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I. PHYSICS

Atomic Collisions

L AND *M* SHELL COULOMB IONIZATION BY HEAVY CHARGED PROJECTILES

R. KARMAKER

Department of Mathematics, Bangladesh Agricultural University, Mymensingh, Bangladesh

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Universal cross sections for *L* and *M* shell ionization have been extracted from the semiclassical approximation (SCA) model in the straight line path approximation of the projectile. It has been shown that it is possible to organise the calculation of the SCA in a suitable way so that it is not necessary to calculate the cross section for different targets. The agreement between the theoretical curve in the SCA model and the available experimental data for different target elements, is reasonably good.

Cross sections for *L* and *M* shell ionization in the straight line path of the projectile in the SCA model for Pb, Au and U targets by the impact of protons have been calculated. The results have been compared with those calculated in the Binary Encounter Approximation (BEA) and the Plane Wave Born Approximation (PWBA) as well as with the available experimental results. The present calculations are in good agreement with the existing theoretical and the experimental results.

Keywords: *L* & *M* **Shell; Coulomb Ionization; Projectiles**

INTRODUCTION

THE production of characteristic X-rays by heavy charged particles has been investigated theoretically and experimentally since the work of Chadwick (1913). A theoretical description of inner shell ionization was first undertaken by Henneberg (1933) who obtained an approximate formula for the *K* shell ionization cross section. Since then, both theoretical and experimental investigations of the inner shell ionization of atoms by proton and other heavy charged particles have been carried out. Lewis *et al.* (1953) and Merzbacher and Lewis (1958) gave a comprehensive description of the theory of the calculations of the *K* and *L* shell ionizations.

An alternative approach is the Semiclassical Approximation (SCA) which describes the bombarding particles as a point charge moving on a classical orbit characterised by its impact parameter. Mott (1931) and Frame (1931) have given partial justification for this approximation. Bang and Hansteen (1959) have calculated the *K* shell ionization cross section in SCA both for straight line trajectories and for hyperbolic Kepler orbits. Hansteen and Mosebekk (1973) have suggested improvement of the SCA model and discussed *K* and *L* shell ionizations. The deflection of the projectile and relativistic effects from the electron wave functions have been discussed. Recently, Hansteen (1975) has given a comprehensive description of the Semiclassical Approximation and stressed the importance of the single as well as multiple coulomb ionization processes. The validity of both the Plane Wave Born Approximation (PWBA) and the SCA in the straight line approximation is limited primarily by neglecting the deflection effect on the incident particle, due to the Coulomb repulsion between the incident particle and the atomic nucleus. The close agreement between the two approximations suggests that a semiclassical calculation at low energies with projectiles moving on hyperbolic Kepler orbits (Bang & Hansteen, 1959) might similarly yield results equivalent to the more quantum mechanical distorted wave Born Approximation.

Another theoretical approach for the inner shell ionization of atoms is the Binary Encounter Approximation (BEA). This model was first proposed by Gryzinski (1959, 1965 *a*, *b*, *c*) and later applied by Garcia (1970). Gryzinski assumed that the dominant interaction producing the inner shell ionization is a direct energy exchange between the projectiles and the atomic electron.

Experimental investigations have been done by Khan *et al.* (1965), Garcia *et al.* (1973), Sellers *et al.* (1969), Johansson *et al.* (1970) and many others. Recently, Vader *et al.* (1976) have measured *K* shell ionization probabilities by impinging α-particles at very small impact parameters on Pb. The data are compared with SCA calculations with relativistic wave functions.

The theoretical predictions made by Bang and Hansteen (1959) in the SCA provides good agreement with both experimental and other theoretical *K* and *L* shell ionization cross sections for light as well as for heavy elements. It is, therefore, desirable to extend the calculations of *K* and *L* shell ionization cross sections in the SCA to the *M* shell calculations.

In the present work, we have calculated cross sections for *L* and *M* shell ionizations in the straight line path of the projectile in the SCA model for Au and U targets respectively by the impact of protons. The results have been compared with those calculated in the BEA and the PWBA as well as with the available experimental results. The present calculations are in good agreement with the existing theoretical and the experimental results.

