Polarization effects in the photoionization of atoms

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The atoms of Ar and Xe are used as examples in considering the various possibilities of obtaining polarized electrons by absorption of circularly polarized, linearly polarized, and unpolarized light by unpolarized atoms. The results are given of a calculation of the degree of electron polarization in the random phase approximation with exchange.

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1. Improvements in the experimental techniques and the use of the coincidence method have made it possible to ensure continuing increase in the detailed information available on collisions of particles with atoms. However, the simplest case of atomic collisions—photoionization—has been considered theoretically so far without allowance for the photoelectron spin orientation. A full quantum-mechanical description of the photoionization of an atom is as follows. Light of known polarization is incident on unpolarized atoms (we shall consider only this case). It is necessary to find the probability of emission of photoelectrons along a given direction $\mathbf{n}$, with spin directed along some vector $\mathbf{s}$, where $\mathbf{n}$ and $\mathbf{s}$ are unit vectors. The polarization of photoelectrons generated by absorption of circularly polarized light in alkali atoms was first considered by Fano.\(^{1,2}\) He showed that near a Cooper minimum the total photoelectron flux is polarized in the direction of the spin vector of the photons because of the spin-orbit interaction in the continuous spectral state. The angular distribution of photoelectrons with this spin orientation was considered by Heinzmann et al.\(^{3}\) It was found that as a consequence of the influence of the spin-orbit interaction the asymmetry coefficient $\beta$ of the angular distribution undergoes a sudden change near a Cooper minimum, whereas in the LS coupling approximation for the $s^2$ subshells it is equal to 2, irrespective of the photon energy. Finally, the general formula for the angular distribution with an arbitrary spin orientation in the Fano effect was obtained by Brehm.\(^{4}\)

The Fano effect also appears in the photoionization of the $s^2$ subshells by circularly polarized light if the photoionization cross section has a Cooper minimum.\(^{5}\) This condition is satisfied, in particular, by the outer $s^2$ subshells of alkaline-earth atoms and atoms of the inert gases, beginning from Ca and Ar, respectively.\(^{6}\)
The Fano effect in the 5s² subshell of Xe is considered in the present author's earlier communication.\textsuperscript{4,5}

The ionization of shells beginning from 1s = 1 is discussed in Ref. 4. The results given there can be used to show that the ionization by polarized or unpolarized light of any subshell (nl)\textsuperscript{N} with \( l > 1 \) and \( 1 < N < 4 l + 2 \) in a state with a given total momentum \( J \) produces polarized photoelectrons corresponding to a specific final state of the ion with the momentum \( J' \). The degree of the electron polarization depends on the angle of emergence of electrons, photon energy, atomic characteristics, and polarization of the incident light. The electron polarization is due to the spin–orbit interaction because the dipole operator does not act on the spin variables. However, the role of the interaction reduces to the energy splitting of the levels, whereas the selection rules of the dipole photoeffect state that the knocking out of an electron with a given spin projection is the more probable or even the only possible event. In the latter case the photoelectrons are totally polarized. The weakness of the spin–orbit interaction usually has the result that the polarization effects induced by this interaction appear when the cross section of the process is small, as—for example—in the case of the elastic and inelastic scattering of electrons by atoms.\textsuperscript{6–10} A typical example is the Fano effect which appears at a minimum of the photoionization cross section. The ionization of the shells with \( l > 1 \) with separate contributions of the individual components of the fine structure is an exception to this rule because the weakness of the spin–orbit interaction is not then important. In fact, the spin–orbit interaction is necessary only for the formation of the initial and final states. If this interaction is sufficiently strong for all the atoms or ions to be in a state with the same value of the total angular momentum, i.e., if the fine splitting of the levels exceeds the thermal energy, the effects in question may appear on absorption of photons of any energy with the necessary monochromaticity. Moreover, we may have a situation in, for example, autoionization resonance when an increase in the photoionization cross section causes an increase in the degree of the electron polarization, reaching 100% at the cross section maximum.\textsuperscript{11,12} This does not apply to the \( s \) subshells for which there is no spin–orbit splitting and, therefore, only the Fano effect is possible.

