Energy and Angular Momentum Distribution of Electrons Emitted from K and L Shells by Proton Impact*

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Explicit expressions for the semiclassical transition probabilities of atomic K- and L-shell electrons into the continuum as a result of proton collisions are obtained as functions of proton-impact parameter and energy transfer, using first-order time-dependent perturbation theory with undeflected proton trajectories. Calculated energy distributions for the ejected electrons are compared with the plane-wave Born-approximation cross sections. The contributions from various partial waves are shown in illustrations. The validity of the calculation is limited by the neglect of the Coulomb deflection of the protons.

I. INTRODUCTION

Theoretical and experimental investigations of the inner-atomic-shell ionization process by the impact of protons and other heavy-charged projectiles have been carried out during the past 50 years, and extensive data now exist on K- and L-shell x-ray yields resulting from such collisions.[1-3] The evaluation of cross sections for these ionization processes has usually been made by the Bethe-Born approximation,[4-6] which employs plane waves for the bombarding particle and hydrogenic wave functions for the atomic electrons. These calculations appear to overestimate the cross section in the region of low-incident energies.

An alternate approach is the semiclassical approximation which describes the bombarding particle as a point charge moving on a fixed classical orbit and exerting a time-dependent perturbation on the atomic electrons. Long ago, Mott and Frame,[7,8] and more recently Bang and Hansteen,[9] have made it plausible that the Born approximation and the semiclassical approximation with undeflected trajectory should give cross sections which agree closely if the incident particle momentum is very large compared to the momentum transfer in the ionizing collision. Bang and Hansteen also evaluated the K-shell ionization cross section in the semiclassical approximation, both for straight-line trajectories and for hyperbolic Kepler orbits, but under the further approximation that only the monopole terms in the proton-electron interaction were retained. They thus considered only transitions from the K-shell to the s-wave electron continuum.

In this paper, the results of a more complete calculation of inner-shell ionization cross sections for a proton on a straight-line trajectory are reported. Explicit expressions for transition probabilities in terms of partial waves are obtained. These formal expressions are used in accurate calculations of the energy distribution of the ejected electrons, including all relevant partial-wave transitions to the continuum. Also, comparisons are made between the semiclassical and the plane-wave Born approximations. The calculations are carried out for electrons which are initially in the K and L shells.

II. ENERGY-TRANSFER CROSS SECTIONS

For an inelastic collision between an incident particle of mass M, charge ze, energy $E=\frac{1}{2}Mv^2$, and an atom at rest, the energy distribution of an ejected electron from the atomic shell (labelled by s) is, according to first-order time-dependent perturbation theory, given by

$$d\sigma_s/dW = [4\pi(ze)^2/\eta_s a_0]\int_0^\infty p\,dp\,|\langle f|M_p|i_s\rangle|^2 \quad (1)$$

with $\langle f|M_p|i_s\rangle = \frac{1}{2}v\int_{-\infty}^{\infty} dt\,e^{i\omega t}\int d^3\vec{r}\,\psi_f^*(\vec{r})\,|\vec{r}-\vec{R}(t)|^{-1}\psi_{i_s}(\vec{r})$. (2)

The energy of the incident particle is measured in terms of the dimensionless quantity

$$\eta_s = mE/M(Z_s^{\,2}\,\mathrm{Ry}) \quad (3)$$

where Z_S is an effective nuclear charge for the s shell which takes screening of the inner electrons summarily into account, and E is in rydbergs. The a_0 is the first Bohr radius of the hydrogen atom, $W=\hbar\omega/(Z_S^{\,2}\,\mathrm{Ry})$ is the energy transferred to the atomic electron in units of $Z_S^{\,2}$ Ry, and p is the impact parameter. The $\vec{r}$ is the electron coordinate, and $\vec{R}(t)$ the coordinate of the heavy projectile, given as a function of time by the assumed classical law of motion; m is the mass of the electron.

