

Semiclassical Approach to **Trajectory** Effects on the **Anisotropy Coefficient** of **L_3 -Subshell X-rays** Induced by Slow Heavy Particles Collisions

E. C. MONTENEGRO and A. C. DE PINHO

Departamento de Física, PUC/RJ, 22453, Rio de Janeiro, Brasil

Recebido em 5 de setembro de 1981

The deflection and the retaraation of a slow bare heavy particle by the repulsive Coulomb field of the target nucleus are known to modify the ionization cross sections of inner shells. In this paper it is shown how to calculate these effects in the magnetic substates of the $2p$ -subshell in the frame of the impact parameter picture. These corrections are essential to understand the energy dependence of the anisotropy coefficient of X-rays emitted in transitions filling an L_3 -subshell vacancy produced by massive particle bombardment.

No âmbito da aproximação semiclássica calculam-se as seções de choque diferenciais e integrais para a ionização dos subestados magnéticos da camada $2p$ por partículas carregadas de baixa energia, incluindo no cálculo os efeitos de aceleração do projétil pelo campo coulombiano do núcleo. Esses efeitos são diferentes nos sub-estados $m=0$ e $|m|=1$ o que afeta fortemente a dependência em energia do coeficiente de anisotropia dos raios- χ ou eletrons Auger emitidos após a produção de uma vacância na sub-camada L , pelo impacto de projéteis pesados lentos. Consegue-se uma descrição satisfatória dos dados experimentais relativos à anisotropia dos raios- χ L_ℓ do ouro e do chumbo.

1. INTRODUCTION

A great deal of interest has been devoted in the last years to the measurement of the polarization and/or the anisotropy of the angular distribution of the X-rays or Auger electrons emitted after the ioniza-

tion of an inner shell by a bare heavy projectile. Even when both the collimated beam and the target are unpolarized, vacancies produced in subshells with $j > 1/2$ can be aligned^{1,2}. This alignment process is responsible for the polarization and anisotropy and it results from the unbalanced population of the magnetic substates of the vacancy produced by the collimated beam^{1,2}. In all measurements of polarization and anisotropy performed up to now the final states of both the ejected electron and the projectile were not observed. The measured anisotropy coefficients³⁻⁶ at low bombarding energies are systematically smaller than the values predicted by the plane wave Born approximation⁷⁻⁸ even after correcting for the transference of unaligned vacancies produced in inner shells to the subshell under consideration by Auger or Coster-Kronig processes.

Many authors^{4,6,9} have suggested that this attenuation is due to the Coulomb interaction of the projectile with the target nucleus. In ref. 6 it is shown that it is essential to take into account both the deflection and the retardation of the projectile by the repulsive nuclear field. Furthermore these effects are not the same for different values of the magnetic quantum numbers $|m|$. Then we need a detailed description of the interaction of the projectile and the ejected electrons, both in the field of the atomic nucleus of the target. This description is most easily performed in the impact parameter formulation of the semiclassical approximation.

If the reduced de Brogliewave length of the projectile is small compared with the Bohr radius of the electron to be ejected a classical hyperbolic trajectory will describe the movement of the projectile. Each trajectory is defined by the energy available in the center-of-mass system, E , and the impact parameter p . The ionization probability for a given value of E can be expressed as a function of p . The impact parameter is related to the scattering angle θ by $\theta = 2 \cot^{-1}(p/d)$ where d is the half-distance of closest approach in a head-on collision, namely:

$$d = Z_1 Z_2 e^2 / 2E$$

where $Z_1 e$ and $Z_2 e$ are the charges of the incident projectile and of the target nucleus, respectively (see Fig. 1). The velocity of the projectile relative to the target nucleus is v .

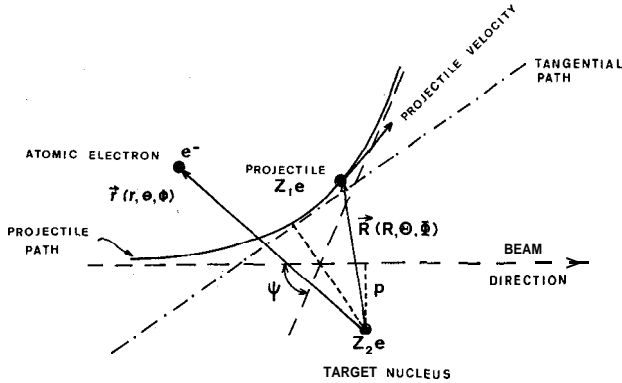


Fig. 1 - Definition of the variables describing the classical trajectory of the projectile in the Coulomb field of the target nucleus.

The most binded inner shell where the alignment can be observed is the $2p\ 3/2$ subshell which is a complete subshell for atoms with $Z \geq 10$. Our objective is to describe the behaviour of the ionization cross sections for the magnetic substates $m_1 = \pm 1/2$ and $m_3 = \pm 3/2$ in the low relative velocity limit where the projectile-target nucleus interaction is more important.

As shown in Fig. 1, $\vec{R}(t)$ and \vec{r} are the position vectors of the projectile and of the atomic electron, respectively. The initial state of the binded electron (\vec{r}) is described by the wave function $\psi_0(\vec{r})$ and its energy is E_0 . Correspondingly, the final continuum wave function is $\psi_n(\vec{r})$ and its energy is E_n . One defines $\omega = (E_n - E_0)/\hbar$. The time dependent Coulomb interaction between the classical charged particle and the electron is treated as a perturbation in a quantum mechanical description of the electronic motion.

