Energy-loss effect in inner-shell Coulomb ionization by heavy charged particles

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The influence of the energy loss of slow projectiles during inelastic collisions on the inner-shell ionization cross sections is treated analytically. The result agrees with available experimental cross sections for K-shell ionization by protons. Residual trends in the data may gauge the quality of wave functions employed in calculations of Coulomb ionization cross sections.

I. INTRODUCTION

During the past decade, the theory of inner-shell Coulomb ionization by heavy charged particles[1] of mass M_1 moving with velocity v_1 and kinetic energy $E_1 = \frac{1}{2}M_1 v_1^2$ has evolved in an approach labeled CPSSR.[2,3] It accounts for the effect of deflection and velocity change of the projectile in the Coulomb field (C) of the target nucleus on the ionization cross section, and describes the electron orbits in the target atom under the influence of the projectile as perturbed stationary states (PSS) with relativistic (R) effects. This theory applies to collison systems such that $Z_1/Z_2 \lesssim \frac{1}{2}\theta_S$, where Z_1 and Z_2 refer to the nuclear charges of the projectile and the target atom, respectively. The observed binding energies ω_{2S} of the electrons removed from the shell S during the collision, in units of the corresponding screened hydrogenic values, are denoted as θ_S. The θ_S values increase with Z_2 from 0.6 to 1.0 for K shells and from 0.4 to 0.8 for L shells. Atomic units are used except where stated otherwise.

The CPSSR theory agrees with the large body of experimental K- and L-shell data that is now available for protons and deuterons, $Z_1 = 1$, on the average to within 30%. This scatter is comparable to the overall uncertainties of the data as they arise in the measurements of absolute Auger-electron or x-ray production cross sections, and in the determination of fluorescence yields for the conversion of x-ray production cross sections to ionization cross sections. We adopt the fluorescense yields recently recommended by Krause.[4] Other contributions not included in the CPSSR theory for direct ionization, such as electron capture by the projectile[5] or target-orbital contraction[6] during the collison, can be neglected for $Z_1 = 1$ projectiles in K-shell ionizations when $Z_2 > 10$ and in L-shell ionizations when $Z_2 > 20$.[3,5]

Renewed analysis of the rapidly accumulating data at low projectile velocities leads us to the conclusion that, at the lowest projectile velocities investigated to date, the calculated ionization cross sections $\sigma_S^{\mathrm{CPSSR}}$ are larger in statistically significant ways than the experimental values σ_S^{expt}. To illustrate this point, Fig. 1 displays some 2300 measured cross sections as inferred from K-shell x-ray production cross sections for protons $(Z_1 = 1)$ in targets covering the range $10 \le Z_2 \le 92$. The data for σ_K^{expt} were culled from the literature in the proton-energy ranges given in Table I (see references therein). The experimental values were divided by $\sigma_K^{\mathrm{CPSSR}}$ calculated according to Ref. 3. The abscissa is given in units of the variable $(\propto E_1^{-1})$

$$\zeta_K \Delta_K = \zeta_K \omega_{2K} M_1 / M E_1 \,, \tag{1}$$

where ζ_K is the factor that accounts for the perturbed stationary states,[2,3] and $\Delta_K \equiv \omega_{2K} M_1 / M E_1$ is the minimum fractional energy loss of the projectile during K-shell ionization in the center-of-mass system with reduced mass $M \equiv (M_1^{-1} + M_2^{-1})^{-1}$. The upper scales give the corresponding values of the reduced velocity variable $\xi_K^R/\zeta_K \propto v_1$ and the ionization cross section $\sigma_K^{\mathrm{CPSSR}}$ for protons ionizing $^{27}_{13}\mathrm{Al}(K)$. Although the cross sections increase in this range of ξ_K^R/ζ_K a million fold, the points in the figure scatter rarely by more than a factor two about the ideal value one. In fact, some 90% of the data agree with the CPSSR prediction to within 30%. The mean of all ratios is, nevertheless, 0.80. The data are close to unity for $\xi_K \gtrsim 1$, but fall systematically below the predictions of the theory when $\xi_K < 1$, the more so the lower the projectile velocity.

We explore to what extent this trend can be attributed to the finite kinetic-energy loss suffered by the projectiles in the inner-shell excitation process.

II. ENERGY-LOSS EFFECT

Consider a projectile of atomic number Z_1, mass M_1, incident energy E_1, and velocity v_1 colliding with a target atom of atomic number Z_2 and mass M_2. In an inelastic collision, the projectile loses the energy

$$E_i - E_f = (M/2)(v_i^2 - v_f^2) = (1/2M)(K_i^2 - K_f^2)\,, \qquad (2)$$

where $E_i = (M/M_1)E_1$ is the initial and E_f the final kinetic energy of the projectile in the center-of-mass system, with corresponding velocities $\vec{v}_i$, $\vec{v}_f$ and momenta $\vec{K}_i = M\vec{v}_i$, $\vec{K}_f = M\vec{v}_f$. The minimum momentum change $q_{\min}$ in such a collision is $[\Delta \equiv (E_i - E_f)/E_i]$

$$q_{\min} \equiv K_i - K_f = 2q_0[1 + (1-\Delta)^{1/2}]^{-1}\,, \qquad (3)$$

while the maximum momentum change $q_{\max}$ becomes

$$q_{\max} \equiv K_i + K_f = 2q_0[1 - (1-\Delta)^{1/2}]^{-1}\,. \qquad (4)$$

The minimum momentum transfer in the limit of vanishing relative projectile-energy losses, $\Delta \to 0$, is denoted by $q_0 = (E_i - E_f)/v_1$.

The calculation of ionization cross sections in the standard plane-wave Born approximation (PWBA) entails an integration over the momentum transfer q form $q_{\min} = q_0$ to $q_{\max} = \infty$. In very slow collisions, however, the relative projectile-energy loss Δ in Eqs. (3) and (4) cannot be neglected, the more so because at low projectile velocities the inelastic cross sections are inversely proportional to high powers of q. Specifically, the differential PWBA ionization cross sections for direct ionization of the target shell S with regard to the final kinetic energy of the ejected electron, $\mathcal{E}_f$, take simple analytical forms.[2,7] When the energy-loss effect is included they can be written as

$$\frac{d\sigma_S^{\mathrm{EPWBA}}}{d\mathcal{E}_f} = \frac{d\sigma^{\mathrm{PWBA}}}{d\mathcal{E}_f}\left[\left(\frac{q_0}{q_{\min}}\right)^{\nu+1} - \left(\frac{q_0}{q_{\max}}\right)^{\nu+1}\right]. \qquad (5)$$

The letter E in the superscript signifies that the q integration was performed between the exact limits Eqs. (3) and (4). For K shells and L_1 shells, $\nu = 9$; for L_2 and L_3 shells, $\nu = 11$.

Integration of Eq. (5) over all final states $\mathcal{E}_f$ yields the ionization cross section[8] in closed form (cf. Appendix A)

$$\sigma_S^{\mathrm{EPWBA}} = f_S(z)\sigma_S^{\mathrm{PWBA}}\,. \qquad (6)$$

The cross sections σ_S^{PWBA} have been calculated for screened hydrogenic (SH) inner-shell wave functions.[9] The energy-loss effect appears through the function $f_S(z)$ of argument $z \equiv (1 - \omega_{2S}M_1/ME_1)^{1/2} \equiv (1-\Delta_S)^{1/2}$,

$$f_S(z) = 2^{-\nu}(\nu-1)^{-1}[(\nu z - 1)(1+z)^{\nu} + (\nu z + 1)(1-z)^{\nu}]\,, \qquad (7)$$