We have used hydrogenic s-shell wave functions $\psi_{i_s}(\vec{r})$ and hydrogenic Coulomb-continuum partial waves as final-state wave functions $\psi_f(\vec{r})$. The latter are normalized per unit energy interval.

Neglecting deflection effects, $\vec{R}(t)$ is chosen to be a straight-line path parallel to the z axis, and traversed by the heavy projectile with constant velocity. The integration over t in the evaluation of Eq. (2) follows the analogous work of Bang and Hansteen.[9] For the radial integration, we employed the method of analytic continuation used by Jamnik and Zupancic[10] in order to reduce the generalized hypergeometric functions to manageable form. The calculation is reasonably straightforward, but involves extensive algebra. We simply quote the final results for the transition probabilities.

For the transition from the K shell to the continuum ($W = k^2+1$),

$$|\langle kl_f m_f|M_p|100\rangle|^2 = |\langle kl_f -m_f|M_p|100\rangle|^2$$

$$= \frac{2\pi m}{\hbar^2}\frac{a_0^2}{Z_K^2}\frac{N_0(k,l_f,m_f)}{1-e^{-2\pi/k}}\left(\frac{4\eta_K}{W^2}\right)^{l_f+4} F_0(p,k,\eta_K,l_f,m_f),\quad (m_f \geq 0), \tag{4}$$

and for the transition from the L shell to the continuum ($W = k^2+\frac{1}{4}$),

$$|\langle kl_f m_f|M_p|200\rangle|^2 = |\langle kl_f -m_f|M_p|200\rangle|^2$$

$$= \frac{2\pi m}{\hbar^2}\frac{a_0^2}{Z_L^2}\frac{N_1(k,l_f,m_f)}{1-e^{-2\pi/k}}\left(\frac{4\eta_L}{W^2}\right)^{l_f+4} F_1(p,k,\eta_L,l_f,m_f),\quad (m_f \geq 0),$$

$$|\langle kl_f m_f|M_p|210\rangle|^2 = |\langle kl_f -m_f|M_p|210\rangle|^2$$

$$= \frac{2\pi m}{\hbar^2}\frac{a_0^2}{Z_L^2}\frac{N_2(k,l_f,m_f)}{1-e^{-2\pi/k}}\left(\frac{4\eta_L}{W^2}\right)^{l_f+5} F_2(p,k,\eta_L,l_f,m_f),\quad (m_f \geq 0),$$

$$|\langle kl_f m_f|M_p|211\rangle|^2 = |\langle kl_f -m_f|M_p|21-1\rangle|^2 \tag{5}$$

$$= \frac{2\pi m}{\hbar^2}\frac{a_0^2}{Z_L^2}\frac{N_3(k,l_f,m_f)}{1-e^{-2\pi/k}}\left(\frac{4\eta_L}{W^2}\right)^{l_f+5} F_3(p,k,\eta_L,l_f,m_f),\quad (m_f \geq 1),$$

$$|\langle kl_f m_f|M_p|211\rangle|^2 = |\langle kl_f -m_f|M_p|21-1\rangle|^2$$

$$= \frac{2\pi m}{\hbar^2}\frac{a_0^2}{Z_L^2}\frac{N_4(k,l_f,m_f)}{1-e^{-2\pi/k}}\left(\frac{4\eta_L}{W^2}\right)^{l_f+5} F_4(p,k,\eta_L,l_f,m_f),\quad (m_f < 1),$$

where $N_0(k,l,m) = n(k,l)\,\dfrac{2(2l+1)(l-m)!}{(l+m)!}\left(\dfrac{(2m)!}{2^{2m}m!}\,\dfrac{(l+1)}{\Gamma(l+\frac{3}{2})}\right)^2,$

$$N_1(k,l,m) = n(k,l)\,\frac{(2l+1)(l-m)!}{(l+m)!}\left(\frac{(2m)!}{2^{2m+2}m!}\,\frac{(l+1)}{\Gamma(l+\frac{3}{2})}\right)^2,$$

