estimate to have no more than a 15% effect. Thus, in comparing with those results, we also omit these terms. The agreement is seen to be rather good in this case as well, which is consistent with the conclusion reached in Ref. 14 and also demonstrated for hydrogenic ions in Ref. 21 that inclusion of the generalized Breit interaction has little effect on ionization until high-impact electron energies $\gtrsim 250$ keV are reached. Our results, like the relativistic calculations of these other workers, are about a factor of 4 smaller than the recent measurements of Ref. 11.

In Table II we give the present results for many additional cases involving ionization from the $1s$, $2s$, $2p_{1/2}$, and $2p_{3/2}$ subshells. In the interest of brevity, closed inactive subshells are omitted in giving the transitions for neonlike ions. The results are given for the reduced ionization cross section Q_R, which is related to the ionization cross section according to Eq. (21). In these cases the branching ratio R is unity except for inner-shell ionization of Li-like ions, where it is $\frac{1}{4}$ and $\frac{3}{4}$ for ionization to the $(1s2s)_0$ and $(1s2s)_1$ states of the He-like ions, respectively. Results of Moores, Golden, and Sampson[22] for the nonrelativistic Coulomb-Born-exchange reduced ionization cross section Q_R^{H} for hydrogenic ions in the

TABLE I. Comparison between present results and recent relativistic calculations by other workers of the cross sections (cm^2) for ionization from various sublevels of various types of ions with various values for the nuclear charge number Z. Here $2p^*$ means $2p_{1/2}$ and $2p$ means $2p_{3/2}$. The present results were obtained using the initial configuration of the target ion in calculating the Dirac-Fock-Slater potential with Eqs. (14)–(16). $x[y]=x\times 10^y$.

Active subshell	Ion type	Z	Source	I (keV)				$u=\varepsilon/I$			
					1.25	1.351	1.448	1.50	1.552	1.737	
$3s$	Na	34	Present	1.036		9.72[−21]	1.09[−20]		1.18[−20]	1.29[−20]	
			Ref. 16	1.036		9.80[−21]	1.09[−20]		1.18[−20]	1.27[−20]	
$2p^*$	Ne	34	Present	2.582	3.33[−21]			4.80[−21]			
			Ref. 16	2.583	3.43[−21]			4.88[−21]			
$2p$	Ne	34	Present	2.539	6.92[−21]			9.97[−21]			
			Ref. 16	2.539	7.14[−21]			9.98[−21]			
							$u=\varepsilon/I$				
					1.05	1.125	1.25	1.50	2.00	2.50	3.00
$3s$	Na	79	Present	8.373		7.70[−23]	1.26[−22]	1.79[−22]	2.13[−22]	2.16[−22]	2.12[−22]
			Ref. 16	8.370		7.72[−23]	1.24[−22]	1.77[−22]	2.11[−22]	2.17[−22]	2.12[−22]
$3s$	Na	92	Present	12.204	1.68[−23]	3.67[−23]					
			Ref. 16	12.202	1.68[−23]	3.70[−23]					
							$u=\varepsilon/I$				
					1.10		1.50		2.00		
$2s$	Li	92	Present	32.96	4.20[−24]		1.24[−23]		1.55[−23]		
			Ref. 12	32.84	4.09[−24]		1.21[−23]		1.51[−23]		
$2s$	Ne	92	Present	25.31					1.34[−23]		
			Ref. 13	25.31					1.30[−23]		
$2p^*$	Ne	92	Present	29.27					4.93[−23]		
			Ref. 13	29.27					4.77[−23]		
$2p$	Ne	92	Present	30.00					3.69[−23]		
			Ref. 13	29.95					3.57[−23]		
$1s$	He	92	Present[a]	130.4	0.54[−24]		1.95[−24]		2.79[−24]		
			Ref. 14	130.2	0.51[−24]		1.76[−24]		2.72[−24]		

[a] Calculated with exchange and interference terms set to zero because that was done in the calculations of Ref. 14.

TABLE II. Comparison of values for the reduced ionization cross section Q_R. Here $2p^*$ means $2p_{1/2}$ and $2p$ means $2p_{3/2}$. Unasterisked entires were obtained using the initial configuration of the target ion in determining the Dirac-Fock-Slater potential with Eqs. (14)–(16), while the asterisked entries were obtained using the configurations of Eqs. (17)–(20) in determining the potential. $x[y]=x\times 10^y$.

