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Atomic L-shell ionization by protons: Dirac-Hartree-Slater calculation of cross sections

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Coulomb ionization of the L subshells of Au and U by slow protons has been calculated in the relativistic plane-wave Born approximation (PWBA), with Dirac-Hartree-Slater (DHS) wave functions. Semiclassical corrections for binding-energy change and Coulomb deflection are applied as developed by Brandt and Lapicki. Considerable improvement is attained in these *ab initio* relativistic PWBA calculations with DHS wave functions, as compared with earlier classical, semiclassical, and PWBA results based on screened hydrogenic wave functions. The predicted subshell ionization cross sections agree well with experimental data. The effect of relativity tends to cancel partially the effects of binding and Coulomb deflection. The calculated energies at which minima occur in $\sigma_{L_1}/\sigma_{L_2}$ and $\sigma_{L_3}/\sigma_{L_2}$ cross-section ratios also agree well with observation. Predicted total L x-ray-production cross sections agree extremely well with experiment. The $L\alpha/L\gamma$ and $L\alpha/L\beta$ x-ray emission rates for $p+$Au agree with measurements if L fluorescence and Coster-Kronig yields are adjusted in accordance with recent relativistic theory.

I. INTRODUCTION

The theory of Coulomb ionization of atomic inner shells by slow, heavy charged particles has progressed beyond calculations based on the plane-wave Born approximation (PWBA) with hydrogenic wave functions[1] (1) by incorporation of the binding effect and Coulomb deflection through the perturbed-stationary-state approach,[2] and (2) by taking account of the effects of relativity on the ionization cross sections, either through a phenomenological approach[3] or by using relativistic hydrogenic wave functions.[4] Even so, substantial discrepancies remain between theory and experiment as shown, e.g., by Rice *et al.*[5] in the case of K-shell ionization cross sections for low-energy collisions.

One obvious question, which we investigate in the present paper, is whether better results can be obtained by using more accurate wave functions in the calculation of inner-shell ionization in low-energy collisions. To look into the effect of more realistic wave functions and of an *ab initio* incorporation of relativity, we have performed a series of relativistic plane-wave Born-approximation (RPWBA) calculations of L-shell ionization cross sections, using Dirac-Hartree-Slater (DHS) wave functions. Here, we report on results for $L_{1,2,3}$-subshell ionization of $_{79}$Au and $_{92}$U by protons, and compare these new theoretical cross sections with earlier calculations and with experiment. Considerable improvement in the calculations has been attained.

II. THEORY

A. Relativistic plane-wave Born-approximation cross sections

In the PWBA,[7] the differential cross section for the collisional ejection of s-shell electrons ($s=1,2,3$) from a closed atomic s shell is

$$\frac{d\sigma}{dE_f}=\frac{4\pi}{\hbar^2}Z_1^2e^4\frac{M_1}{E_1}(2j_s+1)\times\int_{q_{\min}}^{q_{\max}}\frac{dq}{q^3}\,|F_{fi}(q)|^2\,. \quad (1)$$

Here, E_f is the kinetic energy of the ejected electron, $\hbar\vec{q}$ is the momentum transferred to that electron, and Z_1, M_1, and E_1 are the charge, mass, and initial kinetic energy of the projectile, respectively. The exact limits of the momentum transfer,[2,5] used in the present calculations, are (in atomic units)

$$q^2_{\min}=\frac{2M^2E_1}{M_1}\left[1-\left[1-\frac{M_1\epsilon}{ME_1}\right]^{1/2}\right]^2 , \tag{2}$$

$$q^2_{\max}=\frac{2M^2E_1}{M_1}\left[1+\left[1-\frac{M_1\epsilon}{ME_1}\right]^{1/2}\right]^2 . \tag{3}$$

In Eqs. (2) and (3), M is the reduced mass of the system and $\epsilon=E_f+E_{L_i}$ is the energy transferred to the target.

For an atomic-electron shell with quantum numbers l_ij_i, the relativistic form factor pertaining to the l_fj_f partial wave is

$$|F_{fi}(q)|^2=\sum_{l=0}^{\infty}(2l+1)(2j_f+1)\begin{bmatrix} j_f & l & j_i \\ \frac{1}{2} & 0 & -\frac{1}{2}\end{bmatrix}^2 \pi(l_fll_i)\left|\int j_l(qr)(G_iG_f^*+F_iF_f^*)dr\right|^2 , \tag{4}$$

where

$$\pi(l_fll_i)=\begin{cases}0 \text{ if } l_f+l+l_i=\text{odd} ,\\ 1 \text{ if } l_f+l+l_i=\text{even} ,\end{cases} \tag{5}$$

and G and F are the large and small components of the relativistic one-electron wave function.