A Short Survey of the SCA Model

The projectile is taken as a heavy charged particle moving in a classical orbit and the atomic electron before and after scattering is described quantum mechanically. The projectile of charge $Z_1 e$ and velocity v_1 approaches the target atom of charge $Z_2 e$ in a Coulomb field with the potential $\frac{Z_1 Z_2 e^2}{R(t)}$. The geometry of the collision process leading to ionization is considered by placing the coordinate system at the target atom with the origin at the centre of mass of the nucleus. The projectile is considered as a point charge moving along the *Z*-axis in the static electromagnetic field of the nucleus and exerting a time-dependent perturbation on the atomic electrons.

The physical situations for both the straight line and the hyperbolic paths of the projectile are shown in figures 1 & 2.

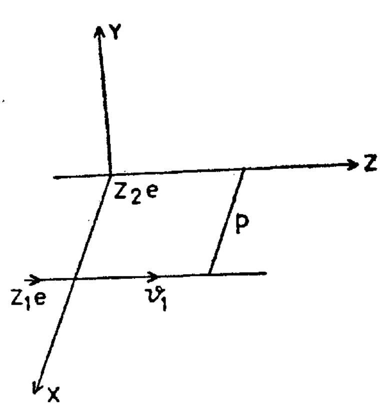


FIG. 1. Straight line path of the projectile.

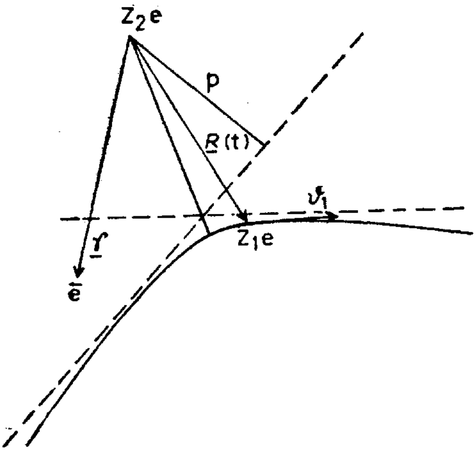


FIG. 2. Hyperbolic path of the projectile.

The condition for the justification of the classical treatment of the projectile is (Bohr, 1948)

$$x = \frac{2Z_1Z_2e^2}{\hbar v_1} \gg 1,$$

which means that the motion of the projectile must be described by a wave packet small compared with the distance of the closest approach to the target nucleus.

A second condition is that the charge of the projectile is much smaller than that of the target nucleus i.e., $Z_1 \ll Z_2$ so that the potential between the incoming particle and the target electron should give a small perturbation of the total electron Hamiltonian.

In the straight line version of the SCA model, the differential cross section for the ejection of an atomic electron from a bound state to continuum states with energies lying in the interval between the energy levels E_f and $E_f + \triangle E_f$ is calculated as (Bang & Hansteen, 1959)

$$\frac{d\sigma}{dE_f} = 4\pi Z_1^2 \frac{M_1}{E_1} \frac{e^4}{\hbar^2} \int_0^\infty p dp \mid M_p \mid^2$$

Here M_1, E_1 and p stand for mass, energy and impact parameter of the projectile.

$$M_p = \int d\tau \psi_i \psi_f^* e^{iq_0z} K_0(q_0\rho)$$

is the matrix element between the initial and the final states ψ_i and ψ_f of the atomic electron and q_0 is the minimum momentum transfer, K_0 is a Bessel function of the third kind and zeroth order.

$$\rho^2 = (x - p)^2 + y^2$$

The expression for the K shell total cross section is

$$\sigma_k = 4\pi Z_1^2 \frac{M_1}{E_1} \frac{e^4}{\hbar^2} \int_0^{E_f} \mathrm{d}E_f \int_0^{\infty} p\mathrm{d}p \mid M_p \mid^2$$

and the ionization probability as a function of the impact parameter p is defined by

$$I_p = \int_0^{\infty} \left(\frac{\mathrm{d}\sigma}{\mathrm{d}E_f}\right)_p \mathrm{d}E_f$$

Thus we may write the total Coulomb ionization cross section as

$$\sigma_k = 2\pi \int p\mathrm{d}pI_p$$

L AND M SHELL IONIZATION

The procedure which was applied to the calculation of the matrix element for the K shell can be extended to calculate M_p for the less bound shells. However, this method yields many different integrals (21 terms for the L shell and 141 terms for the M shell) and consequently the numerical procedure becomes rather complicated.

