Relativistic theory for electron-ion scattering

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(Received 1 February 1988; revised manuscript received 10 April 1989)

A relativistic version of electron-scattering close-coupling theory (in the static approximation) is developed for the $1s_{1/2}$, $2s_{1/2}$, $2p_{1/2}$, and $2p_{3/2}$ states of hydrogenlike (or frozen-core, alkali-metal-like) target ions. Comparisons are made among close-coupling, distorted-wave, and semiclassical distorted-wave results as a function of scattering-electron energy and the charge of the target.

I. INTRODUCTION

A relativistic version of distorted-wave theory for electron scattering from neutral atoms has been available[1] for some time. More recently, relativistic distorted-wave theories have been developed[2,3] for electron scattering from highly stripped ions. Electron-ion scattering has been investigated by use of nonrelativistic close-coupling theory;[4,5] however, little work appears to exist on relativistic close-coupling theory.[6,7] The nonrelativistic work indicates that close-coupling and distorted-wave results tend to merge in a given isoelectronic series with increasing target-ion charge Z, but that optically forbidden cross sections merge more slowly than optically allowed cross sections. Certainly the increase in atomic-level fine-structure splitting with increasing Z opens up new optically forbidden channels which may be significantly coupled to optically allowed channels nearby in energy over a range of Z and, to my knowledge, this phenomenon has not been studied. The usefulness of the present theory, however, is expected to be found not in applications to highly stripped ions, where distorted-wave theory is generally valid, but in applications to medium- to high-Z targets where the ionic charge is small.

There are other advantages for using a relativistic version of close-coupling theory. The electron-target wave function is expanded in eigenstates of the total angular momentum, which is a conserved quantity. Thus a closed radial set occurs for each value of the total angular momentum such that distorted-wave theory following from a perturbative approximation to this theory does not require spherical averaging of the potentials. Further, I investigate use of a semiclassical approximation[8] for relativistic distorted-wave theory. This approximation has already been applied[9] to nonrelativistic distorted-wave theory in the static approximation. Since it obviates the need to generate continuum orbitals, the method is useful in code development for non-local-thermodynamic-equilibrium plasmas, where numerous cross sections are needed. The generalization of the method[8] to relativistic distorted-wave theory is described below.

II. THEORY

The Dirac equation for two electrons in the field of a fixed nucleus (in the absence of all electromagnetic fields) is solved by the substitution of the ansatz[6]

$$\Psi=\sum_j (j0|j_b m_b j_s m_s)\begin{pmatrix} P_{nl_{j_b}}(r_b)\chi_{\kappa_b m_b}(\hat{\mathbf{r}}_b) \\ iQ_{nl_{j_b}}(r_b)\chi_{-\kappa_b m_b}(\hat{\mathbf{r}}_b)\end{pmatrix}\begin{pmatrix} \psi_{k_{nl_{j_b}}l_{j_s}}(r_s)\chi_{\kappa_s m_s}(\hat{\mathbf{r}}_s) \\ i\psi^{(s)}_{k_{nl_{j_b}}l_{j_s}}(r_s)\chi_{-\kappa_s m_s}(\hat{\mathbf{r}}_s)\end{pmatrix}. \tag{1}$$

