ATOMIC THEORY METHODS FOR THE POLARIZATION IN PHOTON AND ELECTRON INTERACTIONS WITH ATOMS

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Received 20 February 2004
Dedicated to 100th anniversary of Professor A.Jucys

An alternative method to the density matrix formalism for the derivation of general expressions for the cross sections of the interaction of polarized atoms with polarized photons and electrons is presented. The expression for the cross section describing the polarization states of all particles taking part in the process are obtained in the form of the expansion via irreducible tensors that have the simplest possible behavior under changes of directions. The ways of the application of the general expressions suitable for the specific experimental conditions are outlined by deriving asymmetry parameters of the angular distributions of photoelectrons and Auger electrons following photoionization as well as the parameters of the angular correlations between photo- and Auger electrons.

Keywords: Photon interactions with atoms, Electron scattering
PACS: 32.80.-t, 34.80.-i

1. Introduction

In collision processes, the differential cross-section is simply a scalar with respect to the joint rotation of incoming and outgoing particles if neither the projection quantum numbers of the incident particle nor the target are resolved. For the derivation of expressions for the spectroscopic characteristics invariant under space rotation, the powerful methods of atomic theory and angular momentum were developed by A.Jucys and his coworkers [1, 2] in the case of the states of atoms described with complex configurations. These methods can be also applied for the study of the interaction of atoms with photons, electrons and other charged particles that is a powerful tool for the investigation of matter and interactions and have both theoretical and practical importance. In any atomic process, but particularly in collisions, energy, momentum and angular momentum are exchanged among the various constituents. All three of these quantities are conserved, and, in a classical theory, all three quantities may simultaneously have fixed values. Quantum states, however, cannot be simultaneously eigenstates of linear and angular momentum. If the state of linear momentum is fixed, as it usually is in collision experiments, then the angular momentum is not. Angular momentum is conserved, but the information about it cannot be used directly. The mean value of products of the components of angular momentum that are proportional to the parameters describing the orientation and alignment can be described. Just these products completely specify atomic states [3]. The measurement of the parameters of the alignment and orientation helps us to learn about the interchange of angular momentum in atomic collisions. Orientation and alignment parameters essentially characterize, respectively, the circulation of the atomic electron around the atomic core and the shape of the excited electron cloud and its direction in space. Orientation and alignment parameters thus allow us to go beyond the cross-section concept, in favorable cases leading to so called perfect scattering experiment,
in which the sets of quantum-mechanical scattering amplitudes and phases are completely determined \[4\].

The studies of the polarization phenomena in the interactions of atoms with charged particles and radiation stimulated the creation of new methods of the investigation of plasmas, ionized gaseous \[5\] and solids \[6\]. One of them is plasma polarization spectroscopy \[5\], since the majority of laboratory and astrophysical plasmas the electron-ion interaction is the dominate mechanism of the radiation emission. Measurements of the polarization of the spectroscopic characteristics of plasma provide a unique possibility for the diagnostics of electron and ion distribution function with high accuracy. The distortion of the Maxwellian distribution function or presence in plasma beams may play a substantial role for the formation of the emission spectra \[6\]. The deviations from the Maxwellian distribution of electrons were directly registered in laser produced \[7\], tokamak \[8\], vacuum spark \[9\] and astrophysical (Solar corona) \[10\] plasmas by observing the polarization of line spectra and continuous radiation. Polarization state of emission and absorption lines could be considered as the consequence of the polarization of atoms due to non equilibrium populations of magnetic sublevels or to ordering of angular momenta of atomic particles in plasma, that is called a self-alignment phenomena caused by the anisotropy properties of plasma sources.

Disentanglement of the geometrical aspects of anisotropy from the dynamical ones is another aspect of alignment and orientation. From the classical radiation theory, it follows that when light is observed, only the components of the source projected onto a plane perpendicular to the direction of observation are imaged. The source must be looked at from different angles to determine its complete electromagnetic configuration. This holds for any measurement of radiation. To see the complete source one must look at it from several angles. Irreducible tensors are selected for the description of polarization precisely because they have the simplest possible behavior under changes of direction (rotation) \[8\].

The experiments on free polarized atoms open up the possibility to disentangle the atomic and solid state effects \[11\]. Because of some atoms \[11, 12\] basic practical importance for the magnetic properties of multilayer systems and of ultra thin films on ferromagnetic substrates they are currently the focus of many investigations. The photoelectron spectroscopy, exploring linear and circular magnetic dichroism \[13\] yields detailed and site-specific information \[11, 12\]. Magneto-optical effects in the VUV and soft x-ray range are very important tool for the investigation of magnetic materials \[13\].

To derive expressions for the parameters suitable to characterize the polarization state in the photoionization of atoms, the density matrix formalism proposed by Fano and Macek \[14, 15\] has been widely used \[16–23\]. In this formalism the polarization state of atoms or ions was described by the statistical tensors (state multipoles) which were the basis for the expansion of atomic density matrix \[24\]. The methods of the density matrix became common, but the work by Fano and Macek \[15\] formulated a transparent method for the light emission in the decay of a stationary state of an atom following the excitation by collision with an electron or photon that used a complete set of mean values of measurable quantities instead of density matrix to characterize a state, thereby by passing the language of the density matrix \[8\]. The Wigner-Eckart theorem \[1\] was used to relate measured quantities to mean values of irreducible tensors constructed from angular momentum operators. In effect, these mean values were proportional to state multipoles, therefore, density matrix elements need never appear. Then the matrix element is expressed as a product of the reduced matrix element invariant under space rotation and the Clebsch-Gordon coefficient depending on the orientation in space.

A further development of the ideas of Fano and Macek \[15\] was accomplished by Kupliauskienė et al. \[25, 26\]. They have used the method based on the atomic theory \[11, 22, 27\] to derive the expressions for the photoionization cross-sections of polarized atoms by polarized radiation. The methods of the theory of an atom \[11, 22, 27\] usually were used to the isolated atom for the derivation of the expressions for the spectroscopic characteristics that are invariant under the rotation of the space. These characteristics were made independent on the magnetic components of the total angular momentum by
using the Wigner-Eckart theorem \[1\]. Then, the matrix element was expressed as a product of reduced matrix element that was invariant under space rotation and the Clebsch-Gordan coefficient depending on the orientation in space. But the Clebsch-Gordan coefficients in the expression for the probability or cross-section can be also used to construct the sums of the spherical tensors for the description of the orientation in space and rotation properties. Until the Vilnius theoreticians have started the application of the atomic theory methods for the investigation of the polarization in atoms \[25, 26\] there have been few applications of this method, and these have been restricted to the polarization parameters for special cases. Fano and Dill \[28\] have obtained the expression for the photoelectron angular distribution parameter $\beta$ expressed as a sum of incoherent contributions corresponding to the different magnitudes of the angular momentum transferred to an unpolarized target. The same method was extended by Klar \[18\] to the angular distribution of spin-polarized photoelectrons from unpolarized atoms. The expression for the angular distribution of Auger electrons following ionization by a beam of unpolarized electrons or protons was also derived without the help of density matrix by Cleff and Mehlhorn \[29\]. Therefore, the formulation of the polarization theory of atoms in general form based on the traditional technique of spherical tensors and wave functions is useful for people working in atomic theory.

The aim of the method based on the atomic theory approach was the derivation of the differential cross-section and parameters describing the interaction of polarized atoms with polarized radiation, electrons or other charged particles in the form of the multiple expansions over spherical tensors by using the graphical technique \[30–35\] for the integration over the angular and spin variables of the matrix elements of the transition operators. Any calculation made using the graphical technique can also be made using conventional algebraic technique \[31\]. To every graphical reduction there is a corresponding algebraic reduction because of the correspondence between graphs and algebraic formulas. However, the graphical method has two advantages over the algebraic methods: (a) the notation is more compact because the undetermined magnetic quantum numbers need not be written explicitly, and (b) reductions can be made by recognizing geometrical patterns. The graphical technique of angular momentum was proposed by Levinson \[30\] to obtain an expression for the reduced matrix element invariant under the rotation of space. The dependence of the matrix element on the magnetic quantum numbers was separated with the help of Wigner-Eckart theorem. In \[25, 26\], the graphical technique was extended to make it suitable for investigating the probability of the process depending on the mutual orientation of the particles participating in the process or on their orientation with respect to the chosen quantization axis.

The present work is devoted to the review of the applications of the alternative method to the density matrix formalism for the investigation of the excitation and ionization of polarized atoms and ions by polarized radiation, electrons and other charged particles with subsequent decay of the formed ions and atoms in two-step approximation. The general expressions for the cross-sections of the excitation of atoms by electrons as well as the radiative and dielectronic recombinations are derived and presented for the first time. The expression for the photoionization cross-section is also written in a more general form more convenient for the practical applications. The photon-atom interaction will be described in Section 2 where the excitation and ionization of polarized atoms by polarized photons as well as the modifications of the expressions for the probabilities or cross-sections in one- and multi-step approximation will be discussed. In Section 3, the electron-atom interactions (excitation and ionization of atoms and ions and radiative recombination) are considered. The radiative and Auger decay processes are described in Section 4. The two-step process – dielectronic recombination – is investigated in Section 5. Section 6 is devoted to demonstrate some applications of the general expressions for the specific experimental conditions. The review ends with concluding remarks that summarize the results and discuss the possibilities of the application of ordinary atomic theory for the
description of the polarization in photon-atom and electron-atom interactions.