$$N_2(k,l,m) = n(k,l)\,\frac{(l-m)!}{(2l+1)(l+m)!}\left(\frac{(2m)!\,(l-m+1)}{2^{2m+1}m!}\,\frac{(l+1)}{\Gamma(l+\frac{3}{2})}\right)^2,$$

$$N_3(k,l,m) = n(k,l)\,\frac{(l-m)!}{2(2l+1)(l+m)!}\left(\frac{(2m-2)!}{2^{2m-1}(m-1)!}\,\frac{(l+1)}{\Gamma(l+\frac{3}{2})}\right)^2,$$

$$N_4(k,l,m) = n(k,l)\frac{(l-|m|)!}{2(2l+1)(l+|m|)!}\left(\frac{(2|m|+2)!}{2^{2|m|+3}(|m|+1)!}\,\frac{(l+1)}{\Gamma(l+\frac{3}{2})}\right)^2,$$

with $n(k,l)=1$, for $l=0$, and $n(k,l)=(1+k^2)(1+2^2k^2)\cdots(1+l^2k^2)$ for $l \geq 1$,

and
$$F_0(p,k,\eta_K,l,m) = (pq_0)^{2m}\left|\sum_{t=0}^{\leq\frac{1}{2}(l-m)} C_{l-m,m+\frac{1}{2}}^{l-m-2t}\sum_{r=0}^{\infty}(-1)^r\,\frac{(l+2)}{r!}r \times A_{2r+1}(l,k)M_{l-m-t+r+2}^{m+1}(pq_0)\left(\frac{4\eta_K}{W^2}\right)^r\right|^2,$$

$$F_1(p,k,\eta_L,l,m) = (pq_0)^{2m}\left|\sum_{t=0}^{\leq\frac{1}{2}(l-m)} C_{l-m,m+\frac{1}{2}}^{l-m-2t}\sum_{r=0}^{\infty}\frac{(-1)^r(l+2)}{r!}r \times [(2r+1)B_{2r}(l,k)+2B_{2r+1}(l,k)]M_{l-m-t+r+2}^{m+1}(pq_0)\left(\frac{4\eta_L}{W^2}\right)^r\right|^2,$$

$$F_2(p,k,\eta_L,l,m) = (pq_0)^{2m}\left|(l+2)\sum_{t=0}^{\leq\frac{1}{2}(l-m+1)} C_{l-m+1,m+\frac{1}{2}}^{l-m+1-2t}\sum_{r=0}^{\infty}\frac{(-1)^r(l+3)}{r!}r \times B_{2r+1}(l,k)M_{l-m-t+r+3}^{m+1}(pq_0)\left(\frac{4\eta_L}{W^2}\right)^r\right.$$
$$\left. + \frac{3(l+m)}{2(l-m+1)}\sum_{t=0}^{\leq\frac{1}{2}(l-m-1)} C_{l-m-1,m+\frac{1}{2}}^{l-m-1-2t}\sum_{r=0}^{\infty}\frac{(\cdot 1)^r(l+2)}{r!}r\left(\frac{2r+3}{3}\right) \times B_{2r+1}(l,k)M_{l-m-t+r+2}^{m+1}(pq_0)\left(\frac{4\eta_L}{W^2}\right)^r\right|^2,$$