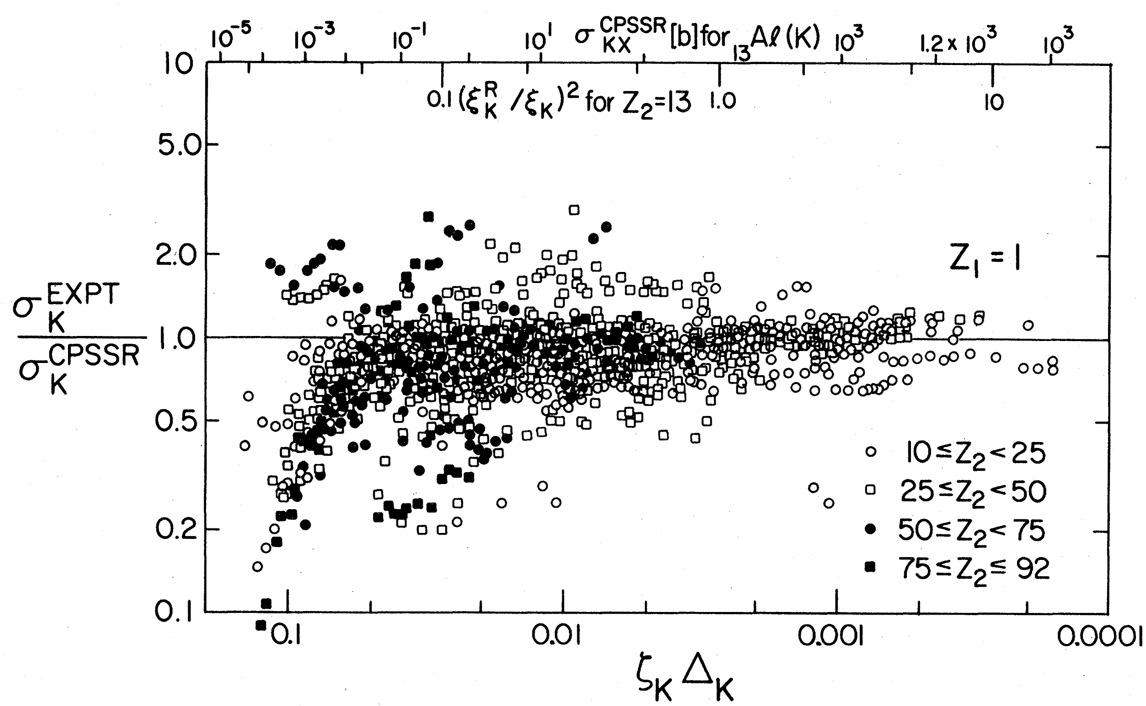

FIG. 1. Ratios of experimental and theoretical cross sections for K-shell ionization by protons vs $\zeta_K\Delta_K$, the effective relative projectile energy loss defined by Eq. (1). The experimental ionization cross sections σ_K^{expt} are measured x-ray production cross sections (cf. Table 1) divided by the fluorescence yields of Ref. 4. The theoretical ionization cross sections $\sigma_K^{\mathrm{CPSSR}}$ are calculated according to Eq. (13).

TABLE I. Ranges of proton energies, from E_1^{min} to E_1^{max} in MeV, for which measured K-shell x-ray production cross sections in various targets of atomic number Z_2 are plotted in Fig. 1, after division by the appropriate fluorescence yield (Ref. 4), as σ_K^{expt}. Papers are cited by the first three letters of the first author and the publication year. The corresponding ranges of the relative projectile-energy loss in the ionizing collision $\zeta_K\Delta_K$, Eq. (1) and Fig. 1, are tabulated in percent. Note that for $\zeta_K\Delta_K > 0.01$, the variable can be calculated to within 3% as $\zeta_K\Delta_K = [(Z_2/300)^2 + (Z_2/330)^3]/E_1$, if the proton energy E_1 is given in MeV. The record energy loss is 17% for 55 keV protons on $_{28}$Ni (Ref. 13).

Target atom	$100\zeta_K\Delta_K$ max	$100\zeta_K\Delta_K$ min	E_1 (MeV) min	E_1 (MeV) max	Ref.[a]
$_{10}$Ne	2.34	0.71	0.048	0.145	Har (1973)
	0.84	0.07	0.125	1.2	Lan (1976)
	0.50		0.2		Lan (1973)
	0.02		5		Bur (1974)
$_{11}$Na	6.99	2.08	0.02	0.065	Shi (1978)
$_{12}$Mg	8.34	2.71	0.02	0.06	Shi (1978)
	6.65	0.08	0.025	1.7	Kha (1965)
	3.28	0.76	0.05	0.2	Bra (1966)
	2.71	0.28	0.06	0.5	Kha (1964)
	0.04		3		Bon (1978)
$_{13}$Al	13.0	3.20	0.015	0.06	Shi (1978)
	9.77	3.50	0.02	0.055	Bru (1973)
	7.80	0.09	0.025	1.7	Kha (1965)
	7.80	0.91	0.025	0.2	Bra (1969)
	7.80	0.05	0.025	2.96	Bas (1973)
	6.49	0.91	0.03	0.2	Bra (1966)
	3.86	0.19	0.05	0.1	Chr (1967)
	3.20	0.34	0.06	0.5	Kha (1964)
	2.73	0.43	0.07	0.4	Nee (1970)
	2.11	0.91	0.09	0.2	Shi (1971)
	0.91		0.2		Web (1977)
	0.22	0.04	0.75	4	Taw (1976)
	0.11		1.5		Ogi (1964)
	0.05		3		Bon (1978)
$_{14}$Si	9.07	3.73	0.025	0.06	Shi (1978)
	0.26	0.05	0.75	4	Taw (1976)
	0.06		3		Bon (1978)
$_{16}$S	0.32	0.08	0.83	3.28	Hop (1975)
	0.08		3.0		Bon (1978)
$_{17}$Cl	0.32		0.95		Mil (1976)
	0.10		3		Bon (1978)
$_{18}$Ar	5.49	2.74	0.068	0.135	Har (1973)
	2.96	0.34	0.125	1	Lan (1976)
	0.32	0.18	1.05	1.88	Mac (1973)
	0.22	0.07	1.5	4.5	Win (1973)
	0.22	0.07	1.5	5	Win (1973)
	0.17		2		Ran (1976)
	0.11		3		Czu (1975)
$_{19}$K	0.41		0.95		Mil (1976)
	0.12		3		Bon (1978)
$_{20}$Ca	2.29	0.89	0.2	0.5	Lop (1979)
	0.89	0.21	0.5	2.0	Lop (1978)
	0.21	0.17	2	2.6	Bis (1970)
	0.21		2		Rai (1977)
	0.14	0.04	3	11	Bon (1978)
$_{21}$Sc	2.54	0.99	0.2	0.5	Lop (1979)
	0.99	0.23	0.5	2	Lop (1978)
	0.73	0.08	0.667	5.67	Hop (1975)
	0.59	0.14	0.83	3.28	Hop (1975)
$_{22}$Ti	14.9	8.05	0.038	0.07	Shi (1978)
	9.40	3.74	0.06	0.15	Zan (1979)
	6.25	2.79	0.09	0.2	Shi (1971)
	5.62	3.74	0.1	0.15	Dug (1972)
	5.62	3.74	0.1	0.15	Zan (1976)
	4.32	1.32	0.13	0.415	Whe (1974)
	3.74	0.51	0.15	1.05	Nik (1976)
	2.79	1.09	0.2	0.5	Lop (1979)
	2.42	1.09	0.23	0.5	Jop (1962)
	1.09	0.26	0.5	2	Lop (1978)
	0.91	0.17	0.6	3	McD (1977)
	0.77	0.25	0.7	2.1	Fah (1973)
	0.53	0.17	1	3	Kha (1975)
	0.35		1.5		Ogi (1964)
	0.35	0.09	1.5	5.5	Lin (1973)
	0.35	0.05	1.5	10.9	Aks (1974)
	0.33	0.13	1.6	3.9	Mer (1958)
	0.26	0.02	2	28	Bis (1970)
	0.17	0.02	3		Bon (1978)
	0.13	0.02	4	22	Pon (1978)
	0.13	0.02	4	22	Pon (1979)
$_{23}$V	6.16	4.09	0.1	0.15	Dug (1972)
	4.09	0.56	0.15	1.05	Nik (1976)
	3.06	1.20	0.2	0.5	Lop (1979)
	1.20	0.29	0.5	2	Lop (1978)
	0.61		0.95		Mil (1976)
	0.29		2		Rai (1977)
$_{24}$Cr	6.72	4.47	0.1	0.15	Dug (1972)
	6.72	4.47	0.1	0.15	Zan (1976)
	3.34	6.11	0.2	1.05	Nik (1976)
	3.34	1.32	0.2	0.5	Lop (1979)
	1.32	0.31	0.5	2	Lop (1978)
	0.72	0.25	0.9	2.5	Kol (1976)
	0.68		0.95		Mil (1976)
	0.31		2		Rai (1977)
	0.24	0.15	2.6	4	Ber (1977)
	0.21	0.05	3	11	Bon (1978)
$_{25}$Mn	7.30	4.85	0.1	0.15	Dug (1972)
	5.61	1.73	0.13	0.415	Whe (1974)
	3.34	1.32	0.2	0.5	Lop (1979)
	1.32	0.34	0.5	2	Lop (1978)
	0.34		2		Rai (1977)
	0.27	0.05	2.5	12	Lie (1973)
	0.23		3		Bon (1978)
$_{26}$Fe	13.1	5.26	0.07	0.15	Zan (1979)
	7.91	5.26	0.1	0.15	Dug (1972)
	7.91	5.26	0.1	0.15	Zan (1976)
	6.10	2.18	0.13	0.36	Whe (1974)
	5.64	0.58	0.14	1.3	Mes (1958)

