PHYSICAL REVIEW A VOLUME 22, NUMBER 1 JULY 1980

Theory of angular distribution and spin polarization of photoelectrons

Keh-Ning Huang
Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556
(Received 9 November 1979)

General formulas of the angular distribution and spin polarization of photoelectrons are derived for arbitrarily polarized incident photons including all multipole effects of the photon fields. Dynamical parameters are given in terms of reduced matrix elements suitable for a general multichannel theory in both the relativistic and nonrelativistic formulations. Low-energy photoionization processes, where the electric-dipole approximation is valid, are dealt with in detail. Simple explicit formulas of the angular distribution and spin polarization of photoelectrons are given for closed-shell atoms. Applications of the present formulation using various relativistic multichannel theories are discussed briefly. A relativistic version of the K-matrix method, by which both closed- and open-shell atoms can be treated, is also given.

I. INTRODUCTION

Photoionization processes have received much attention in recent years. The availability of lasers and synchrotron radiation has especially stimulated advances in photoionization studies. Demands for accurate photoionization data in plasma and fusion research have combined with the traditional astrophysical interest to make these fairly active fields of current research. Low-energy photoionization processes have been reviewed recently by Burke,[1] Manson,[2] Berkowitz,[3] and more recently by Starace[4] on theory and Samson[5] on experiment. The theoretical treatment of high-energy atomic photoionization has been reviewed by Pratt, Ron, and Tseng[6a] and by Cooper.[7] A large body of experimental data for most elements in the periodic system has been made available on photoabsorption cross sections by Hubbell.[8] Scofield[9] has given theoretical photoionization cross sections from 1 to 1500 keV for most elements. In addition, a complete bibliography of original studies of photoionization and photoabsorption has been given by Kieffer[10] for the period 1921 through 1974. These references[1-10] and references therein should be consulted for recent developments in photoionization processes.

The main concerns of most photoionization research are with the cross section and angular distribution of photoelectrons. Nevertheless, a complete analysis of photoionization processes requires the knowledge of the spin polarization as well as the angular distribution of photoelectrons ejected by photons in specific polarization states. In addition, the polarizations, if any, of the target atom and of the residual ion have to be considered if observations are made coincidently with the detection of the photoelectron. Spin polarization of photoelectrons has become increasingly important in recent years, especially because of the utilization of photoionization processes in producing polarized electron beams.[11-14] A notable recent application is the observation of parity nonconservation in inelastic scattering of longitudinally polarized electrons from unpolarized targets.[15,16]

The spin polarization of the total photoelectron flux ejected from unpolarized alkali atoms by circularly polarized photons has been calculated by Fano.[17] General discussions of photoelectron spin polarization have been given by Brehm,[18] Jacobs,[19] Cherepkov,[20] and Lee[21] in the dipole approximation in nonrelativistic formulations. Nevertheless, theoretical formulas of the spin polarization of photoelectrons exist only for unpolarized and linearly and circularly polarized incident photons while many convenient sources of photons are elliptically polarized. Well-known examples are synchrotron radiation and light reflected by metallic mirrors. Additionally, because of the nonrelativistic nature of the above mentioned formulations, the spin-orbit interaction, which plays an essential role, can only be treated in the Pauli approximation or in an *ad hoc* fashion.[20b] Furthermore, only low-energy photoionization processes, in which the electric-dipole approximation remains valid, were considered by these authors. Pratt and coworkers[6b] have calculated polarization correlations between the incident photon and ejected electron in the relativistic single-particle picture; however, no explicit spin-polarization formula of the photoelectron was given.

In this paper, we start with a relativistic multichannel formulation including all multipole fields of the photon and express the total cross section, angular distribution, and spin polarization in terms of dynamical parameters. These dynamical parameters are given as weighted sums of radial integrals. The most general polarization state of the incident photon is assumed; linear, circular,

elliptical, and partial polarizations are special cases and are treated at the same time. However, we will confine ourselves to cases where the target atom is unpolarized, and the polarization of the residual ion is not observed. In other words, we will average over the polarization of the target atom and sum over the polarization of the residual ion. The results for polarized target atoms and residual ions will be reported.

We shall derive photoionization formulas in the helicity formulation. The helicity formulation of collision processes for particles with spin was first introduced by Chou[22] and by Jacob and Wick.[23] The helicity formulation has several advantages[22,23]: (a) Helicity is invariant under ordinary rotations and has simple transformation properties under Lorentz transformations. (b) The helicity formulation does not lead to complications in the relativistic description of spin states. (c) Particles with zero rest mass, e.g., photon, neutrino, or graviton, can be treated on the same footing as massive particles. Especially because of (a), the angular correlation of a scattering process can be absorbed in a single rotation matrix. On the other hand, a bound many-particle system (nucleus, atom, molecule, etc.) is best described in terms of the ordinary angular-momentum eigenstates. Therefore to use the helicity formulation in treating particle scatterings on a many-particle system we have to make the transformation from ordinary angular-momentum eigenstates to helicity eigenstates. It is possible to derive a convenient form for the transition matrix of a certain scattering process by working directly in the helicity formulation. This approach was adopted by Lee[21] in the nonrelativistic formulation of photoionization processes in the electic-dipole approximation. However to make clear the connection between the conventional formulation and the helicity formulation, we shall start from the conventional expression of the transition matrix and proceed to write angular-momentum eigenstates in terms of helicity eigenstates. In this way, we can borrow experiences acquired in working with the conventional method.

In Sec. II, a photon beam of arbitrary polarization is described by the spin density matrix of photons. In Sec. III, the basic transition matrix of photoionization processes is presented and then expressed in terms of helicity eigenstates. The spin density matrix of photoelectrons ejected by a photon beam of arbitrary polarization is introduced in Sec. IV. The angular distribution and spin polarization of photoelectrons are derived in the same section. Additionally, a simple prescription is given for transforming the formulas in jj coupling to those in LSJ coupling. Section V discusses low-energy photoionization processes, where the electric-dipole approximation is valid. In Sec. V A, the angular distribution and spin-polarization formulas are given as functions of photoelectron angles, with all dynamical effects absorbed in five parameters. In Sec. V B, simple explicit formulas for closed-shell atoms are presented. In Sec. VI, applications using various multichannel theories are discussed. Appendix A introduces a convention of the photon-spin polarization used in this work. The phase convention of Dirac orbitals is discussed in Appendix B. Appendix C summarizes multipole interactions and their interaction strengths. In Appendix D, electron and photon helicity eigenstates are presented. Appendix E gives explicit formulas for the transformation of the photoelectron polarization vector between different coordinate systems. In Appendix F, an alternative derivation of the general formulas for the angular distribution and spin polarization of photoelectrons is discussed. Finally, a relativistic multichannel K-matrix method is presented in Appendix G. We note that a letter version of the present work has been reported.[24]

II. PHOTON-SPIN POLARIZATION

There are several equivalent ways of specifying the polarization of a given photon beam. One convenient description is the density matrix of the form

$$\rho=\frac{1}{2}\begin{pmatrix} 1+p\sin 2\alpha & -pe^{-i2\gamma}\cos 2\alpha \\ -pe^{i2\gamma}\cos 2\alpha & 1-p\sin 2\alpha \end{pmatrix}. \tag{2.1}$$

Here the parameter p specifies the degree of polarization, α the type of polarization, and γ the azimuthal orientation of the polarization. This convention is presented in Appendix A. An equivalent description is provided by Stokes parameters[25-27] S_1, S_2, S_3 which are related to p, α, γ as

$$S_1=-p\cos 2\alpha\cos 2\gamma, \tag{2.2}$$

$$S_2=-p\cos 2\alpha\sin 2\gamma, \tag{2.3}$$

$$S_3=p\sin 2\alpha, \tag{2.4}$$

or inversely as

$$p=(S_1^2+S_2^2+S_3^2)^{1/2}, \tag{2.5}$$

$$\sin 2\alpha=S_3(S_1^2+S_2^2+S_3^2)^{-1/2}, \tag{2.6}$$

$$\tan 2\gamma=S_2/S_1. \tag{2.7}$$

Mathematically, Stokes parameters are the expansion coefficients of the density matrix ρ in the complete basis set of 2×2 matrices: the Pauli matrices $\vec{\sigma}$ together with the 2×2 unit matrix; i.e.,

$$\rho = \frac{1}{2}\left(1 + \sum_{i=1}^{3} S_i \sigma_i\right) = \frac{1}{2}\begin{pmatrix} 1+S_3 & S_1 - iS_2 \\ S_1 + iS_2 & 1 - S_3 \end{pmatrix} . \tag{2.8}$$

The Stokes parameters $(S_1 S_2 S_3)$, or equivalently $(p\alpha\gamma)$, can be determined experimentally by three polarization measurements chosen properly. For example: $\frac{1}{2}(1 - S_1)$ is the probability of linear polarization along the X axis; $\frac{1}{2}(1 - S_2)$ the probability of linear polarization along an axis making an angle of $+45°$ with the X axis; and $\frac{1}{2}(1 + S_3)$ the probability of right circular polarization.

III. TRANSITION MATRIX OF PHOTOIONIZATION PROCESSES

It is well known that the basic transition matrix of photoionization processes for a many-electron system has the form, in atomic units,

$$f_{fi} = \left(\frac{4\pi^2 k_\alpha}{\omega c}\right)^{1/2} \langle \psi_f | \sum_{i=1}^{N} \vec{\alpha}_i \cdot \hat{\epsilon} e^{i\vec{k}\cdot\vec{r}_i} | \psi_i \rangle , \tag{3.1}$$

where ψ_i and ψ_f are the initial and final states, respectively, of the many-electron system. The incident photon has the momentum $\vec{k}$ ($|\vec{k}| = \omega/c$) and polarization $\hat{\epsilon}$; the outgoing photoelectron has the momentum $\vec{k}_\alpha$ ($k_\alpha = |\vec{k}_\alpha|$), where the subscript α is the channel index introduced for later convenience. The Dirac matrices $\vec{\alpha}$ have the explicit representation

$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}, \tag{3.2}$$

with $\vec{\sigma}$ the familiar Pauli matrices. The combined final state ψ_f of the photoelectron and residual ion is normalized such that the differential cross section is given by

$$\frac{d\sigma_{fi}}{d\Omega} = |f_{fi}|^2 . \tag{3.3}$$

Now we consider the experimental situation where a photon of polarization $\hat{\epsilon} = \hat{e}_q$ incidents upon a target atom in the polarization state $|J_0 - M_0\rangle_{\hat{k}}$. Here $\hat{e}_q$ is the spherical unit vector[28] with $q = 1$ or -1; the subscript $\hat{k}$ specifies explicitly that the quantization axis of the initial state $|J_0 - M_0\rangle_{\hat{k}}$ is along the direction $\hat{k}$ of the incident photon. The total angular momentum of the initial state is J_0 with the magnetic quantum number $-M_0$. After the photoionization processes, a photoelectron is detected at a macroscopic distance in the direction (θ, ϕ) with respect to the incident photon direction $\hat{k}$. The photoelectron has the linear momentum $\vec{k}_\alpha$ and spin component μ in the direction of the quantization axis $\hat{k}_\alpha$. The residual ion is left in the polarization state $|J_\alpha - M_\alpha\rangle_{\hat{k}_\alpha}$; the subscript $\hat{k}_\alpha$ specifies that the quantization axis of the final state is along the direction $\hat{k}_\alpha$, and the others are obvious notations. The reason for choosing different quantization axes for the initial and final states will become clear when we express (3.1) in helicity eigenstates. The described experimental situation is shown schematically in Fig. 1. For notational purpose, let us represent the initial and final states of the total electron-photon system as $\hat{e}_q e^{i\vec{k}\cdot\vec{r}_i} | \psi_0 \rangle$ and $|\alpha \vec{k}_\alpha^{-}\rangle$, respectively. The superscript "$-$" denotes the fact that for a plane wave $|\vec{k}_\alpha \mu\rangle$ to be detected after the collision the photoelectron-ion system must satisfy the *incoming-wave boundary condition*.[29] We therefore write the basic transition matrix element of this particular photoionization process as

$$f(qM_0 \mu M_\alpha) = \left(\frac{4\pi^2 k_\alpha}{\omega c}\right)^{1/2} \langle \alpha \vec{k}_\alpha^{-} | \sum_{i=1}^{N} \vec{\alpha}_i \cdot \hat{e}_q e^{i\vec{k}\cdot\vec{r}_i} | \psi_0 \rangle . \tag{3.4}$$

The magnetic quantum numbers q, M_0, μ, and M_α on the left-hand side denote the helicities of the photon, target atom, photoelectron, and residual ion, respectively. Except the particular choice of quantization axes, the matrix element (3.4) is just what we would get in a conventional formulation of photoionization processes.