The cross section for the transition $0 \rightarrow n$ is given by

$$\sigma_{0 \rightarrow n} = \int_0^{\infty} 2\pi p |I_n|^2 dp \quad (1)$$

with

$$I_n = -\frac{i}{\hbar} \int_{-\infty}^{+\infty} e^{i\omega t} V_{0n}(t) dt \quad (2)$$

where the time dependent potential energy is

$$V_{0n}(t) = -Z_1 e^2 \int \frac{\psi_n^*(\vec{r}) \psi_0(\vec{r})}{|\vec{r} - \vec{R}(t)|} d^3r \quad (3)$$

When the ejected electron is not observed it is necessary to integrate over all the continuum final states.

Introducing the ionization probability

$$I(p) = \int |I_n|^2 dn \quad (4)$$

it follows that the total ionization cross section is given by

$$\sigma_i = 2\pi \int p I(p) dp \quad (5)$$

2. THE IONIZATION PROBABILITY FOR THE MAGNETIC SUBSTATES OF THE 2p-SHELL

In the frame of an independent electrons atomic model the initial bound state of the electron in the central Coulomb field will be given by

$$\psi_0(\vec{r}) = R_{n\ell}(r) Y_{\ell m}(\theta, \phi)$$

the spin coordinate being not relevant for this problem. For the 2p-subshell

$$\psi_0(\vec{r}) = A_0 r \exp(-br/2) Y_{1m}(\theta, \phi) \quad (6)$$

where the normalization constant is such that

$$|A_0|^2 = b^5/24 \quad (7)$$

with $b = Z'_2/a_0$. The effective nuclear charge as seen by electrons in the L-shell is $Z'e = (Z_2 - 4.15)e$ and a_0 is the fundamental Bohr radius of hydrogen.

For the continuum final wave function the basic assumption is that the outgoing electron has most probably zero angular momentum. This assumption is justified by the fact that the most probable energy transfers are the smallest ones, i.e., collisions which impart no or little kinetic energy to the electron promoted to the continuum are far more probable than collisions ejecting fast electrons. This effect is more pronounced as the bombarding energy of the projectile become smaller. The positive energy wave function was expanded in partial waves and only the $R=0$ component was considered. Retaining terms up to the first power in r in the radial part of the wave function, the Coulomb wave function for the emerging electron with wave number k , in the limit $k \rightarrow 0$, will be written as

$$\psi_n(r) = A_n(1-br) \quad (8)$$

where the normalization function is such that

$$|A_n|^2 = \frac{2\pi b}{k} \quad (9)$$

The wave number is related to the energy transferred to the atom, E , by

$$\left(\frac{k}{b}\right)^2 = W - \frac{1}{4} \quad (10)$$

with $W = \epsilon/Z_2'^2 R_\infty$, where R_∞ is the Rydberg unit of energy.

Then, for a $2p \rightarrow k$ transition the time dependent Coulomb interaction can be written as

$$\begin{aligned} V_{0n} &\equiv V_{2p \rightarrow k} = -Z_1 e^2 A_0 A_n^* \frac{r^3(1-br)e^{-br/2}}{|\vec{r}-\vec{R}(t)|} Y_{1m}(\theta, \phi) dr d\Omega \\ &= -Z_1 e^2 A_0 A_n \left(1 + 2b \frac{\partial}{\partial b}\right) \int \frac{r^3 \exp(-br/2)}{|\vec{r}-\vec{R}(t)|} Y_{1m}(\theta, \phi) dr d\Omega \end{aligned} \quad (11)$$

The appropriate multipole expansion for $|\vec{r}-\vec{R}|^{-1}$ is given by:

$$|\vec{r}-\vec{R}|^{-1} = \sum_{\ell'=0}^{\infty} \frac{4\pi}{2\ell'+1} \frac{r_{<}^{\ell'}}{r_{>}^{\ell'+1}} \sum_{m'=-\ell'}^{\ell'} Y_{\ell'm'}^*(\theta, \phi) Y_{\ell'm'}(\theta, \phi) \quad (12)$$

where Θ and Φ are the polar and the azimuthal angles of the vector \vec{R} and $r_>$ and $r_<$ have the usual meaning. Substituting (12) into (11) and integrating over the coordinates of the electron we get

$$V_{0n} = -\frac{4\pi}{3} Z_1 e^2 A_0 A_n^* Y_{1m}(\Theta, \Phi) \left[1 + 2b \frac{\partial}{\partial b} \right] I(b, R) \quad (13)$$

where

$$I(b, R) = \frac{32}{b^5 R^2} \left[24 - \exp(-bR/2) (24 + 12bR + 3b^2 R^2 + b^3 R^3/2 + b^4 R^4/16) \right] + \frac{4R}{b^2} \exp(-bR/2) (1 + bR/2) \quad (14)$$