2. Photon-atom interactions

2.1. Photoexcitation of atoms

The laser \[36\] and tunable synchrotron radiation allows one not only to ionize an electron of a specific outer or inner shell of an atom but also to excite it to a specific orbital \[37\], \[38\]. The state of the produced atom is polarized if the radiation is polarized. Thus, the excitation of atoms by polarized radiation is one of the ways to produce atoms in polarized states for further measurements \[39\], \[40\]. The photo excitation can be used as a first step to create a resonant state with well defined angular momentum and parity for further investigations of a polarization and angular correlation phenomena \[41\], \[23\].

The general expression for the excitation of polarized atoms by a polarized radiation was obtained \[42\] for the following process:

\[
A(\alpha_0J_0M_0) + h\nu(\hat{\epsilon}_\lambda k_0) \rightarrow A^*(\alpha_1J_1M_1).
\]

Here an atom \(A\) in the state \(\alpha_0J_0M_0\) is excited by the electromagnetic radiation into the state \(\alpha_1J_1M_1\), \(\alpha_0\) and \(\alpha_1\) define the configuration and other quantum numbers, \(J\) is the total angular momentum and \(M\) is its projection. The electromagnetic radiation is described with the wave vector \(\omega/c\) and momentum and parity for further investigations of a polarization and angular correlation phenomena \[41\], \[23\].

The differential cross section of the process (1) can be written as follows \[23\]:

\[
\frac{d\sigma(\alpha_0J_0M_0\hat{\epsilon}_\lambda k_0 \rightarrow \alpha_1J_1M_1)}{d\Omega} = 2\pi^2 \left[ \int \langle \alpha_1J_1M_1|\bf{J}(r)|\alpha_0J_0M_0 \rangle A_{\lambda k_0}(r)dr \right] \times \left[ \int \langle \alpha_1J_1M_1|\bf{J}(r)|\alpha_0J_0M_0 \rangle A_{\lambda k_0}(r)dr \right]^*.
\]

Here \(\bf{J}(r)\) stands for the operator of the current of electrons and \(A_{\lambda k_0}(r)\) is the operator of the vector potential of electromagnetic field. Taking into account that \(kr \ll 1\) and the case of an arbitrary direction of the incidence \(k_0\) of the photon, and inserting the multipole expansion for the \(A_{\lambda k_0}(r)\), the expression in the right brackets of Eq. (2) acquires the form \[23\]:

\[
\int \langle \alpha_1J_1M_1|\bf{J}(r)|\alpha_0J_0M_0 \rangle A_{\lambda k_0}(r)dr = \sum_{p=0,1} \sum_{k=1}^{\infty} \sum_{q=-k}^{q=k} i^k (-i\lambda)^p \left( \frac{k+1}{k} \right)^{1/2} \frac{k_0^{k-1/2}}{(2k-1)!!} D_{pq}^k(\hat{k}_0)
\]

\[
\times \langle \alpha_1J_1M_1|Q_{pq}^k|\alpha_0J_0M_0 \rangle = \sum_{k=1}^{\infty} \sum_{q=-k}^{q=k} \langle \alpha_1J_1M_1|Q_{pq}^k|\alpha_0J_0M_0 \rangle D_{pq}^k(\hat{k}_0),
\]

\[
\langle \alpha_1J_1M_1|Q_{pq}^k|\alpha_0J_0M_0 \rangle = k_0^{k-1/2} \sum_{p=0,1} \left( \frac{k+1}{k} \right)^{1/2} i^k (-i\lambda)^p \frac{k_0^{k-1/2}}{(2k-1)!!} \langle \alpha_1J_1M_1|Q_{pq}^k|\alpha_0J_0M_0 \rangle.
\]
Here $D_{q1}(\hat{k}_0)$ is the Wigner rotation matrix \[43\] for transforming from the helicity frame ($\hat{k}_0$ is the direction of incoming radiation) to the frame common to all particles participating in the process and used for the evaluation of reduced matrix elements. $p = 0$ indicates the operator of the electric multipole transition (E$k$) \[27\]

$$Q^0_{kq} = 1^k C_q^{(k)}$$

and, $p = 1$ shows the operator of the magnetic multipole transition (M$k$)

$$Q^1_{kq} = -\frac{1}{c}[k(2k - 1)]^{1/2}t^{k-1} \left\{ \frac{1}{k + 1} \left[ C^{(k-1)}_q \times L^{(1)}_q \right] + \left[ C^{(k-1)}_q \times S^{(1)}_q \right] \right\}.$$  \(6\)

Here $L^{(1)}$ and $S^{(1)}$ are the operators of the orbital and spin angular momentum, respectively, $C_q^{(k)}$ is the operator of the spherical function normalized to \[4\pi/(2k + 1)\] \[11\].

Note that the parities of the magnetic and electric multipole fields are $(-1)^k$ and $(-1)^{k+1}$, respectively. Only the magnetic (M$k$) and electric (E$k$) part contributes between specific electronic states owing to parity selection rules. Since we are considering pure photon states, there is no need to introduce Stokes parameters explicitly. In electrical dipole approximation, the matrix element (4) is as follows

$$\langle \alpha_1 J_1 M_1 | Q_q^{(1)} | \alpha_0 J_0 M_0 \rangle = \sqrt{2k_0} \langle \alpha_1 J_1 M_1 | Q^0_q | \alpha_0 J_0 M_0 \rangle.$$  \(7\)

The helicity $\lambda = \pm 1$ describes the right-hand and left-hand circular radiation. In the case of any polarization $\epsilon$, the polarization of radiation may be expressed via the circular polarization. Then

$$A_{\epsilon k_0}(r) = \alpha A_{\lambda = +1k_0}(r) + \beta A_{\lambda = -1k_0}(r)$$  \(8\)

that has to be inserted into Eq. (3) to obtain the expression for the excitation cross section (2).

Sometimes it is more convenient to analyze the polarization state of the particle with respect to the direction that differs from the one used for the calculation of the matrix element where all particles of the process (1) should be described in the same coordinate system and their projections of the angular momentum on the same quantization axis. For the transfer from the wave function $|JM\rangle$ defined in the laboratory fixed direction to the wave function $|J\hat{M}\rangle$ of the atomic frame used for the evaluation of reduced matrix elements, the coordinate rotation transformation \[43\] is used

$$|JM\rangle = \sum_{\hat{M}} D^J_{\hat{M}M}(\hat{J}) |J\hat{M}\rangle.$$  \(9\)

Here $D^J_{\hat{M}M}(\hat{J})$ denotes the Wigner rotation matrix \[43\], and the hat on $J$ indicates the rotation by solid angle that transforms the atomic frame into the laboratory one used for the polarization measurements of the characteristics depending on $J$. In the laboratory system of coordinates, the matrix element $\langle \alpha_1 J_1 \hat{M}_1 | Q_q^{(k)} | \alpha_0 J_0 M_0 \rangle$ can be written by taking into account Eq. (9) in the form:

$$\langle \alpha_1 J_1 M_1 | Q_q^{(k)} | \alpha_0 J_0 M_0 \rangle = \sum_{\hat{M}_0, \hat{M}_1, M_1} \langle \alpha_1 J_1 \hat{M}_1 | Q_q^{(k)} | \alpha_0 J_0 \hat{M}_0 \rangle D^J_{\hat{M}_0 \hat{M}_1}(\hat{J}_1) D^k_{\hat{M}_1 M_1}(\hat{J}_0) D^{sJ}_{\hat{M}_1 M_1}(\hat{J}_1).$$  \(10\)