$$F_3(p,k,\eta_L,l,m) = (pq_0)^{2m-2}\left|(l+2)(l-m+2)(l-m+1)\sum_{t=0}^{\leq\frac{1}{2}(l-m+2)} C_{l-m+2,m-\frac{1}{2}}^{l-m+2-2t} \times \sum_{r=0}^{\infty}\frac{(-1)^r(l+3)}{r!}r\,B_{2r+1}(l,k)M^{m}{}_{l-m-t+r+4}(pq_0)\left(\frac{4\eta_L}{W^2}\right)^r\right.$$
$$\left. - \tfrac{3}{2}(l+m)(l+m-1)\sum_{t=0}^{\leq\frac{1}{2}(l-m)} C_{l-m,m-\frac{1}{2}}^{l-m-2t}\sum_{r=0}^{\infty}\frac{(-1)^r(l+2)}{r!}r\left(\frac{2r+3}{3}\right) \times B_{2r+1}(l,k)M^{m}{}_{l-m-t+r+3}(pq_0)\left(\frac{4\eta_L}{W^2}\right)^r\right|^2,$$

$$F_4(p,k,\eta_L,l,m) = (pq_0)^{2|m|+2}\left|(l+2)\sum_{t=0}^{\leq\frac{1}{2}(l-|m|)} C_{l-|m|,|m|+\frac{3}{2}}^{l-|m|-2t} \times \sum_{r=0}^{\infty}\frac{(-1)^r(l+3)}{r!}r\,B_{2r+1}(l,k)M_{l-|m|-t+r+2}^{|m|+2}(pq_0)\left(\frac{4\eta_L}{W^2}\right)^r\right.$$
$$-\frac{3}{2}\sum_{t=0}^{\leq\frac{1}{2}(l-|m|-2)} C_{l-|m|-2,|m|+\frac{3}{2}}^{l-|m|-2-2t}\sum_{r=0}^{\infty}\frac{(-1)^r(l+2)}{r!}r\left(\frac{2r+3}{3}\right)$$

$$\times B_{2r+1}(l,k) M^{|m|+2}_{l-|m|-t+r+1}(pq_0)\left(\frac{4\eta_L}{W^2}\right)^r \Bigg|^2 ,$$

with $q_0 = \left(\frac{W^2}{4\eta_s}\right)^{1/2} \frac{Z_s}{a_0}$, $(n)_r = \frac{\Gamma(n+r)}{\Gamma(n)}$, $C_{n,\nu}^{\;n-2t} = \frac{(-1)^t \Gamma(\nu+n-t) 2^{n-2t}}{\Gamma(\nu) t! (n-2t)!}$,

$$A_n(l,k) = (1-ik)^n \, {}_2F_1(-n, l+1-i/k, 2l+2, -2ik/(1-ik)),$$

$$B_n(l,k) = (\tfrac{1}{2}-ik)^n \, {}_2F_1(-n, l+1-i/k, 2l+2, -ik/(\tfrac{1}{2}-ik)),$$

$$M_n^{\;\nu}(pq_0) = (pq_0)^n K_n(pq_0)/2^{n-1}\Gamma(n+\nu),$$

where q_0 corresponds to the minimum momentum transfer of the incident particle as deduced from the conservation laws, and $K_n(x)$ is the modified Bessel function[11] of the second kind, of order n. The total energy distribution of the ejected electrons from the s shell is given by

$$\frac{d\sigma_s}{dW} = 4\pi \frac{(ze)^2}{\eta_s a_0} \sum_{i_s} \sum_{l_f, m_f} \int_0^\infty p\,dp \, |\langle k l_f m_f | M_p | i_s \rangle|^2, \tag{6}$$

where the sum over i_s signifies summation over all occupied states of the s shell. In the limit $4\eta_s/W \ll 1$,

$$d\sigma_s/dW \approx [8\pi(ze)^2/\eta_s a_0] \int_0^\infty p\,dp \, |\langle k00 | M_p | s00\rangle|^2. \tag{7}$$

