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EXCITATION OF CHARACTERISTIC K X-RAYS BY THE IMPACT OF HEAVY CHARGED PARTICLES

BY

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Synopsis.

The cross section for ejection of K-electrons by slow ions is evaluated in the Born approximation for the incident particles, using relativistic electron wave functions. Numerical results are given for lead (and silver) and compared with experimental cross sections for excitation of characteristic K x-rays. For silver, the relativistic corrections are small, but for lead they are appreciable and improve the agreement with experiment. Still, the theoretical cross sections for Pb as well as for Ag are not in quantitative agreement with the experimental values. The discrepancy is attributed mainly to a failure of the Born approximation.

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I. Introduction.

The characteristic x-rays following the ejection of inner atomic electrons by the impact of heavy charged particles have been investigated by several authors in the past*. Recently, more precise experimental data have become available[1) 2) 3) 4)]. The process has received increasing attention since it yields electrons and x-rays in the same energy range as nuclear transitions following Coulomb excitation of heavy nuclei. From the point of view of the nuclear physicist, the atomic process constitutes an undesirable background, and it is thus necessary to know its dependence on various parameters. On the other hand, it is, at least in principle, accessible to exact calculation and might therefore serve as a reference for calibration of nuclear cross sections.

Following the fundamental stopping power calculations by BETHE, HENNEBERG[5)] has presented a theory of the ionization of the K-shell by the impact of slow protons and α-particles. He neglected the Coulomb interaction between the incident particle and the nucleus. He justified the use of the Born approximation for the impinging particles by proving that the effective part of the product of initial and final wave functions of the heavy particle does not differ appreciably from its plane-wave substitute, though the wave functions themselves are heavily distorted**.

Assuming the Born approximation for the bombarding particles, the cross section for ejection of a K-electron is given by

$$\sigma = \frac{4\pi}{\hbar^2} Z_1^2 e^4 \frac{M}{E_1} \int_{q_{\min}}^{\infty} J \frac{dq}{q^3}. \tag{1}$$

* For historical details, see reference 1.

** One arrives at the same conclusion looking at the collision classically, which is permitted for slow bombarding particles. The main contribution to the cross section should arise from particles with impact parameters of the order of atomic dimensions. If their energy is not too low, these particles are but slightly deflected by the Coulomb field of the nucleus. Thus, the influence of the field is not very important for the calculations and the wave functions for the particles may be described throughout by plane waves.

Here Z_1, M, and E_1 are the charge, mass, and energy of the incoming particle, respectively. The momentum transfer in the collision is given by $\hbar\vec{q} = \hbar(\vec{K}_0 - \vec{K})$, where $\hbar\vec{K}_0$ and $\hbar\vec{K}$ are the momenta of the incident particle before and after the collision, respectively. $q_{\min}$ is defined as $q_{\min} = K_0 - K$ and, if the energy ΔE lost by the heavy particle is small compared to its initial energy E_1, we have approximately

$$q_{\min}^2 \simeq \frac{(\Delta E)^2 M}{2\hbar^2 E_1}\left(1 + \frac{\Delta E}{2E_1}\right). \tag{2}$$

The quantity J is given by

$$J = \sum_f \left[\int e^{i\vec{q}\vec{r}}\,\psi_i(\vec{r})\,\psi_f(\vec{r})\,d\vec{r}\right]^2, \tag{3}$$

where $\psi_i(\vec{r})$ and $\psi_f(\vec{r})$ are the initial and final wave functions of the electron, respectively. The squares of the matrix elements for the different final states are summed, since we are not interested in the angular distribution of the ejected electrons.