The matrix element $\langle \alpha_1 J_1 \hat{M}_1 | Q_q^{(k)} | \alpha_0 J_0 \hat{M}_0 \rangle$ is defined in the atomic frame. The angular momentum part of this matrix element was obtained in \[42\] with the help of the graphical technique of the angular momentum \[11\]. The final expression for the excitation cross-sections is:

$$\frac{d\sigma(\alpha_0 J_0 M_0 \hat{e}_k \hat{k}_0 \rightarrow \alpha_1 J_1 M_1)}{d\Omega} = C \sum_{K_0, K_r, K_1, k, k'} \frac{1}{2K_1 + 1} A^r(K_0, K_r, K_1, k, k') \sum_{N_0, N_r, N_1} \left[ \begin{array}{ccc} K_0 & K_r & K_1 \\ N_0 & N_r & N_1 \end{array} \right]$$
\[ \times T^{sK_0}_{N_0}(J_0, J_0, M_0|\hat{J}_0) T^{sK_r}_{N_r}(k, k', q|\hat{k}_0) T^{K_1}_{N_1N_1'}(J_1, J_1, M_1, M_1|\hat{J}_1) \]  

where

\[ A'(K_0, K_r, K_1, k, k') = (\alpha_1 J_1||Q(k)||\alpha_0 J_0)(\alpha_1 J_1||Q(k')||\alpha_0 J_0)^* \left\{ \begin{array}{ccc} J_0 & K_0 & J_0 \\ k & K_r & k' \\ J_1 & K_1 & J_1 \end{array} \right\} \]

\[ \frac{((2J_0 + 1)(2J_1 + 1)(2k + 1)(2K_1 + 1))^{1/2}}{2}, \]

\[ T^{sK}_{N}(J, J', M|\hat{J}) = (-1)^{J'-M} \left[ \frac{4\pi}{2J+1} \right]^{1/2} \left[ \begin{array}{ccc} J & J' & K \\ M & -M & 0 \end{array} \right] Y^{sK}_{KN}(\theta, \phi), \]

\[ T^{K_1}_{N_1N_1'}(J_1, J_1', M_1, M_1'|\hat{J}_1) = (-1)^{J'-M_1} \left[ \frac{2K_1 + 1}{2J_1 + 1} \right]^{1/2} \left[ \begin{array}{ccc} J_1 & J_1' & K_1 \\ M_1 & M_1' & N_1' \end{array} \right] D^{sK_1}_{N_1N_1'}(\hat{J}_1). \]

In Eq. (12), the relation

\[ (\alpha_1 J_1||Q(k)||\alpha_0 J_0) = [2J_1 + 1]^{1/2}(\alpha_1 J_1||Q(k)||\alpha_0 J_0) \]

is taken into account. In Eq. (11), \( C = 2\pi^2 \). \( \hat{J} \) denotes the angles of \( \hat{J} \) with respect to the \( z \) axis of laboratory frame. In the case when hyperfine structure is important, the reduced matrix element \((\alpha_1 J_1||Q(k)||\alpha_0 J_0)\) should be changed by \((\alpha_1 J_1(I)F_1||Q(k)||\alpha_0 J_0(I)F_0)\) in Eq. (12). A simple relation between these two matrix elements holds:

\[ (\alpha_1 J_1(I)F_1||Q(k)||\alpha_0 J_0(I)F_0) = (-1)^{F_0 - J_1 + I + k' + [(2F_0 + 1)(2J_1 + 1)]^{1/2}} \times \left\{ \begin{array}{ccc} F_0 & k & F_1 \\ J_1 & I & J_0 \end{array} \right\} (\alpha_1 J_1||Q(k)||\alpha_0 J_0). \]

\( I \) is the spin of the nucleus. The values of \( J_0, J_1 \) in (11)–(15) should be changed by \( F_0, F_1 \). The probability \( W(\alpha_0 J_0 M_0 \hat{e}_q \hat{k}_0 \rightarrow \alpha_1 J_1 M_1) \) equals to the cross section (2) divided by the density of the flow of the radiation. Thus the same expression of the cross section can be used for the probability by changing only the definition of the constant \( C \).

### 2.2. Photoionization of atoms

The expression for the differential cross-section of the photoionization process

\[ A(\alpha_0 J_0 M_0 + h\nu(\epsilon_{q0} \hat{k}_0, \hat{e})) \rightarrow A^+(\alpha_1 J_1 M_1) + e^- (p_1, sm_s) \]

was derived by Kupliauskienë et al \[ 20 \] in the case of dipole approximation and the levels \( LS(J)IF \) of an atom. Here the ejected photoelectron has momentum \( p_1 \), and the projection of its spin \( s \) is indicated by \( m_s \).

In the case when the hyperfine structure is small and taking into account of all multipoles, the general expression for the differential cross-section of Eq. (17) can be written as follows:

\[ \frac{d\sigma(J_0 M_0 \hat{e}_q \hat{k}_0 \rightarrow J_1 M_1 p_1 m_s)}{d\Omega_{p_1}} = \pi \sum_{K_0, K_r, K_1, K_L, K_s, K_j, K_k, k_1'} B^{\phi h}(K_1, K_0, K_r, K_L, K_s, K_j, K_k, k_1') \times \sum_{N_0, N_r, N_1, N_L, N_s, N_j, N_k} \left[ \begin{array}{ccc} K_1 & K_j & K \\ N_1 & N_j & N \end{array} \right] \left[ \begin{array}{ccc} K_L & K_s & K_j \\ N_L & N_s & N_j \end{array} \right] \left[ \begin{array}{ccc} K_0 & K_r & K \\ N_0 & N_r & N \end{array} \right] T^{K_1}_{N_1N_1'}(J_1, J_1, M_1, M_1|\hat{J}_1) \times T^{sK_0}_{N_0}(J_0, J_0, M_0|\hat{J}_0) T^{sK_r}_{N_r}(k_1', k_1, q|\hat{k}_0) T^{K_s}_{N_s}(s, m_s|\hat{s}) \sqrt{4\pi} Y_{K_LN_L}(\hat{p}_1), \]

where
\[ B^{ph}(K_1, K_0, K_r, K_\lambda, K_s, K_j, K, k_1, k'_1) = \sum_{\lambda, j, j', j'} (2J + 1)(2J' + 1)(-1)^{j'} \times \begin{aligned} \langle \alpha_1 J_1 \varepsilon_1 \lambda(j) J | Q(k_1) | \alpha_0 J_0 \rangle \langle \alpha_1 J_1 \varepsilon_1 \lambda'(j') J' | Q(k'_1) | \alpha_0 J_0 \rangle^* \\ \times [(2J + 1)(2K_j + 1)((2J_1 + 1)(2K_1 + 1)(2s + 1)(2\lambda + 1)(2\lambda' + 1)(2j + 1)(2j' + 1)]^{1/2} \\ \times \left[ \begin{array}{ccc} \lambda & \lambda' & K_\lambda \\ 0 & 0 & 0 \end{array} \right] \left[ \begin{array}{ccc} J_0 & K_0 & J_0 \\ K_r & K' & J' \end{array} \right] \left[ \begin{array}{ccc} J_1 & K_1 & J_1 \\ K_s & K_s' & J_s \end{array} \right] \lambda \end{aligned} \] \( (\lambda, j, j', j') \). \tag{19} 

In the case of the photoionization as the first step process, the expression for the cross-section should be modified (see Section 2.3). It acquires the form:

\[ \frac{d\sigma_{K_1,N_1}(\alpha_0 J_0 M_0 \hat{e}_q k_0 \to \alpha_1 J_1 \hat{p}_1 m_s)}{d\Omega_{p_1}} = \pi \sum_{K_0, K_r, K_\lambda, K_s, K_j, K, k_1, k'_1} B^{ph}(K_1, K_0, K_r, K_\lambda, K_s, K_j, K, k_1, k'_1) \times \left[ \frac{2K_1 + 1}{2J_1 + 1} \right]^{1/2} \sum_{N_0, N_r, N_s, N_j, N_s} \left[ \begin{array}{ccc} K_1 & N_1 & K_j \\ K & N_j & N \end{array} \right] \left[ \begin{array}{ccc} K_\lambda & K_s & K_i \\ N_\lambda & N_s & N_s' \end{array} \right] \left[ \begin{array}{ccc} K_0 & N_0 & N_r \\ K & N_r & N \end{array} \right] \times T_{N_0}^{K_0}(J_0, M_0) T_{N_j}^{K_j}(k_1, k'_1, q) T_{N_s}^{K_s}(s, s, m_s) \sqrt{4\pi} Y_{K_1,N_1}(\hat{p}_1). \tag{20} \]

Further the general expressions (18)–(20) can be used to obtain some special expressions for specific experimental conditions also investigated by other authors with the help of the density matrix formalism, e.g., the expressions for the angular distribution and spin polarization of photoelectrons in the case of nonpolarized atom.

### 2.3. One- and multi-step processes

The excitation or ionization of an atom by laser or other electromagnetic radiation often is used to prepare it in a polarized state for further investigation. Then the magnetic state of an atom or ion in the final state \( J_1 M_1 \) is not observed, and summation of \( M_1 \) has to be performed coherently. In this case, the excitation (1) is the first step of the multi-step process while the second step is

\[ A^*(\alpha_1 J_1 M_1) + b(\alpha) \rightarrow A(\alpha_2 J_2 M_2) + b'(\alpha'). \tag{21} \]

Here \( b(\alpha) \) stands for impacting particle or electromagnetic radiation in the state \( \alpha \) and \( b'(\alpha') \) indicates ionized and emitted one or more particles. In two-step approximation, the probability of both processes (1) and (21) can be written as coherent sum since the projection \( M_1 \) cannot be observed \( 15 \):

\[ W(\alpha_0 J_0 M_0 \hat{e}_k k_0 \to \alpha_1 J_1 \alpha \to \alpha_2 J_2 M_2 \alpha') = C' | \sum_{M_1} \langle \alpha_2 J_2 M_2 \alpha' | H_2 | \alpha_1 J_1 M_1 \alpha \rangle \langle \alpha_1 J_1 M_1 | H_1 | \alpha_0 J_0 M_0 \rangle |^2 \]

\[ = C' | \sum_{M_1, M'_1} \langle \alpha_2 J_2 M_2 \alpha' | H_2 | \alpha_1 J_1 M_1 \alpha \rangle \langle \alpha_2 J_2 M_2 \alpha' | H_2 | \alpha_1 J_1 M'_1 \alpha \rangle^* \times \langle \alpha_1 J_1 M_1 | H_1 | \alpha_0 J_0 M_0 \rangle \langle \alpha_1 J_1 M'_1 | H_1 | \alpha_0 J_0 M_0 \rangle^* \rangle. \tag{22} \]

The matrix elements in Eq. (22) are defined similar to Eq. (10) allowing the measurement in the direction different from that used for evaluation. \( H_1 \) and \( H_2 \) are the operators of the interaction in the
Auger decay, it is presented by Kupliauskienė and Tutlys (see Eq. (4) in [45]).

