Angular distribution of photoelectrons with a given spin orientation

N. A. Cherepkov

A. F. Ioffe Physico-technical Institute, USSR Academy of Sciences

(Submitted April 4, 1973)
Zh. Eksp. Teor. Fiz. 65, 933–946 (September 1973)

The angular distribution of photoelectrons with a given spin orientation and produced on absorption of polarized light is obtained for the case when there is a single electron in a state with a definite total angular momentum $j = l \pm 1/2$ in the subshell with an orbital momentum $l \geq 1$, or when the shell is filled and the ion produced after absorption of the quantum possesses a definite total angular momentum $J = l \pm 1/2$. If $l = 1$ and $j = J = 1/2$, the photoelectrons produced on absorption of circularly polarized light and emitted in the direction of the quantum angular momentum will in both cases be completely polarized. On deviation from this direction the degree of polarization drops. For a total electron flux with a given energy and definite angular momentum j (or J) the degree of polarization is usually less than 0.5 and attains unity only at the point of the Cooper cross-section minimum. Results of calculation of the degree of polarization are presented for noble gases and in atoms. The possibility of using this process to produce beams of polarized electrons is considered.

1. The production of beams of polarized electrons is of great interest for different branches of physics. Several methods of producing such beams are now known[1-5]. One of them is based on photionization of polarized atoms of alkali metals by unpolarized light[1]. Another method, recently proposed by Fano[2-4], is based on the use of weak spin-orbit interaction of electrons. It is shown in [2] that when circularly-polarized light is absorbed by alkali-metal atoms, the photoelectrons near the minimum of the cross section turn out to be polarized, and the degree of polarization reaches unity.

This paper deals with cases when the splitting of levels with different values of the total angular momentum of the atom due to spin-orbit interaction leads to the possibility of obtaining polarized photoelectrons. These cases include, first, ionization, by circularly polarized light, of atoms having one electron in the outer subshell with orbital angular momentum $l \geq 1$ and a definite total angular momentum $j = l \pm 1/2$ [6]. Second, photoionization of atoms with closed shells with separation of that part of the electrons which corresponds to the final state of the ion with definite total angular momentum $J = l \pm 1/2$ (l is the orbital angular momentum of the electron prior to the absorption of the quantum, $l \geq 1$). Practical interest attaches principally to atoms with one p electron in the outer subshell and to atoms of noble gases with a closed outer p subshell. For these two particular cases it has been shown that at $j = J = 1/2$ the electrons emitted upon absorption of circularly-polarized light in the direction of the quantum polarization vector are fully polarized. The degree of polarization decreases on deviation from this direction.

We obtain also a general formula for the angular distribution of photoelectrons with a specified spin direction for the two types of atoms indicated above. The study of the angular distributions of the photoelectrons is of considerable independent interest for the theory of the atom and makes it possible to obtain additional information in comparison with that obtained from the total photoionization cross section. After absorption of circularly-polarized or unpolarized light, the angular distribution of the electrons takes the form[7,8]

$$I(\vartheta) = \frac{\sigma_{tot}}{4\pi}\left[1 - \frac{\beta}{2}P_2(\cos\vartheta)\right]. \tag{1}$$

Here σ_{tot} is the total cross section of photoionization of the subshell at a given energy, ϑ is the angle between the direction of motion of the electron and the quantum flux, $P_2(\cos\vartheta) = ((3/2)\cos^2\vartheta - 1/2)$ is a Legendre polynomial, and β is the coefficient of angular asymmetry[7]:

$$\beta = \frac{l(l-1)d_{l-1} + (l+1)(l+2)d_{l+1}^2 - 6l(l+1)d_{l-1}d_{l+1}\cos(\delta_{l+1} - \delta_{l-1})}{(2l+1)[ld_{l-1}^2 + (l+1)d_{l+1}^2]}, \tag{2}$$

$d_{l\pm1}$ is the radial part of the dipole matrix element:

$$d_{l\pm1} = \int_0^\infty r^3 R_{nl}(r) R_{\epsilon,l\pm1}(r)\,dr, \tag{3}$$

R_{nl} and $R_{\epsilon,l\pm1}$ are the radial parts of the wave functions, $R_{\epsilon l}(r)$ is normalized to an energy δ function and has the following asymptotic form at large r:

$$R_{\epsilon l}(r) \sim \left(\frac{2}{\pi k}\right)^{1/2}\frac{1}{r}\sin\left(kr - \frac{\pi l}{2} + \delta_l\right), \tag{4}$$

where1) $\epsilon = k^2/2$. As seen from (2), the coefficient β depends on the phase difference of the wave functions of the continuous spectrum (4).

In the last few years, many theoretical and experimental papers have been devoted to the angular distributions of photoelectrons[7-14], and the calculation results agree well with experiment. However, practically no attention has been paid to polarization effects. The formulas derived in the present paper determine the probability with which an electron, after absorbing a polarized quantum, is emitted at a given angle ϑ to the quantum flux and has a spin directed along a certain vector **s**. The quantum energy is assumed to be small enough so that the dipole approximation can be used. The influence of two-electron processes is disregarded.

2. We consider the ionization by circularly polarized light, of an atom having one electron in the outer subshell and in a state with definite total angular momentum $j = l \pm 1$, $l \geq 1$. For the sake of argument, let the projection of the angular momentum of the quantum on the direction of motion be equal to +1, i.e., we assume right-hand circular polarization. We choose the coordinate system with the Z axis in the direction of motion of the quantum flux. Let us find the probability that an electron emitted at an angle ϑ to the quantum flux will have a specified spin projection μ on the Z axis. The wave function of the initial state of the electron in the atom is represented in the form