HENNEBERG obtained his results by using non-relativistic Coulomb wave functions for $\psi_i(\vec{r})$ and $\psi_f(\vec{r})$. He roughly corrected for the screening by adding a constant term to the Coulomb potential and arrived at the following expression for the cross section for excitation of K x-rays*:

$$\sigma = \frac{3{,}51\,Z_1^2}{Z^4\,\Theta}\,\Phi_0(\eta') \times 10^{-16}\ \text{cm}^2. \tag{4}$$

Z is the charge of the nucleus, Θ is the ratio of the observed K-shell ionization energy E_K to the "ideal ionization energy in the absence of outer screening", and $\Phi_0(\eta')$ is defined by

$$\Phi_0(\eta') = \frac{2}{5}\,e^{-\frac{4\eta'}{1+\eta'}}\left(\frac{4\eta'}{1+\eta'}\right)^4\left\{\frac{1}{4} + \frac{1}{12}\left(\frac{4\eta'}{1+\eta'}\right) + \ldots\right\}. \tag{5}$$

The quantity η' is given by

$$\eta' = \frac{4mE_1}{M\Theta E_K},$$

m being the mass of the electron. The above formulae are derived on the assumption that η' is small. Accordingly, the cross section depends mainly on the factor $Z_1^2\,\eta'^4 Z^{-4}$**.

The experiments confirm qualitatively Henneberg's theory, particularly the dependence of the cross section on the energy and mass of the incident

* We quote this formula as given in reference 1.

** A simple derivation of essentially the same result has been given in reference 4.

particle and on the energy of the K-shell. However, there are serious quantitative discrepancies. Especially in heavy elements, the experimental cross sections are up to several times larger than those derived from formula (4).

This deviation is just in the direction expected, considering the neglect of the relativistic effects in the heavy atoms. As it can be seen from expression (2), the value of $1/q_{\min}$ is in cases of interest considerably smaller than the radius of the K-shell. The factor $e^{i\vec{q}\vec{r}}$ in the matrix element (3) is thus a fast oscillating function and any increase in the electron density at the origin, as caused by relativistic effects, will therefore raise the cross section appreciably.

Consequently, it seemed of interest to repeat the calculations, using relativistic wave functions for the electron. In the following chapter the derivation is outlined and the final formulae are given; mathematical details are, however, deferred to the Appendix. In Chapter III, the results are discussed and compared with experiments.

II. Framework of the Calculation.

We insert into the matrix element (3) the stationary[6), 7)] Coulomb solutions of the Dirac equation. They can be written[8)]

$$\psi(\vec{r}) = \begin{pmatrix} -if_\varkappa(r)\,\chi_{-\varkappa}^{\mu}(\vartheta,\varphi) \\ g_\varkappa(r)\,\chi_\varkappa^{\mu}(\vartheta,\varphi) \end{pmatrix} \qquad \varkappa = \mp 1, \mp 2, \ldots$$

with

$$\chi_\varkappa^{\mu} = \sum_{\tau} < l(\varkappa), 1/2, \mu-\tau, \tau \,|\, l(\varkappa), 1/2, j, \mu > \chi_{1/2}^{\tau} Y_{l(\varkappa)}^{\mu-\tau}(\vartheta,\varphi)$$

and

$$\left.\begin{aligned} & j = |\varkappa| - 1/2 \qquad l(\varkappa) = \varkappa \text{ if } \varkappa > 0 \qquad \chi_{1/2}^{1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ & -j \leq \mu \leq j \qquad\quad l(\varkappa) = |\varkappa| - 1 \text{ if } \varkappa < 0 \qquad \chi_{1/2}^{-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \end{aligned}\right\} \tag{6}$$

We write the radial wave functions in the form

$$f_\varkappa(r) = Dr^{-1}\,u(r) \qquad g_\varkappa(r) = Dr^{-1}\,v(r).$$

For a discrete state, these quantities are given by[9)]

$$\left.\begin{aligned} u(r) = & -\sqrt{1-\vartheta}\; r^{\gamma_\varkappa} e^{-\varepsilon_N r}\,[n'\,\Phi(-n'+1, 2\gamma_\varkappa+1, 2\varepsilon_N r) \\ & + (N-\varkappa)\,\Phi(-n', 2\gamma_\varkappa+1, 2\varepsilon_N r)] \\ v(r) = & \sqrt{1+\vartheta}\; r^{\gamma_\varkappa} e^{-\varepsilon_N r}\,[-n'\,\Phi(-n'+1, 2\gamma_\varkappa+1, 2\varepsilon_N r) \\ & + (N-\varkappa)\,\Phi(-n', 2\gamma_\varkappa+1, 2\varepsilon_N r)] \end{aligned}\right\} \tag{7}$$