Active subshell	Type ion	Transition	Z	$I(\mathcal{R})$	$u=\varepsilon/I$					
					1.125	1.25	1.50	2.25	4.00	6.00
$1s$	H[a]				0.283	0.479	0.724	0.978	0.954	0.819
	Li	$1s^22s$-$(1s2s)_1$	8	5.1316[1]	0.2667	0.4598	0.7151	1.0224	1.0542	0.9251
	Li	$1s^22s$-$(1s2s)_0$	8	5.1921[1]	0.2691	0.4643	0.7226	1.0344	1.0673	0.9366
	Li	$1s^22s$-$(1s2s)_0$	8	5.1921[1]	0.2602*		0.6858*			0.8605*
	He	$1s^2$-$1s$	8	5.4259[1]	0.2745	0.4716	0.7293	1.0303	1.0486	0.9139
	Li	$1s^22s$-$(1s2s)_1$	26	6.3881[2]	0.2848	0.4850	0.7396	1.0227	1.0403	0.9269
	Li	$1s^22s$-$(1s2s)_0$	26	6.4108[2]	0.2857	0.4865	0.7421	1.0264	1.0444	0.9305
	He	$1s^2$-$1s$	26	6.4949[2]	0.2866	0.4878	0.7429	1.0245	1.0393	0.9249
	Li	$1s^22s$-$(1s2s)_1$	56	3.1798[3]	0.3086	0.5260	0.8041	1.1346	1.2429	1.2103
	Li	$1s^22s$-$(1s2s)_0$	56	3.1855[3]	0.3091	0.5268	0.8055	1.1368	1.2456	1.2130
	He	$1s^2$-$1s$	56	3.2049[3]	0.3097	0.5277	0.8064	1.1369	1.2447	1.2121
	Li	$1s^22s$-$(1s2s)_1$	92	9.5369[3]	0.3770	0.6427	0.9852	1.4205	1.6817	1.7634
	Li	$1s^22s$-$(1s2s)_0$	92	9.5506[3]	0.3774	0.6435	0.9865	1.4226	1.6851	1.7684
	He	$1s^2$-$1s$	92	9.5865[3]	0.3781	0.6447	0.9881	1.4240	1.6855	1.7684
$2s$	H[a]				0.321	0.532	0.771	0.953	0.847	0.695
	Li	$1s^22s$-$1s^2$	8	1.0139[1]	0.3131	0.5240	0.7743	0.9970	0.9186	0.7646
	Li	$1s^22s$-$1s^2$	8	1.0139[1]	0.2966*		0.7308*			0.7040*
	Ne	$2s^2$-$2s$	26	1.0257[2]	0.2949	0.4947	0.7336	0.9528	0.8908	0.7491
	Li	$1s^22s$-$1s^2$	26	1.5042[2]	0.3198	0.5312	0.7745	0.9720	0.8800	0.7327
	Ne	$2s^2$-$2s$	34	2.0232[2]	0.3028	0.5062	0.7462	0.9589	0.8900	0.7501
	Ne	$2s^2$-$2s$	56	6.6576[2]	0.3126	0.5214	0.7661	0.9808	0.9204	0.7924
	Li	$1s^22s$-$1s^2$	56	7.8134[2]	0.3242	0.5389	0.7875	0.9973	0.9292	0.8011
	Ne	$2s^2$-$2s$	79	1.5083[3]	0.3207	0.5353	0.7882	1.0196	0.9889	0.8890
	Ne	$2s^2$-$2s$	92	2.2051[3]	0.3278	0.5476	0.8078	1.0524	1.0449	0.9596
	Li	$1s^22s$-$1s^2$	92	2.4232[3]	0.3372	0.5624	0.8275	1.0745	1.0680	0.9862
$2p^*$	H[a]				0.409	0.668	0.949	1.135	0.977	0.786
	Li	$1s^22p^*$-$1s^2$	8	9.2544[0]	0.4522	0.7492	1.0780	1.3268	1.1778	0.9614
	Li	$1s^22p^*$-$1s^2$	8	9.2544[0]	0.4140*		0.9826*			0.8566*
	Ne	$2p^{*2}$-$2p^*$	26	9.3633[1]	0.4077	0.6752	0.9801	1.2230	1.1069	0.9189
	Ne	$2p^{*2}$-$2p^*$	26	9.3633[1]	0.3955*		0.9514*			0.8832*
	Li	$1s^22p^*$-$1s^2$	26	1.4684[2]	0.4236	0.6939	0.9894	1.1945	1.0446	0.8531
	Li	$1s^22p^*$-$1s^2$	26	1.4684[2]	0.4132*		0.9659*			0.8298*
	Ne	$2p^{*2}$-$2p^*$	34	1.8980[2]	0.4128	0.6810	0.9822	1.2123	1.0875	0.9021
	Ne	$2p^{*2}$-$2p^*$	56	6.4199[2]	0.4196	0.6912	0.9949	1.2255	1.1112	0.9410
	Li	$1s^22p^*$-$1s^2$	56	7.7192[2]	0.4269	0.7007	1.0030	1.2239	1.1023	0.9338
	Ne	$2p^{*2}$-$2p^*$	79	1.4683[3]	0.4292	0.7089	1.0253	1.2812	1.2031	1.0603
	Ne	$2p^{*2}$-$2p^*$	92	2.1512[3]	0.4357	0.7216	1.0489	1.3270	1.2801	1.1579
	Li	$1s^22p^*$-$1s^2$	92	2.3984[3]	0.4460	0.7372	1.0682	1.3461	1.2986	1.1813
$2p$	H[a]				0.409	0.668	0.949	1.135	0.977	0.786
	Li	$1s^22p$-$1s^2$	8	9.2490[0]	0.4554	0.7494	1.0783	1.3270	1.1779	0.9614
	Ne	$2p^4$-$2p^3$	26	9.2677[1]	0.4097	0.6782	0.9839	1.2263	1.1081	0.9192
	Li	$1s^22p$-$1s^2$	26	1.4563[2]	0.4248	0.6956	0.9914	1.1959	1.0446	0.8526
	Ne	$2p^4$-$2p^3$	34	1.8660[2]	0.4157	0.6853	0.9874	1.2162	1.0886	0.9016
	Ne	$2p^4$-$2p^3$	56	6.1268[2]	0.4265	0.7012	1.0063	1.2332	1.1107	0.9360
	Li	$1s^22p$-$1s^2$	56	7.3934[2]	0.4324	0.7086	1.0118	1.2289	1.1002	0.9273
	Ne	$2p^4$-$2p^3$	79	1.3284[3]	0.4435	0.7295	1.0486	1.2950	1.1961	1.0413
	Ne	$2p^4$-$2p^3$	92	1.8603[3]	0.4566	0.7519	1.0828	1.3457	1.2656	1.1317
	Li	$1s^22p$-$1s^2$	92	2.0876[3]	0.4641	0.7630	1.0962	1.3579	1.2800	1.1483