The initial state consisting of the incident photon and target atom can be expended in terms of helicity states of the composite system as

$$\hat{e}_q e^{i\vec{k}\cdot\vec{r}_i} | \psi_0 \rangle = \sum_J [2\pi^2 (2J+1)]^{1/2} | kqM_0; JM \rangle , \tag{3.5}$$

where $M = q - M_0$. The helicity state of the composite system is given as

$$|kqM_0; JM\rangle = \sum_{jm} \sum_{M_0'} \left(\frac{2j+1}{2J+1}\right)^{1/2} \langle J_0 - M_0\, jq\, | JM \rangle \times \langle J_0 M_0' jm\, | JM \rangle \vec{A}_{kq;\,jm}(\vec{r}_i) | J_0 M_0' \rangle , \tag{3.6}$$

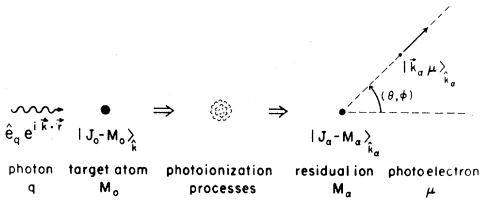

FIG. 1. Schematic diagram of photoionization processes. The symbols q, M_0, M_α, and μ are respective helicities.

where $\langle J_0 - M_0 jq | JM\rangle$, etc. are Clebsch-Gordan coefficients.[28] The atomic state $|J_0 M_0'\rangle$ can be represented in terms of Dirac orbitals, which are described in Appendix B. The multipole interactions of photon fields are discusssd in Appendix C, and the expansion of the photon angular-momentum helicity state $\vec{A}_{kq;jm}$ in terms of photon multipole potentials is given in Appendix D. Appendix D also provides a general prescription for constructing helicity states.

The final state of the photoelectron and residual ion can also be expressed in terms of helicity states as

$$|\alpha \vec{k}_\alpha^-\rangle = \sum_{J'M''} D^{(J')}_{M''M'}(\hat{k}_\alpha)\left(\frac{2J'+1}{4\pi}\right)^{1/2} |k_\alpha^- \mu M_\alpha; J'M''\rangle , \tag{3.7}$$

where $M' = \mu - M_\alpha$. The rotation matrices $D^{(J')}_{M''M'}(\hat{k}_\alpha)$ in (3.7) effect the rotation of the helicity states to align with the direction of the photoelectron and are given explicity as

$$D^{(J')}_{M''M'}(\hat{k}_\alpha) \equiv e^{-iM''\Phi} d^{(J')}_{M''M'}(\theta) , \tag{3.8}$$

where $d^{(J')}_{M''M'}$ are the standard d functions.[28,30,31] The final helicity states must satisfy the incoming-wave boundary condition and are given by

$$|k_\alpha^- \mu M_\alpha; J'M''\rangle = \sum_{\kappa_\alpha}\left(\frac{2l_\alpha+1}{k_\alpha(2J'+1)}\right)^{1/2} i^{l_\alpha}\exp(-i\sigma_{\kappa_\alpha}) \times \langle l_\alpha o s\mu | j_\alpha \mu\rangle \times \langle J_\alpha - M_\alpha j_\alpha \mu | J'M'\rangle |\alpha^- J'M''\rangle , \tag{3.9}$$

where σ_{κ_α} is the Coulomb phase shift of the photoelectron in the particular channel $\kappa_\alpha = (l_\alpha j_\alpha)$. The state $|\alpha^- J'M''\rangle$ is usually called *the open-channel state* and has the asymptotic behavior of containing an outgoing Coulomb spherical wave only in channel α. After substituting (3.5) and (3.7) into (3.4) we can express the transition matrix as

$$f(qM_0\mu M_\alpha) = \left(\frac{2\pi^3 k_\alpha}{\omega c}\right)^{1/2} \sum_J (2J+1) e^{iM\Phi} d^{(J)}_{MM'}(\theta) \times \langle \mu M_\alpha | T^J | qM_0\rangle , \tag{3.10}$$

where we have defined

$$\langle \mu M_\alpha | T^J | qM_0\rangle \equiv \langle k_\alpha^- \mu M_\alpha; JM | \sum_{i=1}^N \vec{\alpha}_i \cdot | kqM_0; JM\rangle . \tag{3.11}$$

In arriving at (3.10), we have used the fact that the electromagnetic interaction is rotationally invariant which implies $J = J'$ and $M = M''$. To evaluate the matrix element $\langle \mu M_\alpha | T^J | qM_0\rangle$, we use (3.6) and (3.9) with the result

$$\langle \mu M_\alpha | T^J | qM_0\rangle = \sum_{\kappa_\alpha}\sum_j \left(\frac{(2l_\alpha+1)(2j+1)}{k_\alpha(2J+1)^2}\right)^{1/2} i^{-l_\alpha}\exp(i\sigma_{\kappa_\alpha}) \times \langle l_\alpha o s\mu | j_\alpha \mu\rangle \langle J_\alpha - M_\alpha j_\alpha \mu | JM'\rangle \langle J_0 - M_0 jq | JM\rangle \times \sum_{mM_0'} \langle J_0 M_0' jm | JM\rangle \langle \alpha^- JM | \sum_{i=1}^N \vec{\alpha}_i \cdot \vec{A}_{kq;jm}(\vec{r}_i) | J_0 M_0'\rangle . \tag{3.12}$$

This expression can be simplified after applying the Wigner-Eckart theorem.[28] Therefore we obtain

$$\langle \mu M_\alpha | T^J | qM_0\rangle = \sum_{\kappa_\alpha j}\left(\frac{(2l_\alpha+1)(2j+1)}{k_\alpha(2J+1)^3}\right)^{1/2} \times \langle l_\alpha o s\mu | j_\alpha \mu\rangle \langle J_\alpha - M_\alpha j\mu | JM'\rangle \times \langle J_0 - M_0 jq | JM\rangle D_q , \tag{3.13}$$

where the reduced matrix element D_q is given explicitly as

$$D_q \equiv D_{jq}[(J_\alpha \kappa_\alpha) JJ_0] \equiv i^{-l_\alpha}\exp(i\sigma_{\kappa_\alpha})\langle \alpha^- J || \sum_{i=1}^N \vec{\alpha}_i \cdot \vec{A}^{(j)}_{kq}(\vec{r}_i) || J_0\rangle . \tag{3.14}$$

In the foregoing derivations, we have implicitly assumed the Coulomb gauge (also called the transverse or radiation gauge) for the photon fields. The appropriate multipole interaction operators in the length gauge[32,33] are given in Appendix C. Using the interaction strength of multipole interactions presented in Appendix C, we can express the reduced matrix element (3.14) in terms of radial integrals. This can be achieved expediently by using a graphical method.[34] With (3.13) we can rewrite the transition matrix element $f(qM_0\mu M_\alpha)$ in terms of reduced matrix elements D_q as

$$f(qM_0\mu M_\alpha) = \sum_{\kappa_\alpha j}\left(\frac{2\pi^3(2l_\alpha+1)(2j+1)}{\omega c(2J+1)}\right)^{1/2} \times e^{iM\Phi} d^{(J)}_{MM'}(\theta)\langle l_\alpha o s\mu | j_\alpha \mu\rangle \times \langle J_\alpha - M_\alpha j\mu | JM'\rangle \langle J_0 - M_0 jq | JM\rangle D_q . \tag{3.15}$$

Because we consider only unpolarized target atoms and do not detect the polarization of the residual ion, it is convenient to define the expression

$$I(q'q;\mu'\mu)=(2J_0+1)^{-1}\sum_{M_0M_\alpha} f(q'M_0\mu'M_\alpha)f^*(qM_0\mu M_\alpha). \tag{3.16}$$

Substituting (3.15) into (3.16), we obtain

$$I(q'q;\mu'\mu)=e^{i(q'-q)\phi}\sum_{\alpha'\alpha l}K_{\alpha'\alpha l}L(q'q;\mu'\mu)D_{q'}D_q^*, \tag{3.17}$$

where

$$\sum_{\alpha' \alpha l}\equiv\sum_{\kappa_\alpha J' j' \kappa_\alpha J j}\sum_{l}, \tag{3.18}$$

$$K_{\alpha'\alpha l}\equiv\frac{2\pi^3(2l+1)}{\omega c(2J_0+1)}[jj_\alpha J][j'j'_\alpha J'](-)^{J_0-J_\alpha+s}\times\begin{Bmatrix}J & J' & l\\ j'_\alpha & j_\alpha & J_\alpha\end{Bmatrix}\begin{Bmatrix}J & J' & l\\ j' & j & J_0\end{Bmatrix}, \tag{3.19}$$

and

$$L(q'q;\mu'\mu)=[l_\alpha l'_\alpha]d^l_{(q-q')(\mu-\mu')}(\theta)\times\begin{pmatrix}0 & s & j_\alpha\\ l_\alpha & \mu & -\mu\end{pmatrix}\begin{pmatrix}0 & j'_\alpha & \mu'\\ l'_\alpha & \mu' & s\end{pmatrix}\times\begin{pmatrix}-\mu & \mu' & \mu-\mu'\\ j_\alpha & j'_\alpha & l\end{pmatrix}\begin{pmatrix}j & j' & l\\ -q & q' & q-q'\end{pmatrix}. \tag{3.20}$$

Here we have used the $3-jm$ coefficients (the Wigner $3-j$ coefficients in the covariant notation[34,35]), and the symbol $[j]\equiv(2j+1)^{1/2}$.