The expression for the second term in Eq. (25) depends on the second-step process. In the case of the first and second processes, respectively. Then the product of two Wigner rotation matrices coming up from the matrix element and its complex conjugate in Eq. (22) should be replaced by

\[
D_{M_1 M_1'}^{J_1}(\hat{J}_1)D_{M_1' M_1}^{* J_1'}(\hat{J}_1) = \sum_{K_1 N_1, N_1'} \left[ J_1' \begin{array}{ccc} \hat{K}_1 & J_1 & K_1 \\ N_1 & M_1 \end{array} \right] T_{N_1 N_1'}^{* K_1}(J_1, J_1', M_1, M_1', \hat{J}_1),
\]

and the summation over \(M_1\) and \(M_1'\) in Eq. (22) is possible to be carried out. From the examination of the expressions (29) in [14] and (11) and (18) of the present work for both terms in Eq. (22) it follows that only the tensors \(T_{N_1 N_1'}^{K_1}(J_1, J_1', M_1, M_1'|\hat{J}_1)\) depend on \(M_1\) and \(M_1'\). The sum over \(M_1, M_1'\) of the product of these tensors is equal to

\[
\sum_{M_1, M_1'} T_{N_1 N_1'}^{K_1}(J_1, J_1, M_1, M_1'|\hat{J}_1) T_{N_1 N_1'}^{* K_1}(J_1, J_1, M_1, M_1'|\hat{J}_1)
\]

\[
= \frac{(2K_1 + 1)(2K_1' + 1)}{2J_1 + 1} D_{N_1 N_1'}^{K_1}(\hat{J}) D_{N_1 N_1'}^{* K_1'}(\hat{J}) \sum_{M_1, M_1'} (-1)^{2J_1 - 2M_1'} \left[ J_1 \begin{array}{ccc} \hat{K}_1 & J_1 & K_1 \\ N_1 & M_1 \end{array} \right] \left[ J_1' \begin{array}{ccc} \hat{K}_1' & J_1' & K_1' \\ N_1' & M_1' \end{array} \right]
\]

Then the quantization axis can be chosen along the \(z\) axis of the laboratory coordinate system, and the sum over \(M_1, M_1'\) in Eq. (22) is changed by the sum over \(K_1, N_1\), i.e. the probability of the two-step process is expanded as the sum of state multipoles. For example, the expressions for the photoexcitation probability (11) and that of the second process slightly change. For the excitation probability, it is

\[
W(\alpha_0 J_0 M_0 \hat{c}_0 k_0 \rightarrow \alpha_1 J_1 \alpha_2 J_2 M_2 \alpha') = \sum_{K_1, N_1} W_{K_1 N_1}(\alpha_0 J_0 M_0 \hat{c}_0 k_0 \rightarrow \alpha_1 J_1) \cdot W_{K_1 N_1}^A(\alpha_1 J_1 \alpha_2 J_2 M_2 \alpha').
\]

Here the sum over \(M_1, M_1'\) in Eq. (22) is changed by the sum over \(K_1, N_1\), i.e. the probability of the two-step process is expanded as the sum of state multipoles. For example, the expressions for the photoexcitation probability (11) and that of the second process slightly change. For the excitation probability, it is

\[
W_{K_1 N_1}(\alpha_0 J_0 M_0 \hat{c}_0 k_0 \rightarrow \alpha_1 J_1) = \frac{C}{[2J_1 + 1]^{1/2}} \sum_{K_0, K_r, k, k'} B^r(K_0, K_r, K_1, k, k') \sum_{N_0, N_r, q} \left[ \begin{array}{ccc} K_0 & K_r & K_1 \\ N_0 & N_r & N_1 \end{array} \right] 
\]

\[
\times T_{N_0}^{* K_0}(J_0, J_0, M_0 | \hat{J}_0) T_{N_r}^{K_r}(k, k', q | \hat{k}_0),
\]

\[
W_{00}(\alpha_0 J_0 k \rightarrow \alpha_1 J_1) = \frac{C}{(2J_0 + 1)(2k + 1)[2J_1 + 1]^{1/2}} |\langle \alpha_1 J_1 | Q^{(k)} | \alpha_0 J_0 \rangle |^2.
\]

The expression for the second term in Eq. (25) depends on the second-step process. In the case of the Auger decay, it is presented by Kupliauskiene and Tutlys (see Eq. (4) in [15]).

The proposed method is easy to generalize for multistep process when intermediate states are not observed. In the case of tree-step process where the fluorescence radiation of the doubly charged ion formed following the photoionization of an atom and Auger decay of the singly charged ion is registered, the summation over intermediate states gives

\[
\sum_{M_1, M_1', M_2, M_2'} W^1(J_0 M_0 k_1 \rightarrow J_1 M_1 M_1' p_1 m_1) W^2(J_1 M_1 M_1' p_1 m_1 \rightarrow J_2 M_2 M_2' p_2 m_2) 
\]

\[
\times W^3(J_2 M_2 M_2' p_2 m_2 \rightarrow J_3 M_3 k_2)
\]
interaction. If the excitation of atoms by electrons is used as the first step process for the preparation

then the summation over \( \sum \) is as follows:

The square root of each multiple \((2K + 1)/(2J + 1)\) in Eq. (28) is also convenient to attribute to both neighbouring terms.

3. Electron-atom interactions

3.1. Excitation of atoms by electrons

The process of the excitation of polarized atoms by polarized electrons can be written as follows:

\[
A(\alpha_0 M_0) + e^{-}(p_0 m_0) \rightarrow A(\alpha_1 M_1) + e^{-}(p_1 m_1).
\] (29)

The expression for the differential cross-section of the process (29) is easy to obtain by the method described in \[20, 44\] and is as follows:

\[
\frac{d^2 \sigma(\alpha_0 M_0 p_0 m_0 \rightarrow \alpha_1 M_1 p_1 m_1)}{d\varnothing d\Omega_1} = 4\pi C \sum_{K, K_0, K_0', K_{\lambda 0}, K_{s 0}, K_1} B^{ex}(K_0, K_0', K_1, K_{\lambda 1}, K_{s 1}, K)
\]

\[
\times \sum_{N_0, N_0', N_{\lambda 0}, N_{s 0}, N_1} \left[ \begin{array}{ccc} K_{\lambda 0} & K_{s 0} & K_{s 0}' \\ N_{\lambda 0} & N_{s 0} & N_0 \\ K \\ \end{array} \right] \left[ \begin{array}{ccc} K_0 & K_0' & K \\ N_0 & N_0' & N_1 \\ K_1 & K_{s 1} & K_{s 1}' \\ \end{array} \right] Y_{K_{\lambda 0} N_{\lambda 0}}(\hat{p}_0) Y_{K_{s 1} N_{s 1}}(\hat{p}_1)
\]

\[
\times T^{*}_{N_0}(J_0, M_0, \hat{J}_0) T^{*}_{N_1}(J_1, M_1, \hat{J}_1) T^{*}_{N_0}(s, s, m_0, \hat{s}) T^{*}_{N_1}(s, s, m_1, \hat{s})
\] (30)

\[
B^{ex}(K_0, K_0', K_1, K_{\lambda 0}, K_{s 0}, K_{\lambda 1}, K_{s 1}, K) = \sum_{\lambda_0, \lambda_0', \lambda_1, j_0, j_0', j_1, j_1'} (2J + 1)(2J' + 1)(2K + 1)(2s + 1)(-1)^{\lambda_0 + \lambda_1}
\]

\[
\times (\alpha_1 J_1, \varepsilon_1 \lambda_1 (j_1) J || H || \alpha_0 J_0, \varepsilon_0 \lambda_0 (j_0) J) (\alpha_1 J_1, \varepsilon_1 \lambda_1 (j_1') J' || H || \alpha_0 J_0, \varepsilon_0 \lambda_0 (j_0') J')^*
\]

\[
\times ((2 \lambda_0 + 1)(2 \lambda_0' + 1)(2 \lambda_1 + 1)(2 \lambda_1' + 1)(2 j_0 + 1)(2 j_0' + 1)(2 j_1 + 1)(2 j_1' + 1)
\]