B. Binding effect

In a classical representation, the binding energy of an atomic electron to be ionized is increased owing to the presence of the slow charged projectile in the vicinity of the nucleus during the collision. This perturbation of the target atomic states by the projectile leads to a reduction in ionization probability. In a treatment employing first-order perturbation theory, Brandt and Lapicki[6] have derived a semiclassical expression for the change in L_i-shell binding energy:

$$\Delta E_{L_i}=\int \psi^*_{L_i}(\vec{r})\frac{Z_1e^2}{|\vec{R}-\vec{r}|}\psi_{L_i}(\vec{r})d\vec{r} , \tag{6}$$

where $\psi_{L_i}(r)$ is the unperturbed L_i-shell wave function, $\vec{R}$ is the projectile coordinate, and $\vec{r}$ is the coordinate of the L_i electron.

Assuming a straight-line trajectory for the projectile and using screened hydrogenic wave functions, Brandt and Lapicki[6] found an average binding-energy shift

$$\langle \Delta E_{L_i}\rangle=2Z_1g_{L_i}(\xi;c)E_{L_i}/(Z_{L_i}\theta_{L_i}) . \tag{7}$$

Here, E_{L_i} is the (unperturbed) L_i-shell binding energy, and $Z_{L_i}=Z_2-4.15$ is the effective nuclear charge seen by an L_i electron in the target atom. The dimensionless reduced binding energy is

$$\theta_{L_i}=4E_{L_i}/Z^2_{L_i}\mathscr{R} , \tag{8}$$

where $\mathscr{R}$ is the Rydberg energy and ξ is a dimensionless quantity defined as

$$\xi=\frac{\hbar Z_{L_i}\mathscr{R}}{e^2E_{L_i}}(2E_1/M_1)^{1/2} . \tag{9}$$

The quantities E_{L_i}, E_1, and M_1 in Eqs. (8) and (9) are in atomic units. In the present RPWBA calculations, we take account of the binding effect by adding $\langle \Delta E_{L_i}\rangle$ as given by Eq. (7) to the L_i-shell binding energy. For the function $g(\xi;c)$ in Eq. (7), we use expressions derived in Ref. 6.

C. Coulomb deflection

In the semiclassical approximation, the ionization cross section for a projectile moving along the classical hyperbolic orbit in the Coulomb field of the target nucleus can be approximated by taking the cross section for a projectile that follows a straight-line path and multiplying this by a correction factor.[7,8] Including the Coulomb-deflection correction factors, the L_i-subshell ionization cross sections can be expressed as follows[2,6]:

$$\sigma^C_{L_i}=C\left[\frac{2dq_{0L_i}\zeta_{L_i}}{z_{L_i}(1+z_{L_i})}\right]\sigma^{\text{PWBA}}_{L_i} , \tag{10}$$

where

$$C\left[\frac{2dq_{0L_i}\zeta_{L_i}}{z_{L_i}(1+z_{L_i})}\right]=\begin{cases}9\mathscr{E}_{10}\left[\dfrac{2\pi dq_{0L_1}\zeta_{L_1}}{z_{L_1}(1+z_{L_1})}\right] \\ \text{for the } L_1 \text{ shell} \\ 11\mathscr{E}_{12}\left[\dfrac{2\pi dq_{0L_i}\zeta_{L_i}}{z_{L_i}(1+z_{L_i})}\right] \\ \text{for the } L_2 \text{ and } L_3 \text{ shells} .\end{cases} \tag{11}$$

In these formulas, ζ_{L_i} and z_{L_i} account for the perturbed-stationary-state and energy-loss effects, respectively,[2,6] d is the half distance between the collision partners at closest approach, q_{0L_i} is the approximate minimum momentum transfer, and $\mathscr{E}_n(x)$ is the exponential integral.[9] In the present calculations, we incorporate the Coulomb-deflection effect in the relativistic plane-wave cross sections through Eqs. (10) and (11).

