

RELATIVISTIC ATOMIC PHOTOEFFECT FROM THE K-SHELL NEAR THRESHOLD

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With the aid of a formalism developed by Pratt et al.^[5], analytic expressions are obtained for the total and differential cross sections of the photoeffect from the K-shell of the atom and for seven non-zero polarization correlations between the incident photons and the outgoing electron at a photon energy close to the K-shell ionization energy. The matrix element is calculated with exact relativistic functions. Terms proportional to $\alpha^6 Z^6$ are discarded from the expression for the total cross section, and terms of the order of $\alpha^5 Z^5$ are discarded from the angular distribution. The correlations were calculated with a relative accuracy on the order of $\alpha^2 Z^2$. The results are applicable at photon energies $k - I_b < m\alpha^4 Z^4 / 2$ (k —photon energy, I_b —binding energy of the K electron). Screening is disregarded.

1. INTRODUCTION

THE relative photoeffect from the K shell at threshold (incident-photon energy close to the K-shell ionization energy) was investigated by Nagel and Olsson^[1], who obtained relativistic corrections of order $\alpha^2 Z^2$ and calculated numerically the total cross section, the angular distribution, and the polarization of the photoelectrons for $Z = 92$. The entire analysis was made in the Coulomb field of the nucleus for the limiting case $p = 0$ (p —momentum of the outgoing electron). Allowance for the relativistic effects leads to a decrease of the cross section by 21% (for uranium), to non-zero cross sections for scattering forward ($\theta = 0$) and backward ($\theta = \pi$; θ —angle between the direction of emission of the electron and the photon propagation direction), and to the appearance of polarization of the photoelectrons. Three numerical calculations for the Coulomb potential, pertaining to the threshold energy region, are given in^[3]. Calculations with different models of the screened potential near threshold are scanty and were made only for the total cross section^[3,4].

In the present paper we use a general formalism developed by Pratt et al.^[5] to obtain analytic expressions for the total cross section of the photoeffect from the K shell in the Coulomb field of the nucleus, the angular distribution of the photoelectrons, and all the non-zero polarization correlations between the incident photon and the outgoing electron at photon energies close to the K-electron binding energy. In this case the natural parameters of the expansions are αZ , k/η , and p/η . Here η —average value of the K-electron momentum ($\eta = m\alpha Z$, m —electron mass), k —photon momentum ($k - I_b < m\alpha^2 Z^2 / 2$; I_b —K-electron binding energy), and p —momentum of the free electron ($p \rightarrow 0$ when $K \rightarrow I_b$). The formulas obtained for the total and differential cross sections are suitable for elements with large Z . The screening effects are disregarded. For the photon energies under consideration ($k - I_b, c < m\alpha^4 Z^4 / 2$, where $I_{b,c}$ is the binding energy of the K electron in the Coulomb field of the nucleus) the difference between the total cross sections for the

Coulomb and screened fields is approximately 3% (the cross sections are compared at identical photon energies; the photoelectron energies are then different, owing to the difference between the binding energies of the K electron for the Coulomb and screened potentials).

The angular distributions and polarizations of the photoelectrons are compared only with the data of the numerical Coulomb calculation^[3,4] for $Z = 92$, in view of the lack of similar calculations for screened fields.

2. GENERAL FORMALISM

In this section we follow^[5]. The differential cross section for the photoeffect is

$$\frac{d\sigma}{d\Omega} = \frac{apE}{2\pi k} \left| \int \psi_f^* \alpha e^{ikr} \psi_i d^3r \right|^2 \tag{1}$$

Here $\hbar = c = 1$, $\alpha = 1/137$; p, E —momentum and energy of the outgoing electron; $k, \mathbf{k}, \mathbf{e}$ —energy, momentum, and polarization vector of the photon; E and k are connected by the energy conservation law:

$$E = k + m\gamma, \tag{1a}$$

where $m\gamma = m\sqrt{1 - \alpha^2 Z^2}$ —energy of bound K electrons; α —Dirac matrix; ψ_i and ψ_f —wave functions of the bound and free electrons:

$$\psi_i = \begin{pmatrix} G(r) \Omega_{JLM}(r/r) \\ iP(r) \Omega_{J'L'M}(r/r) \end{pmatrix} \tag{2}$$