\[
\times (2 J_0 + 1)(2 J_1 + 1)(2 K_0 + 1)(2 K_1 + 1) \right)^{1/2} \left[ \begin{array}{ccc} \lambda_0 & \lambda_0' & K_{\lambda 0} \\ 0 & 0 & 0 \\ \end{array} \right] \left[ \begin{array}{ccc} \lambda_1 & \lambda_1' & K_{\lambda 1} \\ 0 & 0 & 0 \\ \end{array} \right]
\]

\[
\times \left\{ \begin{array}{l} J_0 \\ j_0' \\ \end{array} \right\} \left\{ \begin{array}{l} K_0 \\ K_{\lambda 0} \\ j_0 \\ \end{array} \right\} \left\{ \begin{array}{l} K_0' \\ s \\ j_0' \\ K \\ \end{array} \right\} \left\{ \begin{array}{l} \lambda_0' \\ K_{\lambda 0} \\ j_0 \\ \end{array} \right\} \left\{ \begin{array}{l} \lambda_0 \\ K_{\lambda 0} \\ j_0' \\ \end{array} \right\} \left\{ \begin{array}{l} J_1 \\ j_1' \\ \end{array} \right\} \left\{ \begin{array}{l} K_1 \\ K_{\lambda 1} \\ j_1 \\ K \\ \end{array} \right\} \left\{ \begin{array}{l} J_1' \\ j_1 \\ \end{array} \right\}.
\] (31)

In Eq. (31), \(\alpha_1 J_1, \varepsilon_1 \lambda_1 (j_1) J || H || \alpha_0 J_0, \varepsilon_0 \lambda_0 (j_0) J\) is the reduced matrix element of the electrostatic interaction. If the excitation of atoms by electrons is used as the first step process for the preparation of atoms in polarized excited states for the next step process, the projections \(M_1\) are not registered. Then the summation over \(M_1\) should be performed following the recommendations of Section 2.3.
3.2. Ionization of atoms by electrons

If neither the projection quantum numbers of the incident electron nor the target are resolved, the differential cross-section for the ionization of atoms by electrons is simply a scalar with respect to the joint rotation of the incoming and outgoing electron momenta \( \mathbf{p}_0, \mathbf{p}_1, \) and \( \mathbf{p}_2, \) respectively. This basic symmetry is destroyed by an initial orientation and/or alignment of the target, and can supply more information about the elementary processes in such diverse fields as discharge and plasma physics [37], fusion physics [3], and the physics and chemistry of the upper atmosphere [45]. For the interpretation of recently measured ionization cross-sections of polarized Na atoms [48, 49], the expressions enabling one to describe the polarization states of all particles taking part in the process are necessary.

Recently the general expression for the description of the ionization of polarized atoms by polarized electrons

\[
A(\alpha_0 J_0 M_0) + e^- (p_0 m_0) \rightarrow A^+(\alpha_1 J_1 M_1) + e^- (p_2 m_2) + e^- (p_1 m_1).
\]  

was obtained by Kupliauskienė and Glemza [46]. In Eq. (32), \( p_i \) denotes the momentum of the electron in the initial \( (i = 0) \) and final \( (i = 1, 2) \) states, \( m_i \) indicates the projection of an electron spin. The fine structure splitting was assumed larger than hyperfine one. The expression for the cross-section was derived by using the graphical technique of the angular momentum [11] and is as follows:

\[
\frac{d^3 \sigma(\alpha_0 J_0 M_0 \rightarrow \alpha_1 J_1 M_1 p_2 m_2 p_1 m_1)}{d \varepsilon_2 d \Omega_1 d \Omega_2} = C(4\pi)^{3/2} \sum_{K, K_0, K'_0, K_{s0}, K, K_1, K', K_{\lambda1}, K_{s1}, K_{\lambda2}, K_{s2}} \mathcal{B}^{\text{ion}}(K_0, K_0', K, K_{s0}, K_1, K', K_{\lambda1}, K_{s1}, K_{\lambda2}, K_{s2})
\]

\[
\times \left[ \begin{array}{c} K' \\ N' \\ \end{array} \right] \left[ \begin{array}{c} K_1 \\ N_1 \\ \end{array} \right] \left[ \begin{array}{c} K' \\ N' \\ \end{array} \right] \left| \phi_{K_{\lambda2}N_{\lambda2}}(\hat{p}_2) \right| T_{N_{s1}}^{K_1}(s, s, m_1|\hat{s}) T_{N_{s2}}^{K_2}(s, m_2|\hat{s}), \]

\[
\mathcal{B}^{\text{ion}}(K_0, K_0', K, K_{s0}, K_1, K', K_{\lambda1}, K_{s1}, K_{\lambda2}, K_{s2}) = \sum_{\lambda_0, \lambda'_0, \lambda_1, \lambda'_1, \lambda_2, \lambda'_2, j_0, j'_0, j_1, j'_1, j_2, j'_2, J, j, j'}
\]

\[
\times (2J + 1)(2J' + 1)(2K + 1)(2s + 1)(-1)^{\lambda_0 + \lambda'_0 + \lambda'_1}
\]

\[
\times \langle \alpha_1 J_1, \varepsilon_2 \lambda_2(j_2) \varepsilon_1 \lambda_1(j_1)|j, J||H||\alpha_0 J_0, \varepsilon_0 \lambda_0(j_0)J \rangle
\]

\[
\times \langle \alpha_1 J_1, \varepsilon_2 \lambda'_2(j'_2) \varepsilon_1 \lambda'_1(j'_1)|j', J'||H||\alpha_0 J_0, \varepsilon_0 \lambda'_0(j'_0)J' \rangle^*
\]

\[
\times [(2s + 1)(2\lambda_0 + 1)(2\lambda'_0 + 1)(2\lambda_1 + 1)(2\lambda'_1 + 1)(2\lambda_2 + 1)(2\lambda'_2 + 1)(2j_0 + 1)(2j'_0 + 1)
\]

\[
\times (2j_1 + 1)(2j'_1 + 1)(2j_2 + 1)(2j'_2 + 1)(2j + 1)(2j' + 1)(2J_0 + 1)(2J_1 + 1)(2K'_0 + 1)(2K'_1 + 1)
\]

\[
\times (2K' + 1)(2K'_2 + 1)^{1/2} \left[ \begin{array}{c} \lambda_0 \\ \lambda'_0 \\ K_{s0} \\ \end{array} \right] \left[ \begin{array}{c} \lambda_1 \\ \lambda'_1 \\ K_{s1} \\ \end{array} \right] \left[ \begin{array}{c} \lambda_2 \\ \lambda'_2 \\ K_{s2} \\ \end{array} \right]
\]

\[
\times \left\{ \begin{array}{c} J_0 \\ J'_0 \\ K \\ \end{array} \right\} \left\{ \begin{array}{c} s \\ s \\ j_0 \\ j'_0 \end{array} \right\} \left\{ \begin{array}{c} \lambda_0 \\ \lambda_0 \\ K_{s0} \\ \end{array} \right\} \left\{ \begin{array}{c} J_1 \\ K_{s1} \\ \end{array} \right\} \left\{ \begin{array}{c} \lambda_1 \\ \lambda_1 \\ K_{s1} \\ \end{array} \right\}
\]

\[
\left\{ \begin{array}{c} \lambda_2 \\ \lambda_2 \\ K_{s2} \\ \end{array} \right\} \left\{ \begin{array}{c} j_1 \\ j'_1 \\ K'_1 \\ \end{array} \right\} \left\{ \begin{array}{c} J_2 \\ j_2 \\ j'_2 \end{array} \right\} \left\{ \begin{array}{c} \lambda_0 \\ \lambda_1 \\ \lambda_2 \\ \end{array} \right\}
\]
The reduced matrix element of the electrostatic interaction in Eq. (34) is defined in [2]. In the case of the inner-shell ionization of atoms, the state of the ion is not stable and decays via radiative or Auger transition. Then the expression (33) should be modified following the recommendations of Section 2.3 as it was pointed out in the Section 2.2.