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$$\psi_i=\psi_{nljm_j}(\mathbf{r})=\sum_{m,\mu'}\sqrt{2j+1}(-1)^{1/2-l-m_j}\begin{pmatrix} l & 1/2 & j \\ m & \mu' & -m_j \end{pmatrix}\varphi_{nlm\mu'}(\mathbf{r}), \quad (5)$$

where μ' is the spin projection and $\varphi_{nlm\mu'} = R_{nl}(r)Y_{lm}(\vartheta,\varphi)\chi_{\mu'}$. After absorbing the quantum, the electron moves at large distances from the atom in a definite direction. The wave function of the final state should therefore be chosen to be $\varphi_{\mathbf{k}}^{-}$, which contains in the asymptotic form a superposition of a plane wave propagating in the direction $\mathbf{k}$ and a converging wave:

$$\psi_f=\psi_{\mathbf{k}}^{-}(\mathbf{r})\chi_\mu=\sum_{l',m'}a(l',m')\varphi_{\varepsilon l'm'\mu}(\mathbf{r}), \quad (6)$$

where

$$a(l',m')=4\pi(i)^{l'}e^{-i\delta_{l'}}Y_{lm}^{*}(\mathbf{k}/k), \quad (7)$$

δ_l is the phase defined in (4). We use these wave functions to calculate the dipole matrix element:

$$\langle\psi_f|r\sin\vartheta e^{i\varphi}|\psi_i\rangle=\sqrt{2j+1}(-1)^{1/2-l-m_j}\times\sum_{l',m'}\sum_{m,\mu'}\begin{pmatrix} l & 1/2 & j \\ m & \mu' & -m_j \end{pmatrix}a^{*}(l',m')\langle\varphi_{\varepsilon l'm'\mu}|rC_1^1|\varphi_{nlm\mu'}\rangle; \quad (8)$$

$$C_m^l(\vartheta,\varphi)=[4\pi/(2l+1)]^{1/2}Y_{lm}(\vartheta,\varphi).$$

The matrix element that enters in this expression can be calculated easily [15]:

$$\langle\psi_f|rC_1^1|\psi_i\rangle=\sqrt{2j+1}\sum_{l',m',m}(-1)^{1/2-l-m_j+l'-m'+g}\sqrt{l_>}\,d_{l'}a^{*}(l'\ m')\times\begin{pmatrix} l & 1/2 & j \\ m & \mu & -m_j \end{pmatrix}\begin{pmatrix} l' & 1 & l \\ -m' & 1 & m \end{pmatrix}, \quad (9)$$

where $g=(l-l'+1)/2$ and $l_>=\max\{l,l'\}$.

The cross section of the process as a result of which the photoelectron is emitted at an angle ϑ and has a spin projection μ on the Z axis is proportional to the square of the modulus of this expression, averaged over the initial states:

$$I_j(\vartheta,\mu)\sim\sum_{l_1,l_2,m,m_j}(-1)^{g_1+g_2}\sqrt{l_{1>}l_{2>}}\,d_{l_1}d_{l_2}a^{*}(l_1,m)a(l_2,m)\cdot\times\begin{pmatrix} l & 1/2 & j \\ m-1 & \mu & -m_j \end{pmatrix}^2\begin{pmatrix} l_1 & 1 & l \\ -m & 1 & m-1 \end{pmatrix}\begin{pmatrix} l_2 & 1 & l \\ -m & 1 & m-1 \end{pmatrix}. \quad (10)$$

When summing over l and m, we use the relations given in [7]. As a result of the summation we obtain

$$I_j(\vartheta,\mu)=\frac{\sigma_{tot}^{j}}{8\pi}\left[1+A\operatorname{sign}\mu-\left(\frac{\beta}{2}+\gamma_1\operatorname{sign}\mu\right)P_2(\cos\vartheta)\right], \quad (11)$$

where σ_{tot}^{j} is the photoionization cross section of an atom situated in a state with definite angular momentum j,

$$A=(-1)^{j-l-1/2}\frac{l(l+1)}{2j+1}\frac{d_{l+1}^2-d_{l-1}^2}{ld_{l-1}^2+(l+1)d_{l+1}^2}, \quad (12)$$

$$\gamma_1=(-1)^{j-l-1/2}\frac{2l(l+1)}{(2j+1)(2l+1)}\times\frac{(l+2)d_{l+1}^2-(l-1)d_{l-1}^2+3d_{l+1}d_{l-1}\cos(\delta_{l+1}-\delta_{l-1})}{ld_{l-1}^2+(l+1)d_{l+1}^2} \quad (13)$$

and β has been defined earlier in (2). Replacing the right-hand circular polarization by left-hand polarization, i.e., C_1^1 by C_{-1}^1 in (8), and going through the same steps, we find that in this case the signs of A and γ_1 in the angular distribution (11) are reversed. On this basis we can rewrite the result (11) in more general form. We introduce a unit vector **e** in the direction of the quantum polarization vector, and a unit vector **s** directed along the electron spin. Then

$$I_j(\vartheta,\mu)=\frac{\sigma_{tot}^{j}}{8\pi}\left\{1+A(\mathbf{es})-\left[\frac{\beta}{2}+\gamma_1(\mathbf{es})\right]P_2(\cos\vartheta)\right\}. \quad (14)$$

This expression gives the angular distribution of the electrons with a definite value of the spin projection on the direction of the angular momentum of the circularly polarized quantum.

Let us find the degree of polarization of the electrons as a function of the angle ϑ:

$$P_j(\vartheta)=\frac{I_j(\vartheta,1/2)-I_j(\vartheta,-1/2)}{I_j(\vartheta,1/2)+I_j(\vartheta,-1/2)}=\frac{A-\gamma_1P_2(\cos\vartheta)}{1-1/2\beta P_2(\cos\vartheta)}. \quad (15)$$

Substituting the expressions (12) and (13) for the coefficients A and γ_1, we find that the ratio of the degrees of polarization at $j=l+1/2$ and $j=l-1/2$ is inversely proportional to the statistical weights of these states and does not depend on the energy of the quantum or on the angle:

$$P_{l+1/2}(\vartheta)/P_{l-1/2}(\vartheta)=-l/(l+1). \quad (16)$$

Then, after summing over j, no polarization effects occur, as should be the case, and the angular distribution (14) goes over into (1).