For the K shell, $J = 1/2$, $L = 0$, $L' = 1$, and $M = \pm 1/2$. The radial functions G and F are normalized by the condition

$$\int_0^\infty (G^2 + F^2) r^2 dr = 1 \tag{3}$$

and are given by

$$G = N_i e^{-\gamma r} (2\eta r)^{\gamma-1}, \quad F = -\alpha Z (1 + \gamma)^{-1} G; \tag{4}$$

$$\eta = m\alpha Z, \quad \gamma = (1 - \alpha^2 Z^2)^{1/2}, \quad N_i = [\eta^3 (1 + \gamma) / \Gamma(1 + 2\gamma)]^{1/2}. \tag{4a}$$

The wave function of the outgoing electron ψ_f , in a suitable asymptotic form (plane wave plus a converging spherical wave), will be represented by an expansion in partial waves:

$$\Psi_f = 4\pi \sum_{jlm} \left(\Omega_{jlm}^+ \left(\frac{\mathbf{p}}{p} \right) w \right) l' e^{-i\delta_\kappa} \left(\frac{g_\kappa(r) \Omega_{jlm}(r/r)}{i f_\kappa(r) \Omega_{jlm}(r/r)} \right). \quad (5)$$

Here

$$\begin{aligned} \delta_\kappa &= 1/2\pi(l - \gamma_\kappa) - \arg \Gamma(\gamma_\kappa + i\nu) + \eta_\kappa + \pi/2, \\ e^{2i\eta_\kappa} &= -\frac{\gamma_\kappa - i\nu}{\kappa + i\nu'} = -\frac{\kappa - i\nu'}{\gamma_\kappa + i\nu}, \\ \nu &= \frac{\alpha Z E}{p}, \quad \nu' = \frac{\alpha Z m}{n}, \quad \gamma_\kappa = \sqrt{\nu^2 - \alpha^2 Z^2}, \\ \kappa &= \pm(j + 1/2) \quad \text{when } j = l \mp 1/2, \quad l' = 2j - l; \end{aligned} \quad (6)$$

w -normalized spinor ($w^*w = 1$) defining the polarization of the photoelectron in its rest system. The radial functions g_κ and f_κ behave asymptotically like

$$\begin{aligned} g_\kappa &\approx \sqrt{\frac{E+m}{2E}} \frac{1}{pr} \sin\left(pr - \frac{l\pi}{2} + \delta_\kappa + \nu \ln 2pr\right), \\ f_\kappa &\approx \sqrt{\frac{E-m}{2E}} \frac{1}{pr} \cos\left(pr - \frac{l\pi}{2} + \delta_\kappa + \nu \ln 2pr\right), \end{aligned} \quad (7)$$

and are given by

$$\begin{aligned} g_\kappa &= N_\kappa (2pr)^{\gamma_\kappa - 1} \{ \}_+, \quad f_\kappa = \frac{i\mathbf{p}}{E+m} N_\kappa (2pr)^{\gamma_\kappa - 1} \{ \}_-, \\ N_\kappa &= \sqrt{\frac{E+m}{2E}} e^{\nu\pi/2} \frac{|\Gamma(\gamma_\kappa + i\nu)|}{\Gamma(1 + 2\gamma_\kappa)}, \end{aligned} \quad (8)$$

$$\{ \}_\pm = \{ e^{-i\pi r + i\eta_\kappa} (\gamma_\kappa + i\nu) {}_1F_1(\gamma_\kappa + 1 + i\nu; 1 + 2\gamma_\kappa; 2ipr) \pm \text{c.c.} \}.$$

The photon polarization vector \mathbf{e} will be resolved along the unit vectors \mathbf{e}_1 and \mathbf{e}_2 :

$$\mathbf{e} = e_1 \mathbf{e}_1 + e_2 \mathbf{e}_2, \quad |e_1|^2 + |e_2|^2 = 1; \quad (9)$$

\mathbf{e}_1 lies in the scattering plane (plane containing the photon and electron momenta \mathbf{k} and \mathbf{p}), and \mathbf{e}_2 is perpendicular to this plane (along $\mathbf{k} \times \mathbf{p}$). The triad of orthogonal vectors \mathbf{e}_1 , and \mathbf{e}_2 , and \mathbf{k} form a right-hand system.