IV. ANGULAR DISTRIBUTION AND SPIN POLARIZATION OF PHOTOELECTRONS

We define a fixed (at the target) coordinate system XYZ such that the Z axis is in the direction of the photon flux. The X axis can be chosen in any convenient direction because the photon polarization is determined accordingly. Of course, the best choice would be such that the X axis coincides with the linear polarization vector or with one of the principal axes of elliptically polarized photons. We also define a rotated coordinate system xyz obtained from the fixed coordinate system XYZ by a rotation with the Euler angles $(\phi,\theta,0)$.[28] The rotated coordinate system xyz is chosen such that the z axis, making an angle θ with the Z axis, is in the direction of the outgoing photoelectron, and the y axis is perpendicular to both the Z and z axes. The spin polarization of the photoelectron is defined with respect to the rotated coordinate system xyz. The relative orientation of these two coordinate systems is shown in Fig. 2.

We can easily show that the spin density matrix element $\rho_{\mu'\mu}$ of the photoelectron is related to that of the incident photon $\rho_{q'q}$ by the relation

$$\rho_{\mu'\mu}=\sum_{q'q}\rho_{q'q}I(q'q;\mu'\mu). \tag{4.1}$$

The matrix elements $\rho_{q'q}$ are given explicitly by (2.1) or (2.8) for a general polarization state of the photon. The angular distribution and spin polarization of the photoelectron can be expressed in terms of the spin density matrix $\rho=(\rho_{\mu'\mu})$ as

$$\frac{d\sigma}{d\Omega}=\mathrm{Tr}\{\rho\}, \tag{4.2}$$

$$\vec{P}\equiv\langle\vec{\Sigma}\rangle=\mathrm{Tr}\{\vec{\sigma}\rho\}/\mathrm{Tr}\{\rho\}. \tag{4.3}$$

Here $\mathrm{Tr}\{\}$ denotes the trace of a matrix, and the electron spin operator $\vec{\Sigma}$ is

$$\vec{\Sigma}=\begin{pmatrix}\vec{\sigma} & 0\\ 0 & \vec{\sigma}\end{pmatrix}. \tag{4.4}$$

Evaluation of (4.2) and (4.3) gives the explicit expressions

$$\frac{d\sigma}{d\Omega}=\rho_{\frac12\frac12}+\rho_{-\frac12-\frac12}, \tag{4.5}$$

$$P_x=(\rho_{\frac12-\frac12}+\rho_{-\frac12\frac12})\Big/\left[\frac{d\sigma}{d\Omega}\right], \tag{4.6}$$

$$P_y=i(\rho_{\frac12-\frac12}-\rho_{-\frac12\frac12})\Big/\left[\frac{d\sigma}{d\Omega}\right], \tag{4.7}$$

$$P_z=(\rho_{\frac12\frac12}-\rho_{-\frac12-\frac12})\Big/\left[\frac{d\sigma}{d\Omega}\right], \tag{4.8}$$

It is convenient to define

$$\bar{\rho}_{q'q}\equiv e^{i(q'-q)\phi}\rho_{q'q}. \tag{4.9}$$

Therefore we obtain the "rotated" density matrix

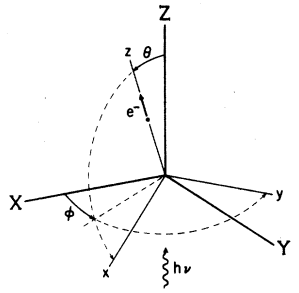

FIG. 2. Geometrical relationships used in spin-polarization formulas. The photon is incident along the Z axis, and the photoelectron is ejected along the z axis.

$$\bar{\rho} \equiv (\bar{\rho}_{q'q})$$

$$= \frac{1}{2} \begin{bmatrix} 1+p\sin 2\alpha & -pe^{i2\bar{\phi}}\cos 2\alpha \\ -pe^{-i2\bar{\phi}}\cos 2\alpha & 1-p\sin 2\alpha \end{bmatrix}, \quad (4.10)$$

where $\bar{\phi} = \phi - \gamma$, the azimuthal angle of the photoelectron direction with respect to the linear polarization vector or with respect to the principal axis $k\cos\alpha$ of elliptically polarized photons. We note that several combinations of the density matrix elements $\bar{\rho}_{q'q}$ are found to be useful:

$$\bar{\rho}_{11} + \bar{\rho}_{-1-1} = 1, \quad (4.11)$$

$$\bar{\rho}_{11} - \bar{\rho}_{-1-1} = p\sin 2\alpha = S_3, \quad (4.12)$$

$$\bar{\rho}_{1-1} + \bar{\rho}_{-11} = -p\cos 2\alpha \cos 2\phi = S_1 \cos 2\phi + S_2 \sin 2\phi, \quad (4.13)$$

$$\bar{\rho}_{1-1} - \bar{\rho}_{-11} = -ip\cos 2\alpha \sin 2\phi = i(S_1 \sin 2\phi - S_2 \cos 2\phi). \quad (4.14)$$

In addition, we define for notational purpose

$$R_{q'q} \equiv \bar{\rho}_{q'q} D_{q'} D_q^*. \quad (4.15)$$

Hence we can rewrite (4.1) as

$$\rho_{\mu'\mu} = \sum_{l\alpha'\alpha} K_{l\alpha'\alpha} \sum_{q'q} L(q'q;\mu'\mu) R_{q'q}. \quad (4.16)$$

To evaluate (4.5)–(4.8) using (4.16) we note the symmetry relations of the coefficients $L(q'q;\mu'\mu)$:

$$L(q'q;-\mu-\mu) = (-)^{l_\alpha + l'_\alpha + 1} L(q'q;\mu\mu), \quad (4.17)$$

$$L(qq;-\mu\mu) = (-)^{l_\alpha + l'_\alpha + l + 1} L(qq;\mu-\mu), \quad (4.18)$$

$$L(-q-q;\mu'\mu) = (-)^{j+j'+1} L(qq;\mu'\mu). \quad (4.19)$$

Hence we obtain the angular distribution and spin polarization of the photoelectron as

$$\frac{d\sigma}{d\Omega} = \sum_{\alpha'\alpha l}^{\pi(l'_\alpha l_\alpha l)} K_{\alpha'\alpha l} \begin{pmatrix} j_\alpha & j'_\alpha & l \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} \left[\begin{pmatrix} j & j' & l \\ 1 & -1 & 0 \end{pmatrix} [R_{11} + (-)^{j+j'+1} R_{-1-1}] P_l(\cos\theta) + \begin{pmatrix} j & j' & l \\ 1 & 1 & -2 \end{pmatrix} [R_{1-1} + (-)^{j+j'+1} R_{-11}] d^l_{20}(\theta) \right], \quad (4.20)$$

$$P_x = \left(\frac{d\sigma}{d\Omega}\right)^{-1} \sum_{\alpha'\alpha l} K_{\alpha'\alpha l} (-)^{l'_\alpha + j'_\alpha - 1/2} \begin{pmatrix} j_\alpha & j'_\alpha & l \\ \frac{1}{2} & \frac{1}{2} & -1 \end{pmatrix} \left[\pi(l'_\alpha l_\alpha l + 1) \begin{pmatrix} j & j' & l \\ -1 & 1 & 0 \end{pmatrix} [R_{11} + (-)^{j+j'+1} R_{-1-1}] d^l_{10}(\theta) - \frac{1}{2} \begin{pmatrix} j & j' & l \\ 1 & 1 & -2 \end{pmatrix} [R_{1-1} + (-)^{l_\alpha + l'_\alpha + j + j' + 1} R_{-11}] [d^l_{21}(\theta) + (-)^{l_\alpha + l'_\alpha + l} d^l_{2-1}(\theta)] \right], \quad (4.21)$$

$$P_y = i\left(\frac{d\sigma}{d\Omega}\right)^{-1} \sum_{\alpha\alpha' l} K_{\alpha\alpha' l} (-)^{l'_\alpha + j'_\alpha - 1/2} \begin{pmatrix} j_\alpha & j'_\alpha & l \\ \frac{1}{2} & \frac{1}{2} & -1 \end{pmatrix} \left[\pi(l_\alpha l'_\alpha l) \begin{pmatrix} j & j' & l \\ -1 & 1 & 0 \end{pmatrix} [R_{11} + (-)^{j+j'+1} R_{-1-1}] d^l_{10}(\theta) - \frac{1}{2} \begin{pmatrix} j & j' & l \\ 1 & 1 & -2 \end{pmatrix} [R_{1-1} + (-)^{l_\alpha + l'_\alpha + j + j'} R_{-11}] [d^l_{21}(\theta) + (-)^{l_\alpha + l'_\alpha + l + 1} d^l_{2-1}(\theta)] \right], \quad (4.22)$$

$$P_z = -\left(\frac{d\sigma}{d\Omega}\right)^{-1} \sum_{\alpha\alpha' l}^{\pi(l_\alpha l'_\alpha l+1)} K_{\alpha\alpha' l} \begin{pmatrix} j_\alpha & j'_\alpha & l \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} \left[\begin{pmatrix} j & j' & l \\ -1 & 1 & 0 \end{pmatrix} [R_{11} + (-)^{j+j'+1} R_{-1-1}] P_l(\cos\theta) + \begin{pmatrix} j & j' & l \\ 1 & 1 & -2 \end{pmatrix} [R_{1-1} + (-)^{j+j'+1} R_{-11}] d^l_{20}(\theta) \right]. \quad (4.23)$$

We can express the d-functions in terms of certain combinations of Legendre polynomials $P_l(\cos\theta)$ as

$$d^l_{10}(\theta) = -[l/(l+1)]^{1/2} \sin^{-1}\theta (-\cos\theta P_l + P_{l-1}), \quad (4.24)$$

$$d^l_{20}(\theta) = l^{1/2}[(l-1)(l+1)(l+2)]^{-1/2} \sin^{-2}\theta \times \{[-(l+1) + (l-1)\cos^2\theta] P_l + 2\cos\theta P_{l-1}\}, \quad (4.25)$$

$$d^l_{21}(\theta) + d^l_{2-1}(\theta) = -4[l(l+1)]^{-1/2} \sin^{-1}\theta d^l_{20}(\theta), \quad (4.26)$$

$$d^l_{21}(\theta) - d^l_{2-1}(\theta) = [2/(l+1)][(l-1)(l+2)]^{-1/2} \sin^{-3}\theta \times \{[(l^2 - l - 4) - l(l-1)\cos^2\theta]\cos\theta P_l + [-(l+2)(l-1) + (l^2 + l + 2)\cos^2\theta] P_{l-1}\}. \quad (4.27)$$

The transformation of components of the polarization vector among different coordinate systems can be carried out easily. The transformation matrix is given in Appendix E.

In deriving the foregoing results, the jj coupling is assumed. To obtain corresponding expressions in the LSJ coupling, we simply make the following substitution:

$$D_q \equiv D_{jq}[(J_\alpha \kappa_\alpha) J J_0] \rightarrow \sum_{LS} [(2L+1)(2S+1)(2j_\alpha+1)(2J_\alpha+1)]^{1/2} \times \begin{Bmatrix} L_\alpha & l_\alpha & L \\ S_\alpha & \frac{1}{2} & S \\ J_\alpha & j_\alpha & J \end{Bmatrix} D_{jq}[(LS)JJ_0]. \quad (4.28)$$

Here the final residual ion is specified by $(L_\alpha S_\alpha) J_\alpha$, and the combined final system by $[(L_\alpha l_\alpha) L (S_\alpha \frac{1}{2}) S] J$.