2. Absorption of circularly polarized light by an occupied subshell \( s l > 1 \) produces electrons whose degree of polarization is

\[ P_{\text{pol}}(s, l) = \frac{A_J(s, l)}{1 - \frac{1}{2} (s \cdot l)^2} \cdot \frac{\text{f}_{1/2}(\text{e}^T) \cdot \text{f}_{1/2}(\text{e}^T)}{\text{f}_{3/2}(\text{e}^T) \cdot \text{f}_{3/2}(\text{e}^T)} \] \hspace{1cm} (1)

where \( s \) is the photon spin vector, \( s \) and \( l \) are the unit vectors in the direction of the electron spin and momentum, respectively; the coefficients \( A_J(s, l) \), \( \gamma^T \), \( \lambda^T \), and \( \delta \) are given by Eqs. (12), (13), (27), and (32) of Ref. 4; \( J \) is the total momentum of the ion in the final state. For linearly absorbed light, the degree of polarization is

\[ P_{\text{pol}}(s, l) = \frac{2 \gamma^T(s \cdot l)}{1 + \frac{1}{2} (s \cdot l)^2} \cdot \frac{\text{f}_{1/2}(\text{e}^T) \cdot \text{f}_{1/2}(\text{e}^T)}{\text{f}_{3/2}(\text{e}^T) \cdot \text{f}_{3/2}(\text{e}^T)} \] \hspace{1cm} (2)

where \( e \) is the photon polarization vector. It follows from this expression that electrons are transversely polarized at right-angles to the plane defined by the vectors \( e \) and \( l \).

Unpolarized light can be regarded as a superposition of the right- and left-polarized components. The terms in Eq. (1) linear in \( s \), are canceled out and the degree of electron polarization due to the absorption of unpolarized light is

\[ P_{\text{pol}}(s, l) = \frac{\text{f}_{1/2}(\text{e}^T) \cdot \text{f}_{1/2}(\text{e}^T)}{\text{f}_{3/2}(\text{e}^T) \cdot \text{f}_{3/2}(\text{e}^T)} \] \hspace{1cm} (3)

where \( k \) is the photon momentum vector. The polarization appears in a direction perpendicular to the plane of the reaction and photoelectrons are again transversely polarized.\textsuperscript{13,14}

Integrating Eqs. (1)–(3) over the angles of emergence of electrons, we find that in the case of linearly polarized and unpolarized light the total electron flux is unpolarized and in the case of circularly polarized light the degree of polarization of the total electron flux is given by the coefficient \( A^l \).

The highest degree of the transverse polarization of electrons formed as a result of absorption of linearly polarized light occurs for angles \( \beta \) between the vectors \( e \) and \( l \), given by

\[ \phi = \arccos \left( \frac{e \cdot l}{\|e\| \|l\|} \right) \] \hspace{1cm} (4)

and it may reach 100%. In the case of unpolarized light the highest degree of the transverse polarization corresponds to the following angle between the vectors \( k \) and \( l \)

\[ \phi = \arccos \left( \frac{e \cdot l}{\|e\| \|l\|} \right) \] \hspace{1cm} (5)

and it may reach \( 70\% \).

3. We can observe the polarization effects in the ionization of \( n^p \) subshells by dividing, in accordance with their energies, the photoelectrons corresponding to the final ion states \( 1\text{P}_{1/2} \) and \( 1\text{P}_{3/2} \). The difference between the energies of these states is 0.18 eV for Ar and 1.3 eV for Xe. In a narrow range between these ionization thresholds there is no need to separate the electrons in accordance with their energy. However, since the lower ionization threshold produces the \( 1\text{P}_{3/2} \) ion, it follows from the expressions for \( A^l \), \( \gamma^T \), and \( \lambda^T \) that the polarization effects in this range are half as strong as for the photoelectrons corresponding to the final ion state \( 1\text{P}_{1/2} \). The polarization effects in the range between the thresholds, where there is a series of autoionization states, were considered by Lee.\textsuperscript{11,12}