$$\left.\begin{aligned} &\vartheta = E/mc^2 = \left[1 + \frac{(\zeta Z)^2}{(n' + \gamma_\varkappa)^2}\right]^{-1/2} \qquad \gamma_\varkappa = \sqrt{|\varkappa|^2 - (\zeta Z)^2} \\ &\varepsilon_N = \frac{Z}{N a_0} \qquad N = \sqrt{n^2 - 2n'(|\varkappa| - \gamma_\varkappa)} \qquad n = n' + |\varkappa| \\ &D = \sqrt{\frac{\Gamma(2\gamma_\varkappa + n' + 1)}{4(n'!)\, N(N - \varkappa)}} \, \frac{(2\varepsilon_N)^{\gamma_\varkappa + 1/2}}{\Gamma(2\gamma_\varkappa + 1)}. \end{aligned}\right\} \tag{7}$$

Here, a_0 is the Bohr radius, ζ the fine structure constant, and E the total energy of the electron. We use the symbol Φ for the confluent hypergeometric function, regular at the origin. For the special case of a K-electron, we have $\varkappa = -1$, $n' = 0$, and

$$\left.\begin{aligned} &f(r) = -\sqrt{1 - \gamma_1}\, C r^{\gamma_1 - 1} e^{-\varepsilon_1 r} \qquad \varepsilon_1 = \frac{Z}{a_0} \\ &g(r) = \sqrt{1 + \gamma_1}\, C r^{\gamma_1 - 1} e^{-\varepsilon_1 r} \qquad C = \frac{(2\varepsilon_1)^{\gamma_1 + 1/2}}{\sqrt{2\Gamma(2\gamma_1 + 1)}}. \end{aligned}\right\} \tag{8}$$

In the continuum, we have[10]

$$\left.\begin{aligned} &u(r) = -2\sqrt{W - 1}\, r^{\gamma_\varkappa} Im\left[e^{-ikr + i\eta}(\gamma_\varkappa + i\alpha)\, \Phi(\gamma_\varkappa + 1 + i\alpha, 2\gamma_\varkappa + 1, 2ikr)\right] \\ &v(r) = 2\sqrt{W + 1}\, r^{\gamma_\varkappa} Re\left[e^{-ikr + i\eta}(\gamma_\varkappa + i\alpha)\, \Phi(\gamma_\varkappa + 1 + i\alpha, 2\gamma_\varkappa + 1, 2ikr)\right] \\ &e^{2i\eta} = -\frac{\varkappa - i\beta}{\gamma_\varkappa + i\alpha} \qquad \beta = \frac{\varepsilon_1}{k} \qquad \alpha = \beta W \qquad W = E/mc^2 = \sqrt{1 + \left(\frac{\hbar k}{mc}\right)^2} \\ &D = \frac{2^{\gamma_\varkappa - 1}}{\Gamma(2\gamma_\varkappa + 1)\hbar}\sqrt{\frac{m}{\pi}}\, k^{\gamma_\varkappa - 1/2} e^{\pi\alpha/2} \left|\Gamma(\gamma_\varkappa + i\alpha)\right|, \end{aligned}\right\} \tag{9}$$

where Im and Re denote the imaginary and the real part of the expression in parentheses, respectively. These wave functions are normalized per unit energy interval.

In the matrix element (3) we integrate over the angles, sum over the final magnetic quantum numbers, and average over the initial magnetic quantum numbers, using standard techniques. We get

$$J = \sum_f |\varkappa_f| \left\{\int j_{l(\varkappa_f)}(qr)\, [f_i f_f^* + g_i g_f^*]\, r^2 dr\right\}^2, \tag{10}$$

$j_l(qr)$ being the spherical Bessel function.