If we substitute (2), (5), and (9) in (1) and direct the z axis along the photon momentum \mathbf{k} , then the integration along the angle variables can be readily performed. In place of the bilinear expressions in \mathbf{e}_1 and \mathbf{e}_2 , which arise in (1), we introduce the quantities (the Stokes parameters)

$$\begin{aligned} \xi_1 &= |e_1|^2 - |e_2|^2, \quad \xi_2 = e_1 e_2^* + e_2 e_1^*, \\ \xi_3 &= i(e_1 e_2^* - e_2 e_1^*). \end{aligned} \quad (10)$$

Then the probability of electron emission with a spin directed in its rest system along $\boldsymbol{\zeta}$, averaged over the polarization of the initial state, is of the form

$$\frac{d\sigma}{d\Omega}(\boldsymbol{\zeta}) = \frac{1}{2} A \sum_{i,j=0}^3 \xi_i \xi_j B_{ij}, \quad (11)$$

$$\xi_0 = \zeta_0 = 1, \quad A = 16\pi\alpha p E / k, \quad (12)$$

where $\xi_1 - \xi_3$ are defined in (10). The three orthogonal unit vectors $\mathbf{e}_2 \times \mathbf{p}/p$, \mathbf{e}_2 , and \mathbf{p}/p form a right-hand coordinate system, in which the projections of the unit vector $\boldsymbol{\zeta}$ are defined:*

$$\zeta_1 = \boldsymbol{\zeta}[\mathbf{e}_2 \times \mathbf{p} / p], \quad \zeta_2 = \boldsymbol{\zeta} \mathbf{e}_2, \quad \zeta_3 = \boldsymbol{\zeta} \mathbf{p} / p.$$

The non-vanishing B_{ij} ($B_{00}, B_{02}, B_{10}, B_{21}, B_{23}, B_{31}$, and B_{33}) are given in [5] (formula (2.25)) and we shall not write out here general expressions for them.

If the photon is linearly polarized, so that^[6] $\mathbf{e} = \mathbf{e}_1 \cos \Phi + \mathbf{e}_2 \sin \Phi$ (Φ -angle between the photon polarization plane and the scattering plane), then $\xi_1 = \cos 2\Phi$, $\xi_2 = -\sin 2\Phi$, and $\xi_3 = 0$. For photons with right-and or left-hand circular polarization $\mathbf{e}_1 = (\mathbf{e}_1 \pm i\mathbf{e}_2)/\sqrt{2}$ and $\xi_1 = \xi_2 = 0$, $\xi_3 = \pm 1$. For unpolarized photons $\xi_1 = \xi_2 = \xi_3 = 0$.

The differential cross section for unpolarized photons, summed over the spins of the outgoing electron, is

$$\left(\frac{d\sigma}{d\Omega} \right)_{\text{unp}} = \frac{d\sigma}{d\Omega}(\boldsymbol{\zeta}) + \frac{d\sigma}{d\Omega}(-\boldsymbol{\zeta}) = AB_{00}, \quad (13)$$

and (11) can be written in a different form:

$$\frac{d\sigma}{d\Omega} = \left(\frac{d\sigma}{d\Omega} \right)_{\text{unp}} \frac{1}{2} \sum_{i,j=0}^3 \xi_i \xi_j C_{ij}, \quad (14)$$

where the polarization correlations C_{ij} are given by

$$C_{ij} = B_{ij} / B_{00}; \quad (15)$$

C_{ij} determines the degree of polarization of the photoelectrons along the ζ_j direction if the state of the photon polarization is described by the Stokes parameter ξ_i .