III. NUMERICAL METHOD

The atomic form factors were calculated with DHS wave functions[10,11] that describe the neutral atom. The continuum wave functions were found by solving the DHS equations in the same atomic potential as for the initial state. For the practical purpose of integrating the differential equations numerically to obtain the continuum solutions, we divided the space into an interior and an exterior region. A logarithmic coordinate was used in the interior region, just as for bound states. In the exterior region, a constant-r mesh was employed. The boundary between the two regions was chosen so that the number of mesh points in one wavelength always exceeded 30 points.[12] The continuum wave functions were normalized by matching them with Coulomb wave functions in the asymptotic region.[12,13]

The spherical Bessel transformation of Eq. (4) was carried out with a technique developed by Talman.[14] First, the properly normalized continuum wave functions was interpolated into the same logarithmic radial mesh that was used for calculating the bound-state wave functions. This interpolation could be safely carried out because the exponential cutoff of the bound-state wave functions limits the important region of integration to the size of the pertinent shell of the target atom. Taking a logarithmic mesh in momentum space as well, the form-factor integral could be evaluated by two successive fast Fourier transforms.[14] Thus, no calculations of Bessel functions were required. The integration over the energy transfer was terminated when the accuracy of the cross section reached 0.5%. This procedure made it economically feasible to carry out systematic calculations of ionization cross sections with relativistic self-consistent-field wave functions. The cross sections could subsequently be corrected for the effects of binding-energy shift and Coulomb deflection as indicated in Sec. II.

A general computer program for calculating RPWBA ionization cross sections with DHS wave functions has been developed. Here, we report on results from this code for the ionization of Au and U L-shells by protons with energies from 0.4 to 18 MeV.

IV. RESULTS AND DISCUSSION

Calculated RPWBA DHS cross sections for L_1-, L_2-, and L_3-subshell ionization of Au and U by protons are listed in Table I. For a critical comparison with other theoretical work and experimental data, we note that measured *total* cross sections for L- (and K-) shell ionization by light ions are found to be in good agreement with any of various theoretical approaches—PWBA, the semiclassical approximation, or the binary-encounter approximation.[15,16] On the other hand, L_1- and L_2-*subshell* ionization induced by protons show significant differences in the projectile-energy dependence. These differences are much better represented by the PWBA calculations than by a classical or semiclassical treatment.[16] Consequently, we compare our RPWBA DHS cross sections with available experimental data for individual subshells, with results from nonrelativistic PWBA calculations,[17] and with RPWBA calculations based on relativistic screened hydrogenic wave functions.[18]

In Figs. 1 and 2, the present theoretical L-subshell ionization cross sections for Au and U are compared with experiment[19] and nonrelativistic calculations based on screened hydrogenic wave functions.[17] Relativity causes the L_1 and L_2 cross sections to increase by a factor of ~ 2 in the low-energy region, while the L_3 cross section is enhanced only slightly. The inflection in the σ_{L_1} curve has been explained as a result of the extra node in the $2s$ radial wave function, as compared with the $2p$ wave function.[15,16,19]

The present RPWBA-DHS results including corrections for binding and Coulomb deflection are seen to agree well with measured cross sections. It is interesting to note that without the binding and deflection corrections the RPWBA-DHS results much exceed experimental cross sections in the low-energy regime. Clearly, the effect of relativity tends to partially cancel the effects of binding and Coulomb deflection. Consequently, the fair agreement with experiment of nonrelativistic PWBA calculations without binding and deflection corrections must be considered accidental. If the binding and deflection corrections were added to the nonrelativistic PWBA results, the low-energy L-subshell ionization cross sections would be underestimated.

In Figs. 3 and 4, the ionization ratios $\sigma_{L_1}/\sigma_{L_2}$

TABLE I. Relativistic plane-wave Born-approximation cross sections (in barns), calculated from Dirac-Hartree-Slater wave functions, for L-subshell ionization of Au and U by protons of energy E_1 (in MeV).