TABLE I. (*Continued*)

Target atom	$100\zeta_K\Delta_K$ max	$100\zeta_K\Delta_K$ min	E_1 (MeV) min	E_1 (MeV) max	Ref.[a]
$_{26}$Fe	3.94	0.73	0.2	1.05	Nik (1976)
	3.94	1.56	0.2	0.5	Lop (1979)
	1.72		0.454		Jop (1962)
	1.56	0.37	0.5	2	Lea (1973)
	1.56	0.37	0.5	2	Lop (1978)
	1.10	0.30	0.7	2.5	Fah (1971)
	0.93	0.22	0.83	3.28	Hop (1975)
	0.81		0.95		Mil (1976)
	0.76	0.13	1	5.5	Lin (1973)
	0.50	0.18	1.5	4.1	Mer (1958)
	0.50		1.5		Ogi (1964)
	0.50	0.07	1.5	10.9	Aks (1974)
	0.49	0.19	1.55	3.9	Bev (1956)
	0.37		2		Rai (1977)
	0.30	0.06	2.5	12	Lie (1973)
	0.25		3		Bon (1978)
	0.25	0.03	3	22	Pon (1979)
	0.18	0.03	4	22	Pon (1978)
	0.01		160		Jar (1962)
$_{27}$Co	8.54	5.68	0.1	0.15	Dug (1972)
	4.25	1.87	0.2	0.45	Nik (1976)
	1.68	0.40	0.5	2	Lea (1973)
	0.83	0.13	1	6	Lin (1973)
	0.55	0.07	1.5	10.9	Aks (1974)
	0.40		2		Rai (1977)
$_{28}$Ni	16.8	3.05	0.055	0.3	Lap (1980)
	11.5	6.12	0.08	0.15	Zan (1979)
	10.2	2.19	0.09	0.415	Whe (1974)
	9.20	6.12	0.1	0.15	Dug (1972)
	4.59	1.05	0.2	0.25	Nik (1976)
	0.94		0.95		Mil (1976)
	0.89	0.17	1	5	Lin (1973)
	0.89	0.29	1	3	Kha (1976)
	0.71		1.25		Sch (1977)
	0.59	0.23	1.5	3.7	Mer (1958)
	0.59	0.08	1.5	10.9	Aks (1974)
	0.44		2		Rai (1977)
	0.35	0.07	2.5	12	Lie (1973)
	0.29		3		Bon (1978)
	0.17	0.03	5	28	Bis (1970)
$_{29}$Cu	7.89	6.57	0.125	0.15	Dug (1972)
	7.59	2.36	0.13	0.415	Whe (1974)
	7.29	1.21	0.1354	0.8	Ben (1978)
	7.05	0.80	0.14	1.2	Mes (1958)
	6.57	1.95	0.15	0.5	Kha (1964)
	4.92	0.79	0.2	1.215	Han (1957)
	4.28	2.15	0.23	0.454	Jop (1962)
	3.94	0.50	0.249	1.9	Bau (1978)
	2.45	0.96	0.4	1	Sin (1957)
	1.95	0.47	0.5	2	Lea (1973)
	1.46	0.16	0.667	5.667	Hop (1975)
	1.39	0.38	0.7	2.5	Fah (1971)
	1.16	0.28	0.83	3.28	Hop (1975)
	1.07	0.38	0.9	2.5	Kol (1976)
	1.01		0.95		Mil (1976)
	0.96	0.47	1	2	Lea (1973)
	0.64		1.5		Ogi (1964)
	0.64	0.08	1.5	10.9	Aks (1974)
	0.47		2		Rah (1976)
	0.47		2		Rai (1977)
$_{29}$Cu	0.38	0.08	2.5	12	Lie (1973)
	0.36	0.23	2.6	4	Ber (1977)
	0.31	0.18	3	5	Fol (1974)
	0.31	0.08	3	11	Bon (1978)
	0.23	0.04	4	22	Pon (1978)
	0.23	0.04	4	22	Pon (1979)
	0.05	0.02	20	50	Ram (1978)
	0.01	0.02	160		Jar (1972)
$_{30}$Zn	10.6	7.05	0.1	0.15	Zan (1979)
	7.05	6.91	0.15	0.153	Whe (1974)
	5.28	2.33	0.2	0.45	Nik (1976)
	2.33	0.51	0.45	2	Lea (1973)
	1.49	0.40	0.7	2.5	Fah (1971)
	1.39	0.23	0.75	4.4	Taw (1974)
	0.51		2		Rai (1977)
$_{31}$Ga	2.24	0.55	0.5	2	Lea (1979)
	0.55		2		Rai (1977)
$_{32}$Ge	2.40	0.58	0.5	2	Lea (1973)
	1.19	0.19	1	6	Lin (1973)
	0.39		3		Bon (1978)
$_{33}$As	2.72	0.62	0.47	2	Lea (1973)
	0.62		2		Rai (1977)
$_{34}$Se	3.41	0.67	0.4	2	Cri (1974)
	1.35	0.67	1	2	Lae (1973)
	0.44		3		Bon (1978)
	0.33	0.06	4	22	Pon (1978)
	0.33	0.06	4	22	Pon (1979)
$_{35}$Br	3.62	0.71	0.4	2	Cri (1974)
$_{36}$Kr	3.07	0.75	0.5	2	Len (1975)
	1.01	0.33	1.5	4.5	Win (1973)
	1.01	0.30	1.5	5	Win (1973)
	0.75		2		Rai (1977)
	0.50		3		Czu (1975)
$_{37}$Rb	4.07	0.80	0.4	2	Cri (1974)
	1.62	0.53	1	3	McD (1977)
	0.08	0.03	20	50	Ram (1978)
$_{38}$Sr	4.31	0.85	0.4	2	Cri (1974)
	0.85		2		Rai (1977)
	0.56		3		Bon (1978)
$_{39}$Y	3.63	0.71	0.5	2.5	Anh (1978)
	3.03	0.90	0.6	2	Cri (1974)
	0.90		2		Rai (1977)
	0.71	0.14	2.5	12	Lie (1973)
	0.59	0.35	3	5	Fol (1974)
	0.44	0.08	4	22	Pon (1978)
	0.44	0.08	4	22	Pon (1979)
$_{40}$Zr	8.36	3.76	0.23	0.51	Jop (1962)
	0.95		2		Rai (1977)
	0.01		160		Jar (1972)
$_{41}$Nb	1.78	0.74	1.13	2.7	Wil (1977)
	1.00		2		Rai (1977)
	0.66		3		Bon (1978)
$_{42}$Mo	8.72	1.76	0.24	1.2	Mes (1958)
	8.52	0.31	0.25	1.61	Han (1957)
	5.32	1.05	0.4	2	Cri (1974)
	4.68		0.454		Jop (1962)
	4.25	0.84	0.5	2.5	Ánh (1978)
	2.12	0.70	1	3	Kha (1976)
	1.05		2		Rai (1977)
	0.87		2.4		Lew (1953)