If ϑ is equal to zero or to π, we obtain from (15)[6]

$$P_j(0)=P_j(\pi)=\frac{A-\gamma_1}{1-\beta/2}=(-1)^{j-l+1/2}\frac{2}{2j+1}. \quad (17)$$

In the particular case $l=1$ and $j=1/2$, it follows from (17) that $P_{1/2}(0)=P_{1/2}(\pi)=1$, i.e., all the electrons emitted along the direction of the quantum flux have spins directed along the quantum polarization vector [16]. Integrating the numerator and denominator of expression (15) with respect to the angle ϑ, we obtain the degree of polarization of the total electron flux at a given energy:

$$P_j=A. \quad (18)$$

Usually $d_{l+1}>d_{l-1}$, and we therefore obtain from (12) that the degree of polarization of the total electron flux is $|P_{l-1/2}|\le 1/2$ and $|P_{l+1/2}|\le l/2(l+1)$. On the other hand, if $d_{l+1}<d_{l-1}$ (this can occur, for example, in the vicinity of the Cooper minimum of the cross section where $d_{l+1}=0$), then $|P_{l-1/2}|\le(l+1)/2l$ and $|P_{l+1/2}|\le 1/2$. We see that at $l=1$ and $d_{l-1}\gg d_{l+1}$ we have $P_{1/2}\lesssim 1$, i.e., the electrons turn out in this case to be almost completely polarized, regardless of the angle ϑ at which they are emitted.

3. We now find the probability that an electron emitted at an angle ϑ has a spin directed along an arbitrary vector **s**. We shall consider, as before, atoms with one electron in the outer shell. We are interested in the states of an atom with a definite total angular momentum j, and only the helicity operator commutes with the total-angular-momentum operator [17]. The wave function of the outgoing electron must therefore be taken with a definite helicity λ, i.e., with a definite projection of the spin on the direction of motion of the electron:

$$\psi_f=\psi_{\mathbf{k}}^{-}(\mathbf{r})\chi_\lambda=\sum_{l',m',\mu}a(l',m')\varphi_{\varepsilon l'm'\mu}D_{\mu\lambda}^{1/2}(\mathbf{k}/k), \quad (19)$$

where $D_{\mu\lambda}^{1/2}$ is the finite-rotation matrix [17]. The dipole matrix element between the wave functions (5) and (19) for right-hand circular polarization of the quantum is equal to

$$\langle\psi_f|rC_1^1|\psi_i\rangle=\sqrt{2j+1}\sum_{l',m',m,\mu}(-1)^{1/2-l-m_j+l'-m'+g}\sqrt{l_>}\,d_{l'}\times a^{*}(l',m')D_{\mu\lambda}^{1/2}\left(\frac{\mathbf{k}}{k}\right)\begin{pmatrix} l & 1/2 & j \\ m & \mu & -m_j \end{pmatrix}\begin{pmatrix} l' & 1 & l \\ -m' & 1 & m \end{pmatrix}. \quad (20)$$

The cross section of the process as a result of which the electron is emitted at an angle ϑ with a spin directed along **s** is proportional to the average value of the spin operator $(1/2)(1+\mathbf{s}\boldsymbol{\sigma})$ (σ is the Pauli-matrix vector), calculated with the wave functions (19), and to the square of the dipole matrix element averaged over the initial states:

$$\begin{aligned} I_j(\vartheta, s) \sim \sum (-1)^{g_1+g_2-m_1'-m_2'} \sqrt{l_{1>} l_{2>}}\, a^*(l_1, m_1') a(l_2, m_2') \\ \times d_{l_1} d_{l_2} D^{1/2}_{\mu_1\lambda_1} (1+\mathrm{s}\boldsymbol{\sigma})_{\lambda_1\lambda_2} D^{1/2*}_{\mu_2\lambda_2} \begin{pmatrix} l & 1/2 & j \\ m_1 & \mu_1 & -m_j \end{pmatrix} \begin{pmatrix} l & 1/2 & j \\ m_2 & \mu_2 & -m_j \end{pmatrix} \\ \times \begin{pmatrix} l_1 & 1 & l \\ -m_1' & 1 & m_1 \end{pmatrix} \begin{pmatrix} l_2 & 1 & l \\ -m_2' & 1 & m_2 \end{pmatrix} \end{aligned} \tag{21}$$

(the summation is over l_1, m_1', l_2, m_2'; m_1, m_2, μ_1, μ_2; λ_1, λ_2, m_j).

We define a coordinate system XYZ such that the Z axis coincides with the direction of the quantum flux, and the electron moves in the XZ plane. We choose the moving system of coordinates $\xi\eta\zeta$ in such a way that the ζ axis coincides with the direction of the electron momentum, and the Y and η axes coincide with each other (see Fig. 1). We denote by ϑ_1 and φ_1 the spherical coordinates of the vector **s** in the system $\xi\eta\zeta$, and by α the angle between the vector **s** and the Z axis. We note immediately that

$$\cos\alpha = \cos\vartheta_1 \cos\vartheta - \sin\vartheta_1 \sin\vartheta \cos\varphi_1, \tag{22}$$

since in accordance with the construction the Z axis has $\varphi = \pi$ in the system $\xi\eta\zeta$. Using the expression for $D^{\mu\lambda}$ [17], we can easily sum over the helicities λ_1 and λ_2.