In Eq. (1), $P_\mu\chi_\nu$ and $iQ_\mu\chi_{\nu'}$ are the large and small components of the eigenfunctions[10] for the bound electron, respectively. Similarly, $\psi_\delta\chi_\epsilon$ and $i\psi^{(s)}_\delta\chi_{\epsilon'}$ are the large and small components of the wave function for the scattering electron, respectively. The radial and angular parts of the position vectors of the electrons are denoted $\mathbf{r}_\sigma$ and $\hat{\mathbf{r}}_\sigma$ where σ is b or s for the bound or scattering electron coordinate, respectively. The vector $\mathbf{j}=\mathbf{j}_b+\mathbf{j}_s$ is the conserved total angular momentum, where $\mathbf{j}_\sigma=\boldsymbol{l}_\sigma+\mathbf{s}_\sigma$ for orbital and spin angular momenta $\boldsymbol{l}_\sigma$ and $\mathbf{s}_\sigma$, respectively, and m_σ is the projection of j_σ. The principal quantum numbers for the bound and scattering electron are n and $k_{nl_{j_b}}$, respectively, and $\kappa_\sigma=l_{j_\sigma}$ or $-l_{j_\sigma}-1$ is the Dirac quantum number. Projection onto the space of $\mathbf{r}_b$ and $\hat{\mathbf{r}}_\sigma$ leads to a set of coupled, first-order differential equations in the radial variable r_s for the large and small components of the scattering electron, where the coupling is the usual Dirac coupling between the large and small components and coupling among subcomponents of either the large or small components induced by the interelectronic Coulomb potential.

Many workers[1,3,6,7] solve the first-order equations. Others[2,11] choose to eliminate the small component, thereby deriving a Schrödinger-like second-order differential equation. The latter approach is used here. This has at least two advantages. First, the Coulomb

Green's function can be used to convert the set of coupled differential equations to a set of coupled integral equations,[12] such that the correct boundary conditions on the scattering wave function appear naturally through the Green's function. Second, the use of Riley's semiclassical theory,[8,9] which makes use of the JWKB approximation to the radial wave functions, requires the Schrödinger form. Although use of the Schrödinger form of the Dirac equation is well known in distorted-wave theory,[11] its use in close-coupling theory has, to my knowledge, not been presented before.

In matrix form, the second-order, close-coupling equations following from the ansatz, Eq. (1), are

$$\left[\left(\frac{d^2}{dr_s^2}-\frac{\kappa_s(\kappa_s+1)}{r_s^2}+k_{nl_{j_b}}^2\right)\underline{I}-\underline{U}\right]\underline{\varphi}=0\ , \tag{2a}$$

$$\underline{U}=\alpha^2(\underline{V}\,\underline{E}+\underline{E}\,\underline{V})-\alpha^2\underline{V}\,\underline{V} -\underline{V}'(\underline{E}-\underline{V}+\underline{I}/\alpha^2)^{-1}\underline{I}\left(\frac{d}{dr_s}+\frac{\kappa_s}{r_s}\right)\ , \tag{2b}$$

where $\underline{I}$ is the identity matrix, $\underline{V}$ is the radial potential matrix, and $\underline{E}$ is the diagonal matrix

$$\underline{E}=\left(\frac{1}{\alpha^4}+\frac{k_{nl_{j_b}}^2}{\alpha^2}\right)^{1/2}\ , \tag{3a}$$

where $k_{nl_{j_b}}^2$ is the channel energy (in rydbergs). For a given transition, the channel energy is defined as

$$k_{nl_{j_b}}^2+E_{nl_{j_b}}=k_{n'l'_{j_b}}^2+E_{n'l'_{j_b}}\ , \tag{3b}$$

where $E_{nl_{j_b}}$ is the target energy (in rydbergs). The primes in Eq. (2b) (and where appropriate) denote derivatives with respect to the scattering electron's radial variable r_s. There is one such set of equations for each j in the expansion given by Eq. (1).

For eigenstates $|j)$ of total angular momentum, a matrix element of the interelectronic Coulomb potential r_{12}^{-1}, is

$$\frac{4\pi}{2\lambda+1}\left(j\left|\frac{r_<^\lambda}{r_>^{\lambda+1}}\sum_\mu Y_{\lambda\mu}Y_{\lambda\mu}^*\right|j\right)=(-1)^{j+j_b+j_b'}(2l_b+1)^{1/2}(2l_b'+1)^{1/2}(2l_s+1)^{1/2} \times(2l_s'+1)^{1/2}(2j_b+1)^{1/2}(2j_b'+1)^{1/2}(2j_s+1)^{1/2}(2j_s'+1)^{1/2} \times\begin{pmatrix}l_b & \lambda & l_b'\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}l_s & \lambda & l_s'\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix}j_b' & j_s' & j\\ j_s & j_b & \lambda\end{Bmatrix}\begin{Bmatrix}j_s & j_s' & \lambda\\ l_s' & l_s & \tfrac{1}{2}\end{Bmatrix}\begin{Bmatrix}j_b & j_b' & \lambda\\ l_b' & l_b & \tfrac{1}{2}\end{Bmatrix}R_\lambda\ , \tag{4}$$