TABLE I. (*Continued*)

Target atom	$100\zeta_K\Delta_K$ max	$100\zeta_K\Delta_K$ min	E_1(MeV) min	E_1(MeV) max	Ref.[a]
$_{42}$Mo	0.84	0.17	2.5	12	Lie (1973)
	0.01		160		Jar (1972)
$_{45}$Rh	2.38	0.90	1.03	2.7	Wil (1977)
	1.22		2		Rai (1977)
	0.01		160		Jar (1972)
$_{46}$Pd	12.0	8.59	0.215	0.3	Lap (1980)
	4.29	1.28	0.6	2	Cri (1974)
	1.28		2		Rai (1977)
$_{47}$Ag	13.5	8.99	0.2	0.3	Lap (1980)
	10.8	1.40	0.249	1.91	Ban (1978)
	10.4	2.24	0.26	1.2	Mes (1958)
	7.43	3.36	0.3628	0.8	Ben (1978)
	6.74	1.10	0.4	2.4	Wil (1977)
	5.39	1.07	0.5	2.5	Anh (1978)
	4.49	2.69	0.6	1	Sin (1957)
	4.49	1.34	0.6	2	Khe (1975)
	2.69	1.34	1	2	Lae (1973)
	2.69	0.89	1	3	Kha (1976)
	1.79	0.24	1.5	10.9	Aks (1974)
	1.57	0.92	1.7	2.88	Lew (1953)
	1.49	0.74	1.8	3.6	Mer (1958)
	1.34	0.09	2	30	Bis (1972)
	1.34	0.48	2	5.5	Lin (1973)
	1.34		2		Rai (1977)
	1.07	0.22	2.5	12	Lie (1973)
	0.89		3		Bon (1978)
	0.66	0.17	4	15	Ber (1978)
$_{48}$Cd	4.69	1.40	0.6	2	Khe (1975)
	1.11	0.23	2.5	12	Lie (1973)
	0.93		3		Bon (1978)
$_{49}$In	4.90	1.22	0.6	2.4	Wil (1977)
	3.26	1.17	0.9	2.5	Kol (1976)
	0.97	0.58	3	5	Fol (1974)
	0.97	0.26	3	11	Bon (1978)
$_{50}$Sn	11.8	2.95	0.26	1.04	Mes (1958)
	6.14	1.22	0.5	2.5	Anh (1978)
	5.12	1.53	0.6	2	Khe (1975)
	2.18	0.69	1.4	4.4	Ish (1974)
	1.53		2		Rai (1977)
	1.31	0.53	2.333	5.667	Hop (1975)
	1.01		3		Bon (1978)
	0.02		160		Jar (1972)
$_{51}$Sb	5.34	1.59	0.6	2	Khe (1975)
	1.59		2		Rai (1977)
$_{53}$I	5.80	1.44	0.6	2.4	Wil (1977)
	1.73		2		Rai (1977)
	1.15	3.08	3	11	Bon (1978)
$_{54}$Xe	0.79	0.71	4.5	5	Win (1973)
$_{55}$Cs	3.33	1.39	1.13	2.7	Wil (1977)
	1.87		2		Rai (1977)
$_{56}$Ba	3.91	1.95	1	2	Khe (1975)
	0.02		160		Jar (1972)
$_{63}$Eu	0.25	0.10	20	50	Ram (1978)
$_{57}$La	5.08	2.02	0.8	2	Khe (1975)
	2.02		2		Rai (1977)
$_{58}$Ce	7.04	1.75	0.6	2.4	Wil (1977)
$_{59}$Pr	8.76	1.74	0.5	2.5	Anh (1978)
	7.30	1.82	0.6	2.4	Wil (1977)
$_{60}$Nd	7.57	1.88	0.6	2.4	Wil (1977)
	1.51	0.90	3	5	Fol (1974)
$_{62}$ Sm	6.50	1.94	0.75	2.5	Anh (1978)
	0.03		160		Jar (1972)
$_{64}$Gd	1.12		4.62		Cel (1979)
	0.74	0.34	7	15	Ber (1978)
$_{65}$Tb	0.03		160		Jar (1972)
$_{67}$Ho	7.69	2.30	0.75	2.5	Anh (1978)
	7.21	1.43	0.8	4	Kam (1977)
$_{69}$Tm	2.04	1.22	3	5	Fol (1974)
$_{70}$Yb	1.58	1.26	4	5	Ber (1978)
$_{72}$Hf	9.01	2.70	0.75	2.5	Anh (1978)
$_{73}$Ta	9.29	2.78	0.75	2.5	Anh (1978)
	6.97	5.57	1	1.25	Mes (1958)
	3.87	2.17	1.8	3.2	Mer (1958)
	3.62	2.21	1.92	3.15	Lew (1953)
	0.99	0.46	7	15	Ber (1978)
	0.04		160		Jar (1972)
$_{74}$W	1.57		4.56		Cel (1979)
$_{75}$Re	9.87	2.95	0.75	2.5	Anh (1978)
$_{78}$Pt	10.8	3.22	0.75	2.5	Anh (1978)
	0.06		160		Jar (1972)
$_{79}$Au	11.1	3.32	0.75	2.5	Anh (1978)
	8.32	2.07	1	4	Kam (1977)
	3.46		2.4		Lew (1953)
	2.77	0.55	3	15	Wal (1973)
	1.10	0.55	7.5	15	Ber (1978)
	0.41	0.16	20	50	Ram (1978)
	0.05		160		Jar (1972)
$_{82}$Pb	12.1	3.62	0.75	2.5	Anh (1978)
	5.66	2.51	1.6	3.6	Mer (1958)
	4.71	3.14	1.92	2.88	Lew (1953)
	3.01	1.81	3	5	Fol (1974)
	2.27	0.60	4	15	Ber (1978)
	0.06		160		Jar (1972)
$_{83}$Bi	12.4	3.72	0.75	2.5	Anh (1978)
$_{90}$Th	2.40	1.10	4.67	10.4	Cel (1979)
	1.60	0.75	7	15	Ber (1978)
$_{92}$U	9.48	4.74	1.25	2.5	Anh (1978)
	8.46	2.96	1.4	4	Kam (1977)
	5.26	3.15	2.25	3.75	Bev (1956)
	4.74	2.11	2.5	5.6	Mer (1958)
	2.40		4.23		Cel (1979)
	0.07		160		Jar (1972)

[a] The K-shell x-ray production cross sections by protons, identified as [Z_2: range of proton energies E_1 (MeV)], stem from the following sources (listed in chronological order): H. W. Lewis, B. E. Simmons, and E. Merzbacher, Phys. Rev. 91, 943 (1953) [42: 2.4; 47: 1.7–2.88; 73: 1.92–3.15; 79: 2.40; 82: 1.92–2.88]; P. R. Bevington and E. M. Bernstein, Bull. Am. Phys. Soc. 1, 198 (1956) [26: 1.55–3.9; 92: 2.25–3.75]; J. M. Hansteen and S. Messelt, Nucl. Phys. 2, 526 (1957) [29: 0.2–1.215; 42: 0.25–1.61]; B. Singh, Phys. Rev. 107, 711 (1957) [29: 0.4–1; 47: 0.6–1]; E. Merzbacher and H. W. Lewis, in *Handbuch der Physik*, edited by S. Flügge (Springer, Berlin, 1958), Vol. 34, p. 119 [22: 1.6–3.9; 26: 1.5–4.1; 28: 1.5–3.7; 47: 1.8–3.6; 73: 1.8–3.2; 82: 1.6–3.6; 92: 2.5–5.6]; S. Messelt, Nucl.

TABLE I. (*Continued*)

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where $\nu=9$ for $S=K$, L_1 and $\nu=11$ for $S=L_2$, L_3. Up to this point, our development is exact.