The total cross section is obtained by integrating (13) over the electron emission angles:

$$\sigma = 2\pi A \int_0^\pi B_{00} \sin \theta d\theta = A \int_{\mathbf{x}} [|R_\kappa^+|^2 + |R_\kappa^-|^2]. \quad (16)$$

The sum is taken over the integer positive and negative κ , $\kappa \neq 0$. The functions R_κ^\pm for positive κ ($\kappa = l$) and negative κ ($\kappa = -l - 1$) are the following radial integrals:

$$\begin{aligned} R_{l^+} &= -\frac{\sqrt{l(l-1)}}{2l+1} \int_0^\infty r^2 dr F g_l (j_{l-1} + j_{l+1}), \\ R_{-l-1}^+ &= \frac{\sqrt{l(l+1)(l+2)}}{2l+1} \int_0^\infty r^2 dr F g_{-l-1} (j_{l-1} + j_{l+1}), \end{aligned} \quad (17)$$

$$R_{l^-} = \frac{\sqrt{l}}{2l+1} \int_0^\infty r^2 dr \{ F g_l [-l j_{l-1} + (l+1) j_{l+1}] - (2l+1) C j_{l-1} \},$$

$$R_{-l-1}^- = \frac{\sqrt{l+1}}{2l+1} \int_0^\infty r^2 dr \{ F g_{-l-1} [-l j_{l-1} + (l+1) j_{l+1}] + (2l+1) G f_{-l-1} j_{l+1} \}.$$

Here $j_l \equiv j_l(kr)$ is the spherical Bessel function that results from the expansion of the exponential factor $\exp(i\mathbf{k} \cdot \mathbf{r})$ in (1) in spherical functions.

If all the R_κ^\pm are calculated, then the problem of finding the cross section, the angular distribution, and all the correlations is solved (the B_{ij} represent infinite sums of bilinear expressions made up of $\exp(i\delta_\kappa) R_\kappa^\pm$, where the phase shifts are defined in (6)). In the next section we shall calculate R_κ^\pm and the total cross section of the photoeffect.

3. CALCULATION OF THE RADIAL INTEGRALS AND OF THE TOTAL CROSS SECTION

Equation (17) contains two types of integrals: of the product of the functions $G f_\kappa j_L$, and of the product $F g_\kappa j_L$. Using (4), (8), and the definition of the spherical Bessel functions

$$j_l(kr) = \sqrt{\frac{\pi}{2kr}} J_{l+1/2}(kr) = \Gamma\left(\frac{3}{2}\right) \sum_{n=0}^{\infty} \frac{(-1)^n (kr/2)^{l+2n}}{n! \Gamma(n+l+3/2)}, \quad (18)$$

* $[\mathbf{e}_2 \times \mathbf{p}/p] \equiv \mathbf{e}_2 \times \mathbf{p}/p$.

we obtain for these integrals

$$\int_0^{\infty} G_{f_{\kappa} j l} r^2 dr = N \frac{m}{E+m} \frac{i}{\nu'} [(-\kappa + i\nu') H_{\kappa l} - (\gamma_{\kappa} - i\nu) H_{\kappa l}^*],$$

$$\int_0^{\infty} F_{g_{\kappa} j l} r^2 dr = -\frac{N}{1+\gamma} [(-\kappa + i\nu') H_{\kappa l} + (\gamma_{\kappa} - i\nu) H_{\kappa l}^*],$$
(19)

where

$$N = e^{-i\eta_{\kappa}} \Gamma(1 + 2\gamma_{\kappa}) N_{\kappa} N_i \frac{\alpha Z}{2\eta^3} \nu^{-\nu_{\kappa}+1},$$
(20)

and η_{κ} , γ_{κ} , ν , and ν' are defined in (6), while γ and η are defined in (4a). The asterisk denotes the complex conjugate. Further,

$$H_{\kappa l} = \left(\frac{E}{m}\right)^{\nu_{\kappa}-1} \frac{2^{\nu_{\kappa}} \Gamma(3/2)}{\Gamma(1+2\gamma_{\kappa})} \sum_{n=0}^{\infty} \frac{(-1)^n \Gamma(c_n)}{n! \Gamma(n+l+3/2)} \left(\frac{k}{2\eta}\right)^{l+2n}$$

$$\times (1+i\mu)^{-c_n} F_1(1+\gamma_{\kappa}+i\nu, c_n; 1+2\gamma_{\kappa}; 2i\mu/(1+i\mu)),$$
(21)

$$c_n = 1 + \gamma + \gamma_{\kappa} + l + 2n, \quad \mu = p/\eta.$$
(22)