where the summations over all projection quantum numbers have been performed analytically. The radial matrix element corresponding to Eq. (4) is

$$R_\lambda=\int_0^\infty dr\,r^2\frac{r_<^\lambda}{r_>^{\lambda+1}}(P_{nl_{j_b}}P_{n'l'_{j_b}}+Q_{nl_{j_b}}Q_{n'l'_{j_b}})\ . \tag{5}$$

Finally, Eq. (2a) is now converted to an integral equation. At large r_s, the leading term on the right-hand side of Eq. (2b) is $-2Z_I\alpha^2\underline{E}/r_s$ where Z_I is the ionic charge. The Coulomb Green's function $\underline{G}$ (in matrix form) for scattered-wave boundary conditions is just the Green's function for the operator of Eq. (2a) with $\underline{U}$ replaced by this term. The integral form of Eq. (2a) is then written as

$$\underline{\varphi}(r)=\underline{F}+\int_0^\infty dr_s'\underline{G}(r_s,r_s')\underline{U}_1(r_s')\underline{\varphi}(r_s')\ , \tag{6a}$$

$$G_{l_{j_s}}=k_{nl_{j_b}}^{-1}F_{l_{j_s}}(k_{nl_{j_b}}r_<)F_{l_{j_s}}^{(i)}(k_{nl_{j_b}}r_>)\ , \tag{6b}$$

where $\underline{F}$ is a diagonal matrix of regular Coulomb functions, $\underline{U}_1$ is $\underline{U}$ after the removal of the Coulombic terms, and F_μ and $F_\mu^{(i)}$ are the regular and irregular Coulomb functions, respectively. Equation (10) is solved numerically[13] for the matrix of radial wave functions $\underline{\varphi}$. Knowing $\underline{\varphi}$ at large r_s the K_j (reactance) matrix is calculated for each total angular momentum j. The integral cross section is then calculated from

$$\sigma_{nl_{j_b}n'l'_{j_b}}=\frac{\pi}{k_{nl_{j_b}}^2}\sum_j(2j+1)|[(\underline{I}-i\underline{K}_j)^{-1}\underline{K}_j]_{nl_{j_b}n'l'_{j_b}}|^2 \tag{7}$$

for a given $nl_{j_b}\to n'l'_{j_b}$ transition. The $\underline{K}_j$ and amplitude matrices [where an element of the latter is given as the argument for the absolute value in Eq. (7)] are symmetric within acceptable numerical accuracy, and this provides a check on our numerical procedures. We remark that the $\underline{V}\,\underline{V}$ term in Eq. (2b) falls off as r_s^{-2} at large r_s. This makes the calculation of the $\underline{K}_j$ matrix nonstandard in that the radial waves of Eq. (2a) must be matched with linear combinations of Coulomb waves of noninteger angular momentum

$$\lambda=-\tfrac{1}{2}+\tfrac{1}{2}\{1+4[\kappa_s(\kappa_s+1)-(Z_I\alpha)^2]\}^{1/2} \tag{8}$$

corresponding to a r_s^{-2} coefficient:

$$\lambda(\lambda+1)=\kappa_s(\kappa_s+1)-(Z_I\alpha)^2\ . \tag{9}$$

A computer code which generates the appropriate Coulomb functions has been provided by Rescigno.[14]