In our new approach, the angular part of the matrix element is transformed into the sum of several terms (Karmaker & Kocbach, 1976) which can be treated by the same method as in the case of K shell. In addition to this, certain relations among the Whittaker functions that occur in the radial integrals, are used to transform the radial integrals into a form similar to that for the K shell.

A short review of the calculation of the matrix elements for the M shell is given here. [For detailed calculations, *see* Karmaker and Kocbach (1976)].

The matrix element M_p can be written as

$$M_p(l_1, m_1, l, m) = \sum_{L=|l-l_1|}^{|l+l_1|} f(l, m, L, M) \times \int_0^{\infty} \mathrm{d}r\, r^2 R_{l_1}(\alpha r) R_l^*(-ikr)$$

$$\times \int_0^{\pi} \mathrm{d}\theta\, e^{iq_0 r \cos\theta} \sin\theta\, P_L^M(\cos\theta) \int_{-\pi}^{\pi} \mathrm{d}\varphi\, e^{-iM\varphi} K_0(q_0\rho)$$

with

$$M = m_1 - m;\ \alpha = \frac{Z_2 e^2 m_e}{n\hbar^2}\ (n = 1, 2, 3, \ldots);$$

$$K = \frac{\alpha_0}{\eta},\ \alpha_0 = \frac{Z_2}{a_0};\ \eta = -\frac{Z_2 e^2}{\hbar v} \text{ and } f(l_1, m, L, M)$$

represents the product of the Clebsch-Gordan coefficients and the normalization constants. $a_0 = 5.2917 \times 10^{-11}$ meter is the Böhr radius.

The φ-integral is transformed into (Karmaker & Kocbach, 1976)

$$\int_{-\pi}^{\pi} e^{-iM\varphi} K_0(q_0\rho)\, d\varphi = 2\pi \int_0^{\infty} dt\, \frac{t}{s^2} J_M(pt)\, J_M(rt \sin\theta)$$

with $s^2 = t^2 + q_0^2$ and J_M is a Bessel Function.

The θ-integral thus leads to (Karmaker & Kocbach, 1976)

$$\int_0^{\pi} d\theta \sin\theta\, e^{iq_0 r\cos\theta} P_L^M(\cos\theta)\, J_M(rt\sin\theta)$$

$$= \left(\frac{2\pi}{rs}\right)^{1/2} i^L \frac{(2M)!}{2^M M!} \left(\frac{t}{s}\right)^M C_{L-M}^{M+1/2}\left(\frac{q_0}{s}\right) J_{L+1/2}(rs)$$

where $C_{L-M}^{M+1/2}$ is a Gegenbauer polynomial.

The radial integral can be written as (Erdélye, 1953)

$$I(r) = \int dr\, r^q e^{-rq} M_{in,l+1/2}(-2ikr)\, M_{0,L+1/2}(2irs) \qquad \text{...(A)}$$

where $q = 0, 1, 2$. The possible L values are given in Table I.

TABLE I

Shell	Initial state	Final state	Possible L values
3*S*	0	l	l
3*P*	1	l	$l-1$
			$l+1$
			$l-2$
3*D*	2	l	l
			$l+2$

In order to evaluate the radial integral we shall take the help of the formula (Erdélye, 1936)

$$\int_0^{\infty} e^{-pz} Z^q M_{k_1,m_1}(\alpha_1 Z)\, M_{k_2 m_2}(\alpha_2 Z)\, dZ$$

$$= (\alpha_1)^{m_1+1/2}(\alpha_2)^{m_2+1/2}\left[p + \frac{\alpha_1+\alpha_2}{2}\right]^{-(q+m_1+m_2+2)} \Gamma(q+m_1+m_2+2)$$

$$\times F_2\left\{q+m_1+m_2+2, \tfrac{1}{2}+m_1-k_1, \tfrac{1}{2}+m_2-k_2, 1+2m_1, 1+2m_2; \frac{\alpha_1}{p+\frac{1}{2}(\alpha_1+\alpha_2)}, \frac{\alpha_2}{p+\frac{1}{2}(\alpha_1+\alpha_2)}\right\}$$

where $F_2\{\ \}$ is a hypergeometric function of two variables, an Appel function. This Appel function can be reduced to hypergeometric functions of one variable (Bang & Hansteen, 1959) if it is of the form

$$F_2\{\alpha + 1, \beta, \beta', \alpha, \alpha', x, y\} \quad \text{...(B)}$$

The possible values of the variable of the function F_2 are given in Table II.