When summing over the remaining indices in expression (21), we separate first the terms with $\mu_1 = \mu_2$. For these terms, the summation is carried out in exactly the same manner as was described in the preceding section, and their contribution is equal to

$$\begin{aligned} I_j^1(\vartheta, s) = \frac{4\pi}{3(2l+1)} \Big\{ [l d_{l-1}^2 + (l+1) d_{l+1}^2] \Big[1 - \frac{\beta}{2} P_2(\cos\vartheta)\Big] \\ - (-1)^{j-l-1/2} \frac{3l(l+1)\cos\alpha}{(2j+1)(2l+1)} [l d_{l-1}^2 - (l+1) d_{l+1}^2 - (l-1) d_{l-1}^2 \cos^2\vartheta \\ + (l+2) d_{l+1}^2 \cos^2\vartheta + d_{l+1} d_{l-1} (3\cos^2\vartheta - 1)\cos(\delta_{l+1} - \delta_{l-1})] \Big\}. \end{aligned} \tag{23}$$

In the terms with $\mu_1 \neq \mu_2$, we change over from the spherical function $Y_{lm}(\mathbf{k}/k)$, which enters in $a(l, m)$, to associated Legendre polynomials, for which the following relations hold:

$$\begin{aligned} \sum_m \frac{(l-m+1)!}{(l+m-1)!} P_{l-1}^m P_{l-1}^{m+1} = \sum_m \frac{(l-m+1)!}{(l+m-1)!} P_{l+1}^m P_{l-1}^{m+1} \\ = -(l-1)l(l+1)\sin\vartheta\cos\vartheta, \end{aligned} \tag{24.1}$$

$$\begin{aligned} \sum_n \frac{(l-m+1)!}{(l+m-1)!} P_{l+1}^m P_{l+1}^{m+1} = \sum_m \frac{(l-m+1)!}{(l+m-1)!} P_{l-1}^m P_{l+1}^{m+1} \\ = l(l+1)(l+2)\sin\vartheta\cos\vartheta. \end{aligned} \tag{24.2}$$

Using these relations, we carry out the summation in (21) for terms with $\mu_1 \neq \mu_2$:

$$\begin{aligned} I_j^2(\vartheta, s) = (-1)^{j-l+1/2} \frac{4\pi l(l+1)}{(2j+1)(2l+1)^2} \{[(l-1) d_{l-1}^2 - (l+2) d_{l+1}^2 \\ - 3 d_{l-1} d_{l+1} \cos(\delta_{l+1} - \delta_{l-1})][\cos^2\vartheta\cos\alpha - \cos\vartheta_1\cos\vartheta] \\ + (2l+1) d_{l+1} d_{l-1} \sin(\delta_{l+1} - \delta_{l-1}) \sin\vartheta\cos\vartheta\sin\vartheta_1\sin\varphi_1\}. \end{aligned} \tag{25}$$

Adding (23) and (25) and reducing the normalization to the form (1), we obtain ultimately

$$\begin{aligned} I_j(\vartheta, s) = \frac{\sigma_{tot}^j}{8\pi} \Big\{ 1 - \frac{\beta}{2} P_2(\cos\vartheta) + A\cos\alpha - \\ - \gamma_1 (3/2 \cos\vartheta_1 \cos\vartheta - 1/2 \cos\alpha) - \gamma_2 \sin\vartheta\cos\vartheta\sin\vartheta_1\sin\varphi_1 \Big\}, \end{aligned} \tag{26}$$

where A, β and γ_1 were defined earlier, and

$$\gamma_2 = (-1)^{j-l-1/2} \frac{3l(l+1)}{2j+1} \frac{d_{l+1} d_{l-1} \sin(\delta_{l+1} - \delta_{l-1})}{[l d_{l-1}^2 + (l+1) d_{l+1}^2]}. \tag{27}$$

When the quantum polarization direction is reversed, the signs of the third and fourth terms of (26) are reversed. This enables us to write the result in more general form, using the unit vectors **e** and **s**, and also $\boldsymbol{\varkappa} = \mathbf{k}/k$—the unit vector in the direction of the electron momentum. For circularly polarized light, the cross section of the process as a result of which the photoelectron is emitted at an angle ϑ and has a spin directed along the vector **s** is given by[2)]

$$\begin{aligned} I_j^{\text{circ}}(\vartheta, s) = \frac{\sigma_{tot}^j}{8\pi} \Big\{ 1 - \frac{\beta}{2} \Big[\frac{3}{2}(\mathbf{e}\boldsymbol{\varkappa})^2 - \frac{1}{2}\Big] + A(\mathbf{es}) \\ - \gamma_1 [3/2 (\mathbf{e}\boldsymbol{\varkappa})(\mathbf{s}\boldsymbol{\varkappa}) - 1/2 (\mathbf{es})] - \gamma_2 (\mathbf{s}[\mathbf{e}\boldsymbol{\varkappa}])(\mathbf{e}\boldsymbol{\varkappa}) \Big\}. \end{aligned} \tag{28}^*$$

We consider an analogous problem for linearly polarized light. We choose the coordinate system XYZ such that the Z axis coincides with the quantum polarization vector **e**, and the Y axis coincides with the direction of the quantum flux. We choose the moving coordinate system $\xi\eta\zeta$ in such a way that the ζ axis coincides with the electron momentum vector (Fig. 2).

In the expression for the dipole matrix element (20), only the projection of the quantum angular momentum changes:

$$\begin{aligned} \langle\psi_f | r C_0^1 | \psi_i\rangle = \sqrt{2j+1} \sum_{l', m', m, \mu} (-1)^{1/2 - l - m_j + l' - n + g} \sqrt{l_>} \\ \times d_{l'} a^*(l', m') D_{\mu\lambda}^{1/2}\Big(\frac{\mathbf{k}}{k}\Big) \begin{pmatrix} l & 1/2 & j \\ m & \mu & -m_j \end{pmatrix} \begin{pmatrix} l' & 1 & l \\ -m' & 0 & m \end{pmatrix}. \end{aligned} \tag{29}$$

The summations are carried out in analogy with the summation considered above. The terms with $\mu_1 = \mu_2$ give a result that does not depend on the direction of the spin:

$$I_j^1(\vartheta, s) = \frac{4\pi}{3(2l+1)} [l d_{l-1}^2 + (l+1) d_{l+1}^2]\{1 + \beta P_2(\cos\vartheta)\}, \tag{30}$$