Although exchange with the target electron is ignored, j-j coupling means that the solution for each j represents a mixture of single and triple scattering, such that Eq. (7)

is the average result for a total of four states of total-spin angular momentum. For example, for each angular momentum l_s of the scattering electron, for zero target-electron orbital angular momentum, there are three values of j consistent with conservation of total angular momentum $\mathbf{j}=\mathbf{j}_s+\mathbf{j}_b$. They turn out to be $j=l_s-1,l_s,l_s+1$ ($j=l_s,l_s+1$ for $l_s=0$) corresponding in ls coupling to $\mathbf{j}=\mathbf{l}+\mathbf{s}$, where l,s are the total spatial, spin angular momentum. For nonzero target-electron orbital angular momentum, l_s and j_s have values consistent with each of these three j values and with conservation of parity. For $j=l_s$ the maximum size of the potential matrix occurs, and for $1s_{1/2},2s_{1/2},2p_{1/2},2p_{3/2}$ target states it is 10×10.

III. RESULTS AND DISCUSSION

Our results are presented in Tables I–V. Collision strengths are defined as cross sections [Eq. (11)] in units of $\pi\alpha_0^2$ scaled by the channel energies $k^2_{nl_{j_b}}$ [Eq. (3b)] in rydbergs. Due to the fine-structure splitting, several inelastic thresholds exist, and the results are presented for collision strengths versus energy in appropriate threshold units $E_j/\Delta E_j$ where $j=1,2,3$ for the cases

$$\frac{k^2_{1s_{1/2}}}{E_{2p_{3/2}}-E_{1s_{1/2}}},\ \frac{k^2_{1s_{1/2}}}{E_{2s_{1/2}}-E_{1s_{1/2}}},\ \frac{k^2_{2s_{1/2}}}{E_{2p_{3/2}}-E_{2p_{1/2}}},$$

respectively, where $E_{2s_{1/2}}$ and $E_{2p_{1/2}}$ are degenerate for hydrogenic targets. For e,He^+, the close-coupling results were checked against the results of Burke *et al.*[15] and found to disagree at worst to within about 2%. The distorted-wave results were checked against the results of Peek and Mann[9] (their numbers are given at $E_1/\Delta E_1=1.35$, with footnote a in Tables and II). For distorted-wave theory the $2p_{1/2}\rightarrow2p_{3/2}$ strength follows the trend[4] of optically forbidden strengths to converge more slowly than optically allowed strengths to the close-coupling results, but does not appear to converge more slowly than the $1s_{1/2}\rightarrow2s_{1/2}$ strength.

TABLE I. Collision strengths for e,He^+ for $E_1/\Delta E_1$ in the close-coupling (CC), distorted-wave (DW), and average (A) approximation. $E_1/\Delta E_1\simeq E_2/\Delta E_2$ is assumed in the table. See text for definition of $E_{j/\Delta}E_j$

$E_1/\Delta E_1$		$1s_{1/2}\rightarrow2s_{1/2}$	$1s_{1/2}\rightarrow2p_{1/2}$	$1s_{1/2}\rightarrow2p_{3/2}$
1.08	CC	0.1147	0.1332	0.2667
	DW	0.1271	0.1300	0.2589
	A	0.1294	0.1286	0.2557
1.33	CC	0.0898	0.1575	0.3173
	DW	0.1256	0.1494	0.2970
		0.12499[a]		
	A	0.1277	0.1505	0.2992
		0.12834[a]		
2.00	CC	0.0900	0.2039	0.4124
	DW	0.1239	0.1978	0.3934
	A	0.1245	0.1995	0.3967

[a]Results from Peek and Mann (Ref. 9) at $E_1/\Delta E_1=1.35$.

TABLE II. Collision strengths for e,C^{5+}. Definitions as in Table I. Numbers in square brackets, denote powers of 10 by which preceding number should be multiplied.