[a] Nonrelativistic Coulomb-Born-Exchange values for hydrogenic ions from Moores, Golden and Sampson, Ref. 22. These values are independent of Z.

limit $Z \rightarrow \infty$ are included for comparison. These are independent of Z.

It is interesting to note that comparisons with other more elaborate calculations and experiments made, for example, in Refs. 22 and 23 indicate the Q_R^H lead to cross sections that are quite accurate for Z satisfying Eq. (1) with $Z \leq 26$. This tends to confirm our expectation that the present relativistic distorted-wave results are accurate for Z satisfying Eq. (1) because one sees from Table II that the present results agree rather well with the corresponding Q_R^H values for low and intermediate Z. Unfortunately, there are no results by the more elaborate relativistic programs of Refs. 12–16, with which we can compare for large Z, barely satisfying Eq. (1). However, the comparisons for Na-like and Ne-like selenium ($Z=34$) ions made in Table I with the results of Ref. 16 do show good agreement for $Z \simeq 3N$ and $3.4N$, which are quite close to $Z=2N$ or $2.5N$.

Initially, all our calculations were done using the initial configuration of the target ion in determining the Dirac-Fock-Slater potential with Eqs. (14)–(16). However, some of the results for Q_R for low Z, especially for ionization from the $2p_{1/2}$ and $2p_{3/2}$ subshells, looked slightly anomalous to us. Hence we decided to do some additional test cases using the configurations given by Eqs. (17)–(20) in determining the potential with Eqs. (14)–(16). This latter procedure is more nearly like that used for excitation in Refs. 3–7. These results are indicated by asterisks as superscripts in Table II. One sees that the effect is quite large for $Z=8$, especially for ionization of the $2p_{1/2}$ electron in Li-like ions in the $1s^2 2p_{1/2}$ configuration,[24] where the asterisked entries are about 10% lower than corresponding unasterisked entries. However, the effect rapidly decreases as Z increases and is seen to be almost negligible ($\sim 2.5\%$) for the same transition when $Z=26$.

It appears that use of results determined using Eqs. (17)–(20) would reduce the "bumpiness" in the data for low Z and would give values for Q_R for any given subshell that vary quite smoothly with ionization energy and for which quite simple fits could be made. In this connection we note that accurate fits of the Q_R^H to simple functions of the impact electron energy in threshold units u that are readily integrated over a Maxwellian electron distribution function to obtain ionization rates have been made in Ref. 22. Since, as noted previously, the present relativistic results for Q_R are generally quite close to those of Ref. 22 for Q_R^H, except for high-Z and/or high-impact electron energies, one would expect that fairly accurate fits of the relativistic results for the reduced cross section could be made, as well, probably using the same functional form given by Eq. (6) of Ref. 22, but allowing the coefficients to be slowly varying functions of an effective Z or of Z and N. This would be very convenient for applications to plasma modeling.

In future work we will attempt to do this. Also, we will consider ionization from additional higher subshells in various types of ions. In addition, we expect to extend the approach to autoionization so that we can treat the excitation-autoionization contribution, which sometimes considerably exceeds the direct contribution to ionization even for high Z, as shown in Ref. 15.

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