# Angular distribution and spin polarization of Auger electrons following photoionization and photoexcitation

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Angular distribution and spin polarization of Auger electrons following photoionization and photoexcitation are presented in concise parametrized expressions. The striking similarity with corresponding expressions for photoelectrons enables one to apply kinematic properties known for photoelectrons in analyzing Auger electrons.

## I. INTRODUCTION

Through collision processes, an atom can be ionized or excited such that the ion or atom is left in an excited state. In the deexcitation of the ion or atom, the transition energy can be carried off either by the emission of photons (fluorescence radiation) or by the ejection of electrons (Auger electrons or autoionization electrons in specific cases) or both. Auger transitions, in particular, are more sensitive to the detailed atomic structure than many other measurable atomic quantities.[1–3] To obtain a complete analysis of the Auger electron, we need to measure its energy or momentum, angular distribution, and spin polarization and compare them with those from theory. Cleff and Mehlhorn[4] have derived angular distribution of Auger electrons following impact ionization by unpolarized projectiles in terms of the relative population of magnetic substates (or equivalently the state multipoles defined by Fano[5]). The quantum-beat phenomena and the effect of hyperfine interactions in the angular distribution have also been treated by Mehlhorn and Taulbjerg[6] and by Bruch and Klar.[7] Spin polarization of Auger electrons has been analyzed by Klar[8] in terms of the state multipoles; however, no convenient expressions were given. By considering a special case, Kabachnik[9] has obtained slightly improved expressions similar to those of Klar.[8] Nevertheless, none of the previous authors has given expressions relating the angular distribution and spin polarization of Auger electrons to the initial excitation processes. We present concise general expressions for the angular distribution and spin polarization of Auger electrons following photoionization or photoexcitation including the quantum-beat phenomena and the effect of hyperfine interactions with the nucleus. These expressions have *exactly* the same form as those for photoelectrons when the initial atom is excited or ionized in the electric dipole transition. This striking similarity enables one to apply kinematic properties known for photoelectrons[10] in analyzing Auger electrons. Here by *kinematic properties,* we mean properties such as the ranges of dynamical parameters, functional forms of measured quantities in terms of dynamical parameters, functional relationship between measured quantities, and transformation properties.

We assume the experimental condition where the incident photon, in an arbitrary polarization state, has a coherent broadband centered around $\omega_i = c|\vec{k}_i|$. The incident photon fields are linear sums of electric multipoles $\vec{A}_m^{(Ej_i)}(k_i \vec{r})$ and magnetic multipoles $\vec{A}_m^{(Mj_i)}(k_i \vec{r})$, where $j_i$ is a positive integer signifying the multipolarity. For examples, $E1$ denotes the electric dipole, $M1$ the magnetic dipole, $E2$ the electric quadrupole, etc. We also assume that the target atom is unpolarized and has a well-defined angular momentum $J_0$, while its unpolarized nucleus is in an angular momentum state $I$. The incident photon either excites or ionizes the target atom and leaves the excited atom or residual ion in a coherent superposition of angular momentum states $J_\alpha$. Here the subscript $\alpha$ is the channel index making the provision for different photoexcitation or photoionization channels. In the case of photoionization, there is, in addition, a total channel phase shift $\sigma_\alpha$ associated with channel $\alpha$. The excitation or ionization processes are characterized by the reduced matrix elements, $D_\alpha^{(Ej_i)}$ and $D_\alpha^{(Mj_i)}$, of multipole transitions.[10]

Because we start from a relativistic formulation, all fine structures of the atomic spectrum are built in from the outset. Assume the excited atomic ensemble has a sufficiently long lifetime such that the electrons can couple with the nucleus through the hyperfine interaction. The coupled electronic and nuclear state has a total electronic enery $E_\alpha$ and is identified by $|(J_\alpha I)FM\rangle$, where $F$ is the total angular momentum of the combined electronic and nuclear system. This excited system will eventually decay, with a decay constant $\gamma_\alpha$, either through Auger processes or by emitting photons. The results for the radiative decay have been presented.[11] We consider here only the Auger processes with one emitted electron. Assume that the Auger electron has a linear momentum $\vec{k}_\beta$, and the final ion is in an angular momentum state $J_\beta$, where $\beta$ is the Auger channel index. Again, we define a total channel phase shift $\sigma_\beta$ and the reduced matrix element $d_{\alpha\beta}$ for the Auger transition.[12]

During the time between excitation and decay the combined electronic and nuclear ensemble will evolve in such a way that each component $|(J_\alpha I)FM\rangle$ of the coherent superposition has a phase $\exp(-iE_\alpha t/\hbar)$. The phase difference, $\exp[-i(E_{\alpha'}-E_\alpha)t/\hbar]$, due to slightly different energies of various components leads to a time modulation, or quantum beats with frequency $\omega_{\alpha'\alpha}\equiv(E_{\alpha'}-E_\alpha)/\hbar$, of the Auger-electron signal.