The radial integration can be carried through, as outlined in the Appendix. The result is a power series in ε_1/q. We may write

$$I = \int j_l(qr)\,[f_i f_f^* + g_i g_f^*]\, r^2\, dr = A q^{-(\gamma_1+\gamma_f+1)}\, S(\varepsilon_1/q)$$

with

$$\left.\begin{aligned}
S(x) &= F \sum_m P_m (-1)^m x^{2m} + G \sum_m Q_m (-1)^m x^{2m+1} \\
F &= \frac{\Gamma(c)}{\Gamma(a+1/2)\Gamma(1-b)}\,, \quad G = \frac{\Gamma(c-1)}{\Gamma(a)\,\Gamma(1/2-b)} \\
A &= BD_f \qquad B = C\frac{\sqrt{\pi}\,\Gamma(a)}{2^{l+1}} \\
P_m &= \frac{(a)_m\,(b)_m}{(c)_m\, m!}\, p_m \qquad Q_m = \frac{(a+1/2)_m\,(b+1/2)_m}{(c+1)_m\, m!}\, q_m \\
a &= \frac{\gamma_1+\gamma_f+l+1}{2} \qquad b = \frac{\gamma_1+\gamma_f-l}{2} \qquad c = 1/2 \\
a_m &= a(a+1)\ldots(a+m-1).
\end{aligned}\right\} \tag{11}$$

The quantities p_m and q_m are different according to whether the final state is in the discrete or in the continuous spectrum. In the discrete spectrum, we have

$$\left.\begin{aligned}
p_m &= [s(N_f-\varkappa_f)\,\mathrm{F}(-2m,\,-n'_f,\,2\gamma_f+1,\,y) \\
&\quad - t n'_f\, F(-2m,\,-n'_f+1,\,2\gamma_f+1,\,y)]\, v^{2m} \\
q_m &= [s(N_f-\varkappa_f)\,F(-2m-1,\,-n'_f,\,2\gamma_f+1,\,y) \\
&\quad - t n'_f\, F(-2m-1,\,-n'_f+1,\,2\gamma_f+1,\,y)]\, v^{2m+1} \\
s &= \sqrt{1+\gamma_1}\sqrt{1+\vartheta_f} + \sqrt{1-\gamma_1}\sqrt{1-\vartheta_f} \\
t &= \sqrt{1+\gamma_1}\sqrt{1+\vartheta_f} - \sqrt{1-\gamma_1}\sqrt{1-\vartheta_f} \\
y &= \frac{2}{1+N_f} \qquad v = 1+\frac{1}{N_f},
\end{aligned}\right\} \tag{12}$$

where F is the usual symbol for the hypergeometric function.

For a final state in the continuum, we have

$$\left.\begin{aligned}
p_m &= 2\,Re\left\{F(-2m,\,\gamma_f+1+i\alpha,\,2\gamma_f+1,\,y)\,v^{2m}\,X\right\} \\
q_m &= 2\,Re\left\{F(-2m-1,\,\gamma_f+1+i\alpha,\,2\gamma_f+1,\,y)\,v^{2m+1}X\right\} \\
y &= \frac{2ik}{\varepsilon_1+ik} \qquad v = 1+i\frac{k}{\varepsilon_1} \\
X &= \left(\sqrt{W+1}\sqrt{1+\gamma_1} - i\sqrt{W-1}\sqrt{1-\gamma_1}\right)(\gamma_f+i\alpha)\,e^{i\eta}.
\end{aligned}\right\} \tag{13}$$

The limit $k = 0$ is not entirely trivial. We get

$$\left.\begin{aligned} p_m &= \sqrt{2(1+\gamma_1)}\,[(\gamma_f+1-\gamma_1-\varkappa_f)\,\Phi(-2m, 2\gamma_f+1, -2) \\ &\quad + \frac{4m}{2\gamma_f+1}\,\Phi(-2m+1, 2\gamma_f+2, -2)] \\ q_m &= \sqrt{2(1+\gamma_1)}\,[(\gamma_f+1-\gamma_1-\varkappa_f)\,\Phi(-2m-1, 2\gamma_f+1, -2) \\ &\quad + \frac{4m}{2\gamma_f+1}\,\Phi(-2m, 2\gamma_f+2, -2)]. \end{aligned}\right\} \quad (14)$$

The radii of convergence of the series S are in the three cases

$$q^2 > \varepsilon_1^2\left(1+\frac{1}{N_f}\right)^2, \quad q^2 > \varepsilon_1^2 + k^2, \quad q^2 > \varepsilon_1^2,$$

respectively.