$E_1/\Delta E_1$		$1s_{1/2}\rightarrow2s_{1/2}$	$1s_{1/2}\rightarrow2p_{1/2}$	$1s_{1/2}\rightarrow2p_{3/2}$
1.08	CC	0.1053[−1]	0.1658[−1]	0.3323[−1]
	DW	0.1287[−1]	0.1599[−1]	0.3188[−1]
	A	0.1300[−1]	0.1631[−1]	0.3254[−1]
1.33	CC	0.1069[−1]	0.1886[−1]	0.3784[−1]
	DW	0.1298[−1]	0.1831[−1]	0.3652[−1]
		0.12878[−1][a]		
	A	0.1303[−1]	0.1860[−1]	0.3711[−1]
		0.13072[−1][a]		
2.00	CC	0.1124[−1]	0.2400[−1]	0.4816[−1]
	DW	0.1308[−1]	0.2362[−1]	0.4712[−1]
	A	0.1305[−1]	0.2374[−1]	0.4737[−1]

[a]Results from Peek and Mann (Ref. 9) at $E_1/\Delta E_1=1.35$.

The collision strengths presented in Tables I–V are converged as l_s wave series to better than four places, with the exception of the $2s_{1/2}\rightarrow2p_{3/2}$ strength for the larger $E_3/\Delta E_3$ value, which is still changing by about one unit in the second decimal place at $l_s^{\max}=17$. The $\Delta n=0$ collision strengths for the optically allowed transitions are expected to be very slowly convergent as the fine-structure splitting decreases to small values; however, it is the larger splittings at high-Z values which are of considerable interest in plasma modeling.[2,3] As the splitting decreases to very small values for low-Z targets, the $\Delta n=0$ optical collision strengths approach the limit of elastic scattering by a point dipole, whose cross section, in distorted-wave theory, is known[16] to diverge as $\ln l_s$ due to the r_s^{-2} range of the potential.

A useful approximation in distorted-wave theory is the use of JWKB wave functions to evaluate the radial matrix element, since obviously the need first to calculate the initial and final distorted waves by numerically solving the radial Schrödinger (in our case Dirac) equation is obviated, reducing the problem to numerical quadrature. The problem of how to evaluate the distorted-wave integral near the turning points of the wave functions was examined by Riley[8] in the context of heavy-particle col-

TABLE III. Collision strengths for e,Ne^{9+}. Definitions as in Table I. Numbers in square brackets denote powers of 10 by which preceding number should be multiplied.

$E_1/\Delta E_1$		$1s_{1/2}\rightarrow2s_{1/2}$	$1s_{1/2}\rightarrow2p_{1/2}$	$1s_{1/2}\rightarrow2p_{3/2}$
1.08	CC	0.3996[−2]	0.6026[−2]	0.1206[−1]
	DW	0.4583[−2]	0.5887[−2]	0.1174[−1]
	A	0.4613[−2]	0.6022[−2]	0.1201[−1]
1.33	CC	0.4085[−2]	0.6850[−2]	0.1371[−1]
	DW	0.4634[−2]	0.6727[−2]	0.1342[−1]
	A	0.4640[−2]	0.6865[−2]	0.1369[−1]
2.00	CC	0.4257[−2]	0.8730[−2]	0.1748[−1]
	DW	0.4697[−2]	0.8652[−2]	0.1726[−1]
	A	0.4670[−2]	0.8721[−2]	0.1740[−1]

TABLE IV. Collision strengths for e,Si^{13+} for $E_1/\Delta E_1$, $E_2/\Delta E_2$, and $E_3/\Delta E_3$. See text for definition of definitions $E_j/\Delta E_j$. The $2p$ fine-structure splitting is 1.75 eV. Numbers in square brackets denote powers of 10 by which preceding number should be multiplied.