With no loss of generality we can choose $\Phi = 0$ since we have cylindrical symmetry around the incident beam direction (z direction). Therefore for the $m=0$ and for the $|m|=1$ states we can write

$$\left[V_{0n} \right]_{m=0} \equiv V_0 = -\sqrt{\frac{4\pi}{3}} Z_1 e^2 A_0 A_n^* \cos \Theta \left[1 + 2b \frac{\partial}{\partial b} \right] I(b, R) \quad (15)$$

$$\left[V_{0n} \right]_{|m|=1} \equiv V_1 = -\sqrt{\frac{2\pi}{3}} Z_1 e^2 A_0 A_n^* \sin \Theta \left[1 + 2b \frac{\partial}{\partial b} \right] I(b, R) \quad (16)$$

The Fourier integrals are then defined by

$$I_m = -(i/\hbar) \int_{-\infty}^{\infty} dt e^{i\omega t} V_m(t) \quad (17)$$

At low impact velocities the minimum momentum transfer is high and the dominant contributions to the ionization cross section come from the high momentum tail of the momentum distribution of the atomic electrons. This corresponds to electrons with $r \ll b^{-1}$. This well known feature of the ionization by heavy particles¹⁰ stresses the importance of the portion of the projectile trajectory in the vicinity of the distance of closest approach to the atomic nucleus. Although the integral along the true trajectory could be performed it simplifies matters if we substitute the hyperbolic path by a straight line tangent at the vertex of the hyperbolic. For the moment we suppose

that this trajectory is described by the projectile with a constant velocity equal to v .

Since

$$R \cos\theta = vt = z \quad (18.a)$$

$$R \sin\theta = p \quad (18.b)$$

and observing that V_0 and V_1 are odd and even functions of \mathbf{t} , respectively, it follows that

$$I_0 = \sqrt{\frac{\pi}{3}} \frac{Z_1 e^2 A_0 A_n^*}{\hbar v} \left[1 + 2b \frac{\partial}{\partial b} \right] \int_0^\infty \frac{z}{R} \sin(az) I(b,R) dz \quad (19)$$

$$I_1 = -i \sqrt{\frac{\pi}{6}} \frac{Z_1 e^2 A_0 A_n^*}{\hbar v} p \left[1 + 2b \frac{\partial}{\partial b} \right] \int_0^\infty \frac{1}{R} \cos(az) I(b,R) dz \quad (20)$$

where $\alpha = \omega/v$. Denoting by K_n the modified Bessel function of order n , we obtain the following results (see Appendix I for mathematical details):

$$I_0 = \sqrt{\frac{\pi}{3}} \frac{Z_1 e^2 A_0 A_n^*}{\hbar v} \alpha \left[1 + 2b \frac{\partial}{\partial b} \right] \left\{ \frac{28.3}{b^5} \sum_{n=3}^{\infty} \left(\frac{pb}{2} \right)^{2n} \frac{K_n p \sqrt{(b/2)^2 + \alpha^2}}{n! (2p \sqrt{(b/2)^2 + \alpha^2})^n} \right\} \quad (21)$$

$$I_1 = -i \sqrt{\frac{\pi}{6}} \frac{Z_1 e^2 A_0 A_n^*}{\hbar v} p^{-1} \left[1 + 2b \frac{\partial}{\partial b} \right] \frac{27.3}{b} \sum_{n=3}^{\infty} \left(\frac{pb}{2} \right)^{2n} \frac{K_{n-1} (p \sqrt{(b/2)^2 + \alpha^2})}{n! (2p \sqrt{(b/2)^2 + \alpha^2})^{n-1}} \quad (22)$$

Only the term with the lowest value of n in the summation over n is compatible with the truncation operated in the radial part of the outgoing electron wave function, then:

$$I_0 \approx \sqrt{3\pi} \frac{Z_1 e^2 A_0 A_n^*}{\hbar v} \alpha b p^3 \frac{K_3 (p \sqrt{(b/2)^2 + \alpha^2})}{[(b/2)^2 + \alpha^2]^{3/2}} \quad (23)$$

and

$$I_1 \approx -i\sqrt{\frac{3\pi}{2}} \frac{Z_1 e^2 A_0 A_n^*}{\hbar v} b p^3 \frac{K_2(p\sqrt{(b/a)^2 + a^2}}{(b/2)^2 + a^2} \quad (24)$$

The following usual definitions will be introduced at this point: the Bohr radius of the $2p$ -shell $a_2 = 4/b$, the Bohr velocity at the $2p$ -shell $v_2 = Z_2' e^2 / 2\hbar$, the scaled energy $\eta = (v/2v_2)^2$, the scaled binding energy $\Theta = I/I_H$ where I is the experimental binding energy of an L -electron and I_H is the hydrogenic binding energy given by $Z_2'^2 R_\infty / n^2$, and the scaled impact parameter $u = p/a_2$.

It results that

$$a = 2W/a_2 \sqrt{\eta} \quad (25)$$

and

$$p[(b/2)^2 + a^2]^{1/2} = 2u[(W^2/\eta)^2 + 1]^{1/2} \quad (26)$$

The minimum value of the energy transfer is $W = \Theta/4$, then at the extreme low energy limit $W^2/\eta \gg 1$.