The arguments of all complex quantities have to be taken between $-\pi$ and $+\pi$.

The screening is taken into account by assuming an effective nuclear charge $Z_{eff} = Z - 0.3$ and by adding to the corresponding Coulomb potential a constant term $e^{-1}V$, representing the effect of the outer electrons. The energy V is the difference between the observed binding energy of the K-electron and the value which this binding energy would have in the absence of outer screening.

The electron wave functions are thus as given above with Z_{eff} instead of Z and the effective energy equal to $E_t - V$, where E_t is the true total energy of the electron. Therefore, the wave functions of the electrons with $E_t < mc^2 + V$ are of the form given for the discrete spectrum, only that n' is in general non-integer.

In order to obtain the total cross section for ionization of the K-shell, we have to square I, given by (11), integrate over q (cf. (1)), sum over different $\varkappa_f$ (cf. (10)) and, finally, integrate over the energies of the outgoing electrons. The last two steps can only be done numerically.

III. Results and Discussion.

The cross section for K x-ray production by protons has been evaluated for two elements, lead and silver, and for the impact energy range in which the experiments were performed, i. e. 1—3 MeV. The numerical work of evaluating the series S was considerable, since the series is alternating with increasing coefficients. We calculated it for three different energies of the ejected electrons and all contributing final $\varkappa$-values, taking into account

up to 15 terms. This was sufficient for $0 < x < 0.3$. In Table I, we give the quantity

$$T = (q/\varepsilon_1)^{4\gamma_1+4} \int_0^{\varepsilon_1/q} x^{2\gamma_1+2\gamma_f+3} S^2(x)\, dx$$

as a function of ε_1/q for lead. Also the normalization factors as calculated from formulae (7) to (9) are listed.

TABLE I.

ΔE / $W_t\,(W_f)$	88,0 keV 1,0000 (0,9749)			101 keV 1,0251 (1,0000)			123 keV 1,0686 (1,0435)		
ε_1/q \ $\varkappa_f$	-1	$+1$	-2	-1	$+1$	-2	-1	$+1$	-2
0.00	0.3542	0	0	0.3333	0	0	0.3414	0	0
0.05	0.5030	0.00023	0.00036	0.4749	0.00055	0.00035	0.4890	0.00071	0.00036
0.10	0.6341	0.00116	0.00236	0.6001	0.00280	0.00232	0.6205	0.00362	0.00240
0.15	0.7266	0.00299	0.00718	0.6889	0.00722	0.00708	0.7145	0.00935	0.00734
0.20	0.7694	0.00557	0.01521	0.7302	0.01354	0.01503	0.7589	0.01759	0.01565
0.25	0.7626	0.00861	0.02574	0.7239	0.02082	0.02549	0.7524	0.02707	0.02660
0.30	0.7150	0.01155	0.03728	0.6781	0.02788	0.03690	0.7028	0.03608	0.03850
$\lvert\varkappa_f\rvert$ A'^2	2.309	8.596	2.804	2.521	4.284	4.304	2.576	4.377	5.758

The quantity T, defined in the text, is given for Pb as a function of ε_1/q and $\varkappa_f$ for three different energies of the ejected electrons. W_t and W_f are defined by $W_t = E_t/mc^2$ and $W_f = (E_t - V)/mc^2$. In the last row the corresponding normalization factor is listed in units of $\varepsilon_1{}^{2\gamma_1+2\gamma_f}\, m/\hbar^2$, i. e. $A^2 = A'^2 \varepsilon_1{}^{2\gamma_1+2\gamma_f}\, m/\hbar^2$. Only those final states which contribute more than 1 % to the total cross section are taken into account.