TABLE II

No. of terms	q	K_1	m_1	K_2	$m_2 = L + \frac{1}{2}$	q	K_2	$4l$
1	0	$-i\eta$	$l + 1/2$	0	$l + 1/2$	0	0	0
2	1	$-i\eta$	$l + 1/2$	0	$l + 1/2$	1	0	0
3	2	$-i\eta$	$l + 1/2$	0	$l + 1/2$	2	0	0
4	1	$-i\eta$	$l + 1/2$	0	$l + 3/2$	1	0	1
5	2	$-i\eta$	$l + 1/2$	0	$l + 3/2$	2	0	1
6	1	$-i\eta$	$l + 1/2$	0	$l - 1/2$	1	0	-1
7	2	$-i\eta$	$l + 1/2$	0	$l - 1/2$	2	0	-1
8	2	$-i\eta$	$l + 1/2$	0	$l + 5/2$	2	0	2
9	2	$-i\eta$	$l + 1/2$	0	$l - 3/2$	2	0	-2

The total cross section for the ionization of a sub-shell in the case of L, M, ... shells with respect to the final energy of the ejected electron is given by

$$\sigma_{\text{sub-shell}} = 4\pi Z_1^2 \frac{M_1}{E_1} \frac{e^4}{\hbar^2} \int_0^{E_f} dE_f \int_0^{\infty} p dp \mid M_p \mid^2$$

with $\mid M_p \mid^2 = \sum_{l,m,m_1} \mid M_p(l_1, m_1; l, m) \mid^2$

Each sub-shell is being specified by the quantum number l_1.

Taking into account the changes introduced by spin the ionization probability is

$$I_p^{(l_1,j)} = C^{(l_1,j)} I_p^{(l_1)}$$

where

$$C^{(l_1,j)} = \frac{2j + 1}{2l_1 + 1}$$

The values of the co-efficients $C^{(l_1,j)}$ up to $l_1 = 2$ are given in Table III.

RESULTS AND DISCUSSION

The SCA model has so far been applied for the calculations of the K and L shells and for $3S$ and $3P$ sub-shells by bombarding specific target elements. By

TABLE III

l_1	j	$C^{(l_1,j)}$
0	1/2	2
1	1/2	2/3
1	3/2	4/3
2	3/2	4/5
2	5/2	6/5

this, we mean that calculations are to be done as many times as the targets are changed.

In order to get rid of this laborious and time-consuming task of repeated calculations for different targets, we propose a way of constructing universal cross sections in the straight line approximation of the SCA theory, from a certain set of universal functions (Karmaker & Kocbach, 1973). The quantities in the expression for the ionization probability have been replaced by the corresponding dimensionless quantities. One such quantity viz., the experimental binding energy E_B has been replaced by a quantity Ⓗ which is defined as the ratio of the experimental binding energy to the ideal binding energy of hydrogen-like atom i.e.

$$Ⓗ = E_B \frac{2m_e}{\hbar^2\alpha^2}$$

A simple variable X is chosen such that

$$X = \frac{Ⓗ Z_2}{\sqrt{E_1}}$$

and this relates the cross section to a universal function

$$F(X) = \sigma Ⓗ Z_2^4$$

This procedure has been extended to the less bound shells (Kocbach, 1973) with proper choice for x, $F(X)$ and Ⓗ. The quantities $Ⓗ_A$, X_A and the function $F(X)$ for the less bound shells are conveniently chosen as follows :

$$Ⓗ_A = \frac{E_B(A) \times n_A{}^2}{13.6\, Z_A{}^2}$$

$$X_A = \frac{Z_A Ⓗ_A}{n_A\sqrt{E_1}}$$

$$\sigma_A\,(\text{barn}) = C_A^{(l_1,j)} \frac{1}{Z_A^4\, Ⓗ_A} F_{n_A l_A}(X_A) \qquad \text{...(C)}$$

Here n_A, l_A are the usual quantum numbers specifying the subshell A and $C_A^{(l_1,j)}$ originates from the Clebsh-Gordan coefficients coupling the spin and the orbital angular momenta.