These monopole excitations give Huus's approximations,[12]

$$\frac{d\sigma_K}{dW} \approx \frac{2^{20}}{5} \pi \frac{z^2 a_0^{\;2}}{Z_K^{\;4}} \frac{\eta_K^{\;4}}{W^{10}}, \quad \frac{d\sigma_L}{dW} \approx \frac{2^{17}}{5} \pi \frac{z^2 a_0^{\;2}}{Z_L^{\;4}} \frac{\eta_L^{\;4}}{W^{10}}, \tag{8}$$

to the lowest order in powers of $4\eta_s/W^2$. Huus's approximation for the K shell has first been derived by Bang and Hansteen[9] using the semiclassical approximations. We note that Huus's approximation is larger than the semiclassical approximation, which includes all partial-wave transitions to the continuum. This can be understood by the fact that the neglected terms in the series expansion of the monopole excitation in deriving Huus' approximation are predominantly negative, and this neglected negative contribution exceeds all the positive higher partial-wave contributions.

The energy distributions for the K and L shell ionization by heavy-charged particles were computed for several values of η_K up to 0.2 and η_L up to 0.03 as functions of the energy transfer W in the region above the minimum energy transfers without outer screening.

For proton impact on copper ($Z_K = 28.7$, $Z_L = 24.87$) and lead ($Z_K = 81.7$, $Z_L = 77.85$), $\eta_K = 0.2$ corresponds to 4.1 and 33.3 MeV of incident energy, respectively, while $\eta_L = 0.03$ corresponds to 462.8 keV and 4.5 MeV of incident energy, respectively. The numerical work of evaluating the transition probabilities, Eqs. (4) and (5), as functions of the impact parameter was considerable, since the series are alternating with increasing coefficients. A PL1 program was written to evaluate the series using the recurrence relations of the coefficient function on the IBM 360 computer. Ten terms of partial waves were found to be sufficient to obtain the total energy distribution within 1% accuracy. Some sample results of the computations of $d\sigma_s/dW$ are given in tabular form in Tables I and II for the K and L shells. In terms of the so-called excitation function[1] $I_S(\eta_S, W_S)$ the tabulated quantities are $I_K/(2^{12}\eta_K)$ in Table I and $I_L/(2^9\eta_L)$ in Table II.

Many of the numerical values for the cross section were compared with the corresponding quantities computed in the plane-wave Born approximation, and agreement to within 1% was found for the entire range of listed values of η and W.

The semiclassical approximation allows us to calculate the ionization corss sections for electrons from the $2s$ and $2p$ subshells of the L shell separately. This option is important since the binding energies of the subshells are significantly different, and outer atomic screening may be partially taken into account - even while employing hydrogenic wave functions - by adjusting the minimum energy transfer appropriately for each subshell.[1] Equations (5) contain the formulas for the subshell cross sections, and Fig. 1 illus-

TABLE I. Energy distribution of K electrons, $(d\sigma_K/dW)/(2^{15}\pi z^2/Z_K^4)a_0^2$.

W	$\eta_K=0.06$	$\eta_K=0.1$	$\eta_K=0.15$	$\eta_K=0.2$
1.01	1.49×10^{-5}	4.86×10^{-5}	9.95×10^{-5}	
1.2	4.49×10^{-6}	1.80×10^{-5}	4.39×10^{-5}	7.19×10^{-5}
1.4	1.38×10^{-6}	6.63×10^{-6}	1.90×10^{-5}	3.49×10^{-5}
1.6	4.65×10^{-7}	2.55×10^{-6}	8.37×10^{-6}	1.71×10^{-5}
1.8	1.70×10^{-7}	1.03×10^{-6}	3.79×10^{-6}	8.55×10^{-6}
2.0	6.67×10^{-8}	4.38×10^{-7}	1.76×10^{-6}	4.31×10^{-6}
2.2	2.80×10^{-8}	1.95×10^{-7}	8.43×10^{-7}	2.21×10^{-6}
2.4	1.25×10^{-8}	9.09×10^{-8}	4.16×10^{-7}	1.16×10^{-6}
2.6	5.88×10^{-9}	4.43×10^{-8}	2.12×10^{-7}	6.16×10^{-7}
2.8	2.91×10^{-9}	2.24×10^{-8}	1.11×10^{-7}	3.36×10^{-7}

trates the results for $\eta_L=0.01$. It should be noted that, in the low-energy transfer limit, the energy distribution of $2p$ electrons is much larger than that of $2s$ electrons.