When considering small momenta of the outgoing electron (in the limit as $p \rightarrow 0$, i.e., $\nu, \nu' \rightarrow \infty$), it is convenient to expand (19)–(21) in terms of p . Using the asymptotic expansion for the Γ function contained in N_{κ} :

$$|\Gamma(\gamma_{\kappa} + i\nu)| = \sqrt{2\pi} \nu e^{-\pi\nu/2} \nu_{\kappa}^{-1} \left\{ 1 + \nu^{-2} \frac{\gamma_{\kappa}}{12} [1 + \gamma_{\kappa}(2\gamma_{\kappa} - 3)] + O(\nu^{-4}) \right\},$$
(23)

and (6) and (8), we find that when $p \rightarrow 0$ we get

$$N \sim O(\nu^{1/2})$$
(20a)

for all κ . The expansion of $H_{\kappa l}$ in terms of p begins with terms $O(1)$ for all κ and l .

In the same limit ($p \rightarrow 0$), the photon momentum approaches $k \rightarrow I_b = m(1-\gamma) \approx m\alpha^2 Z^2/2$, and $k/\eta \rightarrow \alpha Z/2$. Then

$$H_{\kappa l} \sim (k/\eta)^l \approx (\alpha Z/2)^l,$$

and we get for R_{κ}^{\pm} (see (17))

$$R_{\kappa>0, \kappa<0}^{\pm} = R_{l(-l-1)}^{\pm} \sim (k/\eta)^{l-1} \approx (\alpha Z/2)^{l-1} \quad (\kappa \neq 0).$$
(24)

In order to calculate the differential cross section accurate to $\alpha^4 Z^4$, it is necessary to calculate all the R_{κ}^{\pm} up to $l = 5$, i.e., from R_6^{\pm} to R_1^{\pm} (altogether 20; R_0 corresponds to $R_1^+ = R_{-1}^+ = 0$, see (17)). In order to calculate the total cross section with the same accuracy, it will be convenient to have a smaller number of partial waves, up to $l = 3$ (from R_4^{\pm} to R_3^{\pm} , a total of 12), since the sum (16) contains only the squares of R_{κ}^{\pm} .

$H_{\kappa l}$ depends also on the parameter $\alpha^2 Z^2$, which enters in γ_{κ} . Expansion in terms of this parameter will be carried out up to terms of order $\alpha^4 Z^4$.

How far beyond threshold can we advance in such a calculation method? It is seen from (24) that when $k - I_b < I_b$ (i.e., $k < m\alpha^2 Z^2$) one can still guarantee an accuracy up to $\alpha^4 Z^4$. But the expansion in powers of p narrows this region greatly, since in the case of (21) and (23) it is valid when $\nu \gg \gamma_{\kappa}$ (6). When calculating the total cross section, we shall consider energies such that $u = p/\eta < \alpha Z$, and retain as many terms in the expansion in μ as are needed to retain the previous accuracy to $\alpha^4 Z^4$. This limits the range of

variation of k to the inequality

$$k - I_b < m\alpha^4 Z^4/2$$
(25)

(for uranium this is approximately 50 keV above threshold). In calculating the angular distribution we shall consider a still narrower energy region ($\mu < \alpha^2 Z^2$), since it is necessary to take higher κ into account here. With these limitations, we get

$$e^{i\eta_{\kappa}} \int_0^{\infty} G_{f_{\kappa} j l} r^2 dr = -M(1 + a_{\kappa})$$

$$\times \left[\left(1 + \frac{p^2}{8m^2}\right) \text{Re } H_{\kappa l} + \frac{i\mu}{2} (\kappa H_{\kappa l} + \gamma_{\kappa} H_{\kappa l}^*) \right],$$

$$e^{i\eta_{\kappa}} \int_0^{\infty} F_{g_{\kappa} j l} r^2 dr = -\frac{2M}{1+\gamma} (1 + a_{\kappa}) \left[\frac{1}{2} (-\kappa H_{\kappa l} + \gamma_{\kappa} H_{\kappa l}^*) - \frac{1}{\mu} \left(1 + \frac{p^2}{8m^2}\right) \text{Im } H_{\kappa l} - \frac{i\alpha Z p}{4m} H_{\kappa l}^* \right];$$
(26)

Here

$$a_{\kappa} = \mu^2 \frac{\gamma_{\kappa}}{12} [1 + \gamma_{\kappa}(2\gamma_{\kappa} - 3)] + O(\mu^4), \quad M = \frac{2^{\nu-1}}{m} \left[\frac{2\pi(1+\gamma)}{p\Gamma(1+2\gamma)} \right]^{1/2}.$$
(27)