TABLE IV(i)

Values of the universal function for L shell

X	$F_{2S}(X)$	$F_{2P}(X)$
2	2.28 + 09	4.09 + 09
3	4.26 + 09	7.70 + 09
4	6.20 + 09	1.05 + 10
5	7.52 + 09	1.18 + 10
6	8.10 + 09	1.18 + 10
7	8.01 + 09	1.09 + 10
8	7.41 + 09	9.62 + 09
9	6.50 + 09	8.13 + 09
10	5.42 + 08	6.69 + 09
11	4.32 + 09	5.42 + 09
12	3.33 + 09	4.30 + 09
13	2.45 + 09	3.40 + 09
14	1.75 + 09	2.68 + 09
15	1.23 + 09	2.11 + 09
16	8.45 + 08	1.66 + 09
17	5.54 + 08	1.31 + 09
18	3.76 + 08	1.04 + 09
19	3.34 + 08	8.16 + 08
20	1.57 + 08	6.45 + 08
21	1.05 + 08	5.11 + 08
22	7.68 + 07	4.07 + 08
23	6.06 + 07	3.23 + 08
24	5.17 + 07	2.59 + 08
25	4.65 + 07	2.06 + 08
26	4.36 + 07	1.64 + 08
27	4.08 + 07	1.33 + 08
28	3.91 + 07	1.04 + 08
29	3.72 + 07	8.41 + 07
30	3.52 + 07	6.68 + 07
31	3.31 + 07	5.41 + 07
32	3.09 + 07	4.41 + 07
33	2.87 + 07	3.52 + 07
34	2.64 + 07	2.92 + 07
35	2.42 + 07	2.31 + 07

The universal cross section functions for L and M shells for the proton projectile are shown in Figs. 3 & 4 respectively (Kocbach, 1973).

The values of the universal functions $F_{2S}(x)$ and $F_{2P}(x)$ for integral values of X are given in Table IV(i) while the values of the universal functions $F_{3S}(x)$, $F_{3P}(x)$ and $F_{3D}(x)$ for the integral values of X are presented in Table IV(ii).

The L and M shell ionization cross sections have been calculated for Au & U targets respectively by using the formula (C). These are plotted against the incident

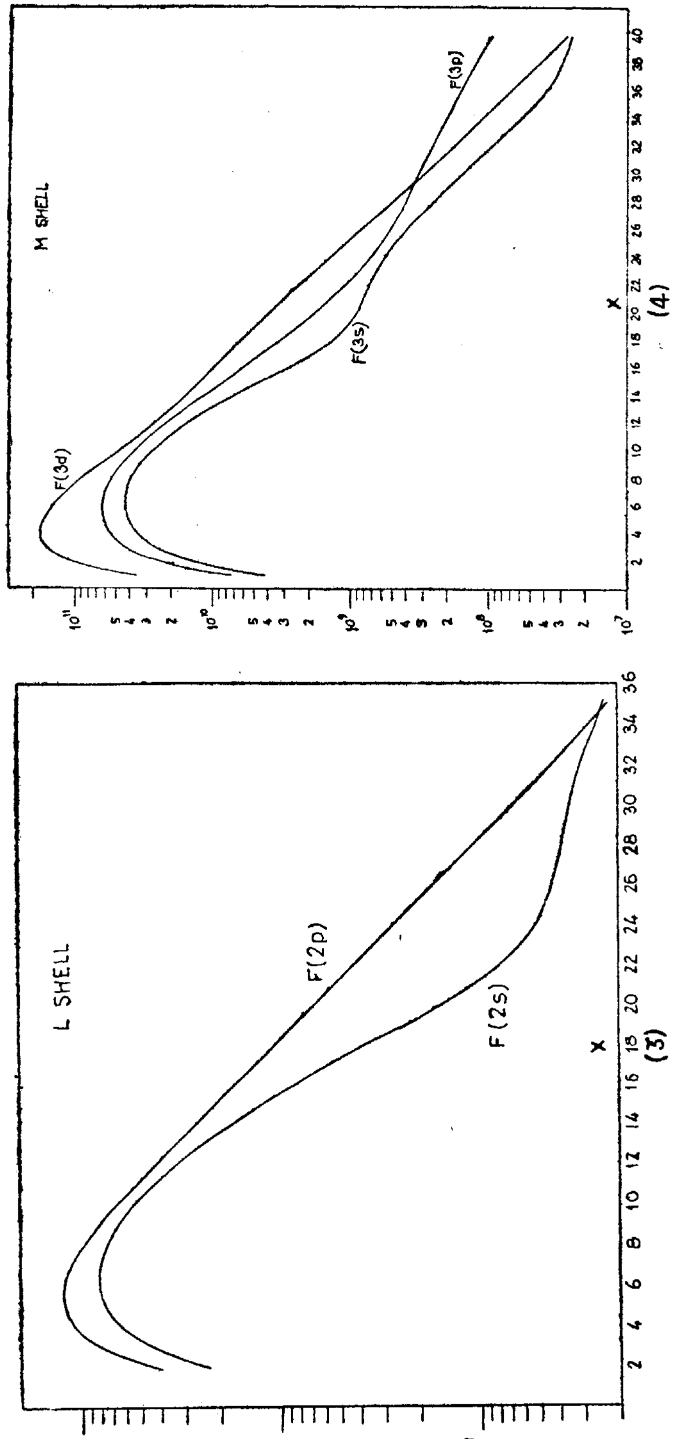
TABLE IV(ii)