The expression (33) for the electron-impact ionization can be also used for the investigation of the ionization of atoms by protons and highly charged ions. Then the expressions for the cross-section of the creation of a vacancy in the outermost closed shell of atoms containing one valence electron, the

\[\sigma_{rr}^{eq}(E_0) = \frac{(\alpha E_1)^2}{2E_0} \frac{g_i}{g_f} \sigma_{i \rightarrow f}^{ph}(E_1).\]

Here \(E_0\) and \(E_1\) are the energy of an electron and emitted photon, respectively, \(g_i\) and \(g_f\) are the statistical weights of the initial and final states, \(\alpha\) is the fine structure constant and \(E_1 = E_0 + I_p\) (\(I_p\) is the ionization energy). Then the general expression for the differential radiative recombination cross-section can be written in the form by using Eq. (18):

\[
d\sigma(J_0 M_0 p_1 m_s \rightarrow J_1 M_1 \hat{e}_q k_{01})
\]

\[
= C\sqrt{4\pi} \sum_{K_0,K_r,K_1,K_s,K_j,K,k_1,k_1'} B^{ph}(K_0, K_1, K_r, K_\lambda, K_s, K_j, K, k_1, k_1') \\
\times \sum_{N_0, N_r, N_1, N_s, N_j, N} \left[ \frac{K_0}{N_0} \frac{K_j}{N_j} \frac{K}{N} \right] \left[ \frac{K_\lambda}{N_\lambda} \frac{K_s}{N_s} \frac{K_j}{N_j} \right] \left[ \frac{K_1}{N_1} \frac{K_r}{N_r} \frac{K}{N} \right] Y^{*}_{K_\lambda,N_\lambda}(\hat{p}_1) T^{sK_0}_{rN_0}(J_0, J_0, M_0, J_0) \\
\times T^{K^r}_{N_r}(k_1', k_1', q_1 | \hat{k}_{01}) T^{sK_1}_{N_s}(s, s, m_s | s) T^{K_1}_{N_1N_1'}(J_1, J_1, M_1, M_1') \hat{J}_1. \tag{37}
\]

Here \(C = (\pi \alpha^2 E_1^2)/E_0\).

If a recombined ion arises in excited state, it can suffer the radiative decay to a lower excited or ground state by emitting a photon. The polarization state of this photon depends on the states of the ion and electron. For the description of the polarization characteristics of the second photon, the expression for the radiative recombination cross-section as that of the first-step process is necessary. It may be obtained following the recommendations of Section 2.3.

### 3.3. Radiative recombination

The process of the radiative recombination of polarized ions with polarized electrons can be written as follows:

\[A^{n+}(\alpha_0 J_0 M_0) + e^- (p_0 m_0) \rightarrow A^{(n-1)+}(\alpha_1 J_1 M_1) + h\nu (e_q k_0).\]  

From the relation of detailed balance, it follows that the cross-section of the radiative recombination \(\sigma_{rr}^{eq}(E_0)\) is related to the cross-section of the photoionization \(\sigma_{i \rightarrow f}^{ph}(E_1)\) through detailed balance (Milne relation) as

\[\sigma_{rr}^{eq}(E_0) = \frac{(\alpha E_1)^2}{2E_0} \frac{g_i}{g_f} \sigma_{i \rightarrow f}^{ph}(E_1).\]

### 4. Decay of excited atoms

In the case of the registration of the decay products of formed ion, much information can be gained not only about the structure of the system under investigation but also about the process itself and many body interactions. Here the Auger decay process is often used [51]. But in the case of the creation of a vacancy in the outermost closed shell of atoms containing one valence electron, the
radiative transition is only way of its decay. The fluorescence and Auger decay of an excited ion or atom are the processes of the second step following inner-shell excitation or ionization of the atom. In the present section, the expressions for the radiative and Auger decay as the second step process will be presented. These expressions were obtained by applying atomic theory methods \[2, 27\] and the graphical technique of the angular momentum \[1\].

4.1. Radiative decay

The radiative decay of an atom or ion is the inverse process to the photoexcitation and can be written in the form:

\[ A(\alpha_1 J_1 M_1) \rightarrow A(\alpha_2 J_2 M_2) + h\nu(q_{k02}) \].

The general expression for the probability of the fluorescence following the photoionization of polarized atoms was obtained by Kupliauskiene and Tutlys \[52\]. In the case of fluorescence as the second step process, the initial state \( M_1 \) is not registered. Then, the expression for the radiative transition probability is as follows:

\[
\frac{dW^{r}_{K_{1}N_{1}}(\alpha_{1}J_{1} \rightarrow \alpha_{2}J_{2}M_{2}q_{k02})}{d\Omega_{2}} = C \sum_{K_{1}^{'},K_{2},k_{2},K_{2}'} A(K_{1},K_{1}^{'},K_{2},k_{2},K_{2}')
\times \sum_{N_{1}',N_{2}} \left[ \begin{array}{ccc} K_{1} & K_{1}' & K_{2} \\ N_{1} & N_{1}' & N_{2} \end{array} \right] T_{N_{2}}^{K_{2}}(J_{2},J_{2},M_{2}|J_{2}) T_{N_{1}'}^{K_{1}'}(k_{2},k_{2}',q_{2}|k_{02}) \right] \right) \right]^{1/2} \left\{ \begin{array}{c} J_{1} \\ k_{2} \\ K_{1} \\ J_{2} \end{array} \right\} \left\{ \begin{array}{c} K_{1}' \\ J_{2} \\ k_{2}' \\ K_{2} \end{array} \right\} \right\} \right].
\]

The reduced matrix element in (40) is equal to

\[
(\alpha_{2}J_{2}||Q^{(k2)}||\alpha_{1}J_{1}) = (2J_{2} + 1)^{1/2}q_{k02}(\alpha_{2}J_{2}||Q^{(k2)}||\alpha_{1}J_{1})
\]

and is defined by Eq. (4). The constant \(C = 1/(2\pi)\).

4.2. Auger decay

 Usually Auger decay is the second step process

\[ A^{+}(\alpha_{1}J_{1}M_{1}) \rightarrow A^{2+}(\alpha_{2}J_{2}M_{2}) + e^{-}(p_{2}, m_{s}') \]

following inner-shell excitation or ionization of atoms and ions. The general expression for the probability of Eq. (42) was obtained by Kupliauskiene and Tutlys \[46, 47\] in the case when the Auger transition follows the photoionization of an atom.

When the state of the intermediate ion is not registered, the Auger transition probability acquires the form \[45\]:

\[
\frac{dW_{K_{1}N_{1}}(\alpha_{1}J_{1} \rightarrow \alpha_{2}J_{2}p_{2}m_{s}')}{d\Omega_{2}} = \sum_{K_{1}',K_{2},K_{1}'} A^{A}(K_{1},K_{2},K_{1}',K_{1}') \sum_{N_{1}',N_{2},N_{1}',N_{2}'} \left[ \begin{array}{ccc} K_{1}' & K_{1}' & K_{1} \\ N_{1}' & N_{1}' & N_{2} \end{array} \right] \left[ \begin{array}{ccc} K_{2} & K_{2}' & K_{1} \\ N_{2} & N_{1}' & N_{2} \end{array} \right] T_{N_{2}}^{K_{2}}(J_{2},J_{2},M_{2}|J_{2}) T_{N_{1}'}^{K_{1}'}(s,s,m_{s}'|s) \right\}
\]

\[
\right\} \sqrt{4\pi Y_{K_{1}'}N_{1}'}(\theta_{2},\phi_{2})
\]

where

\[
A^{A}(K_{1},K_{2},K_{1}',K_{1}',K_{1}') = 2\pi \sum_{\lambda_{1}J_{1},\lambda_{2}J_{2}} \langle \alpha_{2}J_{2}\epsilon_{2}\lambda_{1}(j_{1})J_{1}||H||\alpha_{1}J_{1} \rangle \langle \alpha_{2}J_{2}\epsilon_{2}\lambda_{2}(j_{2})J_{2}||H||\alpha_{1}J_{1} \rangle^{*}
\]
5. Dielectronic recombination

The process of dielectronic recombination (DR) can be written as follows

\[ A^+(\alpha_0 J_0 M_0) + e^- (p_0 m_0) \rightarrow A^{**}(\alpha_1 J_1) \{ \rightarrow A(\alpha_2 J_2 M_2) + h\nu (\epsilon_{q_2}, k_{02}), \quad \rightarrow A^+(\alpha_3 J_3 M_3) + e^- (p_1 m_1). \] (45)

It is an example of a two-step process. The first step is resonant electron capture. The next step is radiative or Auger decay that were described in Section 4. Two-step approximation for DR may be applied if the interference with the radiative recombination is neglected and the summation over intermediate states \( J_1 M_1 \) that usually occurs in second-order perturbation theory, is limited to a single resonance. Then, only a summation over the magnetic substates that are not registered is retained. DR process is finished when the photon is emitted.

In two-step approximation (see Section 2), the cross-section for DR may be written as:

\[
\frac{d\sigma(\alpha_0 J_0 M_0 p_0 m_0 \rightarrow \alpha_1 J_1 \rightarrow \alpha_2 J_2 M_2 \epsilon_{q_2} k_{02})}{d\Omega} = 2\pi \sum_{M_1, M'_1} \langle \alpha_2 J_2 M_2 \epsilon_{q_2} k_{02} | H' | \alpha_1 J_1 M_1 \rangle \langle \alpha_2 J_2 M_2 \epsilon_{q_2}, k_{02} | H' | \alpha_1 J_1 M'_1 \rangle^* \\
\times \langle \alpha_1 J_1 M_1 | H^e | (\alpha_0 J_0 M_0 p_0 m_0) \rangle \langle \alpha_1 J_1 M'_1 | H^e | (\alpha_0 J_0 M_0 p_0 m_0) \rangle^* \times [(E - E_1)^2 + \Gamma^2/4]^{-1}. \] (46)

Here \( H' \) and \( H^e \) is the radiative decay and electrostatic interaction operators, respectively, \( d\Omega \) is the solid angle of the emission of radiation, \( E_1 \) and \( E \) is the energy of the intermediate and initial state of the system atom+electron, respectively, and \( \Gamma \) denotes the decay width of the intermediate state that includes both radiative and nonradiative decay channels.