In the summations in the terms with $\mu_1 \neq \mu_2$ we use the relations

$$\begin{aligned} \sum_m \frac{(l-m+1)!}{(l+m-2)!} (l+m) P_{l-1}^m P_{l-1}^{m-1} \\ = \sum_m \frac{(l-m+2)!}{(l+m-1)!} (l-m+1)^{(l+m)} P_{l+1}\ P_{l+1} = 0, \end{aligned} \tag{31.1}$$

$$\begin{aligned} \sum_m \frac{(l-m+1)!}{(l+m-2)!} (l-m+1) P_{l-1}^{m-1} P_{l+1}^m \\ = -\sum_m \frac{(l-m+2)!}{(l+m-1)} (l+m) P_{l+1}^{m-1} P_{l-1}^m = \frac{1}{2} l(l+1)(2l+1)\sin\vartheta\cos\vartheta. \end{aligned} \tag{31.2}$$

As a result we obtain

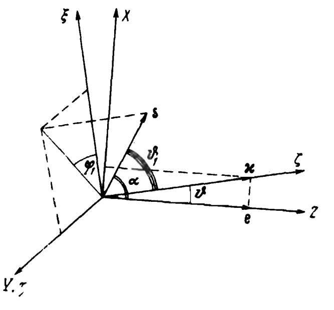

FIG. 1

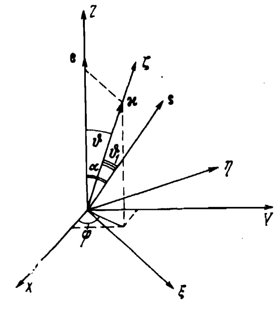

FIG. 2

$$I_j^2(\vartheta, \mathrm{s}) = (-1)^{j-l+{}^1\!/_2} \frac{4\pi l(l+1)}{(2j+1)(2l+1)} d_{l+1} d_{l-1} \sin(\delta_{l+1} - \delta_{l-1}) \sin\vartheta \cos\vartheta \sin\vartheta_1 \sin\varphi_1. \tag{32}$$

The angular distribution of the electrons with a specified spin direction **s**, following absorption of linearly polarized light, is ultimately given by the expression

$$I_j^{\mathrm{lin}}(\vartheta, \mathrm{s}) = \frac{\sigma_{tot}^j}{8\pi}\left\{1 + \beta\left[\frac{3}{2}(\mathbf{e}\varkappa)^2 - \frac{1}{2}\right] - \gamma_2(\mathbf{s}[\mathbf{e}\varkappa])(\mathbf{e}\varkappa)\right\}. \tag{33}$$

It is easy to write down the degree of polarization of the electrons along the direction **s** as a function of the angle ϑ:

$$P_j^{\mathrm{lin}}(\varkappa, \mathrm{s}) = -\frac{\gamma_2(\mathbf{s}[\mathbf{e}\varkappa])(\mathbf{e}\varkappa)}{1 + \beta P_2(\mathbf{e}\varkappa)}. \tag{34}$$

Integrating this expression over all the directions of the vector κ, we find that $P_j^{\mathrm{lin}}(\mathbf{s}) = 0$. Therefore, to observe the polarization it is necessary to separate electrons emitted at a definite angle. In addition, the polarization of the electrons vanishes when the quantity $(\mathbf{s} \cdot \mathbf{e} \times \kappa)(\mathbf{e} \cdot \kappa)$ vanishes, i.e., when the vector **s** lies in a plane defined by the vectors **e** and κ, and also when $\kappa \parallel \mathbf{e}$ and $\kappa \perp \mathbf{e}$.

4. If the orbital angular momentum of the outer electron of the atom is $l = 0$, then, as shown by Fano [2], the electrons become polarized after absorption of circularly polarized light. The Fano effect is based on the fact that the wave functions of the outgoing electron, meaning also the dipole matrix elements, differ from each other for the states with $j = l - 1/2$ and $j = l + 1/2$. It is of interest to obtain the angular distribution of electrons with specified direction of the spin **s** also for the Fano effect. An examination of this process is analogous in many respects to that of the preceding one. The wave function (19) must be transformed in the following manner:

$$\psi_j = \sum (2j+1) \begin{pmatrix} l' & {}^1\!/_2 & j \\ m' & \mu & -m_j \end{pmatrix} \begin{pmatrix} l' & {}^1\!/_2 & j \\ m'' & \mu'' & -m_j \end{pmatrix} \times a(l', m') \varphi^j_{\varepsilon l' m'' \mu''}(\mathbf{r}) D^{{}^1\!/_2 *}_{\mu\lambda}\left(\frac{\mathbf{k}}{k}\right), \tag{35}$$

where one sums over l', m', μ, j, m_j, m'', and μ'', while the index j of the wave function identifies the state $\varphi_{\epsilon l' j m_j}$ from which it is obtained. Since we have alkali atoms in mind, we put immediately $l' = 1$ and $l = 0$. The dipole matrix element between the functions (5) and (35) is, for right-hand circular polarization,

$$\langle\psi_f|rC_1^1|\psi_i\rangle = \sum_{j, m_j, m', \mu} \frac{(2j+1)}{\sqrt{3}} a^*(l', m') D^{{}^1\!/_2}_{\mu\lambda}\left(\frac{\mathbf{k}}{k}\right) d_j \times \begin{pmatrix} 1 & {}^1\!/_2 & j \\ m' & \mu & -m_j \end{pmatrix} \begin{pmatrix} 1 & {}^1\!/_2 & j \\ 1 & \mu'' & -m_j \end{pmatrix}, \tag{36}$$

where

$$d_j = \int_0^\infty R_{ns}(r) R_{\varepsilon p}^j(r) r^3\, dr. \tag{37}$$

The cross section of the process as a result of which the electron is emitted at an angle ϑ with a spin directed along **s** (see Fig. 1) is proportional to the expression

$$I^F(\vartheta, \mathrm{s}) \sim \sum (2j'+1)(2j''+1) a^*(1, m_1) a(1, m_2) d_{j'} d_{j''} \times D^{{}^1\!/_2}_{\mu_1\lambda_1}(1 + \mathbf{s}\sigma)_{\lambda_1\lambda_2} D^{{}^1\!/_2 *}_{\mu_2\lambda_2} \begin{pmatrix} 1 & {}^1\!/_2 & j' \\ m_1 & \mu_1 & -m_j' \end{pmatrix} \begin{pmatrix} 1 & {}^1\!/_2 & j' \\ 1 & \mu'' & -m_j' \end{pmatrix} \times \begin{pmatrix} 1 & {}^1\!/_2 & j'' \\ m_2 & \mu_2 & -m_j'' \end{pmatrix} \begin{pmatrix} 1 & {}^1\!/_2 & j'' \\ 1 & \mu'' & -m_j'' \end{pmatrix} \tag{38}$$