V. LOW-ENERGY PHOTOIONIZATION PROCESSES

A. Angular distribution and spin polarization

For the photoionization of outer subshell electrons, which requires photons with wavelengths $\lambda \gtrsim 100$ Å, the electric-dipole transition dominates. Therefore it is sufficient to retain only the electric-dipole interaction in the multipole expansion of photon fields. In the electric-dipole approximation, we have $j = 1$, and the corresponding reduced matrix element does not depend on q. We then obtain the following simplified expressions:

$$R_{11} + R_{-1-1} = D(\kappa'_\alpha) D^*(\kappa_\alpha), \quad (5.1)$$

$$R_{11} - R_{-1-1} = p \sin 2\alpha D(\kappa'_\alpha) D^*(\kappa_\alpha), \quad (5.2)$$

$$R_{1-1} + R_{-11} = -p \cos 2\alpha \cos 2\bar{\phi} D(\kappa'_\alpha) D^*(\kappa_\alpha), \quad (5.3)$$

$$R_{1-1} - R_{-11} = -ip \cos 2\alpha \sin 2\bar{\phi} D(\kappa'_\alpha) D^*(\kappa_\alpha), \quad (5.4)$$

where we have used the relations (4.11)–(4.14). The reduced matrix element $D(\kappa_\alpha)$ is given explicitly in the Coulomb gauge as

$$D(\kappa_\alpha) = i^{-l_\alpha} \exp(i\sigma_{\kappa_\alpha}) \left\langle J \left\| \sum_{i=1}^{N} \vec{\alpha}_i \cdot \vec{A}^{(E1)}(k\vec{r}_i) \right\| J_0 \right\rangle, \quad (5.5)$$

where the electric-dipole potential is

$$\vec{A}_m^{(E1)}(k\vec{r}) \equiv -\frac{i}{\sqrt{2}} \vec{A}_{1m}^{(E)} = \left(\frac{2}{3\pi}\right)^{1/2} j_0(kr) \vec{Y}_{10m}(\hat{r}) - \left(\frac{1}{3\pi}\right)^{1/2} j_2(kr) \vec{Y}_{12m}(\hat{r}). \quad (5.6)$$

Here $j_l(kr)$ is the spherical Bessel function and $\vec{Y}_{jlm}(\hat{r})$ the vector spherical harmonics.[28] We note that the operator $\vec{A}_m^{(E1)}$ has the long-wavelength limit

$$\vec{A}_m^{(E1)}(k\vec{r}) \underset{kr \ll 1}{\sim} (6\pi^2)^{-1/2} \vec{e}_m. \quad (5.7)$$

When applicable, this considerably simplifies the numerical calculation of radial integrals. Nonrelativistic formulas are obtained by the replacement

$$\vec{\alpha}_i \rightarrow \vec{p}_i \quad (5.8)$$

in Eq. (5.5). When (5.7) is also substituted in (5.5), the matrix element reduces to that of velocity form with an additional factor of $(6\pi^2)^{-1/2}$. A similar simplification can be made in the length gauge, which gives rise to the reduced matrix element of length form in the nonrelativistic limit.

Substituting $j = j' = 1$ and (5.1)–(5.4) into (4.20)–(4.23), we obtain the differential cross section and spin polarization of photoelectrons in the electric-dipole approximation as

$$\frac{d\sigma}{d\Omega}(\theta, \phi) = \frac{\sigma}{4\pi} F(\theta, \phi), \quad (5.9)$$

$$P_x(\theta, \phi) = (\xi p \sin 2\alpha + \eta p \cos 2\alpha \sin 2\bar{\phi}) \sin\theta / F(\theta, \phi), \quad (5.10)$$

$$P_y(\theta, \phi) = \eta (1 + p \cos 2\alpha \cos 2\bar{\phi}) \sin\theta \cos\theta / F(\theta, \phi), \quad (5.11)$$

$$P_z(\theta, \phi) = \zeta p \sin 2\alpha \cos\theta / F(\theta, \phi), \quad (5.12)$$

where

$$F(\theta, \phi) = 1 - \tfrac{1}{2}\beta [P_2(\cos\theta) - \tfrac{3}{2} p \cos 2\alpha \cos 2\bar{\phi} \sin^2\theta]. \quad (5.13)$$

The differential cross section (5.9) in special cases reduces to previous results.[19,36–42] The differential spin polarizations (5.10)–(5.12) also in special cases agree with previous results.[18–21] For comparison, we note particularly that our spin-polarization parameters are related to those of Lee[21] by $\xi = -\delta_k$, $\eta = 2\xi_k$, and $\zeta = \gamma_k$. In (5.9)–(5.13) the dynamical parameters σ, β, ξ, η, and ζ are given as

$$\sigma = \frac{8\pi^4}{\omega c (2J_0 + 1)} \bar{\sigma}, \quad (5.14)$$

$$\beta = -\bar{\sigma}^{-1} (\tfrac{6}{5})^{1/2} \sum_{\kappa_\alpha J, \kappa'_\alpha J'} \begin{pmatrix} j_\alpha & j'_\alpha & 2 \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} C_{\alpha' \alpha 2}, \quad (5.15)$$

$$\xi = \bar{\sigma}^{-1} (3^{1/2}/2) \sum_{\kappa_\alpha J, \kappa'_\alpha J'} (-)^{j'_\alpha + l'_\alpha - 1/2} \times \begin{pmatrix} j_\alpha & j'_\alpha & 1 \\ \frac{1}{2} & \frac{1}{2} & -1 \end{pmatrix} C_{\alpha' \alpha 1}, \quad (5.16)$$

$$\eta = \bar{\sigma}^{-1} i(\tfrac{3}{2}) 5^{-1/2} \sum_{\kappa_\alpha J, \kappa'_\alpha J'} (-)^{j'_\alpha + l'_\alpha + 1/2} \times \begin{pmatrix} j_\alpha & j'_\alpha & 2 \\ \frac{1}{2} & \frac{1}{2} & -1 \end{pmatrix} C_{\alpha'\alpha 2}, \tag{5.17}$$

$$\zeta = \bar{\sigma}^{-1} (\tfrac{3}{2})^{1/2} \sum_{\kappa_\alpha J, \kappa'_\alpha J'} \begin{pmatrix} j_\alpha & j'_\alpha & 1 \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} C_{\alpha'\alpha 1}, \tag{5.18}$$

where we have defined

$$\bar{\sigma} = \sum_{\kappa_\alpha J} D(\kappa_\alpha) D^*(\kappa_\alpha), \tag{5.19}$$

$$C_{\alpha'\alpha l} = (-)^{J_0 - J_\alpha + 1/2} [l]^2 [j_\alpha J j'_\alpha J'] \times \begin{Bmatrix} J & J' & l \\ j'_\alpha & j_\alpha & J_\alpha \end{Bmatrix} \begin{Bmatrix} J & J' & l \\ 1 & 1 & J_0 \end{Bmatrix} D(\kappa'_\alpha) D^*(\kappa_\alpha). \tag{5.20}$$

As noted at the end of Sec. IV, the corresponding formulas in *LSJ* coupling can be obtained by making the substitution (4.28).

In terms of Stokes parameters we can rewrite Eqs. (5.10)–(5.13) as

$$P_x(\theta, \phi) = [\eta(-S_1 \sin 2\phi + S_2 \cos 2\phi) + \xi S_3] \sin\theta / F(\theta, \phi), \tag{5.10'}$$

$$P_y(\theta, \phi) = \eta[1 - S_1 \cos 2\phi - S_2 \sin 2\phi] \sin\theta \cos\theta / F(\theta, \phi), \tag{5.11'}$$

$$P_z(\theta, \phi) = \zeta S_3 \cos\theta / F(\theta, \phi), \tag{5.12'}$$

and

$$F(\theta, \phi) = 1 - \tfrac{1}{2}\beta[P_2(\cos\theta) + \tfrac{3}{2}(S_1 \cos 2\phi + S_2 \sin 2\phi) \sin^2\theta]. \tag{5.13'}$$

It is interesting to note that the functions F, P_xF, P_yF, and P_zF are all *linear functions* of the Stokes parameters S_i. Physically, this fact corresponds to the assertion made by Stokes[25] that *any measurement using polarized light is a linear function of the parameters* S_i. For this reason, the differential cross-section and spin-polarization formulas of four suitably chosen photon polarizations should be sufficient to determine the desired formulas (5.10)–(5.13) for arbitrarily polarized photons. We will discuss this in Appendix F. To write (5.10)–(5.13) in a concise matrix form, we define the column matrices

$$P \equiv \begin{bmatrix} F \\ P_x F \\ P_y F \\ P_z F \end{bmatrix}, \tag{5.21}$$

and

$$S \equiv \begin{bmatrix} 1 \\ S_1 \\ S_2 \\ S_3 \end{bmatrix}. \tag{5.22}$$

Consequently, the angular distribution and spin polarization of photoelectrons are related to the Stokes parameters by the relation

$$P = \Lambda S, \tag{5.23}$$

where the matrix Λ is given as

$$\Lambda = \begin{bmatrix} 1 - \frac{1}{2}\beta P_2(\cos\theta) & -\frac{3}{4}\beta \cos 2\phi \sin^2\theta & -\frac{3}{4}\beta \sin 2\phi \sin^2\theta & 0 \\ 0 & -\eta \sin 2\phi \sin\theta & \eta \cos 2\phi \sin\theta & \xi \sin\theta \\ \eta \sin\theta \cos\theta & -\eta \cos 2\phi \sin\theta \cos\theta & -\eta \sin 2\phi \sin\theta \cos\theta & 0 \\ 0 & 0 & 0 & \zeta \cos\theta \end{bmatrix}. \tag{5.24}$$

The spin polarization with respect to the fixed coordinate system XYZ can be derived by using the transformation formula (E4) in Appendix E. We therefore obtain

$$P_X(\theta, \phi) = \{-\eta(1 + S_1) \sin\phi + [\eta S_2 + (\xi + \zeta) S_3] \cos\phi\} \times \sin\theta \cos\theta / F(\theta, \phi), \tag{5.25}$$

$$P_Y(\theta, \phi) = \{\eta(1 - S_1) \cos\phi + [-\eta S_2 + (\xi + \zeta) S_3] \sin\phi\} \times \sin\theta \cos\phi / F(\theta, \phi), \tag{5.26}$$

$$P_Z(\theta, \phi) = \frac{[\eta(S_1 \sin 2\phi - S_2 \cos 2\phi) - \xi S_3] \sin^2\theta + \zeta S_3 \cos^2\theta}{F(\theta, \phi)}. \tag{5.27}$$

The spin polarization of the total photoelectron flux can easily be obtained from (5.25)–(5.27) by integrating over all angles. The total spin polarization is then given by

$$P_X = P_Y = 0, \tag{5.28}$$

$$P_Z = \delta S_3. \tag{5.29}$$

Here the parameter δ is defined as

$$\delta = \tfrac{1}{3}(\zeta - 2\xi), \tag{5.30}$$

which is to be compared with the spin polarization of photoelectrons ejected by pure circularly polarized photons considered by Fano.[17] Again we see that the total spin polarization P_Z is a *linear function* of the Stokes parameter S_3.

Now we consider special cases of the angular-distribution and spin-polarization formulas (5.9)–(5.12).