	L_1		L_2		L_3	
E_1	RPWBA[a]	RPWBA-BC[b]	RPWBA[a]	RPWBA-BC[b]	RPWBA[a]	RPWBA-BC[b]
			$_{79}$Au			
0.4	0.652	0.152	0.256	0.0574	1.214	0.305
0.6	1.108	0.495	0.973	0.393	4.284	1.822
0.8	1.360	0.806	2.348	1.222	9.682	5.181
1.0	1.501	1.020	4.472	2.674	17.37	10.55
1.2	1.725	1.228	7.328	4.779	27.15	17.88
1.3	1.939	1.380	9.018	6.074	32.71	22.19
1.4	2.252	1.593	10.90	7.54	38.69	26.92
1.5	2.671	1.874	12.91	9.15	45.05	32.03
1.6	3.238	2.259	15.07	10.90	51.88	37.59
1.7	3.954	2.755	17.35	12.78	58.94	43.41
1.8	4.805	3.354	19.76	14.78	66.31	49.55
2.0	7.061	4.996	24.98	19.18	81.84	62.67
2.5	15.56	11.54	39.46	31.77	124.8	99.81
			$_{92}$U			
0.4	0.172	0.0144	0.0291	0.002 52	0.182	0.0214
0.5	0.259	0.0431	0.0622	0.0103	0.384	0.0783
0.6	0.346	0.0890	0.114	0.0286	0.693	0.205
0.8	0.498	0.202	0.291	0.109	1.67	0.698
1.0	0.607	0.320	0.586	0.281	3.19	1.63
1.2	0.677	0.416	1.02	0.567	5.25	3.06
1.4	0.723	0.489	1.61	0.980	7.85	4.96
1.5	0.748	0.529	1.96	1.26	9.33	6.13
1.6	0.776	0.554	2.34	1.53	10.9	7.31
1.8	0.856	0.629	3.22	2.21	14.5	10.1
2.0	0.998	0.741	4.26	3.10	18.4	13.7
2.2	1.215	0.899	5.42	3.99	22.8	16.9
2.4	1.536	1.137	6.69	5.05	27.4	20.9
2.6	1.962	1.454	8.10	6.25	32.4	25.1
2.8	2.521	1.881	9.59	7.53	37.7	29.7
3.0	3.19	2.46	11.2	9.32	43.1	36.0
3.5	5.479	4.234	15.41	12.7	57.8	47.4
4.0	8.540	6.772	19.96	16.8	73.3	61.3
5.0	16.81	13.92	29.61	25.7	106	91.6
6.0	27.3	23.5	39.5	35.3	140	123
8.0	50.81	45.17	58.5	53.3	207	187
12.0	95.2	88.7	90.9	85.4	320	297
18.0	139	138	125	120	431	408

[a]Without corrections.
[b]Corrected for binding-energy difference and Coulomb deflection (BC).

and $\sigma_{L_3}/\sigma_{L_2}$ from the present calculations are compared with experiment[16,19] and PWBA results from screened hydrogenic wave functions.[17,18] The minimum in the $\sigma_{L_1}/\sigma_{L_2}$ ratios is shifted down in energy by ~ 2 keV due to the effect of relativity, and shifted back up by ~ 1 keV by the binding and Coulomb-deflection corrections. The net result is good agreement of the calculated minimum energy with observation.[16,19] The $\sigma_{L_3}/\sigma_{L_2}$ ratios are overestimated by nonrelativistic PWBA calculations with screened hydrogenic wave functions.[17] The effect of relativity tends to reduce these ratios because