From Table I it is seen that the values of T for the important transitions are not sensitive to the energy of the ejected electron and that, consequently, nearly the whole dependence of the cross section on this energy is contained in $q_{\min}$. The interpolation and extrapolation of the data in Table I and the subsequent integration over the energy of the ejected electrons could therefore be performed with sufficient accuracy. The cross sections for production of lead K x-rays, as calculated from the data listed in Table I, are presented in Table II and Figure 1 and compared with experiments and previous theory. The computational accuracy of our results should be better than 5 %. For silver, we had to extrapolate our values for T towards higher values of ε_1/q in order to come into the region covered by the experiments. Hereby, errors of the order of 20 % could easily be introduced. The result-

TABLE II.

Element	E_1 (MeV)	σ_{exp} (cm²)	$\sigma_{th\,1}$ (cm²)	$\sigma_{th\,2}$ (cm²)
Pb	1.00			1.04×10^{-27}
	1.50			3.54
	1.92	3.6×10^{-27}	1.56×10^{-27}	7.0*
	2.00			7.91
	2.17	5.9	2.48	9.9*
	2.40	10.5	3.43	13.1*
	2.50			14.8
	2.88	30.5	6.30	22.0*
	3.00			24.2
Ag	1.70	0.69×10^{-24}	0.76×10^{-24}	
	1.92	1.3	1.15	
	2.17	2.1	1.61	
	2.40	3.0	2.20	
	2.64	4.3	2.77	
	2.88	8.2	3.49	

Experimental[1]) and theoretical cross sections as a function of the proton energy. The last column gives the relativistic cross sections. Those marked with an asterisk have been obtained by graphical interpolation. The last but one column includes cross sections as calculated by LEWIS et al.[1]) according to Henneberg's theory. They have been partially corrected for relativistic effects since a relativistic screening factor Θ is used. A consistent non-relativistic procedure would yield cross sections smaller by ten to fifty per cent. In the case of silver, our relativistic cross sections agree with the semi-relativistic ones within computational errors.

ant cross sections are, however, somewhat accidentally equal to those evaluated by LEWIS et al.[1]) from Henneberg's theory.

It is seen that, as expected, the use of relativistic electron wave functions increases considerably the cross section for heavy elements, and the agreement with the experimental data is thereby improved significantly. Still, there remains a discrepancy between theory and experiment, especially as regards the energy dependence of the cross sections.

Some uncertainty in the theoretical calculations arises from the manner in which the screening effect is taken into account. Work in related fields[11]) indicates that the form of the electron wave functions which we have employed is adequate, since, in the central regions of the atom which contribute to the integral J, the assumed potential is rather accurate. An improvement of the treatment would, however, be obtained by adjusting the normalization factors for the final state wave functions to take into account the modification of the potential at large distances. The effect is found to be small,