(i) For pure or mixed circularly polarized photons, we have $\alpha = \pi/4$ and $\alpha = -\pi/4$, which correspond to the right and left circular polarizations, respectively. Therefore we obtain

$$\frac{d\sigma}{d\Omega}(\theta,\phi) = \frac{\sigma}{4\pi}[1 - \tfrac{1}{2}\beta P_2(\cos\theta)], \tag{5.31}$$

$$P_x(\theta,\phi) = \pm p\frac{\xi\sin\theta}{1 - \tfrac{1}{2}\beta P_2(\cos\theta)}, \tag{5.32}$$

$$P_y(\theta,\phi) = \frac{\eta\sin\theta\cos\theta}{1 - \tfrac{1}{2}\beta P_2(\cos\theta)}, \tag{5.33}$$

$$P_z(\theta,\phi) = \pm p\frac{\zeta\cos\theta}{1 - \tfrac{1}{2}\beta P_2(\cos\theta)}, \tag{5.34}$$

where the + and − signs refer to the right and left circular polarization, respectively (or the positive and negative helicities). In the limiting case $p = 1$, the formulas (5.32)–(5.34) reduce to those for pure circularly polarized incident photons.[21]

(ii) For pure or mixed linearly polarized photons, we have $\alpha = 0$. The formulas (5.9)–(5.12) become

$$\frac{d\sigma}{d\Omega}(\theta,\phi) = \frac{\sigma}{4\pi}F(\theta,\phi), \tag{5.35}$$

$$P_x(\theta,\phi) = p\frac{\eta\sin 2\bar{\phi}\sin\theta}{F(\theta,\phi)}, \tag{5.36}$$

$$P_y(\theta,\phi) = \frac{\eta(1 + p\cos 2\bar{\phi})\sin\theta\cos\theta}{F(\theta,\phi)}, \tag{5.37}$$

$$P_z(\theta,\phi) = 0, \tag{5.38}$$

with

$$F(\theta,\phi) = 1 - \tfrac{1}{2}\beta[P_2(\cos\theta) - \tfrac{3}{2}p\cos 2\bar{\phi}\sin^2\theta]. \tag{5.39}$$

For pure linearly polarized incident photons, the degree of polarization p equals 1, and we can rewrite $F(\theta,\phi)$ as

$$F(\theta,\phi) = 1 + \beta P_2(\cos\bar{\theta}), \tag{5.40}$$

where $\bar{\theta}$ is the polar angle of the photoelectron direction referring to the photon polarization vector. We can also simplify the nonvanishing components of the spin polarization as

$$P_x(\theta,\phi) = \frac{2\eta\sin\bar{\phi}\cos\bar{\theta}}{1 + \beta P_2(\cos\bar{\theta})}, \tag{5.41}$$

$$P_y(\theta,\phi) = \frac{2\eta\cos\bar{\phi}\cos\bar{\theta}\cos\theta}{1 + \beta P_2(\cos\bar{\theta})}. \tag{5.42}$$

By a rotation of the coordinate system xyz on the xy plane through an angle $\psi = -\tan^{-1}(\tan\bar{\phi}/\cos\theta)$, we can make the new y' axis coincide with the direction of the photoelectron polarization vector $\vec{P} = P_x\hat{e}_x + P_y\hat{e}_y$. In this new coordinate system $x'y'z'$ we have

$$P_{y'}(\theta,\phi) = \frac{2\eta\sin\bar{\theta}\cos\bar{\theta}}{1 + \beta P_2(\cos\bar{\theta})}, \tag{5.43}$$

$$P_{x'}(\theta,\phi) = P_{z'}(\theta,\phi) = 0. \tag{5.44}$$

We note that when the photon polarization vector coincides with the X axis, i.e., $\gamma = 0$, we have $\bar{\phi} = \phi$. Consequently, the y' axis lies on the YZ plane (and, of course, the xy plane) and is perpendicular to the Xz plane. To compare with the pure linear polarization result of Lee,[21] we note that his x' and y' axes correspond to our $-x'$ and $-y'$ axes, respectively.

(iii) For unpolarized incident photons, we simply take $p = 0$, and the angular-distribution and spin-polarization formulas (5.9)–(5.12) become

$$\frac{d\sigma}{d\Omega}(\theta,\phi) = \frac{\sigma}{4\pi}[1 - \tfrac{1}{2}\beta P_2(\cos\theta)], \tag{5.45}$$

$$P_x(\theta,\phi) = P_z(\theta,\phi) = 0, \tag{5.46}$$

$$P_y(\theta,\phi) = \frac{\eta\sin\theta\cos\theta}{1 - \tfrac{1}{2}\beta P_2(\cos\theta)}. \tag{5.47}$$

The spin-polarization formulas (5.46) and (5.47) agree with previous results.[20,21]

The maximum photoelectron polarization attainable by any photons incident on a specific target atom can be derived by considering (5.10)–(5.12). The total spin polarization of photoelectrons at certain angles (θ,ϕ) is given by

$$P(\theta,\phi) \equiv |\vec{P}(\theta,\phi)| = [P_x^2(\theta,\phi) + P_y^2(\theta,\phi) + P_z^2(\theta,\phi)]^{1/2}. \tag{5.48}$$

The maximum of $P(\theta,\phi)$ is best obtained numerically because of the large number of parameters involved. However, the maxima of spin-polarization components P_x, P_y, and P_z for specific cases can readily be calculated. We give a few examples as follows.

(a) Circularly polarized photons:

$$|P_x|_{\max} = |\xi| \begin{cases} \dfrac{4}{4+\beta}, & -1 \le \beta \le \frac{4}{5}, \quad \text{at } \theta = \dfrac{\pi}{2} \\ \left[\dfrac{2}{3\beta(2-\beta)}\right]^{1/2}, & \frac{4}{5} \le \beta \le 2 \quad \text{at } \sin\theta = \left[\dfrac{4-2\beta}{3\beta}\right]^{1/2} \end{cases} ; \tag{5.49}$$

$$|P_y|_{\max} = |\eta| \left[\frac{2}{(2-\beta)(4+\beta)}\right]^{1/2}, \quad \text{at } \sin\theta = \left[\frac{4-2\beta}{8-\beta}\right]^{1/2} ; \tag{5.50}$$

$$|P_z|_{\max} = |\xi| \left[\frac{2}{2-\beta}\right], \quad \text{at } \theta = 0, \ \pi . \tag{5.51}$$

(b) Linearly polarized photons:

$$|P|_{\max} = |P_{y'}|_{\max} = |\eta| \left[\frac{2}{(1+\beta)(2-\beta)}\right]^{1/2}, \quad \text{at } \sin\bar{\theta} = \left[\frac{2+2\beta}{4+\beta}\right]^{1/2} . \tag{5.52}$$

(c) Unpolarized photons:

$$|P|_{\max} = |P_y|_{\max} = |\eta| \left[\frac{2}{(2-\beta)(4+\beta)}\right]^{1/2}, \quad \text{at } \sin\theta = \left[\frac{4-2\beta}{8-\beta}\right]^{1/2} . \tag{5.53}$$

Because the polarization vector P must have a length less than or equal to 1 at all angles (θ, ϕ), we can establish interesting kinematic relations between the angular-distribution parameter β and the spin-polarization parameters ξ, η, and ζ:

$$|\xi| \le \begin{cases} (4+\beta)/4, & -1 \le \beta \le \frac{4}{5} \\ [3\beta(2-\beta)/2]^{1/2}, & \frac{4}{5} \le \beta \le 2 \end{cases} \tag{5.54}$$

$$|\eta| \le [(1+\beta)(2-\beta)/2]^{1/2}, \tag{5.55}$$

$$|\zeta| \le (2-\beta)/2 , \tag{5.56}$$

and also

$$|\delta| \le \begin{cases} 1, & -1 \le \beta \le \frac{4}{5} , \\ (2-\beta)/6 + [2\beta(2-\beta)/3]^{1/2}, & \frac{4}{5} \le \beta \le 2 . \end{cases} \tag{5.57}$$

These relations can serve as checks on the self-consistency in the measurement of the angular distribution and spin polarization of photoelectrons. It is also interesting to note that when β reaches its maximum value 2 the spin polarization must be zero, and that when β attains its minimum value -1 there will be no spin polarization perpendicular to the reaction plane defined by the Z and z axes. These are demonstrated in Fig. 3.

The maximum number of independent dynamical parameters for photoionizations in the electric-dipole approximation is *five*. However, there are cases in which this number is *less than five*. Examples will be given in the next subsection, where we consider the photoionization of closed-shell atoms.

B. Explicit formulas for closed-shell atoms

Because of special interests in closed-shell atoms, we present explicit expressions of the five dynamical parameters σ, β, ξ, η, and ζ in this section. The total cross section (5.14) for closed-shell atoms is given as

$$\sigma = \frac{8\pi^4}{\omega c}\bar{\sigma}, \tag{5.58}$$

where

$$\bar{\sigma} = |D_{j-1}|^2 + |D_j|^2 + |D_{j+1}|^2 . \tag{5.59}$$

Here for brevity we have used the notation $j \equiv J_\alpha$, $D_{j-1} \equiv D(\kappa_\alpha)_{j_\alpha = J_\alpha - 1}$, etc. The other parameters for closed-shell atoms are

$$\beta = \left\{ \frac{(2j-3)}{2(2j)} |D_{j-1}|^2 - \frac{(2j-1)(2j+3)}{(2j)(2j+2)} |D_j|^2 + \frac{2j+5}{2(2j+2)} |D_{j+1}|^2 - \frac{3}{2j}\left[\frac{2j-1}{2(2j+2)}\right]^{1/2} (D_{j-1}D_j^* + \text{c.c.}) \right.$$
$$\left. - \frac{3}{2}\left[\frac{(2j-1)(2j+3)}{2j(2j+2)}\right]^{1/2} (D_{j-1}D_{j+1}^* + \text{c.c.}) + \frac{3}{2j+2}\left[\frac{2j+3}{2(2j)}\right]^{1/2} (D_j D_{j+1}^* + \text{c.c.}) \right\} \Big/ \bar{\sigma} , \tag{5.60}$$

$$\xi = (-)^{l+j+1/2} \left\{ -\frac{3(2j-1)}{4(2j)} |D_{j-1}|^2 - \frac{3(2j+1)}{2(2j)(2j+2)} |D_j|^2 + \frac{3(2j+3)}{4(2j+2)} |D_{j+1}|^2 \right.$$
$$\left. + \frac{3}{4(2j)}\left[\frac{(2j-1)(2j+2)}{2}\right]^{1/2} (D_{j-1}D_j^* + \text{c.c.}) - \frac{3}{4(2j+2)}\left[\frac{2j(2j+3)}{2}\right]^{1/2} (D_j D_{j+1}^* + \text{c.c.}) \right\} \Big/ \bar{\sigma} \tag{5.61}$$

$$\eta = i(-)^{l+j+1/2}\left\{-\frac{3}{4}\left[\frac{2j-1}{2(2j+2)}\right]^{1/2}(D_{j-1}D_j^* - \text{c.c.}) + \frac{3}{4}\left[\frac{(2j-1)(2j+3)}{2j(2j+2)}\right]^{1/2}(D_{j-1}D_{j+1}^* - \text{c.c.}) - \frac{3}{4}\left[\frac{2j+3}{2(2j)}\right]^{1/2}(D_jD_{j+1}^* - \text{c.c.})\right\} \Big/ \bar{\sigma}, \tag{5.62}$$

$$\zeta = \left\{-\frac{3}{2(2j)}|D_{j-1}|^2 + \frac{3}{(2j)(2j+2)}|D_j|^2 + \frac{3}{2(2j+2)}|D_{j+1}|^2 - \frac{3}{2(2j)}\left[\frac{(2j-1)(2j+2)}{2}\right]^{1/2}(D_{j-1}D_j^* + \text{c.c.}) - \frac{3}{2(2j+2)}\left[\frac{2j(2j+3)}{2}\right]^{1/2}(D_jD_{j+1}^* + \text{c.c.})\right\} \Big/ \bar{\sigma}, \tag{5.63}$$

where $(-)^l$ gives the parity of the residual ion. The expression for β agrees with previous results.[33,43] The parameter δ for the total spin polarization can be obtained from (5.61) and (5.63) as