The expansion of $H_{\kappa l}$ (21) is in terms of $k/\eta = a/2 + a^3/8 + a\mu^2/2 + O(a^5)$, $\mu = p/\eta$, and $a = \alpha Z$. The main difficulty lies in the expansion of the hypergeometric function contained in $H_{\kappa l}$ in powers of p , since one of its parameters is of the order of $1/p$. This expansion is best carried out by using the integral representation for the hypergeometric function. After long and laborious calculations, which we shall omit here, we obtain for the total cross section of the photoeffect from the K shell the following sample expression¹⁾

$$\sigma = \sigma_0 \{ Q(\mu) - 0.393a^2 - 0.144a^4 + 1.023\mu^2 a^2 + O(a^6) \},$$
(28)

where

$$\sigma_0 = \frac{2^9 \pi^2 a e^{-4}}{3mk} = \frac{335.8}{m/k} \text{ [b]}$$
(28a)

(k should be specified in units of the electron mass),

$$Q(\mu) = \frac{1}{(1+\mu^2)^3} \exp \left[4 \left(1 - \frac{\arctg \mu}{\mu} \right) \right] = 1 - \frac{5}{3} \mu^2 + \frac{94}{45} \mu^4 + O(\mu^6),$$
(28b)

$$a = \alpha Z, \quad \mu = p/\eta, \quad \eta = m\alpha Z;$$
(28c)

μ is determined from the energy conservation law.

$$E = \sqrt{m^2 + p^2} = k + m\gamma$$

$$(\gamma = \sqrt{1 - \alpha^2 Z^2}).$$

When $p = 0$, the last term in the curly brackets of (28) vanishes, and the first equals unity. In this limit we get for uranium

$$\sigma = 0.793\sigma_0.$$

¹⁾Nagel and Olsson give [1] for the total cross section the formula $\sigma = \sigma_0(1 - 0.36 a^2)$ (in the limit where $p = 0$).

Table I

| Z | k, keV | σ | |
|----|--------|-----------|----------|
| | | from (28) | from [2] |
| 82 | 102 | 1420 | 921 |
| | 120 | 921 | |
| 92 | 132 | 1030 | 1026 |
| | 140 | 882 | 887 |

Table II

| Z | k, keV | σ | | |
|----|--------|-----------|----------|----------|
| | | from (28) | from [1] | from [2] |
| 50 | 35,3 | 4600 | 3160 | 3168 |
| | 40 | 3260 | | |
| 60 | 52,1 | 3030 | 2040 | |
| | 60 | 2080 | | |
| 74 | 81 | 1840 | 1370 | 1804 |
| | 90 | 1400 | | |
| 82 | 102 | 1420 | 812 | |
| | 125 | 834 | | |
| 92 | 132 | 1030 | 731 | 725 |
| | 150 | 738 | | |
| | 175 | 532 | | |

The exact numerical calculation by Nagel and Olsson^[1] yields for this case

$$\sigma = 0.789\sigma_0.$$

The difference is only 0.5%. With increasing distance from the threshold, the error in (28) increases.

Comparison of the total cross sections calculated from (28) with the numerical Coulomb calculations of Hultberg, Nagel, and Olsson^[3] (there are only three such calculations) is shown in Table I, and comparison with the numerical calculations in screened fields, by Schmickley and Pratt^[4] and by Racavy and Ron^[3] is given in Table II. For each element, the first number in the table is the cross section at the Coulomb threshold. As seen from these tables, the difference between the cross sections does not exceed 1% in the first case and about 3% in the second, with the exception of $k = 175$ keV for $Z = 92$, where the difference reaches 8%. But this energy value lies far beyond the Coulomb threshold (43 keV above threshold), where the accuracy of formula (28) is much worse.