We shall give the results of a calculation of the coefficients \( A^l \), \( \gamma^T \), \( \lambda^T \), for \( J = 1 \)–1/2 carried out in the random phase approximation with exchange, as described in detail earlier.\textsuperscript{11,12} In the case of Ar, we allowed for the influence of the 3s\(^2\) and 2p\(^6\) electrons on the 3p\(^6\) subshell under consideration. The calculated values of the asymmetry of the angular distribution of \( \beta \) were in good agreement...
The dependence of the parameters $\beta$, $\alpha'$, $\gamma'$, and $\ell'$ on the photoelectron energy $\varepsilon$ for $J=1/2$ and the 3p subshell of Ar calculated in the random phase approximation with exchange. The points are the experimental results obtained in the determination of the parameter $\beta$ (Ref. 10).

Since it is difficult to generate circularly polarized light in the range of photon energies under consideration, we shall consider in greater detail the absorption of unpolarized and linearly polarized light (in the latter case, synchrotron radiation can be used). In both cases the polarization is governed by the coefficient $\gamma'$. We can see from Fig. 1 that this coefficient changes its sign twice. At the electron energy $\varepsilon=1.3$ Ry the change in the sign of $\gamma'$ is due to the change in the sign of the sine of the phase difference, whereas at $\varepsilon=2.45$ Ry there is a Cooper minimum of the cross section at which the matrix element $d_{1+}$ changes its sign. The good agreement between the calculated photoionization cross sections and the asymmetry coefficient $\gamma$ of the angular distribution with the experimental data suggests that the same matrix elements and phases are used in their calculation.

Figure 2 shows the dependence of the degree of polarization of photoelectrons on the photon energy in the case of unpolarized and linearly polarized light. The angles at which the degree of polarization in Fig. 2 is achieved are given by Eqs. (4) and (5).
at transferred energies of the order of a few tens of electron volts simulates very well the photoabsorption in the part of the spectrum where it is difficult to find high-power sources. Experiments of this type are based on the coincidence of fast electrons scattered through a small angle and suffering a fixed energy loss with a slow electron emerging at some angle \( \theta \).

The Born approximation can be used to describe the scattering of fast electrons and since the scattering through zero angle corresponds to small transferred momenta \( q \), the exponential function \( \exp(iq \cdot r) \) occurring in the Born amplitude can be expanded as a series and only the first nonvanishing term \( q 
abla r \cdot \mathbf{E} \) need be retained.\(^{111} \) This means that the inelastic scattering of fast electrons through zero angle is equivalent to the absorption of linearly polarized light. The degree of polarization of cell electrons is governed by Eq. (2), when we have to replace the polarization vector \( \mathbf{e} \) by a unit vector in the direction of the momentum \( q \), the exponential function \( \exp(iq \cdot r) \) occurs symmetrically in Eq. (2) and therefore, averaging-over the directions of the vector \( q \) (or in this case \( q \)), and also over the directions of the vector \( \mathbf{e} \), destroys the polarization effect. It follows that to observe polarization of slow electrons in the case of inelastic scattering of fast electrons through zero angle it is necessary to select conditions ensuring that the momentum \( q \) transferred to an atom is fixed in direction. Let \( E \) be the energy of a fast electron and \( \Delta E \) be the energy transferred to an atom, where \( \Delta E < E \). Then, \( |q| = \Delta E / (2E)^{1/2} \) and the scattering angle of a fast electron is \( \theta \propto q/p, \) where \( p \) is the momentum of the fast electron. We can ensure that the vector \( q \) is directed mainly from the vector \( p \), by satisfying the condition

\[
\Delta E = 10 \text{ keV}.
\]

For example, in Ref. 19 use is made of electrons of \( E = 10 \text{ keV} \). For \( \Delta E = 20 \text{ eV} \), we find that from Eq. (6) \( \theta < 10^{-5} \) whereas apparatus is available for measurements down to angles of \( \theta < 2 \times 10^{-4} \), which is quite satisfactory for the observation of the polarization of slow electrons.

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