(i) $l = j + \frac{1}{2}$:

$$\delta = \left\{\frac{2j-2}{2(2j)}|D_{j-1}|^2 + \frac{1}{2j}|D_j|^2 - \tfrac{1}{2}|D_{j+1}|^2 - \frac{1}{2j}\left[\frac{(2j-1)(2j+2)}{2}\right]^{1/2}(D_{j-1}D_j^* + \text{c.c.})\right\} \Big/ \bar{\sigma}, \tag{5.64}$$

(ii) $l = j - \frac{1}{2}$:

$$\delta = \left\{-\tfrac{1}{2}|D_{j-1}|^2 - \frac{1}{2j+2}|D_j|^2 + \frac{2j+4}{2(2j+2)}|D_{j+1}|^2 - \frac{1}{2j+2}\left[\frac{2j(2j+3)}{2}\right]^{1/2}(D_jD_{j+1}^* + \text{c.c.})\right\} \Big/ \bar{\sigma}. \tag{5.65}$$

It is of interest to note that in the case of ($l = 1$, $j = \frac{1}{2}$) different components combine *incoherently* as indicated in (5.64).

The corresponding formulas in *LSJ* coupling can be derived with the substitutions (4.28). With the short-hand notation

$$D_{LS} \equiv D[(LS)JJ_0], \tag{5.66}$$

we have explicitly:

(i) $l = j + \frac{1}{2}$:

$$D_{j-1} = [4(2j)]^{-1/2}\{[2(2j-1)]^{1/2}D_{10} - (2j-1)^{1/2}D_{11} + (2j+3)^{1/2}D_{21}\}, \tag{5.67}$$

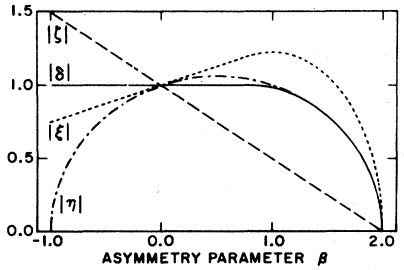

FIG. 3. Maximum ranges of spin-polarization parameters plotted against the angular distribution parameter β.

$$D_j = [2(2j)(2j+2)]^{-1/2}\{-\sqrt{2}D_{10} + (2j+1)D_{11} + [(2j-1)(2j+3)]^{1/2}D_{21}\}, \tag{5.68}$$

$$D_{j+1} = [4(2j+2)]^{-1/2}\{[2(2j+1)]^{1/2}D_{10} + (2j+1)^{1/2}D_{11} + (2j+5)^{1/2}D_{21}\}. \tag{5.69}$$

(ii) $l = j - \frac{1}{2}$:

$$D_{j-1} = [4(2j)]^{-1/2}\{[2(2j+1)]^{1/2}D_{10} + (2j+1)^{1/2}D_{11} - (2j-3)^{1/2}D_{21}\}, \tag{5.70}$$

$$D_j = [2(2j)(2j+2)]^{-1/2}\{\sqrt{2}D_{10} + (2j+1)D_{11} - [(2j-1)(2j+3)]^{1/2}D_{21}\}, \tag{5.71}$$

$$D_{j+1} = [4(2j+2)]^{-1/2}\{[2(2j+3)]^{1/2}D_{10} - (2j+3)^{1/2}D_{11} - (2j-1)^{1/2}D_{21}\}. \tag{5.72}$$

It is clear that the maximum number of independent dynamical parameters is *five* because there are at most *three* dipole amplitudes and *two* relative phases. For cases with $j = \frac{1}{2}$, there are only *two* dipole amplitudes and *one* relative phase; hence only *three* independent dynamical parameters are possible. For examples in the $np_{1/2}$ or $ns_{1/2}$ subshell photoionization, we can choose σ, β, and η to be the three independent parameters and obtain

$$\xi^2 = (1 - \beta/2)(1 + \beta) - \eta^2, \tag{5.73}$$

$$\zeta = 1 - \beta/2. \tag{5.74}$$

Note that in these cases when β reaches its minimum value -1 only the longitudinal spin polarization is possible with the corresponding parameter $\zeta = 1.5$.

VI. APPLICATIONS

All the dynamical properties of photoionization processes are contained in the reduced matrix elements (3.14). These reduced matrix elements may be calculated in separate single-channel calculations or a multichannel calculation. Several

relativistic multichannel theories have been developed, e.g., the relativistic random-phase approximation,[33,44] relativistic quantum-defect theory,[45] relativistic R-matrix theory,[46] and the relativistic equation-of-motion method.[47] In addition, we introduce a relativistic version of the K-matrix theory,[48] which is outlined in Appendix G. When relativistic effects are not important, nonrelativistic multichannel theories may also be used in computing the reduced matrix element (3.14) with the nonrelativistic replacement (5.8). Also we note that the LSJ coupling may be more suitable in a nonrelativistic calculation, in which case we would need the transformation formula (4.28). Nonrelativistic multichannel theories have been reviewed recently,[4] and references therein should be consulted. Nevertheless, the spin-orbit interactions have to be treated to observe polarization effects.

The present formulation for the spin polarization of photoelectrons has been applied using the nonrelativistic K-matrix method with the spin-orbit interactions included[49] and using the relativistic random-phase approximation.[50-52] Excellent agreement with experiments[53,54] has been obtained.

ACKNOWLEDGMENT

The author acknowledges the support by the National Science Foundation under Grant No. PHY79-09229 and by a Cottrell Research Grant from the Research Corporation.

APPENDIX A: A CONVENTION OF PHOTON SPIN POLARIZATION

To make unambiguous the meaning of parameters p, α, and γ used in this work, we will introduce briefly our convention. We choose a coordinate system XYZ such that the Z axis is in the direction of the photon flux. The X axis can be chosen in any convenient direction because the photon polarization is determined accordingly. A *pure polarization state* (*completely polarized*) can be characterized by the polarization vector $\hat{\epsilon}$ which has the general form

$$\hat{\epsilon} = \hat{e}_{+1} e^{-i\gamma} \cos(\alpha - \tfrac{1}{4}\pi) + \hat{e}_{-1} e^{i\gamma} \sin(\alpha - \tfrac{1}{4}\pi) . \quad \text{(A1)}$$

Here $\hat{e}_{+1}$ and $\hat{e}_{-1}$ are the spherical unit vectors[28] in the coordinate system XYZ and correspond to the positive and negative helicity states, respectively. We shall refer to e_{+1} as right circular and to e_{-1} as left circular polarization; *in optics the converse definition is usually adopted.* It is sufficient to restrict the parameters in Eq. (A1) to the ranges $-\pi/2 < \alpha < \pi/2$ and $0 \leq \gamma < \pi$. The case $\alpha = 0$ denotes linear polarization at an angle γ to the X axis, the cases $\alpha = \pi/4$ and $-\pi/4$ denote right and left circular polarizations, respectively,

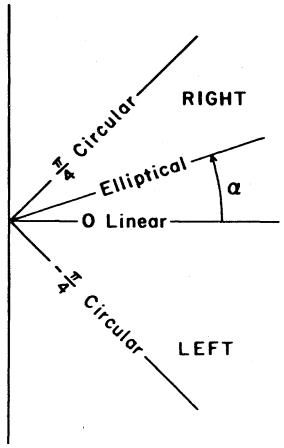

FIG. 4. Types of photon polarization as determined by parameter α. Right and left circular polarizations correspond to positive and negative helicity states, respectively.

and cases with arbitrary α correspond to elliptical polarizations with the principal axis $k\cos\alpha$ at an angle γ to the X axis. In general, the parameter α specifies the type of polarization, which is illustrated in Fig. 4. The parameter γ specifies the azimuthal orientation of the polarization, and this is best illustrated by the general case of elliptical polarization, where the ellipse traced out by $\mathrm{Re}\{\vec{E}\}$ is rotated through an angle γ (see Fig. 5). The density matrix corresponding to the polarization state (A1) is

$$\rho = \frac{1}{2} \begin{pmatrix} 1+\sin 2\alpha & -e^{-i2\gamma}\cos 2\alpha \\ -e^{i2\gamma}\cos 2\alpha & 1-\sin 2\alpha \end{pmatrix} . \quad \text{(A2)}$$

An incoherent sum of equal amounts of two mutually orthogonal polarization states is a *completely unpolarized state*; a notable example is the natural light. The most general polarization state can be

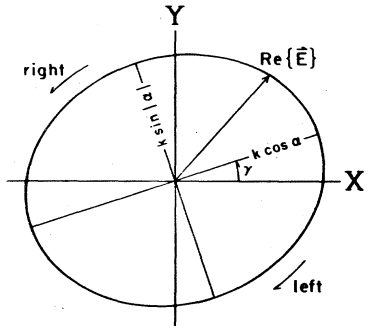

FIG. 5. Precession of the electric field at a given point in space for an elliptically polarized photon. The ellipse traced out by the electric field $\vec{E}$ is oriented with one of its principal axes making an angle γ with the X axis. The direction (right or left) of precession depends on the sign (positive or negative) of parameter α.

regarded as a mixture of completely polarized and completely unpolarized states. The probability p $(0 \leq p \leq 1)$ of complete polarization is referred to as the degree of polarization of the photon. The most general polarization state cannot be described by a polarization vector but rather by a density matrix:

$$\rho = \frac{1}{2}\begin{pmatrix} 1+p\sin 2\alpha & -pe^{-i2\gamma}\cos 2\alpha \\ -pe^{i2\gamma}\cos 2\alpha & 1-p\sin 2\alpha \end{pmatrix}. \tag{A3}$$

Note that when $p=1$, we recover the completely polarized state (A2). The three parameters p, α, and γ completely specify an arbitrary polarization state of the photon.