$E_2/\Delta E_2$		$1s_{1/2}\rightarrow 2s_{1/2}$	$1s_{1/2}\rightarrow 2p_{1/2}$	$E_1/\Delta E_1$	$1s_{1/2}\rightarrow 2p_{3/2}$	$E_3/\Delta E_3$	$2s_{1/2}\rightarrow 2p_{3/2}$	$2p_{1/2}\rightarrow 2p_{3/2}$
1.001	CC	0.2112[−2]	0.2935[−2]	1.0001	0.5857[−2]	1.12	0.3389	0.5354[−1]
	DW	0.2339[−2]	0.2887[−2]		0.5747[−2]		0.3418	0.5153[−1]
	A	0.2351[−2]	0.2970[−2]		0.5915[−2]		0.3069	0.5654[−1]
1.081	CC	0.2114[−2]	0.3089[−2]	1.08	0.6167[−2]	92.6	0.4026	0.4808[−1]
	DW	0.2352[−2]	0.3043[−2]		0.6059[−2]		0.4048	0.4638[−1]
	A	0.2358[−2]	0.3103[−2]		0.6178[−2]		0.3855	0.5009[−1]

lisions. He proposed that the lower limit of integration be the turning point of the average local kinetic energy of the two JWKB wave functions. Thus the method is referred to as the average approximation. Peek and Mann[9] applied the method to nonrelativistic electron scattering (their numbers appear with footnotes a in Tables I and II). It turns out to be accurate over a wide range of energies, as inspection of Tables I–V shows. Some care had to be taken to get the Dirac equations in the appropriate second-order Schrödinger form for use of standard JWKB theory. This was discussed earlier. In the average approximation[8] the radial distorted-wave matrix element is written as

$$M_{12}\simeq\tfrac{1}{2}\int_{\bar r}^{\infty}\left[\frac{U_{12}}{\bar K(r)}\cos\left[\int_{\bar r}^{r}dr'\frac{1}{2}\frac{[K_1^2(r')-K_2^2(r')]}{\bar K(r')}\right]+\tilde U_{12}\sin\left[\int_{\bar r}^{r}dr'\frac{1}{2}\frac{[K_1^2(r')-K_2^2(r')]}{\bar K(r')}\right]\right]dr\ , \tag{10a}$$

$$K_j(r)^2=k_j^2-U_j(r)-\frac{(\kappa_j+\frac{1}{2})^2}{r^2}\ , \tag{10b}$$

$$\bar K(r)^2=\tfrac{1}{2}[K_1(r)^2+K_2(r)^2]\ , \tag{10c}$$

where $\bar r$ is the turning point of $\bar K(r)$.[2] U_j is a diagonal element of Eq. (2b), with the negative derivative term replaced by $\frac{1}{4}\tilde U_j^2+\frac{1}{2}\tilde U_j'$, where $\tilde U_j$ is a diagonal element of the matrix multiplying the derivative in Eq. (2b). These terms arise from the wave-function transformation which removes the derivative term from the distorted-wave equations (for example, for scattering in a potential V, they are the familiar terms,[2,11]

$$\tfrac{3}{4}(V')^2\left[E-V+\frac{1}{\alpha^2}\right]^{-2}+\tfrac{1}{2}V''\left[E-V+\frac{1}{\alpha^2}\right]^{-1}\ .$$

In Eq. (2b), off diagonally, the derivative term is approximated by ignoring the operation on the prefactor in the JWKB wave function (see Ref. 8). Thus U_{12} is the off-diagonal element in Eq. (2b) less the derivative term, and $\tilde U_{12}$ is the off-diagonal element of the matrix multiplying the derivative. Equation (10) gives the average approximation.

Equation (10a) depends only on the low-frequency (i.e., phase difference) contribution to the matrix element, the high-frequency part having been dropped as unimportant.[17] Thus the accuracy of the JWKB approximation should improve with increasing energy as the integrand develops a smaller rather than larger number of oscillations. Tables I–V show that the average approximation[8,9] gives, with several exceptions near threshold, reasonably accurate distorted-wave results over a wide range of energy and ion charge.