In two step approximation \( (E \approx E_1) \), the general expression for DR (46) in the case of the interaction of a polarized ion with a polarized electron may be obtained by applying the methods described in [26, 45] and is as follows:

\[
\frac{d\sigma(\alpha_0 J_0 M_0 p_0 m_0 \rightarrow \alpha_1 J_1 \rightarrow \alpha_2 J_2 M_2 \epsilon_{q_2} k_{02})}{d\Omega} = \frac{2\pi}{p_0^2} \sum_{K_1, N_1} W_{K_1, N_1} W_{K_1, N_1}^c \left( \frac{(E - E_1)^2 + \Gamma^2/4}{4} \right)^{-1}. \] (47)

The resonant electron capture cross-section \( W^c \) is reversed to that of Auger decay and is defined by Eq. (43). The expression for the radiative decay probability \( dW^r/d\Omega \) is the same as in Eq. (39).

The DR process is similar to that of resonant electron transfer and excitation (RTE). When highly charged ions interact with low-Z atoms, the differential cross-section for RTE may be determined by using the cross-section of DR and momentum approximation for the distribution of electron charge in the atom [53, 54]. Angular distribution of radiation emitted after RTE in collisions of nonpolarized
U^{90+} with a graphite target was investigated in [55]. The process of DR with emission of two and more photons was also treated both in nonrelativistic [56] and fully relativistic [57] approximations.

6. Practical applications

General expression for the differential cross section and probability of the excitation and ionization of polarized atoms and ions by polarized electrons or radiation can be used to obtain many more simple expressions applicable for specific experimental conditions. The authors who used the density matrix formalism to derive the expressions for various parameters describing the polarization usually started from the very beginning by formulating the problem dealing the specific experiment. Below a limited number of the most important papers are reviewed.

In the case of the photoionization of polarized atoms by polarized radiation, Jacobs [16] obtained the general expression for the differential cross-section, the asymmetry parameters $\beta$ of the angular distribution and $\gamma$, $\delta$ and $\xi$ for the spin polarization of photoelectrons. The statement that the photoion was not detected was assumed from the very beginning. The angular distribution of photoelectrons from nonpolarized atoms was investigated in [58, 59]. The investigation of the angular distribution of photoelectrons with specific spin orientation in the case of nonpolarized atoms by polarized dipole radiation was carried out by Cherepkov [60]. General expression for the angular distribution and polarization of photoelectrons from nonpolarized atoms in the region of autoionizing states was obtained in [17]. Here the photons of any multipolarity were treated. Later on, the expressions for the cross-sections and asymmetry parameters for the angular distribution of photoelectrons from polarized atoms exposed to polarized radiation in both resonant [20] and nonresonant [18, 13] case were obtained. These expressions also found their applications for the investigation of magnetic dichroism in the angular distributions of photoelectrons [61]. Recently, dramatic nondipole effects in low-energy photoionization were discovered both theoretically and experimentally [62].

Much larger number of papers is devoted to the investigation of Auger and fluorescence decay of atoms following ionization by electrons and photons. In 1972 and 1974, three papers presented calculations on angular distributions of ionized atom decay products. The polarization of characteristic radiation excited by electron impact [65] and angular distribution of Auger electrons following photoionization [66, 29] were calculated did not applying the density matrix formalism. Later on, Kabachnik and coworkers [17, 67, 68, 69, 70, 41, 71], Lohman et al [72, 73] and Bartschat and Grum-Grzhimailo [74] obtained numerous expressions describing the angular distribution and spin polarization of Auger electrons for various specific experimental conditions. As the expressions were hinted to the applications of noble gaseous the initial state of the atom was considered randomly orientated. The atoms could be ionized by polarized dipole photons [67] or nonpolarized electrons [51, 68, 72, 73]. Angular distribution of Auger electrons ejected by electron-impact from laser-excited and polarized atoms was described in [70]. A resonant cascade model based on a stepwise approach was suggested [41] for the analysis of the angular correlation in the decay of core-excited resonances produced by photoabsorption. The model was applied to the description of angular distributions of Auger electrons and fluorescence.

The alignment of atoms and ions in radiative electron capture (REC) into ground and excited states of ions is recently formed field for the polarization investigation in electron-ion interactions [75, 76, 77]. The angular distribution of the decay radiation of recombed ions may provide useful information about the ionic sublevels following electron capture from atoms [78], molecules and solids. But the parameters of the resonant electron transfer and excitation (RETE) are similar to those of dielectronic recombination. Some special cases of RETE were investigated in [55, 79].

The general expressions presented in Sections 2–5 can be used for the description of the processes mentioned above that were investigated with the help of the density matrix formalism. These general expressions are written in the invariant form of the expansions over the state multipoles, i.e. they are
integration over the angles leads to

$$q \neq 0 \text{ usually is represented as a sum of equal parts of the left- and right-polarized radiation since the helicity that only the tensor } T_d \text{ dipole radiation } (kP) \text{ in Eq. (51),} \quad \text{and averaging over the components of the atoms is necessary. From the application of Eq. (48) in (18) follows that}$$

$$K(0) = 0 \Rightarrow \lambda = 1 \Rightarrow N0 = 0 \Rightarrow$$

$$\sum_j T_N^K(J, J, M\dot{J}) = \delta(K, 0)\delta(N, 0). \quad (48)$$

Integration over the angles leads to

$$\int_0^{2\pi} d\phi Y_{KN}(\theta, \phi) = \sqrt{4\pi}\delta(K, 0)\delta(N, 0). \quad (49)$$

A more complicated case occurs with the polarization of radiation. The nonpolarized radiation usually is represented as a sum of equal parts of the left- and right-polarized radiation since the helicity \( q \neq 0 \). Thus for the nonpolarized dipole photon we have:

$$\sum_{q=\pm 1} T_N^K(1, 1, q|\mathbf{k}_0) = \frac{1}{3} \delta(K, 0)\delta(N, 0) + \sqrt{4\pi} \frac{1}{3} \left[ \begin{array}{ccc} 1 & 1 & 2 \\ 1 & -1 & 0 \end{array} \right] Y_{2N}(\theta, \phi)\delta(K, 2). \quad (50)$$

This expression can also be used in the case when the polarization of the emitted radiation is not detected.

6.1. The angular distribution of photoelectrons from unpolarized atoms

If the initial state of atoms is randomly orientated, the final state of ions and the spin of the photoelectrons are not registered, the summation over the components of the ion state and the spin of photoelectron, and averaging over the components of the atoms is necessary. From the application of Eq. (48) in (18) follows that \( K_0 = K_1 = K_s = 0, \quad K_r = K_\lambda = K_j = K \). The use of these values in Eq. (18) and the choice of the z axis along the direction of incoming radiation allows us to write the differential cross-section

$$\frac{d\sigma(\alpha_0 J_0 q \rightarrow \alpha_1 J_1)}{d\Omega_p} = \frac{\pi}{2J_0 + 1} \sum_{K,k,k'} B^{ph}(0, 0, K, K, 0, K, k, k')(1)^{k-q} \left[ \begin{array}{ccc} \frac{2J_1 + 1}{2k + 1} \\ k & q & -q \end{array} \right] \frac{1}{2} P_K(\cos \theta) \quad (51)$$

In Eq. (51), \( P_K(\cos \theta) \) stands for a Legendre polynomial. For the circular polarization of incoming dipole radiation \( (k = k' = q = 1) \), the cross-section may be written:

$$\frac{d\sigma(\alpha_0 J_0 \rightarrow \alpha_1 J_1)}{d\Omega_p} = \frac{\sigma(J_0 \rightarrow J_1)}{4\pi} \left[ 1 - \frac{1}{2} \beta P_2(\cos \theta) \right] \quad (52)$$

where

$$\beta = \frac{1}{\sqrt{2}} B^{ph}(0, 0, 0, 0, 0, 0, 0, 0, 1, 1), \quad (53)$$

$$\sigma(\alpha_0 J_0 \rightarrow \alpha_1 J_1) = \frac{4\pi}{3} \frac{[2J_1 + 1]^{1/2}}{2J_0 + 1} B^{ph}(0, 0, 0, 0, 0, 1, 1). \quad (54)$$

The expressions for \( \beta \) (53) and \( \sigma \) (54) differ from those obtained in [26] and used in the calculations of the angular distribution of 2p photoelectrons from Na atoms in the ground [80] and excited states.
The spin polarization parameters \(\gamma, \delta\) and \(\xi\) were also calculated for the 2p photoionization of Na in the ground and first excited states \[83\].