III. PARTIAL-WAVE CONTRIBUTIONS

As η_S becomes larger, the contributions of the higher partial waves will be significant. This may be seen from Eq. (4) and (5).

Figures 2(a) and (b) show the contributions of the partial waves to $d\sigma_K/dW$ for $\eta_K=0.06$ and 0.15, respectively.

Above $\eta_K=0.15$, the contribution of the p-wave continuum transition is comparable to that of s-wave continuum transition. The partial-wave contributions for $2s$ and $2p$ states are shown in Fig. 3(a) and (b) for $\eta_L=0.01$. The curve corresponding to $l=0$ in Fig. 3(a) is the monopole excitation for $2s$ states. Again the contributions of the higher partial waves such as p and d waves are dominant for low-energy transfers.

IV. CONCLUSIONS

The angular momentum and energy distributions of electrons ejected from K and L shell by the impact of a heavy charged particle, given by explicit expressions for the transition probabilities, Eq. (4) and (5), are the main results of this paper. The semiclassical approximation, which treats the projectile as moving uniformly on a straight line, was found to agree with the plane-wave Born approximation in the region of low incident energy. The validity of both approximations is limited primarily by neglecting the deflection effect of the incident particle, due to the Coulomb repulsion between the incident particle and the atomic nu-

TABLE II. Energy distribution of L electrons, $(d\sigma_L/dW)/(2^{12}\pi z^2/Z_L^4)a_0^2$.

W	$\eta_L=0.01$	$\eta_L=0.03$
0.250	9.00×10^{-3}	
0.255		1.23×10^{-1}
0.285		6.51×10^{-2}
0.350	8.12×10^{-4}	
0.395		8.32×10^{-3}
0.450	1.05×10^{-4}	
0.485		2.01×10^{-3}
0.550	1.81×10^{-5}	
0.585		4.96×10^{-4}
0.650	3.92×10^{-6}	
0.685		1.40×10^{-4}
0.750	1.02×10^{-6}	
0.785		4.39×10^{-5}
0.850	3.07×10^{-7}	
0.885		1.52×10^{-5}
0.950	1.04×10^{-7}	
0.985		5.71×10^{-6}
1.050	3.94×10^{-8}	
1.085		2.32×10^{-6}
1.150	1.60×10^{-8}	

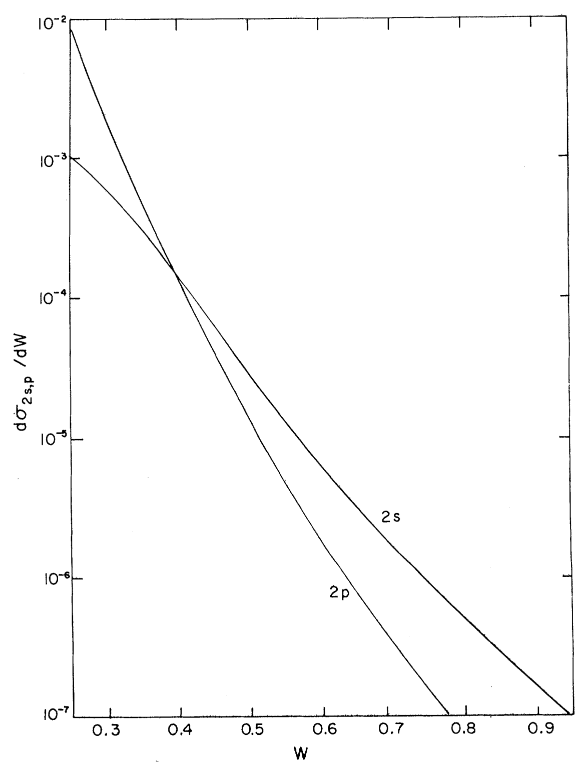

FIG. 1. Energy distributions $d\sigma_{2s,p}/dW$ of $2s$ and $2p$ electrons in units of $2^{12}\pi z^2 a_0^2/Z_L^4$, for $\eta_L=0.01$ as functions of the energy transfer W in units of Z_L^2 Ry.