Values of the universal functions for M shell

X	$F_{3S}(X)$	$F_{3P}(X)$	$F^{*}_{3D}(X)$
1	4.15 + 09	7.31 + 09	3.63 + 10
2	1.39 + 10	2.44 + 10	1.09 + 11
3	2.60 + 10	4.35 + 10	1.63 + 11
4	3.55 + 10	5.63 + 10	1.80 + 11
5	4.11 + 10	6.33 + 10	1.69 + 11
6	4.34 + 10	6.40 + 10	1.45 + 11
7	4.23 + 10	6.06 + 10	1.16 + 11
8	3.88 + 10	5.40 + 10	8.85 + 10
9	3.35 + 10	4.57 + 10	6.52 + 10
10	2.72 + 10	3.68 + 10	4.73 + 10
11	2.10 + 10	2.85 + 10	3.46 + 10
12	1.53 + 10	2.14 + 10	2.58 + 10
13	1.06 + 10	1.58 + 10	1.98 + 10
14	6.90 + 09	1.15 + 10	1.55 + 10
15	4.38 + 09	8.31 + 09	1.23 + 10
16	2.80 + 09	6.04 + 09	9.75 + 09
17	1.85 + 09	4.37 + 09	7.78 + 09
18	1.33 + 09	3.20 + 09	6.21 + 09
19	1.05 + 09	2.40 + 09	4.97 + 09
20	9.20 + 08	1.81 + 09	3.80 + 09
21	8.21 + 08	1.39 + 09	3.02 + 09
22	7.45 + 08	1.10 + 09	2.37 + 09
23	6.60 + 08	8.82 + 08	1.83 + 09
24	5.71 + 08	7.35 + 08	1.41 + 09
25	4.85 + 08	6.21 + 08	1.10 + 09
26	4.03 + 08	5.34 + 08	8.38 + 08
27	3.19 + 08	4.66 + 08	6.45 + 08
28	2.56 + 08	4.11 + 08	5.02 + 08
29	2.01 + 08	3.84 + 08	3.84 + 08
30	1.56 + 08	3.24 + 08	2.95 + 08
31	1.20 + 08	2.88 + 08	2.29 + 08
32	9.24 + 07	2.57 + 08	1.79 + 08
33	7.17 + 07	2.28 + 08	1.40 + 08
34	5.67 + 07	2.02 + 08	1.09 + 08
35	4.59 + 07	1.79 + 08	8.56 + 07
36	3.81 + 07	1.59 + 08	6.73 + 07
37	3.27 + 07	1.40 + 08	5.29 + 07
38	2.91 + 07	1.23 + 08	4.21 + 07
39	2.66 + 07	1.08 + 08	3.35 + 07
40	2.49 + 07	9.50 + 07	2.67 + 07

energies of the protons and the resulting graphs are displayed in figures 5 & 6 showing the cross sections for the subshells and the total cross sections for each shell.

The ionization cross sections are converted into X-ray production cross sections (Bush *et al.*, 1973; and Karmaker, 1974). σ_L X-ray and σ_M X-ray for Pb are com-



FIGS. 3 & 4. *L* and *M* shell universal cross section functions for proton projectile.