### 6.2. Angular distribution of Auger electrons for unpolarized atoms

The process of the photoionization of an atom \(A\) with following Auger decay of a photoion \(A^+\) in a two-step approximation can be written as follows:

\[
A(\alpha_0 J_0 M_0) + h\nu(\epsilon_q, \mathbf{k}_{01}) \rightarrow A^+(\alpha_1 J_1 M_1) + e^- (\mathbf{p}_1, m_s) \rightarrow A^{2+}(\alpha_2 J_2 M_2) + e^- (\mathbf{p}_1, m_s) + e^- (\mathbf{p}_2, m'_s).
\]  

In Eq. (55), \(\alpha_0, \alpha_1\) and \(\alpha_2\) indicate the configuration and other quantum numbers, \(J_0 M_0, J_1 M_1\) and \(J_2 M_2\) describe the total angular momenta and their magnetic components of the electron cloud of an atom in the initial state, intermediate photoion and doubly charged ion in the final state, respectively. The photo- and Auger electrons have the momentum \(\mathbf{p}_1\) and \(\mathbf{p}_2\), the projection of their spin \(s\) is \(m_s\) and \(m'_s\), respectively. The wave vector of incoming radiation is indicated by \(\mathbf{k}_{01}\) \(|\mathbf{k}_{01}| = \omega_1/c\), where \(\omega_1\) is the frequency of radiation.

An expression for the cross-section of the processes (55) was derived by Kupliauskiene and Tutlys \[45, 44\] and can be written in the form:

\[
\frac{dW(\alpha_0 J_0 M_0 \epsilon_q \mathbf{k}_{01} \rightarrow \alpha_1 J_1 \mathbf{p}_1 m_s \rightarrow \alpha_2 J_2 \mathbf{p}_2 m'_s)}{d\Omega_1 d\Omega_2} = \sum_{K_1, N_1} \frac{d\sigma_{K_1 N_1}(\alpha_0 J_0 M_0 \epsilon_q \mathbf{k}_{01} \rightarrow \alpha_1 J_1 \mathbf{p}_1 m_s)}{d\Omega_1} \cdot \frac{dW_{K_1 N_1}(\alpha_1 J_1 \rightarrow \alpha_2 J_2 \mathbf{p}_2 m'_s)}{d\Omega_2}.
\]  

Here \(d\Omega_1\) and \(d\Omega_2\) indicate the solid angles of the emission of the photoelectron and Auger electron, respectively.

The probability describing the angular distribution of Auger electrons from unpolarized atoms simplifies as a result of the summation of (56) over the magnetic components of the spins of photo- and Auger electrons, the total angular momentum of a doubly charged ion, integration over the angles of photoelectron and averaging over the magnetic components of an atom. In the case of dipole approximation, it acquires the following form:

\[
\frac{dW(J_0 \rightarrow J_1 \rightarrow J_2 \mathbf{p}_2)}{d\Omega_2} = \sum_{K_1} A^A(K_1, 0, K_1, 0, K_1) B(K_1) P_{K_1}(\cos \theta_2)
\]

\[
= A^A(0, 0, 0, 0, 0) B(0)[1 + \beta P_2(\cos \theta_2)],
\]

Here

\[
B(K_1) = \frac{4\pi}{2J_0 + 1} \left[ \frac{2K_1 + 1}{3} \right]^{1/2} \left[ \begin{array}{cc} 1 & 1 \\ 1 & -1 \end{array} \right] K_1 \left[ \begin{array}{c} 1 \\ 0 \end{array} \right] B(K_1, 0, K_1, 0, 0, 0, K_1, 1, 1),
\]

\[
\beta = \frac{A^A(2, 0, 0, 0, 0) B(2)}{A^A(0, 0, 0, 0, 0) B(0)} = \frac{A^A(2, 0, 2, 0, 2)}{A^A(0, 0, 0, 0, 0)} A_2
\]

where \(A_2\) is the alignment \[26\]. Its expression coincides with that presented by Kabachnik and Sazhina \[69\] if the expressions for \(B(K_1)\) would be inserted.

In the case of unpolarized atoms, the expression for the probability describing angular correlations between photo- and Auger electrons is obtained by summation of Eq. (56) over magnetic components of the spins of photo- and Auger electrons, the angular momentum of a doubly charged ion and averaging over magnetic components of an atom. For circularly polarized dipole ionizing radiation, it has the following expression:
\[
\frac{dW(J_0 \rightarrow J_1 \text{p}_1 \rightarrow J_2 \text{p}_2)}{d\Omega_1 \, d\Omega_2} = \sum_{K_1N_1} A(K_1, 0, K_1, 0, K_1) \left[ \frac{4\pi}{2K_1 + 1} \right]^{1/2} \, Y_{K_1N_1}(\theta_2, \phi_2) 
\times \sum_{K_rN_r, K_\lambda} B'(K_1, K_\lambda, K_r) \sum_{N_rN_\lambda} \left[ \begin{array}{ccc} K_1 & K_\lambda & K_r \\ N_1 & N_\lambda & N_r \end{array} \right] \frac{4\pi}{\sqrt{2K_r + 1}} \, Y^*_{K_rN_r}(\theta_0, \phi_0) \, Y_{K_\lambdaN_\lambda}(\theta_1, \phi_1).
\] (60)

Here
\[
B(K_1, K_\lambda, K_r) = \frac{1}{2J_0 + 1} \left[ \frac{(2K_1 + 1)(2K_r + 1)}{3} \right]^{1/2} \left[ \frac{2K_1 + 1}{3} \right]^{1/2} \left[ \begin{array}{ccc} 1 & 1 & K_r \\ 1 & -1 & 0 \end{array} \right] 
\times \mathcal{B}(K_1, 0, K_r, K_\lambda, 0, K_\lambda, 1, 1).
\] (61)

More examples of the practical application of the general expressions can be found in Refs. [26, 42, 44, 45, 46, 52].

7. Concluding remarks

A method for the derivation of general expressions for the cross-section and transition probability describing the polarization states of all particles participating in the interaction of polarized photons and electrons with polarized atoms is developed. It is alternative to the density matrix formalism. The graphical technique of the angular momentum applied for the integration over angular and spin variables of the matrix elements as well as for the expansion of the cross-sections and probabilities over the spherical tensors enables us to obtain the most general expressions for the cross-sections. Irreducible tensors are selected for the description of polarization because they have the simplest possible behavior under changes of directions. The method is also generalized for the multistep processes.

The following processes playing very important role in plasma are investigated:

- excitation and ionization of atoms by photons;
- excitation and ionization of atoms by electron impact;
- radiative recombination of an ion and electron;
- radiative and Auger decay of excited and ionized atoms.

The dielectronic recombination of an ion with an electron is an example of two-step process.

The practical application of the general expressions for the description of more simple processes under specific experimental conditions is easy to accomplish. The asymmetry parameter of the angular distribution of photoelectrons and Auger electrons following photoionization of unpolarized atoms as well as the parameters describing the angular correlations between the photo- and Auger electrons are obtained. These examples demonstrate the way for the derivation of more simple expressions. All expressions are presented in a similar form convenient for development of computer software and practical applications.

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ATOMO TEORIJOS METODAI ATOMU SĄVEIKAI SU FOTONAIS IR ELEKTRONAI TIRTI

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Santrauka

Sklaidos uždaviniuose sklaidomosios dalelės kryptis yra apibrėžta, todėl reakcijos produktų būsenų užpildai budinga asimetrinė šios krypties atžvilgiu. Iki šiol tokia polarizacija ir asimetrija buvo tiriamos tankio matricos metodais. Prieš ketvertą metu poliarizacijos reiškiniams, kai atomai ir jona sąveikauja su elekronais ir fotonais, nagrinėti buvo pritaikyti atomo teorijos metodai, kurie iki šiol buvo taikomi izoliuotų atomų skerspjūviams neatsižvelgiant į išskirtą kryptį erdvėje. Apžvelgti darbai, skirti poliarizuotų atomų sąveikos su poliarizuotais fotonais ir elektronais skerspjūvių bendravimams įsiraškoms nereliatyvinių artėjimų surasti. Judėjimo kiekio momento grafinė technika šulio pritaikyta šulio operatorių matricinių elementų kvadratams integruoti kampinių ir sumauti sukininių kintamųjų atžvilgiu. Skerspjūvių įsiraškų uzrašytos daugialypiiais sferinių multipolių skleidiniais, kadangi sferiniai tensoriai transformuojasi paprasčiausiai, keičiant matavimo kryptis. Pateiktas būdas fotonų ar elektronų spinduliuiotei po atomo ar jonų jonizacijos, sužadinimo ar rekombinacijos dvipakopui artėjimu nagrinėti.
Išnagrinėti svarbiausi plazmoje vykstantys vyksmai: atomų ir jonų sužadinimas ir jonizacija fotonais bei elektronais, jono ir elektrono fotorekombinacija, spinduliavimo ir Auger šuoliai sužadintuose ir jonizuotuose atomuose. Dvipakopų vyksmą iliustruoja dvielektronė rekombinacija. Taip pat parodyta, kaip galima surasti skerspjūvinių įrašiškas konkretiems eksperimentams aprašyti. Visų įrašiškų forma paprasta, patogi kompiuterinėms programoms rašyti.