APPENDIX B: DIRAC ORBITALS

We review briefly the Dirac orbital and its phase convention used here. Dirac orbitals in central field can be completely specified by the quantum numbers n, κ, and m. For a definite κ, the total-angular-momentum quantum number j and the orbital-angular-momentum quantum number l of the large component, which determines the parity of the Dirac orbital, are given as

$$j = |\kappa| - \tfrac{1}{2}, \quad l = \begin{cases} \kappa, & \kappa > 0 \\ -\kappa - 1, & \kappa < 0 \end{cases}. \tag{B1}$$

For example, the values $\kappa = -1$, 1, -2, and 2 correspond to $s_{1/2}$, $p_{1/2}$, $p_{3/2}$, and $d_{3/2}$ orbitals, respectively. The magnetic quantum number m is associated with the z component J_z of the total angular momentum. Dirac orbitals with definite $n\kappa m$ have the explicit form

$$U_{n\kappa m} = \frac{1}{r}\begin{pmatrix} G_{n\kappa}(r) & \Omega_{\kappa m} \\ iF_{n\kappa}(r) & \Omega_{-\kappa m} \end{pmatrix}. \tag{B2}$$

Here the radial functions $G_{n\kappa}$ and $F_{n\kappa}$ are the large and small components, respectively, and satisfy the orthonormality condition

$$\int_0^\infty dr(G_{n\kappa}G_{n'\kappa} + F_{n\kappa}F_{n'\kappa}) = \delta_{nn'}. \tag{B3}$$

The angular functions $\Omega_{\kappa m}$ in (B2) are normalized spherical spinors defined as

$$\Omega_{\kappa m} \equiv \Omega_{jlm} = \sum_{M\mu} \langle lM\tfrac{1}{2}\mu | jm\rangle Y_{lM}(\hat{r})\chi_\mu, \tag{B4}$$

where Y_{lM} is the spherical harmonics, and χ_μ the spin eigenfunction with $s=\frac{1}{2}$ and $s_z=\mu$, given, for example, by the two-component Pauli spinor.

Note that the phase convention (B2) used here is different from that of Ref. 34, namely,

$$U_{n\kappa m} = \frac{1}{r}\begin{pmatrix} iG_{n\kappa}(r) & \Omega_{\kappa m} \\ F_{n\kappa}(r) & \Omega_{-\kappa m} \end{pmatrix}. \tag{B5}$$

Therefore to use formulas presented in Ref. 34, where the convention (B5) is used, we have to make the substitution

$$G_{n\kappa} \to -G_{n\kappa}, \text{ or } F_{n\kappa} \to -F_{n\kappa}. \tag{B6}$$

APPENDIX C: MULTIPOLE INTERACTIONS AND THEIR INTERACTION STRENGTHS

We shall first define the normalized magnetic, electric, and longitudinal multipole potentials

$$\vec{A}^{(M)}_{jm} = i^j\left(\frac{2}{\pi}\right)^{1/2} j_j(kr)\vec{Y}_{jjm}(\hat{r}), \tag{C1}$$

$$\vec{A}^{(E)}_{jm} = i^j\left(\frac{2}{\pi}\right)^{1/2}\left[\left(\frac{j+1}{2j+1}\right)^{1/2} j_{j-1}(kr)\vec{Y}_{j(j-1)m}(\hat{r}) - \left(\frac{j}{2j+1}\right)^{1/2} j_{j+1}(kr)\vec{Y}_{j(j+1)m}(\hat{r})\right], \tag{C2}$$

$$\vec{A}^{(L)}_{jm} = i^j\left(\frac{2}{\pi}\right)^{1/2}\left[\left(\frac{j}{2j+1}\right)^{1/2} j_{j-1}(kr)\vec{Y}_{j(j-1)m}(\hat{r}) + \left(\frac{j+1}{2j+1}\right)^{1/2} j_{j+1}(kr)\vec{Y}_{j(j+1)m}(\hat{r})\right], \tag{C3}$$

where Y_{jlm} are vector spherical harmonics,[28] and the radial functions $j_l(kr)$ are spherical Bessel functions (of the first kind). The multipole potentials are normalized such that

$$\int d^3r\vec{A}^{(a')}_{j'm'}\cdot\vec{A}^{(a)*}_{jm} = \frac{1}{k^2}\delta(k'-k)\delta_{a'a}\delta_{j'j}\delta_{m'm} \tag{C4}$$

with $a = M$, E, or L. The multipole interaction operators are given in the Coulomb (or transverse) gauge by

(i) magnetic multipole interactions:

$$T^{(M)}_{jm} = -\vec{\alpha}\cdot\vec{A}^{(M)}_{jm}, \tag{C5}$$

(ii) electric multipole interactions:

$$T^{(E,v)}_{jm} = -\vec{\alpha}\cdot\vec{A}^{(E)}_{jm}, \tag{C6}$$

where the superscript v signifies that the interaction reduces to that of velocity form in the nonrelativistic limit. Multipole interaction operators in other gauges can be obtained by making gauge transformations. One particular choice is the length gauge[32,33]:

(i) Magnetic multipole interactions are the same as in the Coulomb gauge.

(ii) Electric multipole interactions:

$$T^{(E,l)}_{jm} = ik\chi_{jm} - \vec{\alpha}\cdot[\vec{A}^{(E)}_{jm} + \vec{\nabla}\chi_{jm}], \tag{C7}$$

where the gauge function χ_{jm} is

$$\chi_{jm} = -i^j\left(\frac{2}{\pi}\right)^{1/2}\frac{1}{k}\left(\frac{j+1}{j}\right)^{1/2} j_j(kr)Y_{jm}(\hat{r}). \tag{C8}$$

Note that

$$\vec{\nabla}\chi_{jm} = -\left(\frac{j+1}{j}\right)^{1/2}\vec{A}^{(L)}_{jm}. \tag{C9}$$

After substituting (C8) and (C9) into (C7) we get

$$T^{(E,l)}_{jm} = i^j\left(\frac{2}{\pi}\right)^{1/2}\left[-i\left(\frac{j+1}{j}\right)^{1/2} j_j(kr)Y_{jm}(\hat{r}) + \left(\frac{2j+1}{j}\right)^{1/2} j_{j+1}(kr)\vec{\alpha}\cdot\vec{Y}_{j(j+1)m}\right]. \tag{C10}$$

Here the superscript l signifies that the interaction reduces to that of length form in the nonrelativistic limit.

The interaction strength of a tensor interaction T_{jm} of rank j is defined by the Wigner-Eckart theorem[28] as

$$\langle j_a m_a | T_{jm} | j_b m_b\rangle = \begin{pmatrix} j_a & m & m_b \\ m_a & j & j_b \end{pmatrix} X_j(a;b), \tag{C11}$$

where the vector-coupling coefficient is in the covariant notation,[34] and the interaction strength $X_j(a;b)$ can be expressed in terms of radial integrals. The interaction strengths of the multipole interactions $T^{(M)}_{jm}$, $T^{(E,v)}_{jm}$, and $T^{(E,l)}_{jm}$ can easily be evaluated using formulas given in Ref. 34. We present here only the results:

(i) Interaction strength of magnetic multipoles:

$$X^{(M)}_j(a;b) = i^{j-1}\pi^{-1}\left(\frac{2j+1}{2j(j+1)}\right)^{1/2}(\kappa_a+\kappa_b)C_j(ab) \times \langle j_j V_{ab}\rangle^{\text{odd}}. \tag{C12}$$

(ii) Interaction strength of electric multipoles:

$$X^{(E,v)}_j(a;b) = i^{j-1}\pi^{-1}\left(\frac{j(j+1)}{2(2j+1)}\right)^{1/2} C_j(ab) \times [\langle j_{j-1}P_{ab}\rangle^{\text{even}} - \langle j_{j+1}Q_{ab}\rangle^{\text{even}}], \tag{C13}$$

$$X^{(E,l)}_j(a;b) = i^{j-1}\pi^{-1}\left(\frac{(2j+1)(j+1)}{2j}\right)^{1/2} C_j(ab) \times [\langle j_j W_{ab}\rangle^{\text{even}} - \langle j_{j+1}Q_{ab}\rangle^{\text{even}}]. \tag{C14}$$

In (C12), (C13), and (C14), the notations used are defined in Ref. 34 with the modification of phase (B6) in Appendix B.

APPENDIX D: HELICITY STATES

Angular-momentum helicity states (or *spherical helicity states*) $|k\lambda;jm\rangle$ with helicity λ can be constructed from *linear-momentum helicity states* (or *linear helicity state*) $|\vec{k}\lambda\rangle$, and vice versa. They are related by the following[22,23,35]:

$$|k\lambda;jm\rangle = \left(\frac{2j+1}{4\pi}\right)^{1/2}\int d\hat{k} D^{(j)}_{m\lambda}(\hat{k})^* |\vec{k}\lambda\rangle, \tag{D1}$$

and

$$|\vec{k}\lambda\rangle = \sum_{jm}\left(\frac{2j+1}{4\pi}\right)^{1/2} D^{(j)}_{m\lambda}(\hat{k})|k\lambda;jm\rangle, \tag{D2}$$

where $D^{(j)}_{m\lambda}(k)$ are rotation matrices. Here the helicity states are normalized such that

$$\langle\vec{k}\lambda|\vec{k}'\lambda'\rangle = \delta^3(\vec{k}-\vec{k}')\delta_{\lambda\lambda'}, \tag{D3}$$

$$\langle k\lambda;jm|k'\lambda';j'm'\rangle = \left(\frac{1}{k^2}\right)\delta(k-k')\delta_{\lambda\lambda'}\delta_{jj'}\delta_{mm'}. \tag{D4}$$

Photon helicity states. The linear-momentum helicity state is given as

$$\vec{A}_{\vec{k}q} = (2\pi)^{-3/2}\hat{e}_q e^{i\vec{k}\cdot\vec{r}}. \tag{D5}$$

The angular-momentum helicity state can be obtained by

$$\vec{A}_{kq;jm} = \left(\frac{2j+1}{4\pi}\right)^{1/2}\int d\hat{k} D^{(j)}_{mq}(\hat{k})^*\vec{A}_{\vec{k}q}. \tag{D6}$$

In terms of the normalized electric and magnetic multipole potentials we get

$$\vec{A}_{k\pm1;jm} = \mp(1/\sqrt{2})(\vec{A}^{(M)}_{jm} \pm i\vec{A}^{(E)}_{jm}), \tag{D7}$$

where $q = \pm 1$ correspond to the positive and negative helicity states, respectively, of the photon. We may also define the helicity state

$$\vec{A}_{k0;jm} = \vec{A}^{(L)}_{jm}, \tag{D8}$$

which, however, is *not a physical state* of the photon.

Electron helicity states. The linear-momentum helicity state is given by

$$\langle\vec{r}|\vec{k}\mu\rangle = (2\pi)^{-3/2}\begin{pmatrix}1\\ \dfrac{c\vec{\sigma}\cdot\vec{k}}{E+c^2}\end{pmatrix}\chi_\mu e^{i\vec{k}\cdot\vec{r}}, \tag{D9}$$

where χ_μ is the spin eigenfunction with the quantization axis chosen in the $\vec{k}$ direction, $s_{\vec{k}} = \mu$. The angular-momentum helicity state can be obtained by

$$\langle\vec{r}|k\mu;jm\rangle = \left(\frac{2j+1}{4\pi}\right)^{1/2}\int d\hat{k} D^{(j)}_{m\mu}(\hat{k})^*\langle\vec{r}|\vec{k}\mu\rangle = \sum_l i^l\left(\frac{2l+1}{k(2j+1)}\right)^{1/2}\langle los\mu|j\mu\rangle\langle\vec{r}|\kappa m\rangle, \tag{D10}$$

where $\langle\vec{r}|\kappa m\rangle$ is the usual angular-momentum eigenstate,

$$\langle\vec{r}|\kappa m\rangle \equiv \psi_{\kappa m}(\vec{r}) \equiv \frac{1}{r}\begin{pmatrix}G_{\kappa m} & \Omega_{\kappa m}\\ iF_{\kappa m} & \Omega_{-\kappa m}\end{pmatrix}. \tag{D11}$$

In the Pauli approximation, we have

$$\langle\vec{r}|\kappa m\rangle \equiv \langle r|(ls)jm\rangle = \sum_{m\nu}\langle lm s\nu|jm\rangle\langle\vec{r}|lm\rangle\chi_\nu, \tag{D12}$$

where χ_ν is the spin eigenfunction with $s_z = \nu$.