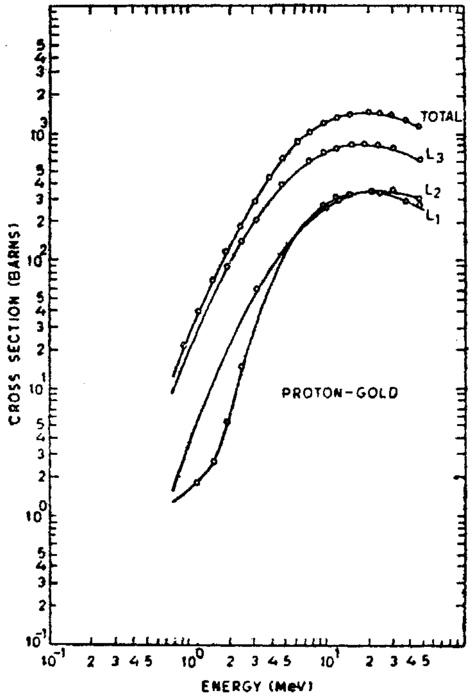


FIG. 5. The L_1, L_2, L_3 subshell and the total L shell cross sections for proton projectile on Au-target as a function of incident energy.

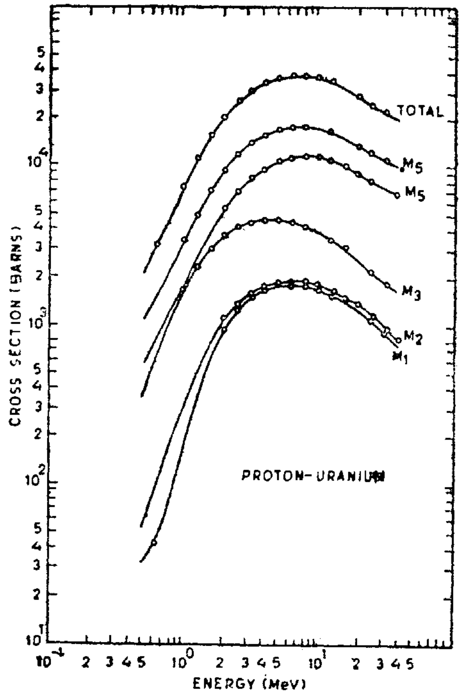


FIG. 6. The M_1, M_2, M_3, M_4, M_5 subshell and the total M shell cross sections for proton projectile on U-target as a function of incident energy.

pared with the experimental results of Bush *et al.* (1973) and the comparison is shown in figures 7 and 8. The present calculation for σ_L X-ray is about 2–10 per cent higher for proton energies up to 14 MeV and that for σ_M X-ray is about 2–10 per cent lower for proton energies up to 4 MeV and about 15–35 per cent lower for proton energies from 5 MeV to 14 MeV. The discrepancy between the present calculation and the experimentally measured values for σ_M X-ray may be due to the inaccuracy of the fluorescence yields, the non-availability of sufficient sub-shell yields and Coster-Kronig transitions. However, if the Coulomb deflection of the projectile is taken into account, the cross section for the L shell becomes lower in value and the agreement with the experiment may be even better.

The present calculation for M shell ionization cross sections for U targets by proton projectile is compared with that of Choi (1972) and the comparison is displayed in figure 9.

The present calculation for L X-ray is compared with that made in both PWBA & BEA. The theoretical data for PWBA & BEA have been taken from figure 2 of Bush *et al.* (1973) and the comparison is shown in figure 10. The SCA calculation seems to be higher by about 20 per cent than that in PWBA and about 40 per cent than that in BEA for proton energies up to 4 MeV. For higher energies (8–14 MeV) SCA & PWBA give about the same result. However, after correction

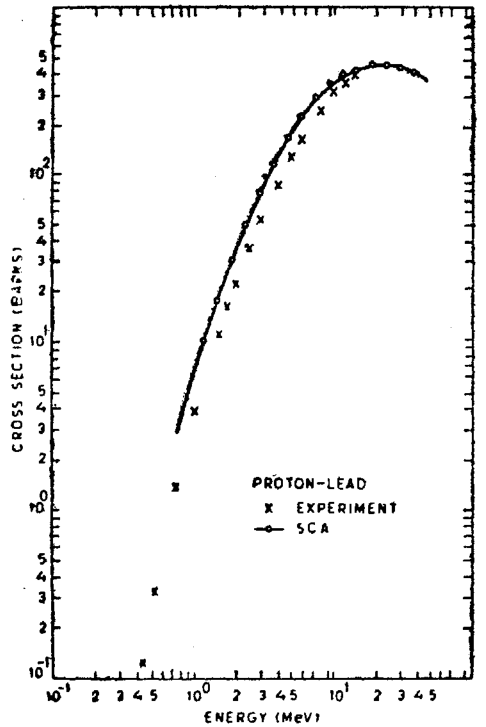


FIG. 7. Comparison of the L shell total cross section (SCA) with the experimentally measured L shell total cross section for proton projectile and Pb-target.