In terms of the semiclassical approximation (SCA), which is equivalent to the PWBA, Eq. (6) pertains to a straight projectile trajectory. The Coulomb interaction between the projectile and the target nucleus becomes important in reducing the ionization probability just in a low projectile-velocity range where also the energy-loss effect can diminish the ionization cross sections noticeably. The ratio of the differential ionization cross section calculated in SCA for the hyperbolic trajectory $(d\sigma_S/d\mathcal{E}_f)^{\rm hyp}$ and for the straight-line trajectory $(d\sigma_S/d\mathcal{E}_f)^{\rm sl}$ determines the Coulomb-deflection factor $C\equiv(d\sigma_S/d\mathcal{E}_f)^{\rm hyp}/(d\sigma_S/d\mathcal{E}_f)^{\rm sl}$. The argument of $C=C(dq_0)$ is the product of the half distance between the collision partners at closest approach, $d\equiv Z_1Z_2/Mv_1^2$, and of q_0. The minimum value of q_0, at $\mathcal{E}_f=0$, is $q_{0S}\equiv\omega_{2S}/v_1$. The classical approximation for the treatment of a projectile is justified if $2d$ is large compared to the de Broglie wavelength $1/K_i$ of the projectile,[10] i.e., when Bohr's parameter κ,

$$\kappa\equiv 2dK_i=2Z_1Z_2/v_1=4dq_{0S}/\Delta_S\,, \tag{8}$$

becomes $\ll 1$. This condition obtains in the entire low-velocity range where the energy-loss effect is important. At higher velocities the Coulomb-deflection factor approaches unity and a plane wave or straight-line approximation for the projectile applies.

The argument dq_0 of the Coulomb-deflection factor in the presence of energy loss must be replaced by[11]

$$Z_1Z_2M(K_f^{-1}-K_i^{-1})=\frac{Z_1Z_2}{Mv_iv_f}(K_i-K_f)\,. \tag{9}$$

One recognizes that Eq. (9) is the product of the symmetrized half-distance of closest approach, Z_1Z_2/Mv_iv_f, and of $q_{\rm min}$ given by Eq. (3). In consequence, the Coulomb-deflection factor with energy loss C^E follows from C by a change of argument,

$$C^E=C\left(\frac{2dq_0}{(1-\Delta)^{1/2}[1+(1-\Delta)^{1/2}]}\right). \tag{10}$$

In the notation $q_{0S}\equiv\omega_{2S}/v_1=q_0\Delta_S/\Delta$, and $z^2\equiv 1-\Delta_S$, the energy-loss function with Coulomb deflection becomes

$$f_S^C(z,dq_{0S})\simeq\frac{\nu\Delta_S^\nu}{2^{\nu+1}}\int_{\Delta_S}^1\left(\frac{1+(1-\Delta)^{1/2}}{\Delta}\right)^{\nu+1}\times C\left(\frac{2dq_{0S}\Delta}{\Delta_S[(1-\Delta)^{1/2}+(1-\Delta)]}\right)d\Delta\,. \tag{11}$$

We separate Eq. (11) into a Coulomb-deflection factor and the straight-line energy-loss function $f_S(z)$, Eq. (7), by writing

$$f_S^C(z,dq_{0S})=C_S\left(\frac{2dq_{0S}}{z(1+z)}\right)f_S(z)(1+\delta_S)\,. \tag{12}$$

As demonstrated in Appendix A, the error δ_S incurred in the factorization can be neglected for the known expressions of C.

III. COMPARISON WITH EXPERIMENT

The CPSSR cross section for direct ionization of an S shell is given by

$$\sigma_S^{\mathrm{CPSSR}} = C_S(dq_{0S}\zeta_S)\sigma_S^{\mathrm{PWBA}}(\xi_S^R/\zeta_S,\ \zeta_S\theta_S)\,, \tag{13}$$

where C_S represents the Coulomb-deflection effect, and the factor ζ_S accounts for the perturbed stationary-state effect.[2,3,12] The projectile-velocity variable $\xi_S^R = [m_S^R(\xi_S/\zeta_S)]^{1/2}\xi_S$ is the product of $\xi_S \equiv v_i/\frac{1}{2}\theta_S v_{2S}$ (v_{2S} = orbital velocity in S shell) and the function $(m_S^R)^{1/2}$ that introduces relativistic effects in the range of impact parameters, of order q_{0S}^{-1}, where excitation takes place with high probability. The development in the preceding section permits us to incorporate the energy-loss effect (E) according to Eq. (13) as

$$\sigma_S^{\mathrm{ECPSSR}} = C_S\left(\frac{2dq_{0S}\zeta_S}{z_S(1+z_S)}\right) f_S(z_S)\sigma_S^{\mathrm{PWBA}}(\xi_S^R/\zeta_S,\ \zeta_S\theta_S)\,, \tag{14}$$

where

$$z_S^2 \equiv 1 - \zeta_S\Delta_S = 1 - \frac{4}{M\zeta_S\theta_S}\left(\frac{\zeta_S}{\xi_S}\right)^2 . \tag{15}$$

We wish to compare Eq. (14) with the K-shell data displayed in Fig. 1. To isolate and exhibit trends in a managable but statistically significant manner, we divided the data into groups within five equal intervals in each decade of the logarithmic abscissa scale in Fig. 1. Each group contains, then, some 150 data points for which the $\zeta_K\Delta_K$ variable changes by approximately 60%. The arithmetic-mean value of each group of points is plotted in Fig. 2 midway within the abscissa interval and marked with an error bar determined by the 95% confidence limit, corresponding to two times the standard deviation for the group. These mean values should hover around the ordinate value one if the projectile-energy loss in the ionizing collision were unimportant. The two curves represent the calculated energy-loss effect as

$$\sigma_S^{\mathrm{ECPSSR}}/\sigma_S^{\mathrm{CPSSR}} = (C_S^E/C_S) f_S(z_S)\,, \tag{16}$$

where $C_S^E = C_S[2dq_{0S}\zeta_S/z_S(1+z_S)]$. For $S=K$ we set $C_K(dq_{0K}) = 9E_{10}(\pi dq_{0K})$, corresponding to the choice $\gamma = 1$ in Eq. (28) of Ref. 3. The curves clearly reproduce the trend of the K-shell ioniza-

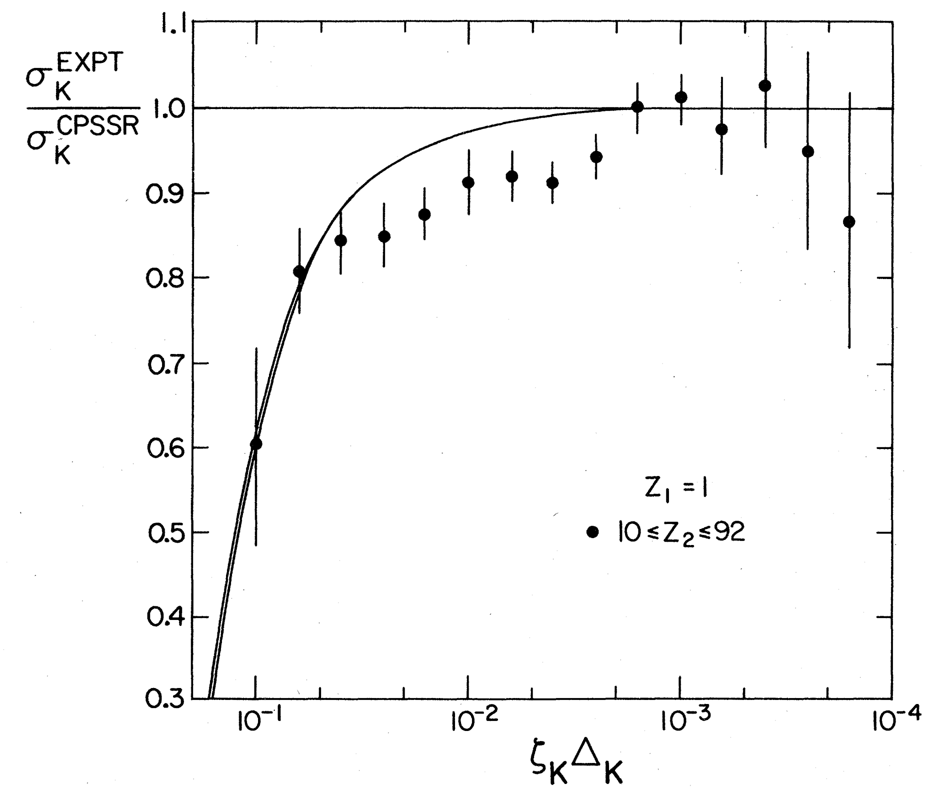

FIG. 2. Ratios as in Fig. 1 after a statistical analysis described in the text. Had the energy loss effect been negligably small, $\sigma_K^{\mathrm{expt}}/\sigma_K^{\mathrm{CPSSR}}$ would have been equal to one. The two curves bracket the values of $\sigma_K^{\mathrm{ECPSSR}}/\sigma_K^{\mathrm{CPSSR}}$ [Eq. (16)] for all elements included in Fig. 1. The evaluation of Eq. (16) is illustrated in Appendix B.