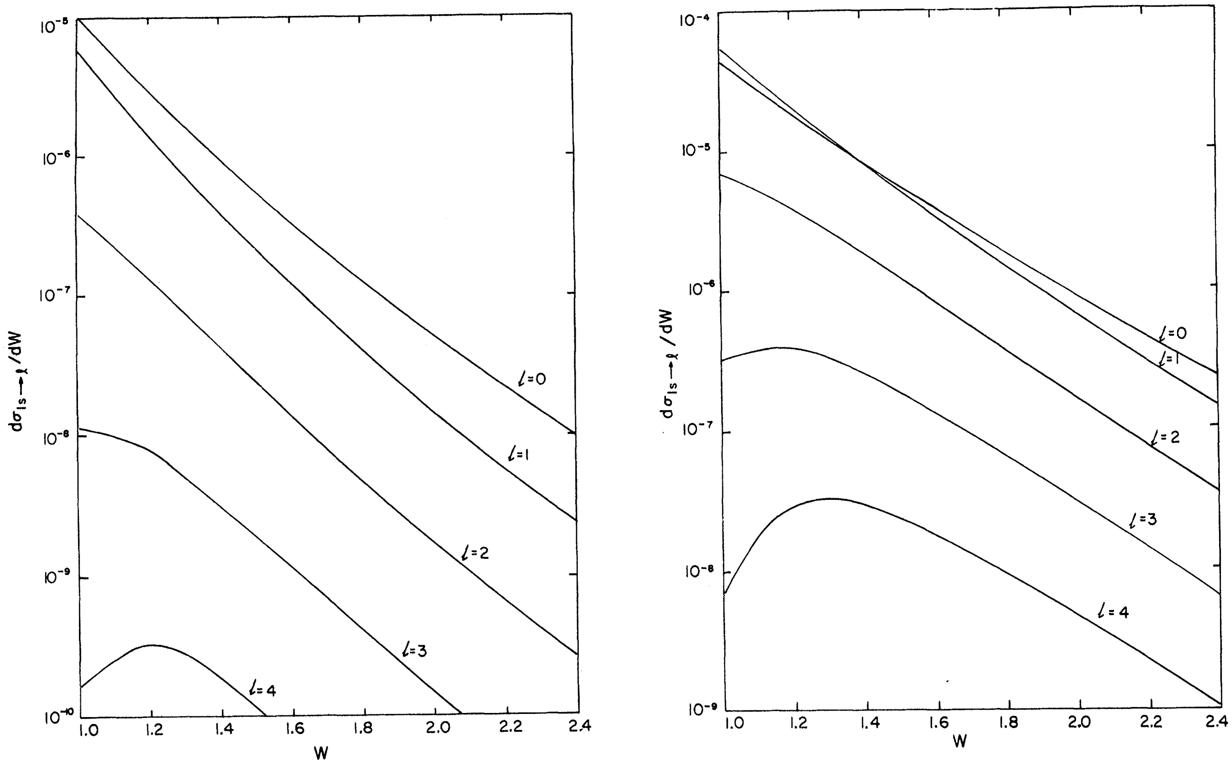

FIG. 2. Partial-wave contributions $d\sigma_{1s\to l}/dW$ in units of $2^{15}\pi z^2 a_0^2/Z_K^4$, as functions of the energy transfer W in units of Z_K^2 Ry, (a) for $\eta_K = 0.06$, (b) for $\eta_K = 0.15$.