Substituting the normalization factors given by equations (7) and (9) and noting that at the extreme adiabatic limit the argument of the Bessel functions reduce to $2uW\eta^{-1/2}$, we get finally:

$$|I_0|^2 = \frac{2^{10} \pi^2 Z_1^2 a_2^2}{Z_2'^2} \frac{\eta u^6}{k} \frac{[K_3(2uW\eta^{-1/2})]^2}{W^4} \quad (27)$$

and

$$|I_1|^2 = \frac{2^9 \pi^2 Z_1^2 a_2^2}{Z_2'^2} \frac{\eta u^6}{k} \frac{[K_2(2uW\eta^{-1/2})]^2}{W^4} \quad (28)$$

The integral over the final states is easily performed noting that with the normalization we have adopted:

$$dn = \frac{1}{(2\pi)^3} k^2 dk d\Omega_k$$

and

$$dW = 2k dk/b^2$$

Then

$$I_m(\eta, u) = \frac{4b^2}{\pi^2} \int_{W_{\min}}^{W_{\max}} k [I_m(\eta, u, W)]^2 dW$$

and the ionization probabilities are given by:

$$I_0(\eta, u) = \frac{2^{12} Z_1^2}{Z_2'^2} \eta u^6 \int_{\Theta/4}^{\infty} \frac{[K_3(2uW\eta^{-1/2})]^2}{W^4} dW \quad (29)$$

and

$$I_1(\eta, u) = \frac{2^{11} Z_1^2}{Z_2'^2} \eta u^6 \int_{\Theta/4}^{\infty} \frac{[K_2(2uW\eta^{-1/2})]^2}{W^4} dW . \quad (30)$$

3. THE IONIZATION CROSS SECTIONS FOR THE MAGNETIC SUBSTATES OF THE 2p-SHELL

From equations (5), (29) and (30) and remembering that $p = u\alpha_2$ the total cross sections for $m=0$ and $|m| = 1$ can be obtained. Inverting the order of the integrals over the energy transfer and the impact parameter, we get:

$$\sigma_0 = \frac{2^5 \pi \alpha_2^2 Z_1^2}{Z_2'^2} \eta^5 \int_{\Theta/4}^{\infty} \frac{dW}{W^{12}} \int_0^{\infty} x^7 K_3^2(x) dx \quad (31)$$

and

$$\sigma_1 = \frac{2^4 \pi \alpha_2^2 Z_1^2}{Z_2'^2} \eta^5 \int_{\Theta/4}^{\infty} \frac{dW}{W^{12}} \int_0^{\infty} x^7 K_2^2(x) dx \quad (32)$$

where we have introduced $x = 2uW\eta^{-1/2}$:

The fact that $d\sigma_m/dW$ is proportional to W^{-12} in the adiabatic limit justifies the approximations done in section 2 since it is transparent that the main contributions to the cross sections come from the smallest values of W which correspond to values of the electron kinetic energy close to zero.

Performing the integrations we find

$$\sigma_0 = (2^{38} \times 3^2 / 7 \times 11) \pi \alpha_2^2 (Z_1 / Z_2^2)^2 \eta^5 \Theta^{-11} \quad (33)$$

$$\sigma_1 = \sigma_0 / 12 \quad (34)$$

These results agree with those obtained within the PWBA⁶ what is quite natural since the PWBA is equivalent to the limit of a straight line path in the SCA in the calculation of the total cross section.

4. THE WEIGHT FUNCTIONS

The momentum transfer to the atom in units of \hbar is the vector \vec{q} . The minimum value of the magnitude of \vec{q} is

$$q_0 = \frac{\Theta}{2 a_2 \sqrt{\eta}} \quad (35)$$

The dominant contributions to the cross section in the adiabatic limit is by far those in the close vicinity of $W = \Theta/4$. Then, we define

$$x_0(u, \eta) = x(u, \eta, W = \frac{\Theta}{4}) = pq_0 \quad (36)$$

Normalizing the integrals

$$\int N_0 [x_0^6 K_3^2(x_0)] x_0 dx_0 = 1 \implies N_0 = \frac{7}{1152}$$

and

$$\int N_1 [x_0^6 K_2^2(x_0)] x_0 dx_0 = 1 \implies N_1 = \frac{7}{192},$$

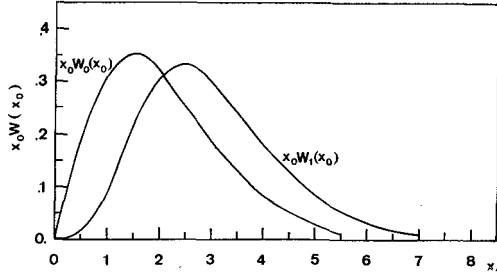


Fig. 2 - The functions $x_0 W(x_0)$ for $m=0$ and $m=\pm 1$

we can define the weight functions

$$W_0 = \frac{7}{1152} x_0^6 K_3^2(x_0) \quad (37)$$

and

$$W_1 = \frac{7}{192} x_0^6 K_2^2(x_0) \quad (38)$$

for the $m=0$ and $m=\pm 1$ substates, respectively. These weight functions are essential for calculating average values of impact parameter dependent quantities. (See Figure 2).