Under the experimental condition mentioned above, we define a fixed (at the target) coordinate system $XYZ$ such that the $Z$ axis is in the direction $\vec{k}_i$ of the incident photon. The $X$ axis can be chosen in any convenient direction because the Stokes parameters $S_X$, $S_Y$, and $S_Z$ of the incident photon are determined accordingly. A simple relationship between the Stokes parameters and the degree, type, and orientation of the photon polarization has been given.[10] We also define a coordinate system $xyz$ associated with the emitted electron, where the $z$ axis, making an angle $\theta$ with the $Z$ axis, is in the direction $\vec{k}_\beta$ of the Auger electron, and the $y$ axis is perpendicular to the scattering plane, i.e., $\hat{y}=\hat{Z}\times\hat{z}/|\hat{Z}\times\hat{z}|$. The spin polarization of the Auger electron is defined in the $xyz$ coordinate system as $P_x(\theta,\phi)$, $P_y(\theta,\phi)$, and $P_z(\theta,\phi)$, where $(\theta,\phi)$ defines the orientation of $\vec{k}_\beta$ with respect to the fixed $XYZ$ coordinate system.

In such defined coordinate systems, we obtain angular distribution and spin polarization of Auger electrons following photoionization or photoexcitation including all multiple transitions; the expressions are similar to those for the fluorescence radiation.[11] The detailed derivation and explicit expressions will be reported. For the present purpose, we discuss only the important case where the initial atom is excited or ionized in the electric dipole transition.

When the size of the atomic system is small and when the photon energies are low, the initial excitation is predominantly due to electric dipole transitions. The angular distribution and spin polarization of Auger electrons following electric dipole photoexcitation or photoionization are given by

$$\frac{dW(\theta,\phi)}{d\Omega}=\frac{W}{4\pi}F(\theta,\phi)\ , \tag{1}$$

where the angular distribution function is

$$F(\theta,\phi)=1-\tfrac{1}{2}\beta[P_2(\cos\theta)+\tfrac{3}{2}(S_X\cos2\phi+S_Y\sin2\phi)\sin^2\theta]\ , \tag{2}$$

and

$$P_x(\theta,\phi)F(\theta,\phi)=[\xi S_Z+\eta(S_Y\cos2\phi-S_X\sin2\phi)]\sin\theta\ , \tag{3}$$

$$P_y(\theta,\phi)F(\theta,\phi)=\eta(1-S_X\cos2\phi-S_Y\sin2\phi)\sin\theta\cos\theta\ , \tag{4}$$

$$P_z(\theta,\phi)F(\theta,\phi)=\zeta S_Z\cos\theta\ . \tag{5}$$

Here $W$ is the total Auger rate per incident photon flux, $\beta$ is the angular asymmetry parameter for Auger electrons (not the same quantity as the photoelectron $\beta$), and $(\xi,\eta,\zeta)$ are the spin-polarization parameters. These five dynamical parameters have the explicit forms when the initial atom is photoionized

$$W=\frac{8\pi^5c}{\omega_i[J_0]^2}\overline{W}\ , \tag{6}$$

where we have used the notation $[J_0]\equiv(2J_0+1)^{1/2}$, and

$$\overline{W}=\sum_{\substack{JJ_\alpha\kappa_\beta\\ \kappa_\alpha F}}\frac{1}{[J_\alpha]^2}d^2_{\alpha\beta}D^2_\alpha\left[\frac{[F]^2}{[J_\alpha]^2[I]^2}\right]e^{-\gamma_\alpha t}\ , \tag{7}$$

and

$$\beta=-(\tfrac{6}{5})^{1/2}\sum_{\substack{\alpha'\beta'\\ \alpha\beta}}\begin{pmatrix} j'_\beta & j_\beta & 2\\ \tfrac{1}{2} & -\tfrac{1}{2} & 0\end{pmatrix}C_2\cos\sigma_{\alpha'\beta'\alpha\beta}\ , \tag{8}$$

$$\xi=-\frac{\sqrt{3}}{2}\sum_{\substack{\alpha'\beta'\\ \alpha\beta}}(-)^{l'_\beta+j'_\beta+\frac{1}{2}}\begin{pmatrix} j'_\beta & j_\beta & 1\\ -\tfrac{1}{2} & -\tfrac{1}{2} & 1\end{pmatrix}C_1\cos\sigma_{\alpha'\beta'\alpha\beta}\ , \tag{9}$$

$$\eta=-\frac{3}{2\sqrt{5}}\sum_{\substack{\alpha'\beta'\\ \alpha\beta}}(-)^{l'_\beta+j'_\beta+\frac{1}{2}}\begin{pmatrix} j'_\beta & j_\beta & 2\\ -\tfrac{1}{2} & -\tfrac{1}{2} & 1\end{pmatrix}C_2\sin\sigma_{\alpha'\beta'\alpha\beta}\ , \tag{10}$$

$$\zeta=(\tfrac{3}{2})^{1/2}\sum_{\substack{\alpha'\beta'\\ \alpha\beta}}\begin{pmatrix} j'_\beta & j_\beta & 1\\ \tfrac{1}{2} & -\tfrac{1}{2} & 0\end{pmatrix}C_1\cos\sigma_{\alpha'\beta'\alpha\beta}\ . \tag{11}$$