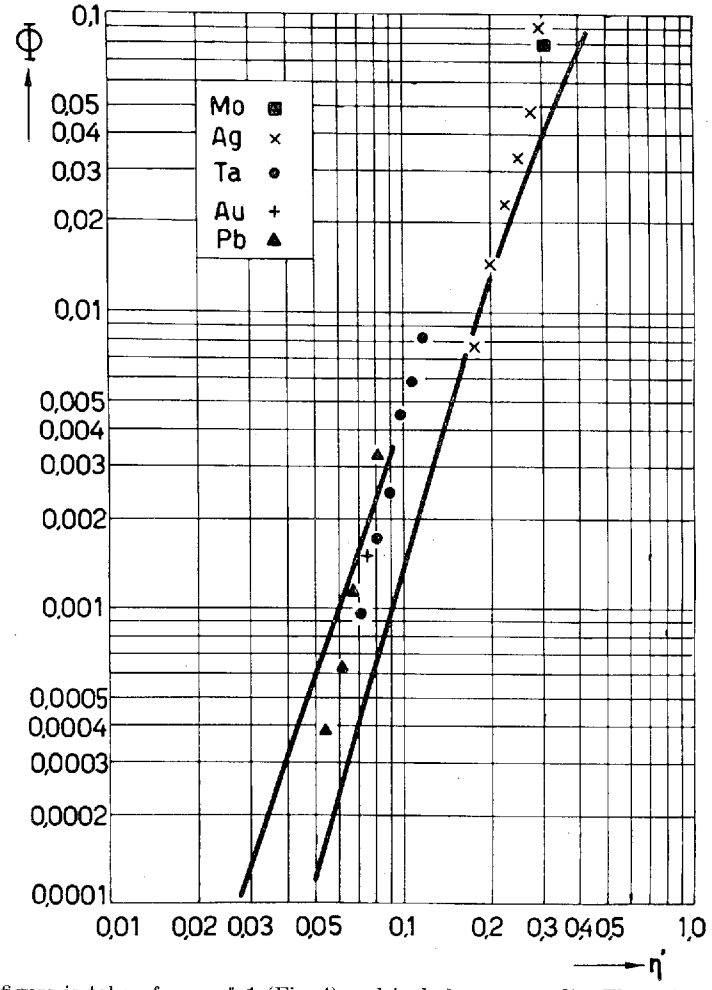

Fig. 1. The figure is taken from ref. 1 (Fig. 4) and includes our results. The points give the experimental quantity $\Phi = Z^4\Theta/3{,}51\ \sigma \times 10^{16}\ \mathrm{cm}^{-2}$ as a function of η'. The left-hand curve represents the function Φ obtained in the same way from the relativistic cross sections for lead. The right-hand curve represents the function Φ_0. In the case of silver, both curves coincide within computational errors. Relativistic screening factors Θ are used throughout.

except for very low electron energies, as is also indicated by the results obtained for the screening effect in other problems, such as internal conversion[12]. Still, since the low energy end of the spectrum of the ejected electrons contributes most of the total cross section, the correction might be significant. While no quantitative estimates have been made, it can be seen that the effect tends to decrease the cross section. In fact, the correct

normalization factor is expected to be smaller than that in (7), which corresponds to bound states. Moreover, the effect on the energy dependence of the total cross section appears to be small. It thus seems unlikely that the discrepancies between theory and experiment can be removed by improving the electron wave functions and their normalization factors.

Another source of error arises from the use of the Born approximation for the bombarding particles, which neglects the deflections of the incident particle in the Coulomb field of the nucleus.

The deflection prevents particles with low energy from coming close enough to the nucleus and thus decreases the cross section for K-shell ionization. One is tempted to consider the quantity $r_0 q_{\min}$, where $r_0 = Z_1 Ze/E_1$ is the distance of closest approach, as a measure of the significance of this deflection* rather than the less stringent criteria of HENNEBERG. It would seem that, if $r_0 q_{\min} > 1$, the ionization cross section must be considerably less than predicted by the Born approximation and that, only if $r_0 q_{\min} \ll 1$, can the influence of the Coulomb field on the incident particle be neglected. Now, for electrons ejected with zero energy, we have $r_0 q_{\min} = 1$ at a proton energy of about 1.1 MeV in lead and about 0.3 MeV in silver. It should thus be understandable that, at proton energies of this order of magnitude or smaller, the cross sections fall below the predictions of the Born approximation.

While thus the failure of the Born approximation may account for the small cross sections observed at low energies and for the rapid energy dependence, it seems more difficult to explain the large experimental cross sections at higher bombarding energies. Additional measurements, especially of the absolute cross sections for silver, would therefore be of value as a further test of the theoretical calculations.

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* This has been suggested to us by A. BOHR.

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Appendix.

We have to evaluate the integral

$$I = \int j_l(qr)\,[f_i f_f^* + g_i g_f^*]\,r^2\,dr\,.$$

The functions f_i and g_i are defined in formula (8). We write the derivation for the case when the final wave functions f_f and g_f are as given in (9). The other case is analogous. We express $j_l(qr)$ as a confluent hypergeometric function

$$j_l(qr) = \frac{\sqrt{\pi}}{\Gamma(l+3/2)\,2^{l+1}}\,(qr)^l\,e^{-iqr}\,\Phi(l+1, 2l+2, 2iqr)\,.$$