Since at this limit $\sigma_1 = \sigma_0/12$ it follows that, for both L_2 and L_3 -subshells,

$$\begin{aligned} W_{L_2, L_3} &= [\sigma_0/(\sigma_0+2\sigma_1)]W_0 + [2\sigma_1/(\sigma_0+2\sigma_1)]W_1 \\ &= (6/7)W_0 + (1/7)W_1 = \frac{1}{192} x_0^6 [K_2^2(x_0) + K_3^2(x_0)] \end{aligned} \quad (39)$$

which agrees with a result given by Brandt and Lapicki¹¹. Following these authors, it is convenient for numerical computations to substitute the functions (37) and (38) by fitted polynomials in the intermediate region of the argument. In the following we will adopt the approximations:

$$W_0 = \frac{7}{18} (1 + 2x_0 + 2x_0^2 + 0.8x_0^3 + 0.16x_0^4 + \frac{\pi}{128} x_0^5) e^{-2x_0} \quad (40)$$

$$W_1 = \frac{7}{48} (1 + 1.96x_0 + 1.52x_0^2 + \frac{\pi}{8} x_0^3) x_0^2 e^{-2x_0} \quad (41)$$

5. THE POLARIZATION OF THE RADIATION FOLLOWING THE CREATION OF A VACANCY IN THE L_3 -SUBSHELL.

As mentioned in the introductory section, the measurement of the polarization coefficient of the dipole radiation emitted by the atom after the ionization of the L_3 -subshell by a bare heavy projectile is the main reason of interest in the calculation of the σ_m -partial cross sections.

We suppose that all the ionizing particles are moving along the z direction. The collimated beam defines a cylindrical symmetry. If the scattered projectile or the ejected electron are not observed and if θ denotes the angle between emitted dipole X -rays and the z direction, adopted as the quantization axis of the whole system, the angular distribution of the radiation is a linear function of $\cos^2\theta$, viz.,

$$W(\theta) \propto 1 - P \cos^2\theta \quad (42)$$

where $P(j_i, j_f, E) = (I_{\parallel} - I_{\perp}) / (I_{\parallel} + I_{\perp})$ is the "degree of polarization"¹². The intensities I_{\parallel} and I_{\perp} are both measured at right angles to the z -axis and correspond to radiation with the electric vector aligned parallel or perpendicular to the quantization axis, respectively.

The polarization coefficient is related to the cross sections $\sigma_{m_i}^{j_i}$ (the m_i are the $2j_i+1$ magnetic substates corresponding to j_i) by

$$P = \frac{3 A_2}{A_2 - 2} \quad (43)$$

where, for a vacancy created in the j_i -subshell and then filled by an electron coming from a j_f -subshell,

$$A_2 = \frac{\sum_{m_i} \frac{1}{2} \left[3(j_f + 1 m_i \ 0 | j_i m_i) - 1 \right] \sigma_{m_i}^{j_i}(E)}{\sum_{m_i} \sigma_{m_i}^{j_i}(E)} \quad (44)$$

Parity invariance of the process requires that $\sigma_{-m_i}^{j_i} = \sigma_{m_i}^{j_i}$

We will consider, as an example, a vacancy produced in the $2p_{3/2}$ subshell and filled by an electron coming from the $3s_{1/2}$ subshell. The emitted radiation is called the L_R -line. For low energy bombarding protons ($E \approx 600$ keV) values of P as large as $\approx 25\%$ has been measured for gold³⁻⁵ and lead⁶. They are however considerably smaller than the predictions of the PWBA. Furthermore, the PWBA predicts a regular increase in the value of P toward the limit $P \rightarrow 33/67$ as $\eta \rightarrow 0$. When the attenuation due to Coster-Kronig transfer of unaligned vacancies produced in the L_2 - and L_1 - subshells is taken into account the value of P is reduced by an energy-dependent factor. Of course the limit $\eta \rightarrow 0$ is meaningless, but even when $\eta \rightarrow \eta_{min}$, where η_{min} corresponds to $E=I$, neither the magnitude of the experimental data nor their trend as the bombarding energy decreases are correctly described by the PWBA.

Taking into account the spin of the electron, and with an obvious notation, one can write for the ionization cross sections:

$$\sigma_{L_3}(m=\pm 3/2) = \sigma_{2p}(m=\pm 1) \quad (45a)$$

$$\sigma_{L_3}(m=\pm 1/2) = [2\sigma_{2p}(m=0) + \sigma_{2p}(m=\pm 1/2)]/3 \quad (45b)$$

Then the L_3 ionization cross section will be given by

$$\sigma_{L_3} = \sum_{m_i} \sigma_{m_i} = \frac{4}{3} (2\sigma_1 + \sigma_0) \quad (46)$$

For an initial vacancy in the L subshell eq. (44) reduces to

$$A_2 = \alpha(j_f) \frac{\sigma_1(E) - \sigma_0(E)}{2\sigma_1(E) + \sigma_0(E)} \alpha(j_f) A_2(E) \quad (47)$$

Normally the quantity that is compared with the theoretical calculations is the anisotropy coefficient $A_2(E)$ since it is the same for all transitions filling a given initial vacancy. For the particular transition L_β we have $\alpha(s1/2) = 1/2$. For the more intense complex line L_α we have $\alpha(d5/2) = 1/10$ and $\alpha(d3/2) = -2/5$, for the L_{α_1} and L_{α_2} components, respectively.