(the sum is over j', m_j', j'', m_j''; m_1, m_2, μ_1, μ_2; λ_1, λ_2, μ''). Substituting here the numerical values of the 3j-symbols and summing, we obtain

$$I^F(\vartheta, \mathrm{s}) = \frac{\sigma_{tot}}{8\pi}\left\{1 - \frac{b}{2} P_2(\cos\vartheta) + a\cos\alpha - \gamma\left(\frac{3}{2}\cos\vartheta_1 \cos\vartheta - \frac{1}{2}\cos\alpha\right)\right\}, \tag{39}$$

where

$$b = \frac{2|d_3 + d_1|^2 - 2d_1^2}{2d_3^2 + d_1^2}, \quad a = \frac{3d_3^2 - {}^1\!/_3|2d_3 + d_1|^2}{2d_3^2 + d_1^2}, \quad 2\gamma = \frac{{}^1\!/_3|2d_3 + d_1|^2 - 3d_1^2}{2d_3^2 + d_1^2}. \tag{40}$$

The subscript 3 or 1 of the dipole matrix element denotes respectively $j = 3/2$ or $j = 1/2$. The angular distribution (39) can be written in a different form, using the unit vectors defined above[3)]:

$$I^F(\vartheta, \mathrm{s}) = \frac{\sigma_{tot}}{8\pi}\left\{1 - \frac{b}{2}\left[\frac{3}{2}(\mathbf{e}\varkappa)^2 - \frac{1}{2}\right] + a(\mathbf{es}) - \gamma\left[\frac{3}{2}(\mathbf{e}\varkappa)(\mathbf{s}\varkappa) - \frac{1}{2}(\mathbf{es})\right]\right\}. \tag{41}$$

The photoionization cross section of alkali atoms, starting with Na, has a minimum close to zero near the ionization thresholds, and this minimum is due to the reversal of the sign of the dipole matrix element. When the spin-orbit interaction is taken into account, the wave functions of the states with $j = 3/2$ and $j = 1/2$ turn out to be somewhat different. Therefore the matrix elements d_3 and d_1 vanish at different quantum energies, and the total photoionization cross section never vanishes rigorously. At the point where $d_3 = -2d_1$, we obtain from (40) $b = 0$, $a = 1$, and $\gamma = 0$. This means that all electrons are polarized in the direction of the vector **e** independently of their emission angle ϑ, and the angular distribution is isotropic.

We note that formula (41) is also valid in the case of ionization of the ns^2 subshell. The only change in the derivation lies in the fact that the wave function of the final state is the product of the functions (5) and (35), while the wave function of the initial state constitutes a linear combination of s-states with different spin projections, yielding the same dipole matrix element (36). The photoionization cross section of the alkaline-earth atoms also has a minimum near the ionization threshold (see, e.g., [18-20]), and the cross section at the minimum is larger for these atoms than for the preceding alkali atoms.

5. Let us consider the ionization, with polarized light, of a closed shell of an atom with $l \geq 1$. We obtain the angular distribution of the electrons with a specified spin direction **s**, assuming that after absorption of the quantum the ion remains in a state having definite values of the orbital angular momentum L, the spin S, and the total angular momentum J. The wave function of such a final state is given by

$$\psi_f = \psi_{\mathbf{k}}^-(\mathbf{r}) \chi_\lambda \varphi_{LSJM} = \sum_{M_L, M_S} (-1)^{S-L-M} \begin{pmatrix} L & S & J \\ M_L & M_S & -M \end{pmatrix} \sqrt{2J+1} \times \psi_{LM_LSM_S} \sum_{l', m', \mu} a(l', m') \varphi_{\varepsilon l' m' \mu}(\mathbf{r}) D^{{}^1\!/_2}_{\mu\lambda}\left(\frac{\mathbf{k}}{k}\right). \tag{42}$$

We calculate with this wave function the dipole matrix element for the right-hand circular polarization of the quantum

$$\langle\psi_f|rC_1^1|\psi_i\rangle = \sum_{M_L, M_S} (-1)^{S-L-M} \begin{pmatrix} L & S & J \\ M_L & M_S & -M \end{pmatrix} \sqrt{2J+1} \times \sum_{l', m', \mu} a^*(l', m') D^{{}^1\!/_2 *}_{\mu\lambda} \langle\varphi_{\varepsilon l' m' \mu} \psi_{LM_LSM_S}|rC_1^1|\psi_0\rangle, \tag{43}$$

where ψ_0 is the wave function of the ground state of the atom. We connect the angular momenta of the ion and of the electron, and change over in the final state to the wave function $\psi(l'1/2, LS; L'M_L'S'M_S')$. The dipole matrix element is then expressed in the following manner [21]:

$$\langle\psi(l'{}^1/_2, LS; L'M_L'S'M_S')|rC_1{}^1|\psi_0\rangle = \delta_{S'0}\delta_{M_S'0}(-1)^{L'-M_L'+L+l'+1+g} \times [(2L'+1)l_> \cdot 2(2l+1)]^{1/2} d_{l'} \begin{pmatrix} L' & 1 & 0 \\ -M_{L'} & 1 & 0 \end{pmatrix} \begin{Bmatrix} 0 & 1 & L' \\ l' & L & l \end{Bmatrix}. \quad (44)$$