4. ANGULAR DISTRIBUTION AND POLARIZATION CORRELATIONS

In order to calculate the angular distribution of the photoelectrons and their polarization, it is necessary to know the expressions for $[\exp(i\delta_\kappa)]R_\kappa^\pm$ (δ_κ —phase shift defined in (6)). Since (26) defines $[\exp(i\eta_\kappa)]R_\kappa^\pm$, we get for $\delta_\kappa - \eta_\kappa$

$$\delta_\kappa - \eta_\kappa = \frac{\pi}{2}(l - \gamma_\kappa) - \arg \Gamma(\gamma_\kappa + i\nu) = \frac{\pi}{2}(l - 2\gamma_\kappa) + \mu b_\kappa \left(1 - \frac{b_\kappa \mu^2}{2}\right) + O(\mu^5), \quad (29)$$

$$b_\kappa = \frac{1}{2}\gamma_\kappa(\gamma_\kappa - 1). \quad (29a)$$

We have left out from (29) all the terms which do not depend on the summation index κ (or l), since they are grouped in one common phase factor preceding the wave function.

We now write out, again omitting all the intermediate calculations, the expressions for the functions B_{ij} , which determine the differential cross section and the

polarization correlations (see (11), (13)–(15)):

$$C_{ij} = B_{ij} / B_{00}, \quad B_{ij} = D b_{ij}, \quad D = 4 / m^2 p; \quad (30)$$

$$b_{00} = q^2 [1 - \frac{5}{3}\mu^2 - 0.393a^2 + 4ta(\mu - \frac{1}{15}\pi a^2) - a^4(0.340 + 0.020q^2)] + a^4(0.141 + \Delta(\theta)), \quad (30a)$$

$$b_{10} = q^2 [1 - \frac{5}{3}\mu^2 - 0.393a^2 + 4ta(\mu - \frac{1}{15}\pi a^2) - a^4(0.420 + 0.020q^2)], \quad (30b)$$

$$b_{02} = -\frac{1}{6}\pi a^2 q [t - a(0.503 + 0.221q^2) - ta^2(0.839 - 0.207q^2)], \quad (30c)$$

$$b_{12} = -\frac{1}{6}\pi a^2 q [t - a(0.503 + 0.221q^2) - ta^2(0.339 - 0.207q^2)], \quad (30d)$$

$$b_{21} = \frac{1}{6}\pi a^2 q [1 - ta(0.503 - 0.640q^2) - a^2(0.339 - 0.336q^2)], \quad (30e)$$

$$b_{23} = a^2 q^2 [-0.101 + 0.335q^2 + O(a^2)], \quad (30f)$$

$$b_{31} = -\frac{1}{2}a^2 q [q^2 [1 + a^2(0.837 - 0.670q^2)] - 0.180 + \frac{4}{15}\pi ta - 0.048a^2], \quad (30g)$$

$$b_{33} = \frac{1}{2}a^2 t [q^2 [1 + a^2(0.010 - 0.670q^2)] + 2a^2(0.141 + \Delta(\theta))]. \quad (30h)$$

Here

$$a = \alpha Z, \quad \mu = p / ma, \quad q = \sin \theta, \quad t = \cos \theta,$$

θ —angle between the electron emission direction and the photon incidence direction, and

$$\Delta(\theta) = -0.176ta(1 - 0.756q^2) + 0.0207a^2(1 - 1.733q^2 + 0.927q^4). \quad (31)$$

The inclusion of the term $\Delta(\theta)$ makes it possible to calculate B_{00} and B_{33} at small angles and at angles close to 180° , with a relative accuracy on the order of a^2 . At other angles, this term is very small and does not change the result noticeably.

In (30c)–(30h) there are no terms linear in μ , and the terms $O(\mu^2)$ have been left out (as already mentioned, we are considering here an energy region such that $\mu^2 < a^4$). The relative accuracy is on the order of a^4 for the coefficients B_{00} and B_{10} , on the order of a for B_{23} , and on the order of a^2 for the remaining B_{ij} .

Having all the B_{ij} , we can calculate the angular distribution of the photo-electrons and their polarization. If we are not interested in the spin of the outgoing electron (the detector counts all the electrons), then the differential cross section for linearly polarized photons is

$$(d\sigma / d\Omega)_{lp} = K(b_{00} + \xi_1 b_{10}) = K[2b_{10} \cos^2 \Phi + a^4(0.141 + 0.080q^2 + \Delta(\theta))], \quad (32)$$

Φ —angle between the plane of polarization of the photon and the scattering plane

$$K = 2^6 \pi \alpha / e^4 m k = 40.1 m / k \quad [\text{b/sr}]. \quad (33)$$

For unpolarized particles we have

$$(d\sigma / d\Omega)_{unp} = K b_{00}. \quad (34)$$

We see from (32) that, unlike the nonrelativistic case, photoemission in a direction perpendicular to the photon polarization vector does not vanish ($\sim a^4$). Formula (34) gives a nonzero ($O(a^4)$) electron emission both forward ($\theta = 0$) and backward ($\theta = \pi$).