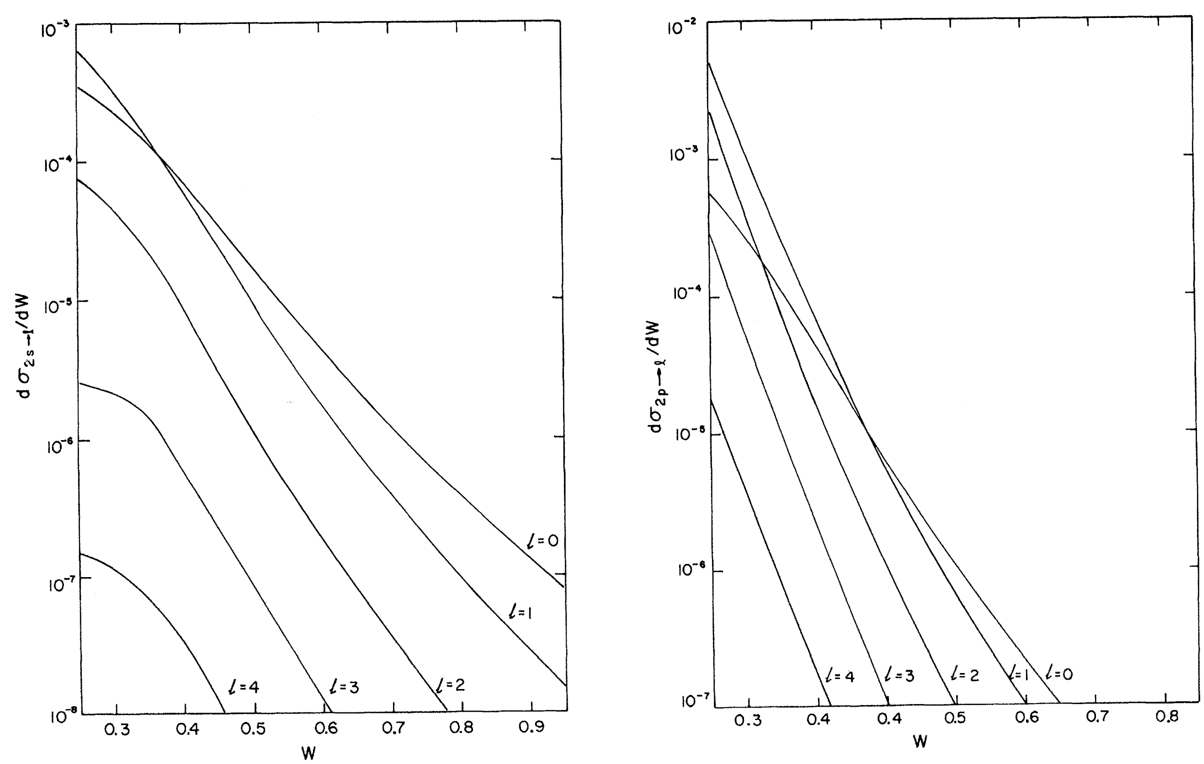

FIG. 3. Partial-wave contributions for $\eta_L = 0.01$ as functions of the energy transfer W in units of Z_L^2 Ry. (a) $d\sigma_{2s\to l}/dW$, (b) $d\sigma_{2p\to l}/dW$, in units of $2^{12}\pi z^2 a_0^2/Z_L^4$.

cleus. The close agreement between the two approximations suggests that a semiclassical calculation at low energies with projectiles moving on hyperbolic Kepler orbits[9] might similarly yield results equivalent to the more fully quantum-mechanical distorted-wave Born approximation. More accurate calculations of cross sections which take the Coulomb deflection into account are desirable. The application of Eqs. (5) to the calculation of angular distributions of the emitted L-shell electrons will be reported elsewhere.[13]

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[13]Further numerical values of partial and differential ionization cross sections, as described in this paper, may be obtained upon request from the authors by specifying the relevant experimental parameters (incident energy, kind of projectile, target atom).