IV. CONCLUSION

Tables I–V show that relativistic close-coupling and distorted-wave results tend to converge with increasing Z, in agreement with earlier nonrelativistic results.[4] The new aspect of the present theory is that the target and scattering electrons are treated fully relativistically. Thus fine-structure splitting opens new channels, such as the $2p_{1/2}\rightarrow 2p_{3/2}$, which are optically forbidden and strongly coupled to optically allowed channels energetically near-

TABLE V. Collision strengths for e,Ar^{17+}. See Table IV for definitions. The $2p$ fine-structure splitting is 4.81 eV. Numbers in square brackets denote powers of 10 by which preceding number should be multiplied.

$E_2/\Delta E_2$		$1s_{1/2}\rightarrow 2s_{1/2}$	$1s_{1/2}\rightarrow 2p_{1/2}$	$E_1/\Delta E_1$	$1s_{1/2}\rightarrow 2p_{3/2}$	$E_3/\Delta E_3$	$2s_{1/2}\rightarrow 2p_{3/2}$	$2p_{1/2}\rightarrow 2p_{3/2}$
1.001	CC	0.1308[−2]	0.1804[−2]	1.0001	0.3672[−2]	1.069	0.2085	0.3188[−1]
	DW	0.1436[−2]	0.1766[−2]		0.3509[−2]		0.2097	0.3105[−1]
	A	0.1429[−2]	0.1797[−2]		0.3570[−2]		0.1872	0.3388[−1]
1.081	CC	0.1317[−2]	0.1878[−2]	1.08	0.3739[−2]	56.3	0.2425	0.2874[−1]
	DW	0.1444[−2]	0.1860[−2]		0.3697[−2]		0.2435	0.2801[−1]
	A	0.1436[−2]	0.1884[−2]		0.3744[−2]		0.2312	0.3001[−1]

by. Thus, as the $1s \rightarrow 2s$ channel studied earlier,[4] the fine-structure channels show slower convergence of close coupling to distorted-wave results with increasing Z.

Except for the fine-structure channel, relativistic effects on the scattering are small as measured by adding fine-structure component cross sections and comparing the results with nonrelativistic cross sections. However, the present study was confined to $Z = 2-18$ targets because of the abundance of nonrelativistic results in this range of Z. For example, comparison with the pseudostate results for Ar^{17+} of Oza *et al.*[18] shows that our relative values for coupled versus distorted-wave results are in reasonable agreement with their relative values. Also, we infer the error in our results, relative to their results, due to omission of exchange. At $E_1/\Delta E_1 = 2$ this error is about 18% for $1s \rightarrow 2s$ and about 7% for $1s \rightarrow 2p$ cross sections. Although exchange becomes less important with increasing Z (being about 5% or less for the $2s \rightarrow 2p$ cross sections of Ref. 3), the size of the error remains fairly large in the optically forbidden channels, even for the $Z = 54$ target[19] of Ref. 3. Thus, although relativistic effects such as orbital contraction[3] and the importance of the small component of the continuum orbital are expected to be more important than exchange for high Z (at least for target excitation as opposed to ionization), it would be useful nonetheless to include exchange in the present theory by use of a suitable local-exchange approximation.

The tables also show that the average method[8] is a reliable approximation to distorted-wave theory over a wide range of energy, in general agreement with earlier nonrelativistic results.[9] It should be emphasized that the potential functions used in the relativistic version of the average method, as defined by Eq. (2b), are quite different from those used in its nonrelativistic version. Since they account fully for relativistic effects in the distortion and coupling, these potential functions become more appropriate with increasing Z. The form of the theory makes it clear that relativistic effects contribute to the coupling, both in its close-coupling and distorted-wave versions. In conventional relativistic distorted-wave theory,[2,3] however, relativistic effects are absent in the coupling and appear only in the distortion.

ACKNOWLEDGMENTS

For helpful discussions the author wishes to thank L. Collins, A. Hazi, K. T. Cheng, M. Chen, J. Scofield, M. Riley, J. Peek, M. Pindzola, D. Griffin, and Yong-Ki Kim. A special thanks to T. Rescigno for supplying and helping with the Coulomb code and to L. Minner for expert programming assistance in making this code compatible with my existing codes. Work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

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