In Eqs. (8)–(11), we have defined

$$C_l = (-)^{J_0+J'+J-J_\beta+j_\alpha+l+\frac{1}{2}} \frac{1}{\overline{W}} [J j_\beta J' j'_\beta][l]^2 \begin{Bmatrix} J' & J & l \\ 1 & 1 & J_0 \end{Bmatrix}$$

$$\times \begin{Bmatrix} J' & J & l \\ J_\alpha & J'_\alpha & j_\alpha \end{Bmatrix} \begin{Bmatrix} J'_\alpha & J_\alpha & l \\ j_\beta & j'_\beta & J_\beta \end{Bmatrix} d_{\alpha'\beta'} d_{\alpha\beta} D_{\alpha'} D_\alpha \left[ \frac{[F'F]^2}{[I]^2} \begin{Bmatrix} F' & F & l \\ J_\alpha & J'_\alpha & I \end{Bmatrix}^2 \right] \exp[-(\gamma_{\alpha'}+\gamma_\alpha)t/2] \ , \qquad (12)$$

$$\sigma_{\alpha'\beta'\alpha\beta} = \sigma_{\alpha'} - \sigma_\alpha + \sigma_{\beta'} - \sigma_\beta + \omega_{\alpha'\alpha} t \ , \qquad (13)$$

$$\sum_{\substack{\alpha'\beta' \\ \alpha\beta}} = \sum_{J'J'_\alpha \kappa'_\beta F'} \ \sum_{JJ_\alpha \kappa_\beta F} \ \sum_{\kappa_\alpha} \ , \qquad (14)$$

$$D_\alpha = D_\alpha^{(E1)} \ . \qquad (15)$$

If the initial atom is photoexcited, the corresponding dynamical parameters can be obtained from Eqs. (7)–(15) by setting $j_\alpha$ and $\sigma_\alpha = 0$, and removing all quantities having a $(j_\alpha l_\alpha)$ signature. If we are not interested in the effect of hyperfine interactions or if the nuclear spin $I$ vanishes, we can either set $I=0$ or ignore quantities inside large square brackets in Eqs. (7) and (12) and disregard summations over $F$. If the experimental resolution of the Auger electrons is not high enough to see the quantum beat, a time average of the parameters can easily be performed. When the incident photon has a well-defined energy or is in an incoherent energy state, no quantum-beat phenomena can be observed. In that case, we set $J'_\alpha = J_\alpha$, $F'=F$, $\gamma'_\alpha = \gamma_\alpha$, and $\omega_{\alpha'\alpha}=0$, and eliminate the summations over $J_\alpha$ and $F$.

It is of interest to note that the angular distribu tion and spin polarization of Auger electrons, Eqs. (1)–(5), have *exactly* the same forms as corresponding ones for photoelectrons.[10] Consequently, *all the kinematic properties known for photoelectrons in the electric dipole transition also apply to corresponding Auger electrons.* In the fixed coordinate system $XYZ$, the spin polarization of Auger electrons is given by Eqs. (5.25)–(5.27) of Ref. 10. The spin polarization of the total Auger-electron flux is then given by

$$P_X = P_Y = 0 \ , \qquad (16)$$

$$P_Z = \delta S_Z \ , \qquad (17)$$

where the total spin-polarization parameter $\delta$ is given by

$$\delta = \tfrac{1}{3}(\zeta - 2\xi) \ . \qquad (18)$$

Examples of special cases of Eqs. (1)–(5) are given by (5.31)–(5.47) of Ref. 10. The maximum Auger-electron polarization can be analyzed as in Eqs. (5.48)–(5.53) of the same reference. It is obvious that the range of $\beta$ is restricted by $-1 \leq \beta \leq 2$. Kinematic relations between the angular distribution parameter $\beta$ and the spin-polarization parameters $\xi$, $\eta$, and $\zeta$ are

$$|\xi| \leq \begin{cases} 1+\frac{1}{4}\beta, & -1 \leq \beta \leq \frac{4}{5} \\ [3\beta(1-\beta/2)]^{1/2}, & \frac{4}{5} \leq \beta \leq 2 \ , \end{cases} \qquad (19)$$

$$|\eta| \leq [(1+\beta)(1-\beta/2)]^{1/2} \ , \qquad (20)$$

$$|\zeta| \leq 1 - \tfrac{1}{2}\beta \ , \qquad (21)$$

and also

$$|\delta| \leq \begin{cases} 1, & -1 \leq \beta \leq \frac{4}{5} \\ \frac{1}{6}(2-\beta) + [\frac{2}{3}\beta(2-\beta)]^{1/2}, & \frac{4}{5} \leq \beta \leq 2 \ . \end{cases} \qquad (22)$$

We note that when $\beta$ reaches its maximum value 2 the spin polarization must be zero, and that when $\beta$ attains its minimum value $-1$ there will be no spin polarization perpendicular to the scattering plane defined by the $Z$ and $z$ axes.

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