In the low energy region of the PWBA, A_2 is an universal func-

tion of the adimensional parameter η/θ^2 . Taking into account the attenuation introduced by the Coster Kronig transfer of unaligned vacancies oriedefines

$$A'_2 = F(E, Z_2) A_2(E) \quad (48)$$

with

$$F^{-1} = 1 + f_{23} \frac{\sigma_{L_2}}{\sigma_{L_3}} + (f_{13} + f_{12} f_{23}) \frac{\sigma_{L_1}}{\sigma_{L_3}} \quad (49)$$

where the f_{ij} are the Coster-Kronig transition probabilities. For gold and lead the attenuation factor F is well determined experimentally⁶. In the Figure 3 the measured values of A'_2 are compared with the results obtained with equation (48) calculated with the experimental values of F and the PWBA results for A_2 (dashed line). Curves for $Z_2 = 79$ and $Z_2 = 82$ are equal within 2% in the range of energy considered

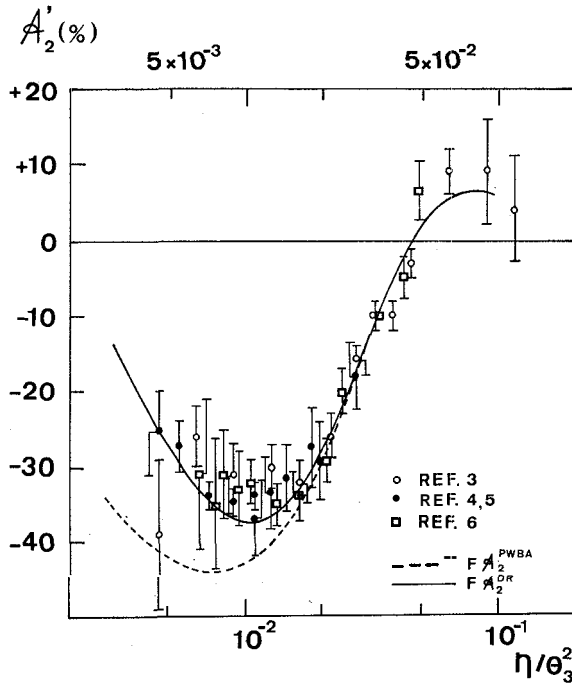


Fig. 3 - The experimental values of the anisotropy coefficient A'_2 for Ar and Pb plotted against the dimensionless parameter η/θ_3^2 . Curves are predictions of the PWBA (----) and of the PWBA corrected for the deflection and the retardation of the projectile as described in the text (—). Both curves take into account the attenuation due to Coster-Kronig transfers of vacancies.

A considerable improvement in the description of the experimental data is attained by incorporating into the theory an *ad hoc* correction due to the Coulomb repulsion of the impinging particle by the target nucleus. This correction will be treated in the frame of the impact parameter description introduced for the magnetic substates. The repulsion by the Coulomb field leads to a deflection from the straight line trajectory and to a retardation of the projectile. For a given incident energy, E , there exist an infinite family of classical trajectories each one characterized by its own impact parameter. The ionization can occur at any point of the classical trajectory. Therefore a double average must be performed. Firstly an average over each trajectory in order to define the most probable direction and magnitude of the velocity vector $\vec{v}(p)$ and secondly an average over p taking into account the weight functions.

The angle of observation of the emitted radiation with respect to the velocity direction is

$$\cos \theta' = \cos \theta \cos \alpha + \sin \theta \sin \alpha \cos \beta$$

where β is the angle between the plane of the trajectory of the scattered projectile and the direction of observation (azimuthal angle) and α is the polar angle of \vec{v} . Since the emerging particles are not observed the cylindrical symmetry is preserved and the average over β is trivial. From symmetry considerations it is evident that the relevant polar angle is $\alpha = \psi/2$, the average value of α along the hyperbolic trajectory. Therefore the "rotation" of the radiation pattern characteristic of the dipole transitions associated with the filling of the $m=0$ and $|m|=1$ initial vacancies will be differently affected because ψ depends on x , and the \bar{W}_m functions are not the same for the two magnetic substates. It has been stressed along this paper that the main contributions to the cross section come from values of W near $\theta/4$, therefore the following approximation is adopted:

$$d\sigma_m/dx_0 \approx \sigma_m x_0 \bar{W}_m(x_0)$$

where σ_m is the PWBA cross sections. It results that the anisotropy coefficient corrected for the deflection effect is expressed by

$$A_2^D = \frac{\sigma_1 \langle P_2(\cos(\psi/2)) \rangle_1 - \sigma_0 \langle P_2(\cos(\psi/2)) \rangle_0}{2 \sigma_1 + \sigma_0} \quad (50)$$

where P_2 is the second Legendre polynomial and the average values correspond to:

$$\langle P_2(\cos(\psi/2)) \rangle_m = \int_0^\infty P_2(\cos(\psi/2)) x_0 W_m(x_0) dx_0 \quad (51)$$

where $\psi/2 = \cot^{-1}(x_0/dq_0)$.