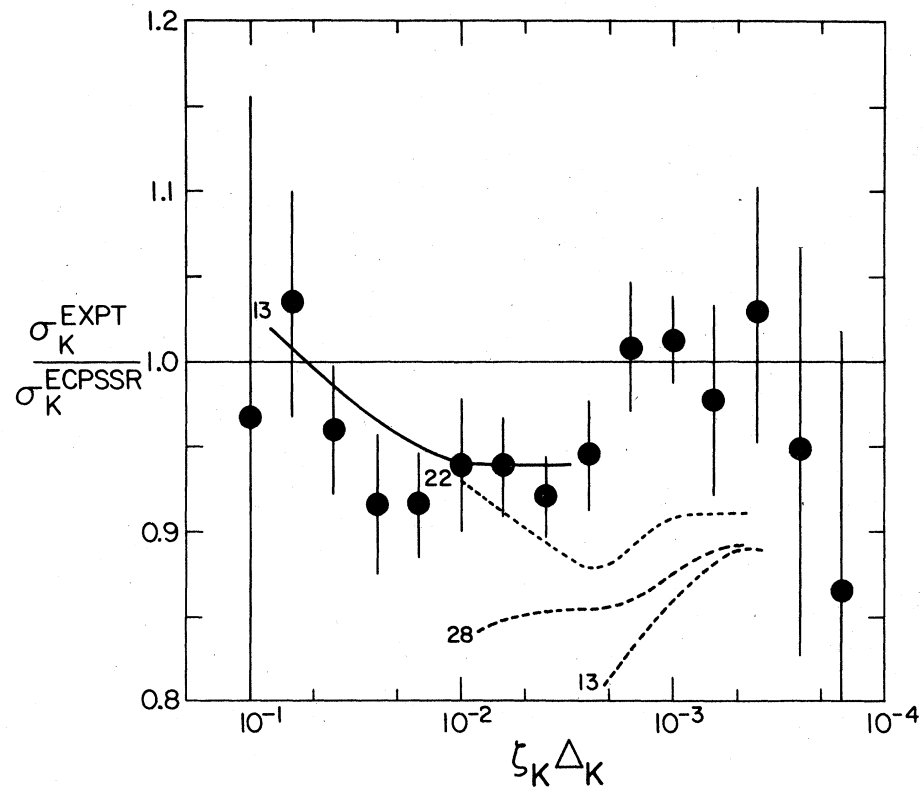

FIG. 3. Ratios as in Fig. 2, but presented relative to $\sigma_K^{\mathrm{ECPSSR}}$ [Eq. (14)], which accounts for the energy loss effect in both the Coulomb deflection factor and the PSSR cross section. The curves represent the ratios of PWBA cross sections calculated with Hartree-Slater (HS) wave functions and those calculated with screened hydrogenic (SH) wave functions (Ref. 9) as currently used in our analysis. The solid curve is from Basbas, Brandt, and Laubert (1973) in Ref. 2 for the K-shell ionization of $_{13}$Al by protons. The dashed curves, identified by the respective Z_2 values, depict the calculations of Ford. *et al*. (1977) in Ref. 14 for the K-shell ionization of $_{13}$Al, $_{22}$Ti, and $_{28}$Ni by protons.

tion measurements with protons or target elements ranging from neon ($Z_2 = 10$) to uranium ($Z_2 = 92$).

This comparison supports the conclusion reached in Refs. 3 and 13, namely that the Coulomb-deflection factor, if calculated in the lowest, the monopole approximation [$\gamma = 2$, Eq. (28) of Ref. 3], overpredicts the deflection effect as deduced from experimental data. The form $\nu E_{\nu+1}(\pi d q_{0S})$ underlying the present treatment agrees closely with all known data.

In order to pursue, if cautiously, the discussion to the limit of the statistical significance of the data, we have replotted, in Fig. 3, the average points relative to the solid curve in Fig. 2, i.e., in the form $\sigma_K^{\mathrm{expt}}/\sigma_K^{\mathrm{ECPSSR}}$ on a twofold enlarged ordinate scale. Theory and experiment agree, on the average, to within $\pm 10\%$. Time will sort out to what extent residual deviations are real and systematic, i.e., in the nature of a significant fine structure superimposed on the millionfold change of the cross sections with projectile velocity according to Eq. (14) in the abscissa range displayed in Fig. 3. Such fine structure can signify the extent to which interconnected quantum mechanical effects on ionization cross sections are represented by the factorization in Eq. (14). In our comparison, moreover, the function σ_K^{PWBA} in Eq. (14) was calculated with SH wave functions.[9] The curves drawn in Fig. 3 display the changes one calculates if one improves the basis through the use of Hartree-Slater (HS) wave functions. The solid curve gives $\sigma_K(\mathrm{HS})/\sigma_K(\mathrm{SH})$ according to our calculation for Al(K) of 1973.[2] The dashed curves are based on later calculations by Ford *et al.*[14] for $_{13}$Al(K), $_{22}$Ti(K), and $_{28}$Ni(K). Apparently, experiment and theory now converge in a domain where the measurements can test atomic wave functions.

ACKNOWLEDGMENT

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APPENDIX A: DERIVATION OF ENERGY-LOSS FUNCTION

When integrated over final states, Eq. (5) takes the form

$$\sigma_S^{\mathrm{EPWBA}} = \sigma_S^{\mathrm{PWBA}} \frac{\nu\Delta_S^\nu}{2^{\nu+1}} \int_{\Delta_S}^1 \left[\left(\frac{1+(1-\Delta)^{1/2}}{\Delta}\right)^{\nu+1} - \left(\frac{1-(1-\Delta)^{1/2}}{\Delta}\right)^{\nu+1}\right] d\Delta \tag{A1}$$

in terms of the minimum relative kinetic energy loss Δ_S, Eq. (1). The projectile emerges from the collision with the residual relative kinetic energy $z^2 \equiv 1-\Delta_S$. In the low-velocity limit represented by Eq. (5), the cross sections σ_S^{PWBA} are analytical functions of the projectile velocity v_1.[2,7]

With the substitution $(1-\Delta)\equiv u^2$, the first term integral in Eq. (A1) becomes

$$_1f_2(z) = \frac{\nu(1-z^2)^\nu}{2^\nu} \int_0^z \frac{u\,du}{(1-u)^{\nu+1}} = 2^{-\nu}(\nu-1)^{-1}[(\nu z-1)(1+z)^\nu + (1-z^2)^\nu], \tag{A2}$$

and the second-term integral

$$_2f_S(z) = 2^{-\nu}(\nu-1)^{-1}[(1-z^2)^\nu - (\nu z+1)(1-z)^\nu]. \tag{A3}$$

Subtraction, $f_S(z) \equiv {_1f_S(z)} - {_2f_S(z)}$, yields the analytical function Eq. (7) that accounts for the energy-loss effect.