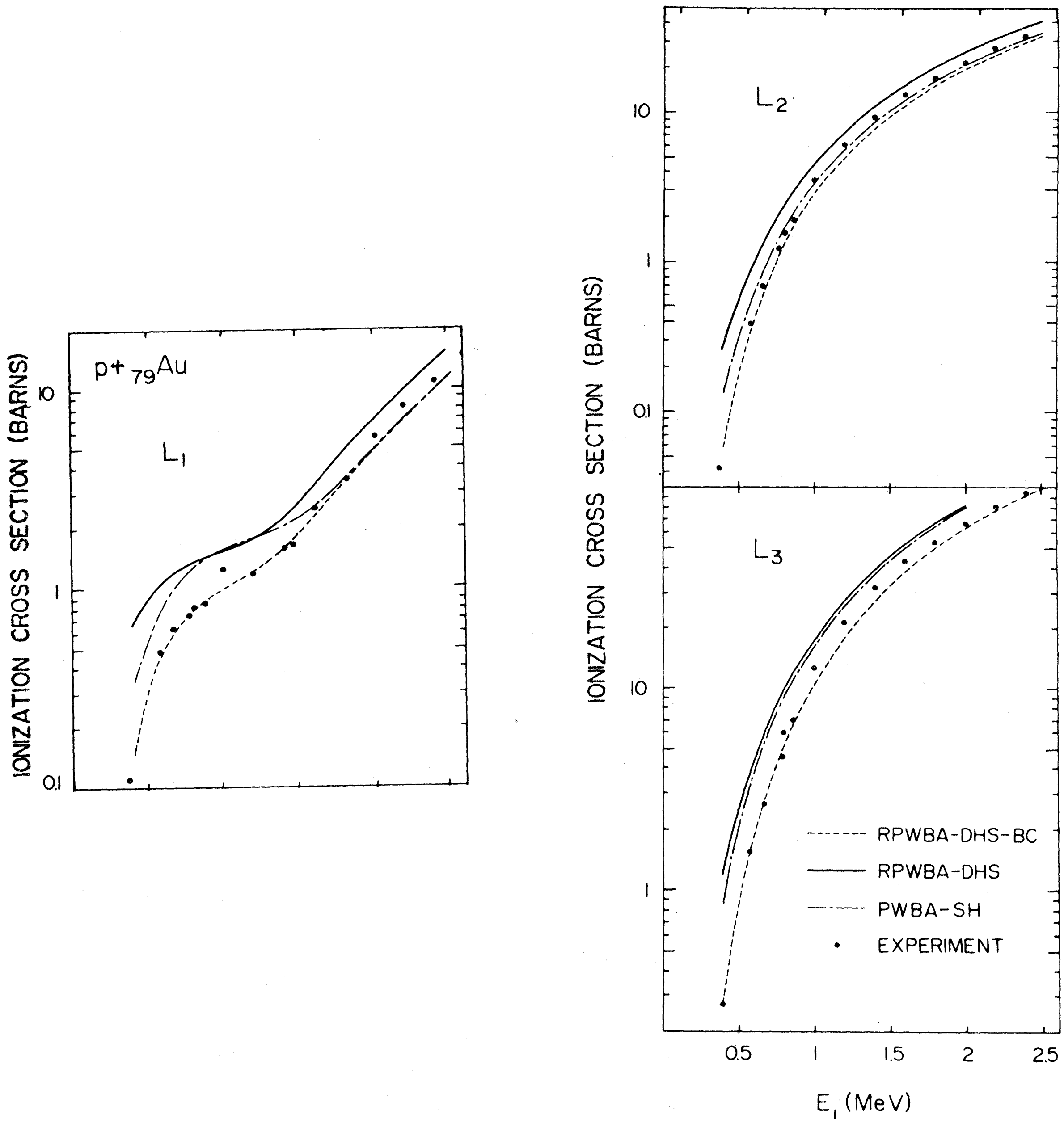

FIG. 1. Cross sections for L-subshell ionization of Au by protons. Results of the present relativistic plane-wave Born-approximation calculations with DHS wave functions, without corrections (RPWBA-DHS) and with corrections for binding-energy change and Coulomb deflection (RPWBA-DHS-BC) are compared with nonrelativistic plane-wave Born-approximation calculations based on screened hydrogenic (SH) wave functions (PWBA-SH) from Ref. 17 and with experimental data from Datz *et al.* (Ref. 19).

relativity affects the L_2 wave functions more than the L_3 wave functions. Comparison of the present RPWBA results from DHS wave functions with RPWBA calculations with screened hydrogenic wave functions[18] reveals that the more accurate DHS wave functions lead to an $\sim 8\%$ reduction in the L-subshell ionization cross-section ratios, for low proton energy (0.4—1.0 MeV), yielding fair agreement with experiment.[16,19]

Predicted total L x-ray-production cross sections can be calculated from theoretical L-subshell ionization cross sections, fluorescence yields ω_i and