The retardation effect is considered in a similar way. We begin by choosing an average value for the magnitude of \vec{v} along the trajectory. Following Kocbach¹³ the best choice is the arithmetic mean between the asymptotic velocity v and the velocity at the vertex of the hyperbola. Being ϵ the eccentricity of the hyperbola,

$$\bar{v}(p) = (v/2) [1 + \sqrt{(\epsilon-1)/(\epsilon+1)}] \quad (52)$$

where $\epsilon = \sqrt{1 + (x_0/dq_0)^2}$

We now average $\bar{v}(p)$ with the convenient weight functions obtaining $\langle \bar{v} \rangle_n$ and $\langle \bar{v} \rangle_1$. Since η is proportional to the square of the projectile velocity we define $\eta_m = (\langle \bar{v} \rangle_m / 2v_2)^2$ and calculate the RWBA cross sections with this "effective" value of the reduced energy. The resulting partial cross sections will be denoted by σ_m^* .

The final value for the anisotropy coefficient with both deflection and retardation effects included is

$$A_2^{DR} = \frac{\sigma_1^* \langle P_2(\cos(\psi/2)) \rangle_1 - \sigma_0^* \langle P_2(\cos(\psi/2)) \rangle_0}{2 \sigma_1^* + \sigma_0^*} \quad (53)$$

This theoretical value of the anisotropy coefficient must replace $A(E)$ in the equation (48).

In Figure 3 the solid line represents the function FA_2^{DR} . The improvement in the description of the experimental results is outstanding. As mentioned before curves for $Z=79$ and $Z=82$ are not distinguishable.

If the scattered projectile is observed, in an angular correlation p^1-X experiment, the average over the impact parameter will be avoided. On the other hand, with a fixed azimuthal angle there will be no axis of symmetry. Much more information concerning the ionization mechanism can be learned.

6. CONCLUSIONS

A complete description of differential and integral ionization cross sections for the magnetic substates of the $2p$ -shell in the adiabatic limit was obtained in the frame of a semiclassical picture. The formulation in terms of the impact parameter allows the introduction of corrections due to the repulsion of a bare heavy ion by the Coulomb field of the target nucleus in the basic PWBA formulation. These corrections are essential to describe the anisotropy of the dipole radiation emitted after the production of a vacancy in the L subshell by a collimated beam.

This work was financed by grants from the CNPq and FINEP.

APPENDIX

This appendix is intended to put together some mathematical formulae involving the modified Bessel functions of order n , $K_n(x)$, in order to make easier to the reader to obtain the ionization probabilities given by equations (21) and (22).

Let^{14,15}

$$\int_0^m \frac{\exp[-\beta(\gamma^2+x^2)^{1/2}]}{(\gamma^2+x^2)^{1/2}} x \sin ax \, dx = \alpha \gamma \frac{K_1[\gamma(\alpha^2+\beta^2)^{1/2}]}{(\alpha^2+\beta^2)^{1/2}}, \quad (\text{A.1})$$

$$\int_0^{\infty} \frac{\exp[-\beta(\gamma^2+x^2)^{1/2}]}{(\gamma^2+x^2)^{1/2}} \cos ax \, dx = K_0[\gamma(\alpha^2+\beta^2)^{1/2}] \quad , \quad (\text{A.2})$$

$$\int_0^{\infty} \frac{x \sin ax}{(\gamma^2+x^2)^{3/2}} \, dx = a K_0(\gamma a) \quad , \quad (\text{A.3})$$

and

$$\int_0^{\infty} \frac{\cos ax}{(\gamma^2+x^2)^{3/2}} \, dx = \frac{a}{\gamma} K_1(\gamma a) \quad . \quad (\text{A.4})$$

On the other hand

$$\frac{d}{dz} [z^n K_n(z)] = -z^n K_{n-1}(z) \quad (\text{A.5})$$

$$\frac{d}{dz} [z^{-n} K_n(z)] = -z^{-n} K_{n+1}(z) \quad (\text{A.6})$$

Taking the derivatives of both sides of equations (A.1) and (A.2) with respect to y we find

$$\begin{aligned} & \beta \int_0^{\infty} \frac{\exp[-\beta(\gamma^2+x^2)^{1/2}]}{(\gamma^2+a^2)} x \sin ax \, dx + \int_0^{\infty} \frac{\exp[-\beta(\gamma^2+x^2)^{1/2}]}{(\gamma^2+a^2)^{3/2}} x \sin ax \, dx = \\ & = a K_0[\gamma(\alpha^2+\beta^2)^{1/2}] \end{aligned} \quad (\text{A.7})$$

and

$$\begin{aligned} & \beta \int_0^{\infty} \frac{\exp[-\beta(\gamma^2+x^2)^{1/2}]}{(\gamma^2+a^2)} \cos ax \, dx + \int_0^{\infty} \frac{\exp[-\beta(\gamma^2+x^2)^{1/2}]}{(\gamma^2+a^2)^{3/2}} \cos ax \, dx = \\ & = \frac{(\alpha^2+\beta^2)^{1/2}}{\gamma} K_1[\gamma(\alpha^2+\beta^2)^{1/2}] \end{aligned} \quad (\text{A.8})$$