The cross sections, Eq. (6), have a low-energy threshold in that $f_S(z)$ vanishes when $\Delta_S = 1$, or $z=0$, i.e., when all the initial energy of projectiles is transferred to the ejected electron, and the projectile comes to rest. The cross sections rise from the threshold, for $z^2 \equiv (1-\Delta_S) \ll 1$, as

$$\frac{\sigma_S^{\mathrm{EPWBA}}}{\sigma_S^{\mathrm{PWBA}}} = f_S(z) = \frac{(\nu+1)\nu}{3\cdot 2^{\nu-1}} z^3\left(1+\frac{(\nu-2)(\nu-3)}{2} z^2 + \cdots\right). \tag{A4}$$

For small $\Delta_S \equiv 1-z^2$, the energy-loss function takes the form

$$\sigma_S^{\mathrm{EPWBA}}/\sigma_S^{\mathrm{PWBA}} = f_S(z) = 1 - \tfrac{45}{16}\Delta_S + \tfrac{45}{16}\Delta_S^2 - \tfrac{75}{64}\Delta_S^3 + \tfrac{45}{256}\Delta_S^4 - \cdots$$

$$\text{for } \nu = 9 \; (S = K, L_1) \tag{A5}$$

and

$$\sigma_S^{\mathrm{EPWBA}}/\sigma_S^{\mathrm{PWBA}} = f_S(z) = 1 - \tfrac{33}{10}\Delta_S + \tfrac{33}{8}\Delta_S^2 - \tfrac{77}{32}\Delta_S^3 + \tfrac{165}{256}\Delta_S^4 - \cdots$$

$$\text{for } \nu = 11 \; (S = L_2, L_3). \tag{A6}$$

These expansions are accurate to within 1% if one retains terms to order Δ_S^P such that $P > 10\Delta_S$. For the discussion of current experiments ($\Delta_S < 0.2$), it suffices to calculate the energy-loss effect by truncating the series beyond the Δ_S^3 terms.

Since the second term in Eq. (A1) contributes negligibly, we can set $f_S = {_1f_S}$ in the z range of interest[15] and derive Eqs. (A5) and (A6) from Eq. (A1) by calculating

$$_1f_S(z) = \frac{\nu(1-z^2)^\nu}{2^{\nu+1}} \int_{1-z^2}^1 \left(\frac{1+(1-\Delta)^{1/2}}{\Delta}\right)^{\nu+1} d\Delta, \tag{A7}$$

with the substitution

$$y \equiv \Delta/\Delta_S[(1-\Delta) + (1+\Delta)^{1/2}], \tag{A8}$$

through series expansion and term-by-term integration

$$f_S(z) = {_1f_S(z)} = \frac{\nu}{2^\nu} \int_{[z(1+z)]^{-1}}^\infty \frac{[1+(1-z^2)y]^{\nu-2}}{y^{\nu+1}} dy = \frac{\nu}{2^\nu} \sum_{\mu=0}^{\nu-2} \binom{\nu-2}{\mu} (1-z^2)^\mu \int_{[z(1+z)]^{-1}}^\infty \frac{dy}{y^{\nu+1-\mu}} = \left(\frac{z(1+z)^\nu}{2}\right) \sum_{\mu=0}^{\nu-2} \binom{\nu-2}{\mu} \frac{\nu}{\nu-\mu} \left(\frac{1-z}{z}\right)^\mu. \tag{A9}$$

We retrieve leading terms given by Eqs. (A5) and (A6).

The Coulomb-deflection factor varies approximately as $\exp(-\gamma\pi d q_0)$, where the parameter γ has values in the range $1 \leq \gamma \lesssim 2$ depending on the underlying approximations.[3,11] For this form the energy-loss function with Coulomb deflection f_S^C can be factorized as given in Eq. (12), and as demonstrated presently. In the expression

$$f_S^C(z, dq_{0S}) = \frac{\nu(1-z^2)^\nu}{2^{\nu+1}} \int_{1-z^2}^1 \left[\left(\frac{1+(1-\Delta)^{1/2}}{\Delta}\right)^{\nu+1} - \left(\frac{1-(1-\Delta)^{1/2}}{\Delta}\right)^{\nu+1}\right] \exp\left(-\frac{2\gamma\pi d q_{0S}}{1-z^2} \frac{\Delta}{(1-\Delta)+(1-\Delta)^{1/2}}\right) d\Delta, \tag{A10}$$

only the first term under the integral is important. We integrate in the manner of Eqs. (A7) to (A9),

$$ {}_1f_S^C(z,dq_{0S})=\left(\frac{z(1+z)}{2}\right)^{\nu}\sum_{\mu=0}^{\nu-2}\binom{\nu-2}{\mu}\nu E_{\nu+1-\mu}\left(\frac{2\gamma\pi dq_{0S}}{z(1+z)}\right)\left(\frac{1-z}{z}\right)^{\mu} . \tag{A11} $$

The function $E_n(t)=\int_1^\infty r^{-n}e^{-tr}dr$ is the exponential integral of order n. In the straight-line limit $dq_{0S}\to 0$, Eq. (A11) reduces to Eq. (A9).

We wish to separate Eq. (A11) into a Coulomb-deflection factor and the straight-line energy-loss factor $f_S(z)$ [Eq. (7)]. Since[16]

$$ E_{\nu+1}\le E_{\nu+1-\mu}\le\frac{\nu}{\nu-\mu}E_{\nu+1} , \tag{A12} $$

Eqs. (A9) and (A11) imply that

$$ {}_1f_S^C(z,dq_{0S})<\nu E_{\nu+1}\left(\frac{2\gamma\pi dq_{0S}}{z(1+z)}\right){}_1f_S(z) . \tag{A13} $$

Similarly,

$$ {}_2f_S^C(z,dq_{0S})<\nu E_{\nu+1}\left(\frac{2\gamma\pi dq_{0S}}{z(1-z)}\right){}_2f_S(z) . \tag{A14} $$

Factorization, therefore, is uncertain within the limits

$$ \nu E_{\nu+1}\left(\frac{2\gamma\pi dq_{0S}}{z(1+z)}\right)f_S(z)<f_S^C(z,dq_{0S})<\nu E_{\nu+1}\left(\frac{2\gamma\pi dq_{0S}}{z(1+z)}\right){}_1f_S . \tag{A15} $$

We write Eq. (A15) in the form of Eq. (12), where

$$ C_S^E=\nu E_{\nu+1}[2\gamma\pi dq_{0S}/z(1+z)] \tag{A16} $$

with $\nu=9$ for $S=K,L_1$, $\nu=11$ for $S=L_2,L_3$, and $1\le\gamma\le 2$, where $\gamma=1$ represents the standard approximation and $\gamma\sim 2$ the monopole approximation to the Coulomb-deflection factor.[2,3] The error δ_S incurred through the factorization Eq. (12) is bounded as

$$ 0<|\delta_S|<{}_2f_S(z)/f_S(z) \tag{A17} $$

and can always be neglected, for it is less than 10^{-9} under present experimental conditions, and it remains less than 10^{-2} as long as $z>0.3$, or $\Delta_S<0.9$. At even smaller velocities, the Coulomb deflection, through C_S^E, makes the cross section vanishingly small before the threshold at $\Delta_S=1$ is reached. Although based on the analytical form of the differential cross section Eq. (5) that is strictly valid in the low-velocity limit, numerical calculations show that Eq. (12) is accurate to within 0.3% or less for all velocities.

APPENDIX B: SAMPLE CALCULATION OF ENERGY-LOSS EFFECT IN *K*-SHELL IONIZATION

We illustrate the effect by evaluating Eq. (14) for protons (${}_1^1H: Z_1=1$, $M_1=1836m\simeq 1u$) and deuterons (${}_1^2H: Z_1=1$, $M_1\simeq 2u$) impinging with energy $E_1/M_1=25$ keV/u $=0.025$ MeV/u on aluminum (${}_{13}^{27}Al: Z_2=13$, $M_2\simeq 27u$). The Al(K) binding energy, $\hbar\omega_{2K}=1559.6$ eV, corresponds to $\theta_K=0.711$. For ready reference to the previous work,[2,3] we denote the papers by Basbas, Brandt, and Laubert of 1973 as KI, of 1978 as KII, those by Brandt and Lapicki of 1974 as LI, of 1979 as LII, and the present paper as E. We retain enough digits in this example to make rounding-off errors unimportant for the final results.