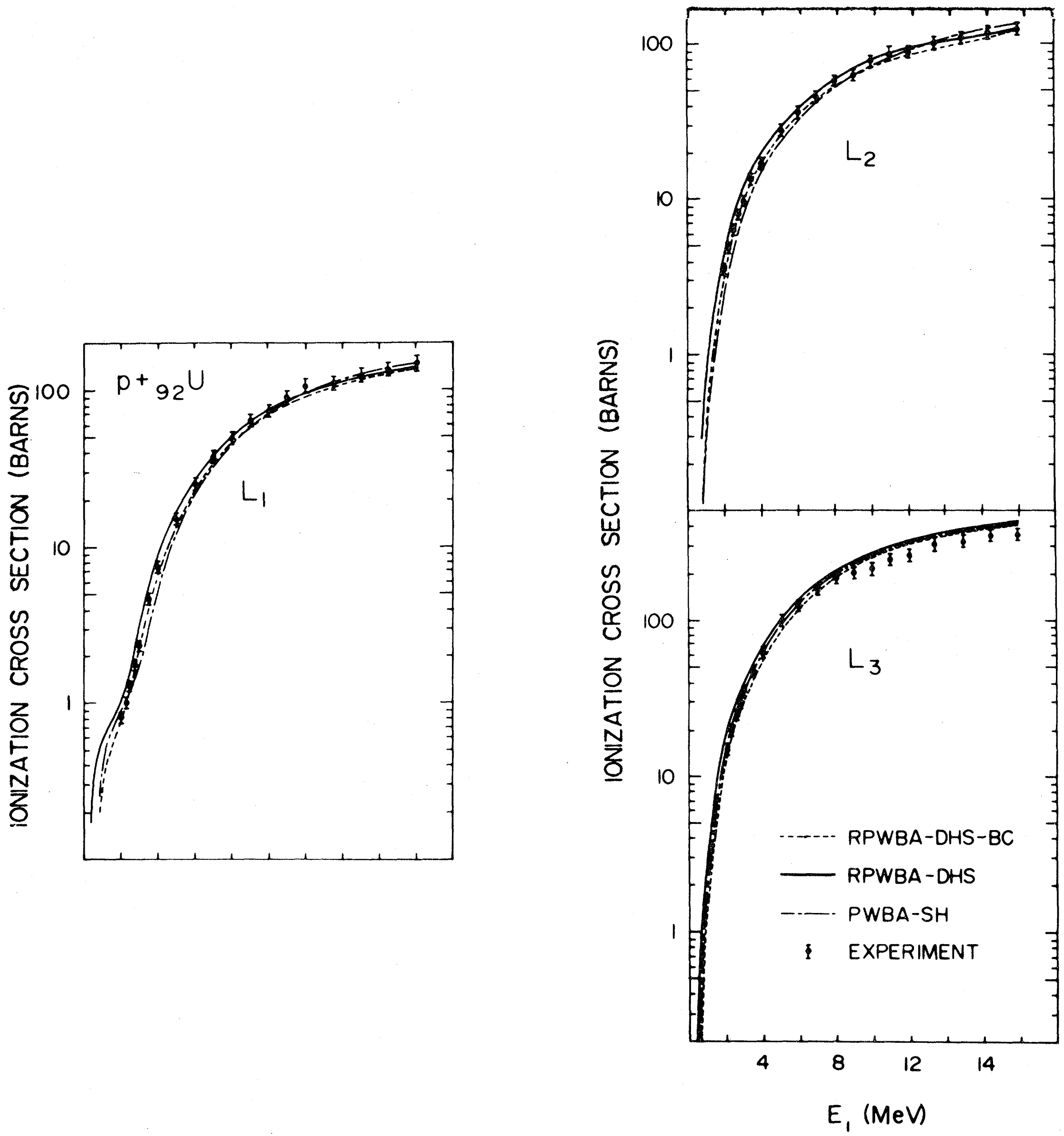

FIG. 2. Cross sections for L-subshell ionization of U by protons. Results of the present relativistic plane-wave Born-approximation calculations with DHS wave functions, without corrections (RPWBA-DHS) and with corrections for binding-energy shift and Coulomb deflection (RPWBA-DHS-BC) are compared with nonrelativistic plane-wave Born-approximation calculations based on screened hydrogenic wave functions (PWBA-SH) from Ref. 17 and with experimental data from Li *et al.* (Ref. 16).