Using integral representations for the occurring confluent hypergeometric functions we are able to carry out the radial integration and arrive at the following expression:

$$I = \frac{\sqrt{\pi}\,\Gamma(2a)}{\Gamma(l+3/2)}\,CD\left(\frac{q}{2}\right)^l Re\left\{X(\varepsilon_1+ik+iq)^{-2a}\,F_2\left(2a, l+1, \gamma_f+1+i\alpha, 2l+2,\right.\right.$$
$$\left.\left. 2\gamma_f+1; \frac{2iq}{\varepsilon_1+ik+iq}, \frac{2ik}{\varepsilon_1+ik+iq}\right)\right\}.$$

Here, the definition of the various quantities is the same as in the text. F_2 is the symbol for one of the Appell functions as defined in reference 13, page 230.

We may transform F_2 into H_4 using the equation[14]

$$F_2(\alpha, \beta, \beta', 2\beta, \gamma'; x, y) = \left(1-\frac{x}{2}\right)^{-\alpha} H_4\left(\alpha, \beta', \beta+\frac{1}{2}, \gamma'; \frac{x^2}{4(2-x)^2}; \frac{2y}{2-x}\right)$$

and get

$$I = \frac{\sqrt{\pi}\,\Gamma(2a)}{\Gamma(l+3/2)}\,CD\left(\frac{q}{2}\right)^l Re\left\{X(\varepsilon_1+ik)^{-2a}\,H_4\left(2a,\ \gamma_f+1+i\alpha,\ l+3/2,\right.\right.$$
$$\left.\left. 2\gamma_f+1; -\frac{q^2}{4(\varepsilon_1+ik)^2}, \frac{2ik}{\varepsilon_1+ik}\right)\right\}.$$

We require the analytical continuation for large values of q. It can be obtained in the following way. Using the notation of reference 13, we have

$$H_4(\alpha,\beta,\gamma,\delta;x,y)=\sum_{m,n}\frac{(\alpha)_{2m+n}(\beta)_n}{(\gamma)_m(\delta)_n\,m!\,n!}x^m y^n=\sum_{m,n}\frac{(\alpha/2)_m\left(\frac{\alpha+1}{2}\right)_m(\alpha+2m)_n(\beta)_n}{(\gamma)_m(\delta)_n\,m!\,n!}(4x)^m y^n$$

$$=\sum_m\frac{(\alpha/2)_m\left(\frac{\alpha+1}{2}\right)_m}{(\gamma)_m\,m!}F(\alpha+2m,\beta,\delta,y)(4x)^m$$

$$=\frac{\Gamma(\delta)}{\Gamma(\beta)\Gamma(\delta-\beta)}\int_0^1 u^{\beta-1}(1-u)^{\delta-\beta-1}(1-yu)^{-\alpha}F\left(\frac{\alpha}{2},\frac{\alpha+1}{2},\gamma,\frac{4x}{(1-yu)^2}\right)du.$$

Applying here the equation for analytic continuation of the ordinary hypergeometric function and working the same way backward, we arrive at

$$H_4(\alpha,\beta,\gamma,\delta;x,y)$$

$$=\frac{\Gamma(1/2)\Gamma(\gamma)}{\Gamma\left(\frac{\alpha+1}{2}\right)\Gamma\left(\gamma-\frac{\alpha}{2}\right)}(-4x)^{-\frac{\alpha}{2}}\left[\sum_m\frac{(\alpha/2)_m\left(1-\gamma+\frac{\alpha}{2}\right)_m}{(1/2)_m\,m!}F(-2m,\beta,\delta,y)(4x)^{-m}\right]$$

$$+\frac{\Gamma(-1/2)\Gamma(\gamma)}{\Gamma(\alpha/2)\Gamma\left(\gamma-\frac{\alpha+1}{2}\right)}(-4x)^{-\frac{\alpha+1}{2}}\left[\sum_m\frac{\left(\frac{\alpha+1}{2}\right)_m\left(3/2-\gamma+\frac{\alpha}{2}\right)_m}{(3/2)_m\,m!}F(-2m-1,\beta,\delta,y)(4x)^{-m}\right].$$

Applying this result to the matrix element I, we get the final expression, given in formulae (11)—(14).

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