For the screened ${}_{13}^{27}Al$ nuclear charge $Z_{2K}=13-0.3=12.7$, the velocity parameter [KII, Eq. (4)] becomes $\xi_K=(160)^{1/2}(0.025)^{1/2}(0.711\times 12.7)^{-1}=0.222$. The PSS factor [KII, Eq. (45)], with $c_K=\frac{3}{2}$, $g_K(0.222,1.5)=0.922$ [KII, Eq. (39) and Table V], and $h\propto I(1.5/0.222)=I(6.76)\simeq 0$ [KII, Eq. (27)] has the value

$$ \zeta_K=1+\frac{2\times 0.922}{0.711\times 12.7}=1.204 , \tag{B1} $$

so that $\xi_K/\zeta_K=0.222/1.204=0.184$ and $\zeta_K\theta_K=1.204\times 0.711=0.856$. Given the mass $M({}_1^1H, {}_{13}^{27}Al)=1836(1^{-1}+27^{-1})^{-1}=1770$ in the center-of-mass system, we calculate the energy-loss parameter [E, Eqs. (1) and (15) and Figs. 1–3]

$$ \zeta_K\Delta_K=\frac{4}{M\zeta_K\theta_K}\left(\frac{\zeta_K}{\xi_K}\right)^2=\frac{4}{1770\times 0.856\times(0.184)^2}=0.0780 . \tag{B2} $$

For $\nu=9$ and the value of the argument $z_K=(1-\zeta_K\Delta_K)^{1/2}=0.960$, the energy-loss function [E, Eq. (7)], reduces the cross section by the factor $f_K(0.960)=0.796$.

The Coulomb-deflection variable [KI, Eq. (33a) with Eq. (2)] with $\gamma=1$

$$ \pi dq_{0K}\zeta_K=4\pi Z_1M^{-1}(\zeta_K\theta_K)^{-2}(\xi_K/\zeta_K)^{-3}(Z_2/Z_{2K})=1.59 \tag{B3} $$

gives for the Coulomb-deflection factor [KII, Eq. (49)], without considering the projectile energy loss, the value[16] $C_K=9E_{10}(1.59)=0.171$. When the energy loss is included, the argument becomes [E, Eqs. (14) and (15)]

$$ \frac{2\pi dq_{0K}\zeta_K}{z_K(1+z_K)}=\frac{2\times 1.59}{0.960\times 1.960}=1.69 , \tag{B4} $$

which yields $C_K^E=9E_{10}(1.69)=0.153$. The energy-loss effect, then, reduces the CPSSR cross section [LII, Eq. (29), and E, Eq. (13)] by the factor [E, Eq. (16)]

$$\frac{\sigma_K^{\text{ECPSSR}}}{\sigma_K^{\text{CPSSR}}}=\frac{C_K^E}{C_K}f_K(z_K)=\frac{0.153}{0.171}\times 0.796=0.712 \quad \text{(B5)}$$

as displayed in Fig. 2 by the solid curves at the abscissa value $\zeta_K\Delta_K=0.0780$. In the monopole approximation, corresponding to $\gamma\simeq 2$, the ratio Eq. (B5) has a smaller value.

Under the given conditions, the relativistic effect increases $\xi_K=0.222$ to $\xi_K^R\equiv[m_K^R(0.184)]^{1/2}\times 0.222=(1.019)^{1/2}\times 0.222=0.224$ [LII, Eqs. (6) and (22)]. The straight-line K-shell ionization cross section [KI, Appendix B, Table V; LII, Eq. (23)] is

$$\begin{aligned}\sigma_K^{\text{PSSR}}&=(\sigma_{0K}/\zeta_K\theta_K)\times F_K(\xi_K^R/\zeta_K)\\&=(0.270\times 10^5/0.856)\times 1.296\times 10^{-5}\text{ b}\\&=0.409\text{ b}\,,\end{aligned}\quad \text{(B6)}$$

since $\xi_K^R/\zeta_K=0.186$ and $F_K(\xi_K)=(2^9/45)\xi_K^8/(1+1.72\xi_K^2)^4$ for $\xi_K<1$. [LI, Eq. (7) and the following discussion therein]. This cross section is reduced by the Coulomb deflection and the energy-loss effects [E, Eq. (14)] to the value

$$\begin{aligned}\sigma_K^{\text{ECPSSR}}&=C_K^E f_K(z_K)\sigma_K^{\text{PSSR}}\\&=0.153\times 0.796\times 0.409\text{ b}=0.0498\text{ b}\,.\end{aligned}\quad \text{(B7)}$$

Taking the fluorescence yield $\omega_K=0.039$ as recommended by Krause,[4] the predicted Al(K) x-ray production cross section for 25-keV protons becomes

$$\begin{aligned}\sigma_{KX}&=\omega_K\sigma_K^{\text{ECPSSR}}\\&=0.039\times 0.0498\text{ b}=1.9\times 10^{-3}\text{ b}\,.\end{aligned}\quad \text{(B8)}$$

The experimental value [KI, Table I] is $\sigma_{KX}^{\text{expt}}=(2.0\pm 0.5)\times 10^{-3}$ b.

The isotope effect in the cross sections depends on the projectile energy loss as follows. Deuterons of $E_1=50$ keV or 0.025 MeV/u have the same velocity as 25-keV protons so that $\xi_K=0.222$, $\zeta_K=1.204$, $\zeta_K\theta_K=0.856$, $\xi_K^R/\zeta_K=0.186$, and, hence, $\sigma_K^{\text{PSSR}}(\xi_K^R/\zeta_K,\zeta_K\theta_K)=0.409$ b [see Eq. (B6)]. The reduced mass, however, increases from $M({}^1_1\text{H},{}^{27}_{13}\text{Al})=1770$ to $M({}^2_1\text{H},{}^{27}_{13}\text{Al})=1836(2^{-1}+27^{-1})^{-1}=3419$, so that now $\pi d q_{0K}\zeta_K=1.59\times 1770/3419=0.823$ and $C_K=0.400$. Moreover, the relative energy loss during the collision is reduced to $\zeta_K\Delta_K=0.0780\times 1770/3419=0.0404$. With $z_K=(1-0.0404)^{1/2}=0.980$, the energy-loss function has the value $f_K(0.980)=0.893$. The Coulomb-deflection factor becomes $C_K^E=9E_{10}(2\times 0.823/0.980\times 1.980)=0.389$. For deuterons, then, the energy loss reduces the cross section merely by the factor

$$\frac{C_K^E}{C_K}f_K(z_K)=\frac{0.389}{0.400}\times 0.893=0.868\,. \quad \text{(B9)}$$

From the cross section for direct ionization by deuterons, $\sigma_K^{\text{ECPSSR}}=0.389\times 0.893\times 0.409$ b $=0.142$ b, we calculate, with the same fluorescence yield $\omega_K=0.039$, the x-ray production cross section $\sigma_{KX}=\omega_K\sigma_K^{\text{ECPSSR}}=0.039\times 0.142\text{ b}=5.5\times 10^{-3}$ b. The experimental value [KI, Table II] is $\sigma_{KX}^{\text{expt}}=(5.7\pm 1.4)\times 10^{-3}$ b.

The projectile energy loss enhances the isotope effect, as expressed through the cross section ratio [KI, Eq. (30)], from $\sigma_K^{\text{CPSSR}}({}^2_1\text{H})/\sigma_K^{\text{CPSSR}}({}^1_1\text{H})=0.166\text{ b}/0.0724\text{ b}=2.29$ [KI, Coulomb curve in Fig. 6] to $\sigma_K^{\text{ECPSSR}}({}^2_1\text{H})/\sigma_K^{\text{ECPSSR}}({}^1_1\text{H})=0.142\text{ b}/0.0498\text{ b}=2.85$. For constant ω_K, these results are to be compared with the ratio of the experimental values $\sigma_{KX}^{\text{expt}}({}^2_1\text{H})/\sigma_{KX}^{\text{expt}}({}^1_1\text{H})=(5.71\pm 1.43)\times 10^{-3}\text{ b}/(2.02\pm 0.50)\times 10^{-3}\text{ b}=2.8\pm 1.0$.

The differences between the dashed curves and the experimental points in Figs. 3 and 4 recently reported by Chang *et al.*[17] are fully accounted for by the energy-loss effects as developed here.

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