Coster-Kronig yields f_{ij}.[20,21] We have

$$\sigma_{L\,\text{x ray}}=\sigma_{L_1}\omega_1+(\sigma_{L_1}f_{12}+\sigma_{L_2})\omega_2 +[(f_{13}+f_{12}f_{23})\sigma_{L_1}+\sigma_{L_2}f_{23}+\sigma_{L_3}]\omega_3 \,. \tag{12}$$

In Fig. 5, we compare theoretical L x-ray-production cross sections for protons on Au with results from other calculations and experiment.[15,22] The present RPWBA-DHS predictions including binding and Coulomb-deflection corrections agree extremely well with experiment[15,22] (Fig. 5). Fluorescence and Coster-Kronig yields from the compilation of Krause[21] were used to derive these x-ray-production cross sections from the calculated

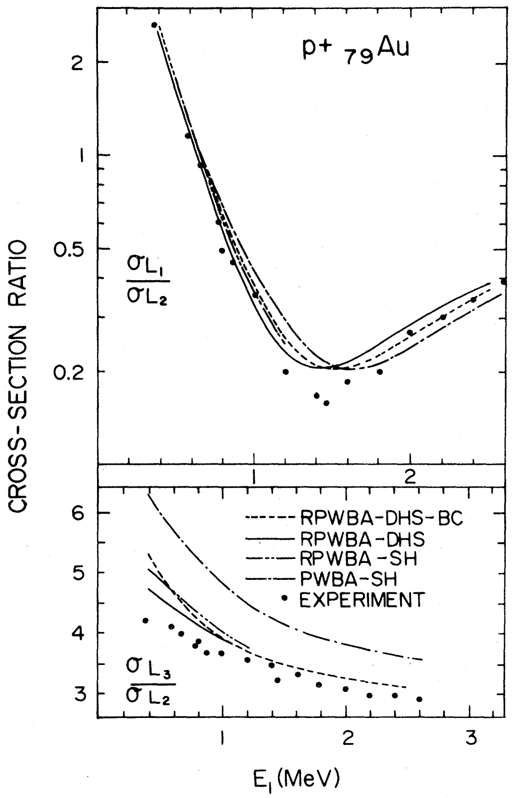

FIG. 3. Ratios of L-subshell cross sections for ionization of Au by protons. The present RPWBA results with corrections for binding and Coulomb deflection (RPWBA-DHS-BC) and without corrections (RPWBA-DHS) are compared with RPWBA calculations based on screened hydrogenic wave functions (RPWBA-SH, Ref. 18), with nonrelativistic PWBA calculations from screened hydrogenic wave functions (PWBA-SH, Ref. 17), and with experimental data (Ref. 19).

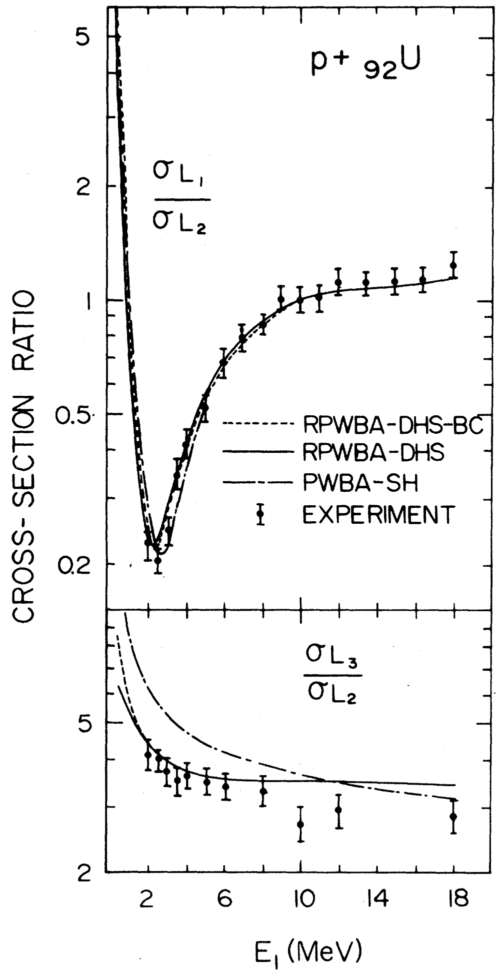

FIG. 4. Ratios of L-subshell cross sections for ionization of U by protons. Present RPWBA results with corrections for binding and Coulomb deflection (RPWBA-DHS-BC) and without corrections (RPWBA-DHS) are compared with nonrelativistic PWBA calculations based on screened hydrogenic wave functions (PWBA-SH, Ref. 17) and with experimental data (Ref. 16).

ionization probabilities. If binding and Coulomb-deflection corrections are omitted, the predictions become much larger than experimental data. The nonrelativistic PWBA predictions from screened hydrogenic wave functions[17] seem to agree with experiment above $E_1 = 0.7$ MeV, but this agreement is fortuitous, caused by accidential cancellation between the effects of relativity and the effects of binding and Coulomb deflection. Below $\sim$0.7-MeV proton energy, the PWBA predictions[17] deviate significantly from measured x-ray yields.