In Fig. 1 we compare the angular distributions of the photoelectrons for $Z = 92$ and a photon energy $k = 132$ keV, obtained from formula (34), and numerically in^[1]. The electron polarizations along the axis defined by the unit vectors e_2 , p/p , and $e_2 \times p/p$

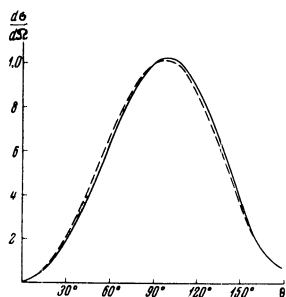


FIG. 1. Angular distribution of photoelectrons for $Z = 92$ at a photon energy equal to the K-electron Coulomb binding energy ($k = 132$ keV). The solid curve is plotted from (34), and the dashed curve is calculated numerically by Nagel and Olsson^[1]. The curves are normalized to unity at $\theta = \pi/2$.

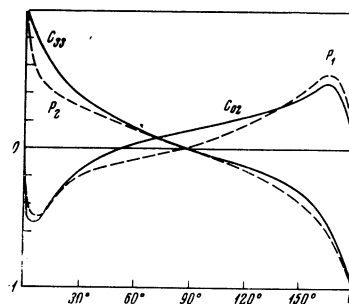
(C_{02} , C_{33} , and C_{31} ; in the notation of Nagel and Olsson^[1] - P_1 , P_2 , and $-P_3$), calculated from formulas (30c), (30g), (30h), and (30), (30a) as well as numerically in^[1] for the case of cyclically polarized photons with energy $k = 132$ keV and $Z = 92$, are in good qualitative agreement (see Fig. 2). Quantitatively the agreement is much poorer than for the angular distribution. This is connected with the fact that the accuracy of formulas (30c)–(30h) is small, especially at those angles, at which the principal term vanishes, and for heavy elements we can count only on a qualitative agreement with the exact calculations. On the other hand, there are no numerical calculations for other Z , and we therefore do not present any plots for all the possible C_{ij} in the region of small and medium Z , where good quantitative agreement may possibly be expected. The values of C_{ij} for such Z , can be readily obtained from (30a)–(30h). These formulas represent correctly the behavior of the polarization correlations at all angles, including the ends of the interval (angles $\theta = 0$ and $\theta = \pi$), if B_{00} , which enters in the denominators of all the C_{ij} , is taken with the maximum accuracy given by (30a).

In conclusion we note that in^[1] are given also analytic expressions for the polarizations P_1 , P_2 , and P_3 (in the case of circular polarization of a photon) in the first non-vanishing order in αZ , suitable for angles that are far from $\theta = 0$ and $\theta = \pi$:

$$P_1 = -\frac{\pi}{6} a^2 \operatorname{ctg} \theta, \quad P_2 = 0.40 a^2 \cos \theta,$$

$$P_3 = 0.40 a^2 \frac{\sin^2 \theta - 0.058}{\sin \theta}$$

FIG. 2. Polarizations of photoelectrons for $Z = 92$ and cyclically polarized photons with energy $k = 132$ keV. The transverse polarization C_{02} , perpendicular to the scattering plane, and the longitudinal polarization C_{33} , calculated from (30c) and (30h), are shown by solid lines. The same polarizations, obtained numerically in^[1], are shown by the dashed lines (P_1 and P_2).



($a = \alpha Z$). For these polarizations we get from (30), in the same approximation, somewhat different expressions:

$$C_{02} = -\frac{\pi}{6} a^2 \operatorname{ctg} \theta, \quad C_{33} = 0.50 a^2 \cos \theta,$$

$$-C_{31} = 0.50 a^2 \frac{\sin^2 \theta - 0.180}{\sin \theta}.$$

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