Substituting these expressions in the matrix element (43), we obtain for the cross section of the sought process

$$I_J(\vartheta, s) = (2J+1) \sum (-1)^{g_1+g_2-m_1-m_2}\sqrt{l_{1>}l_{2>}}\, a^*_\cdot(l_1, m_1)\, a(l_2, m_2) \times \begin{pmatrix} l & {}^1/_2 & J \\ M_L' & \mu_1 & -M \end{pmatrix} \begin{pmatrix} l & {}^1/_2 & J \\ M_L'' & \mu_2 & -M \end{pmatrix} \begin{pmatrix} l_1 & 1 & l \\ -m_1 & 1 & M_L' \end{pmatrix} \begin{pmatrix} l_2 & 1 & l \\ -m_2 & 1 & M_L'' \end{pmatrix} \quad (45)$$
$$\times D^{1/2}_{\mu_1\lambda_1}(1+s\sigma)_{\lambda_1\lambda_2} D^{1/2}_{\mu_2\lambda_2}\, d_{l_1} d_{\cdot_2}$$

(the sum is over l_1, m_1, l_2, m_2; μ_1, μ_2, λ_1, λ_2; M_L', M_L'', M). This expression coincides with (21), and therefore we obtain after summing over all the indices the same formulas (28) and (33), with j replaced by J, and also with another factor in front of the curly bracket:

$$\frac{\sigma_{tot}}{8\pi}\,\frac{(2J+1)}{2(2l+1)}$$

where σ_{tot} is the total cross section for the photoionization of the considered subshell. Thus, upon absorption of polarized light, the angular distribution of the electrons with a specified spin orientation, for atoms with one electron in the outer shell and angular momentum $l \geq 1$ and with a definite total angular momentum $j = l \pm 1/2$, coincides with the analogous angular distribution for atoms with a closed shell having the same angular momentum l, when the remaining ion has a definite total angular momentum J = j.

6. The angular distributions of the photoelectrons for atoms of noble gases were measured, and the contributions of the processes in which the ion in the final state has angular momenta J = 1/2 and J = 3/2 were separated[9,12]. The coefficient β turned out to be close to zero near the ionization thresholds of the atoms Ar, Kr, and Xe, and even negative in the case of Ne[11,13,14]. With decreasing β, the number of electrons emitted at small angles to the quantum flux, where the degree of polarization is largest, is increased. Therefore the region of low energies near the ionization threshold is of greatest interest for the study of polarization effects in these atoms.

The results of the calculations of the photoionization cross sections and of the coefficients β for noble-gas atoms, with allowance for many-electron correlations, were published earlier in [14,22]. The values of the parameters A, γ_1, and γ_2 obtained with their aid at certain values of the energy are given in Table I, while Fig. 3 shows the dependence of the degree of polarization of the electron on the angle ϑ for the atoms Ne, Ar, and Xe, obtained from formula (15) for a spin parallel to the quantum polarization vector.

The same figure shows the dependence of the total electron flux on the angle, obtained from formula (1) (in arbitrary units). As seen from the figure, for all atoms at J = 1/2 the degree of polarization $P_{1/2}(\vartheta) > 0.7$ in the angle interval $\vartheta = 0-20°$, whereas the intensity of the electron flux is practically independent of the angle. The dependence of the degree of polarization on the angle is almost the same for all the atoms, and changes little with increasing energy far from the region of the Cooper minimum. As seen from Table I, the degree of polarization of the total energy flux, equal to the coefficient A, reaches the largest absolute value for Xe near the ionization threshold.

TABLE I. Values of the parameters for noble-gas atoms

Atom ($J = {}^1/_2$)	Ne, $\varepsilon = 0.25$ Ry	Ar, $\varepsilon = 0.16$ Ry	Kr, $\varepsilon = 0.1225$ Ry	Xe, $\varepsilon = 0.1225$ Ry
A	−0.21	−0.36	−0.36	−0.38
γ_1	−1.32	−1.18	−1.18	−1.08
γ_2	−0.34	−0.38	−0.35	−0.54
β	−0.21	0.35	0.36	0.60

TABLE II. Values of the parameters at j – 1/2 and photoionization cross section of the In atom

ε, Ry	σ_{tot}, 10^{-18} cm²	A	γ_1	γ_2	β
0.01	23.3	−0.40	−0.90	−0.52	1.00
0.16	9.9	−0.37	−0.60	−0.34	1.56

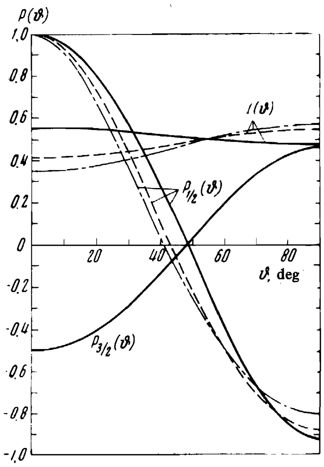

FIG. 3

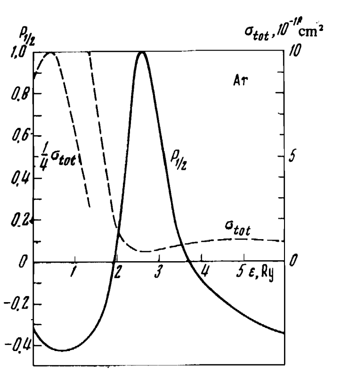

FIG. 4

FIG. 3. Angular dependence of the degree of polarization $P_J(\vartheta)$ and of the total electron flux $I(\vartheta)$. Solid line–Ne. $\epsilon = 0.25$ Ry; dashed = Ar, $\epsilon = 0.16$ Ry; dash-dot–Xe, $\epsilon = 0.1225$ Ry, $I(\vartheta)$ is in arbitrary units.

FIG. 4. Dependence of the degree of polarization of the total electron flux $P_{1/2}$ on the energy for the Ar atom. σ_{tot} is the photoionization cross section of the $3p^6$ subshell of Ar.