We have calculated $L\alpha/L\gamma$ and $L\alpha/L\beta$ x-ray emission rates for $p+$Au from the present theoretical subshell ionization cross sections, the fluorescence and Coster-Kronig yields compiled by Krause,[21] and Scofield's theoretical x-ray branching ratios.[23] In Fig. 6, we compare these x-ray intensity ratios with experiment[15] and with calculations based on screened hydrogenic wave functions.[17,18] The present DHS calculations are seen to represent a drastic improvement over the older PWBA results. We note that excellent agreement between theory and experiment can be attained if, in the calculations based on the present work, the L_3 fluorescence yield is reduced by 6%, the L_2 fluorescence yield is increased by 7%, and the L_1 fluorescence yield is increased by $\sim$5% with respect to the

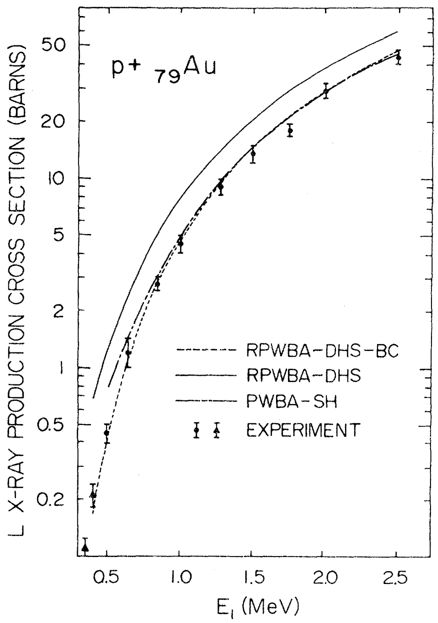

FIG. 5. L x-ray production cross section for protons on Au. Present relativistic results with corrections for binding and Coulomb deflection (RPWBA-DHS-BC) and without corrections (RPWBA-DHS) are compared with results from nonrelativistic PWBA calculations based on screened hydrogenic wave functions (PWBA-SH, Ref. 17) and with experimental data from Refs. 15 (dots) and 22 (triangles).

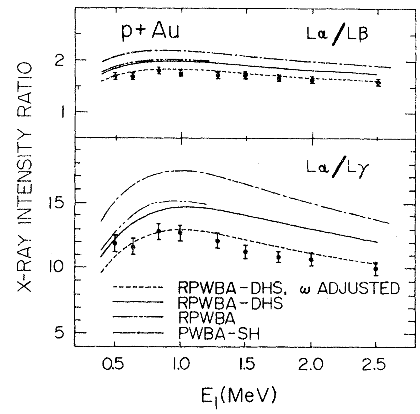

FIG. 6. $L\alpha/L\beta$ and $L\alpha/L\gamma$ x-ray-emission ratios for L-shell ionization of Au by protons. Results from the present RPWBA-DHS calculations with adjusted L fluorescence yields (as described in the text) and with fluorescence yields from Ref. 21 are compared with relativistic PWBA calculations based on screened hydrogenic wave functions (RPWBA-SH, Ref. 18), nonrelativistic PWBA calculations based on screened hydrogenic wave functions (PWBA-SH, Ref. 17) and with experiment (Ref. 15).

values of Ref. 21 (Fig. 6). These adjustments of the fluorescence yields are consistent with results from our new relativistic L-subshell calculations.[24] It can be concluded that the residual discrepancies between observed L x-ray intensity ratios and the present RPWBA-DHS calculations of ionization cross sections are mostly due to uncertainties in fluorescence and Coster-Kronig yields.

Note added in proof. It has come to our attention that the cancellation between the effects of relativity and those of Coulomb repulsion, discussed in Sec. III, was first noted for K-shell ionization by George Basbas, cf. Proceedings of the Conference on The Application of Small Accelerators, Denton, Texas, October 25—27, 1976 [The Institute of Electrical and Electronic Engineers, Nuclear and Plasma Science Society, Conference Record Publication No. 76CH1175-9NTS], p. 142.

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