Now we take the first and the second derivatives of the same equations with respect to β and find

$$\int_0^{\infty} \exp[-\beta(\gamma^2+x^2)^{1/2}] x \sin ax \, dx = a\beta\gamma^2 \frac{K_2[\gamma(\alpha^2+\beta^2)^{1/2}]}{\alpha^2+\beta^2}, \quad (\text{A.9})$$

$$\int_0^{\infty} \exp[-\beta(\gamma^2+x^2)^{1/2}] \cos ax \, dx = \beta\gamma \frac{K_1[\gamma(\alpha^2+\beta^2)^{1/2}]}{(\alpha^2+\beta^2)^{1/2}}, \quad (\text{A.10})$$

$$\begin{aligned} \int_{-\infty}^{\infty} (\gamma^2+x^2)^{1/2} \exp[-\beta(\gamma^2+x^2)^{1/2}] x \sin ax \, dx &= -a\gamma^2 \frac{K_2[\gamma(\alpha^2+\beta^2)^{1/2}]}{(\alpha^2+\beta^2)} \\ + \frac{a\beta^2\gamma^2 K_3[\gamma(\alpha^2+\beta^2)^{1/2}]}{(\alpha^2+\beta^2)^{3/2}} \end{aligned} \quad (\text{A.11})$$

and

$$\begin{aligned} \int_0^{\infty} (\gamma^2+x^2)^{1/2} \exp[-\beta(\gamma^2+x^2)^{1/2}] \cos ax \, dx &= -\gamma \frac{K_1[\gamma(\alpha^2+\beta^2)^{1/2}]}{(\alpha^2+\beta^2)^{1/2}} + \\ + \frac{\beta^2\gamma^2 K_2[\gamma(\alpha^2+\beta^2)^{1/2}]}{(\alpha^2+\beta^2)} \end{aligned} \quad (\text{A.12})$$

In the equations (19) and (20) we have integrals of the following type

$$\int_0^{\infty} f(R) \frac{z \sin az}{(p^2+z^2)^{1/2}} \, dz \quad \text{and} \quad \int_0^{\infty} f(R) \frac{\cos az}{(p^2+z^2)^{1/2}} \, dz$$

where $R = (p^2+z^2)^{1/2}$ and $f(R)$ stands for a function of the type R^n or $R^n \exp(-bR/2)$. These integrals can be evaluated with the help of the above results.

Furthermore use was made of the integral representation of the modified Bessel functions:

$$\begin{aligned}
 K_n(z) &= \frac{1}{(2z)^n} \int_0^{\infty} \exp \left[-\left(z^2 x^2 + \frac{1}{4x^2} \right) \right] \frac{dx}{x^{2n+1}} = \\
 &= (2z)^n \int_0^{\infty} \exp \left[-\left(z^2 x^2 + \frac{1}{4x^2} \right) \right] x^{2n-1} dx = K_{-n}(z)
 \end{aligned} \tag{A.13}$$

to write

$$K_0(pa) = \sum_{n=0}^{\infty} \left(\frac{pb}{2} \right)^{2n} \frac{K_n [p(b^2/4 + a^2)^{1/2}]}{n! [2p(b^2/4 + a^2)^{1/2}]^n}$$

and

$$K_1(pa) = \frac{1}{2pa} \sum_{n=0}^{\infty} \left(\frac{pb}{2} \right)^{2n} \frac{K_{n-1} [p(b^2/4 + a^2)^{1/2}]}{n! [2p(b^2/4 + a^2)^{1/2}]^{n-1}}$$

REFERENCES

1. W. Mehlhorn, Phys. Lett. 26A, 166 (1968).
2. E.G. Berezko and N.M. Kabachnik, J. Phys. B: Atom. Molec. Phys. 10, 2467 (1977).
3. W. Jitschin, H. Kleinpoppen, R. Hippler and H.O. Lutz, J. Phys. B.: Atom. Molec. Phys. 12, 4077 (1979).
4. J. Pálinkás, L. Sarkadi and B. Schlenk, J. Phys. B: Atom. Molec. Phys. 13, 3829 (1980).
5. J. Pálinkás, B. Schlenk and A. Valek, J. Phys. B: Atom. Molec. Phys. 14, 1157 (1981).
6. C.V. Barros Leite, N.V. de Castro Faria, R.J. Horowicz, E.C. Montenegro and A.G. de Pinho (to be published in Phys. Rev. A).
7. S.C. McFarlane, J. Phys. B: Atom. Molec. Phys. 5, 1906 (1972).
8. M. Kamiya, Y. Kinefuchi, H. Endo, A. Kuwako, K. Ishii, and S. Morita, Phys. Rev. A 20, 1820 (1979).

9. W.Jitschin, H.O.Lutz and K.Kleinpoppen, International Conference on X-ray processes and inner shell ionization, (Glasgow), Abstract n? 32, (1980).
10. D.Madison and E.Merzbacher, in *Atomic Inner-Shell Processes*, ed. by B. Crasemann (New York, Academic Press), (1975).
11. W. Brandt and G. Lapicki, Phys. Rev. A20, 465 (1979) (foot note n? 36).
12. N.F.Mott and H.S.Massey, *Theory of Atomic Collisions*. (London, Oxford University Press), 3rd edition (1965).
13. L. Kocbach, Physica Norvegica 8, 187 (1976).
14. I.S. Gradshteyn and I.M. Ryzhik. *Table of integrals, series and products* (New York, Academic Press) (1965).
15. *Handbook of Mathematical Functions*, ed. by M. Abramowitz and I. A. Stegun (New York, Dover Publications) (1970).