Figure 4 shows a plot of the coefficient A against the energy for the Ar atom. It also shows the photoionization cross section of the $3p^6$ subshell of the atom. At the Cooper-minimum point, the degree of polarization $P_{1/2} = A$ reaches unity, from which it follows that at this energy all the electrons with J = 1/2 turn out to be polarized independently of the angle ϑ. At the Cooper minimum there should also appear the Fano effect connected with the difference between the wave functions of the photoelectron in the states $d_{3/2}$ and $d_{5/2}$, but now against the background of the nonvanishing transition ns → εp. The cross section of the transition np → εp never vanishes rigorously, and the influence of the Fano effect is determined by the minimum of the cross section ratio $\sigma_{p\to d}/\sigma_{p\to s}$. Using the method described in the paper, we can obtain formulas for this case, too.

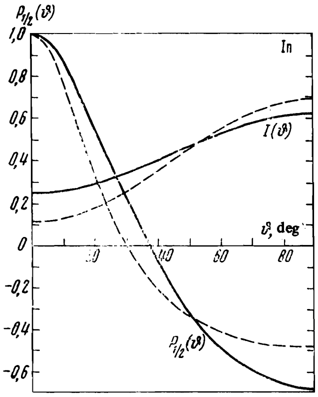

FIG. 5

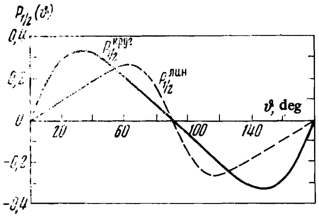

FIG. 6

FIG. 5. Dependence of the degree of polarization $P_{1/2}(\vartheta)$ and of the total electron flux $I(\vartheta)$ on the angle for the In atom. Solid lines–ϵ = 0.01 Ry, dashed–ϵ = 0.16 Ry; $I(\vartheta)$ is in arbitrary units.

FIG. 6. Dependence of the degree of polarization on the angle for the In atom at $s \perp e$ and $s \perp \mathcal{H}$. $j = 1/2$. Solid line–circular polarization of the light, dashed–linear polarization of the light.

By way of example of an atom with one p electron in the outer shell, we have considered In. Table II gives the values of the parameters, and also the photoionization cross section of In at electron energy values $\epsilon = 0.01$ Ry and 0.16 Ry ($j = 1/2$), obtained in the Hartree-Fock approximation with dipole matrix elements of the coordinate [22]. Figure 5 shows the dependence of the degree of polarization, obtained from formula (15), and also of the total electron flux, on the angle for the same energies. The degree of polarization decreases here with increasing angle more rapidly than in noble-gas atoms.

To explain the influence of the last term in the angular distribution (28), let us consider the situation in which $\mathbf{s} \perp \mathbf{e}$ and $\mathbf{s} \perp \kappa$. The degree of polarization is then given by

$$P_j^{\mathrm{circ}}(\varkappa, \mathbf{s}) = -\frac{\gamma_2(\mathbf{s}[\mathbf{e}\varkappa])(\mathbf{e}\varkappa)}{1 - {}^1/_2\beta P_2(\mathbf{e}\varkappa)}. \tag{46}$$

Let the vector $\mathbf{s}$ coincide with the η axis (see Fig. 1). Then $\vartheta_1 = \varphi_1 = \pi/2$, and in formula (46) there remains only the dependence on the angle ϑ. For linear polarization of the quantum at $\mathbf{s} \perp \mathbf{e}$ and $\mathbf{s} \perp \kappa$, and at a vector $\mathbf{s}$ coinciding with the η axis (see Fig. 2), we also have $\vartheta_1 = \varphi_2 = \pi/2$, and the angular distribution is given by formula (34). The dependence of the degree of polarization on the angle ϑ for these two cases, obtained at an electron energy $\epsilon = 0.01$ Ry and $j = 1/2$ in the In atom, is shown in Fig. 6. We see that under definite conditions this term can also make a noticeable contribution. It appears that an analogous situation takes place also in other atoms with one p electron in the outer subshell.

The results show that to obtain a beam of polarized electrons it is more convenient to use noble-gas atoms. The largest splitting between the $^2P_{1/2}$ and $^2P_{3/2}$ levels of the ion is found in Xe and amounts to 0.096 Ry. The photoionization cross section at $\epsilon = 0.1225$ Ry is equal to 75×10^{-18} cm^2, which exceeds by three orders of magnitude the photoionization cross section of the Cs atom near the minimum of the cross section, where the Fano effect is observed. Following absorption of circularly-polarized light, the electrons that leave the ion in the state $^2P_{1/2}$ and are emitted at angles $\vartheta = 0$–$20°$, constitute 0.7% of the total electron flux at this energy, and have a degree of polarization equal to 0.84. In comparison with the Fano effect in the Cs atom [4], in the considered case the flux of the polarized electrons, at the same light-source intensity, should be larger by at least one order of magnitude. If the electrons emitted in the angle interval $\vartheta = 0$–$10°$ are separated, then the degree of polarization for them turns out to be 0.95, but the flux of the polarized electrons then decreases by a factor of 4. As already noted, the degree of polarization depends little on the energy, and therefore the width of the spectrum of the light source is limited only by the spacing between the $^2P_{1/2}$ and $^2P_{3/2}$ levels of the ion.

In principle one can consider the angular distribution of the photoelectrons with a specified spin orientation in an arbitrary atom. However, to observe the polarization it is necessary to separate the electrons corresponding to the definite total angular momentum of both the initial atom and of the final ion. In such a situation it is impossible to perform all the manipulations in general form.

The author is sincerely grateful to M. Ya. Amus'ya for useful remarks, and also to V. G. Gorshkov and G. F. Drukarev for discussions.

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*$[\mathbf{e}\kappa] = \mathbf{e} \times \kappa$.

[1)] The atomic system of units with $\hbar = m = e = 1$ is used.

[2)] The invariance of expression (28) under inversion and time reversal is obvious (with the exception of the last term). In the case of time reversal, all the vectors of the last term reverse sign, but γ_2 contains the sine of a phase difference and also reverses sign, so that even this term remains invariant.

[3)] This expression was first derived in [16] by another method. For $\mathbf{e} \parallel \mathbf{s}$, the angular distribution was considered in [3].

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Translated by J. G. Adashko
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