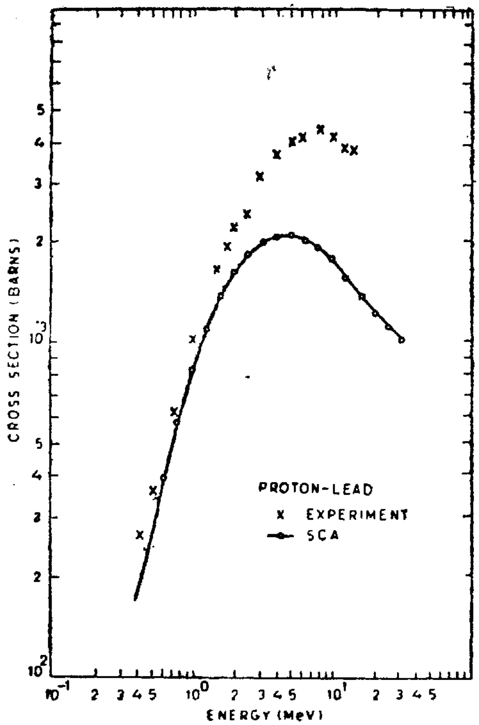


FIG. 8. Comparison of the M shell total cross section (SCA) with the experimentally measured M shell total cross section for proton projectile on Pb-target.

for Coulomb deflection of the projectile, which means lower values of the cross section, there may be a close agreement among the three theories.

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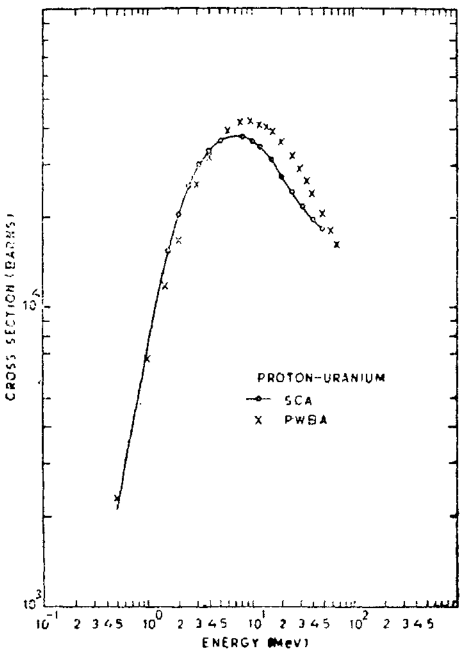

FIG. 9. Comparison of the M shell total cross section (SCA) with that of PWBA for proton projectile on Pb-target.

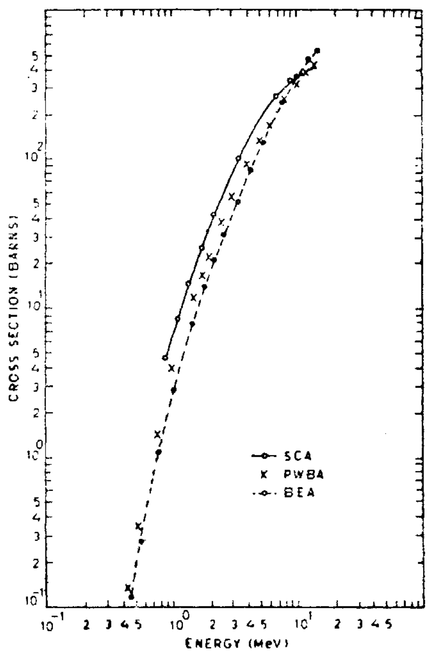

FIG. 10. Comparison of the L shell total X-ray cross section with those of PWBA and BEA for proton projectile on Pb-target.

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