APPENDIX E: TRANSFORMATION OF THE POLARIZATION VECTOR P

The polarization vector $\vec{P}=(P_X, P_Y, P_Z)$ in a coordinate system XYZ can be expressed in terms of components $P_{X'}$, $P_{Y'}$, $P_{Z'}$ along axes of a rotated coordinate system $X'Y'Z'$. Assume that the coordinate system $X'Y'Z'$ is obtained from the coordinate system XYZ by a rotation with Euler angles (ϕ,θ,ψ); this is illustrated by Fig. 6. Hence the components of the same polarization vector P in these two coordinate systems are related by the relation

$$P'=AP, \quad \text{or} \quad P=A^{-1}P', \tag{E1}$$

where

$$P\equiv\begin{bmatrix}P_X\\P_Y\\P_X\end{bmatrix}, \quad P'\equiv\begin{bmatrix}P_{X'}\\P_{Y'}\\P_{Z'}\end{bmatrix}, \tag{E2}$$

and the transformation matrix A is

$$A=\begin{bmatrix}\cos\phi\cos\theta\cos\psi-\sin\phi\sin\psi & \sin\phi\cos\theta\cos\psi+\cos\phi\sin\psi & -\sin\theta\cos\psi\\ -\cos\phi\cos\theta\sin\psi-\sin\phi\cos\psi & -\sin\phi\cos\theta\sin\psi+\cos\phi\cos\psi & \sin\theta\sin\psi\\ \cos\phi\sin\theta & \sin\phi\sin\theta & \cos\theta\end{bmatrix}. \tag{E3}$$

Note that the transformation matrix A is orthogonal, $A^{-1}=\tilde{A}$.

Consider, for example, the two coordinate systems XYZ and xyz related by the Euler angles $(\phi,\theta,0)$ as illustrated in Fig. 2. We can obtain the components in the fixed coordinate system XYZ by the transformation formula

$$\begin{bmatrix}P_X\\P_Y\\P_Z\end{bmatrix}=\begin{bmatrix}\cos\phi\cos\theta & -\sin\phi & \cos\phi\sin\theta\\ \sin\phi\cos\theta & \cos\phi & \sin\phi\sin\theta\\ -\sin\theta & 0 & \cos\theta\end{bmatrix}\begin{bmatrix}P_x\\P_y\\P_z\end{bmatrix}. \tag{E4}$$

APPENDIX F: AN ALTERNATIVE DERIVATION OF THE GENERAL FORMULAS (5.9)–(5.12)

As mentioned in Sec. V, any measurement using polarized light is a linear function of the parameters S_i. Consequently, the differential-cross-section and spin-polarization formulas for four suitably chosen photon polarizations should be sufficient to determine the desired formulas (5.9)–(5.12) for arbitrarily polarized photons. As examples, we shall first show that the differential cross-section formula (5.9) can be derived in this way. Because the differential cross section is a linear function of the parameters S_i, we assume the general form

$$\frac{d\sigma}{d\Omega}=a+bS_1+cS_2+dS_3. \tag{F1}$$

Suppose that we know explicit formulas for four different photon polarization as follows:

(i) Right circular polarization: $(S_1=0, S_2=0, S_3=1)$ or $(p=1, \alpha=\pi/4)$

$$\frac{d\sigma}{d\Omega}=\frac{\sigma}{4\pi}[1-\tfrac{1}{2}\beta P_2(\cos\theta)]\equiv a+d. \tag{F2}$$

(ii) Left circular polarization: $(S_1=0, S_2=0, S_3=-1)$ or $(p=1, \alpha=-\pi/4)$

$$\frac{d\sigma}{d\Omega}=\frac{\sigma}{4\pi}[1-\tfrac{1}{2}\beta P_2(\cos\theta]\equiv a-d. \tag{F3}$$

(iii) Linear polarization along the Y axis: $(S_1=1, S_2=0, S_3=0)$ or $(p=1, \alpha=0, \gamma=\pi/2)$

$$\frac{d\sigma}{d\Omega}=\frac{\sigma}{4\pi}\{1-\tfrac{1}{2}\beta[P_2(\cos\theta)+\tfrac{3}{2}\cos2\phi\sin^2\theta]\}$$
$$\equiv a+b. \tag{F4}$$

(iv) Linear polarization along an axis making an angle of $-\pi/4$ with the X axis: $(S_1=0, S_2=1, S_3=0)$ or $(p=1, \alpha=0, \gamma=-\pi/4)$

$$\frac{d\sigma}{d\Omega}=\frac{\sigma}{4\pi}\{1-\tfrac{1}{2}\beta[P_2(\cos\theta)+\tfrac{3}{2}\sin2\phi\sin^2\theta]\}$$
$$\equiv a+c. \tag{F5}$$

From (F2)–(F5) we can easily solve for a, b, c,

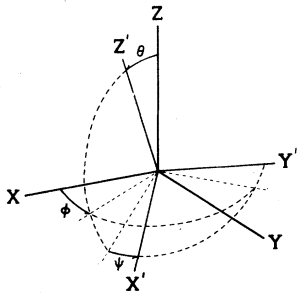

FIG. 6. Coordinate system $X'Y'Z'$ is obtained from coordinate system XYZ by a rotation with Euler angles (ϕ,θ,ψ).

and d; therefore the general formula (5.9) is obtained. Consider another example. We assume

$$P_x F = a + bS_1 + cS_2 + dS_3 , \tag{F6}$$

and the following explicit formulas:

$$P_x F = \begin{cases} \xi \sin\theta = a + d, \quad S_1 = 0, S_2 = 0, S_3 = 1 & \text{(F7)} \\ -\xi \sin\theta = a - d, \quad S_1 = 0, S_2 = 0, S_3 = -1 & \text{(F8)} \\ -\eta \sin 2\phi \sin\theta = a + b, \quad S_1 = 1, S_2 = 0, S_3 = 0 & \text{(F9)} \\ \eta \cos 2\phi \sin\theta = a + c, \quad S_1 = 0, S_2 = 1, S_3 = 0. & \text{(F10)} \end{cases}$$

Again after a, b, c, and d being solved from (F7)–(F10), the general formula (5.10′) is obtained.

APPENDIX G: RELATIVISTIC MULTICHANNEL K-MATRIX METHOD

The underlying idea of the K-matrix method[48] is to obtain eigenstates of an improved Hamiltonian H using a complete set of basis states from an approximate Hamiltonian H_0. We denote the basis states by $|\alpha E\rangle$ where α is the basis-state index (called *the channel index*) and E the total energy. The residual interaction is defined by

$$V = H - H_0 . \tag{G1}$$

The multichannel K matrix $\langle \alpha' E' | K(E) | \alpha E \rangle$ is defined by the integral equation

$$\langle \alpha' E' | K(E) | \alpha E \rangle = \langle \alpha' E' | V | \alpha E \rangle + \sum_{\alpha''} \mathcal{P} \int dE'' \frac{\langle \alpha' E' | V | \alpha'' E'' \rangle \langle \alpha'' E'' | K(E) | \alpha E \rangle}{E - E''} , \tag{G2}$$

where $\langle \alpha' E' | V | \alpha E \rangle$ is the matrix element of the residual interaction (G1). In (G2), the symbol $\mathcal{P}$ indicates that the Cauchy principal value of the integral is to be taken. The integration symbol $\int dE''$ denotes implicitly both a summation over the discrete spectrum and an integration over the continuum spectrum. By diagonalizing the on-the-energy-shell K matrix, we obtain

$$\sum_{\alpha'} \langle \alpha E | K(E) | \alpha' E \rangle U_{\alpha' a}(E) = \lambda_a(E) U_{\alpha a}(E), \tag{G3}$$

where $\lambda_a(E)$ and $U_{\alpha a}(E)$ are the ath eigenvalue and the associated eigenvector, respectively. The eigenstates $|aE\rangle$ of the improved Hamiltonian H, called *the eigenchannel states*, are given by

$$|aE\rangle = \sum_{\alpha} \left[|\alpha E\rangle + \sum_{\alpha'} \mathcal{P} \int dE' \frac{|\alpha' E'\rangle \langle \alpha' E' | K(E) | \alpha E \rangle}{E - E'} \right] \times U_{\alpha a}(E) \cos\eta_a(E) , \tag{G4}$$

where $\eta_a(E)$ is called *the eigenphase shift* and related to the eigenvalue $\lambda_a(E)$ by the relation

$$\lambda_a(E) = -(1/\pi) \tan\eta_a(E) . \tag{G5}$$

The open-channel state $|\alpha E^-\rangle$, which has the asymptotic behavior of containing an outgoing Coulomb wave only in channel α, is given by

$$|\alpha E^-\rangle = \sum_a e^{-i\delta_\alpha(E)} U_{\alpha a}(E) e^{-i\eta_a(E)} |aE\rangle . \tag{G6}$$

Here $\delta_\alpha(E)$ is the phase shift of channel $|\alpha E\rangle$ with respect to the Coulomb wave. The open-channel state $|\alpha E^-\rangle$ defined in (G6) should be substituted for $|\alpha^- J' M'\rangle$ in (3.9) in a relativistic multichannel K-matrix calculation.

For the present purpose, the complete set of relativistic orbitals may be Dirac-Fock or Dirac-Slater orbitals or orbitals from a model potential. The basis channel states constructed are linear combinations of Slater determinants, having definite parity and total angular momentum. Practically, the eigenchannel states of an improved Hamiltonian are computed within a restricted Hilbert space spanned by a finite number of chosen basis channels. For a parity-conserved and rotationally-invariant residual interaction, these chosen basis channels should have the same parity and total angular momentum. Certain relativistic interactions[34,55] are suggested.

[1] P. G. Burke, in *Atomic Processes and Applications*, edited by P. G. Burke and B. L. Moiseiwitsch (North-Holland, Amsterdam, 1976), pp. 199–248.

[2] S. T. Manson, Adv. Electron. Electron. Phys. 41, 73 (1976); 44, 1 (1977).

[3] J. Berkowitz, *Photoabsorption, Photoionization, and Photoelectron Spectroscopy* (Academic, New York, 1979).

[4] A. F. Starace, in *Handbuch der Physik*, edited by W. Mehlhorn (Springer, Berlin, in press), Vol. 31.

[5] J. A. R. Samson, in *Handbuch der Physik*, edited by W. Mehlhorn (Springer, Berlin, in press), Vol. 31.

[6] (a) R. H. Pratt, A. Ron, and H. K. Tseng, Rev. Mod. Phys. 45, 273 (1973); (b) R. H. Pratt, R. D. Levee, R. L. Pexton, and W. Aron, Phys. Rev. 134, A916 (1964); R. D. Schmickley and R. H. Pratt, Phys. Rev. 164, 104 (1967).

[7] J. W. Cooper, in *Atomic Inner-Shell Processes*, edited by B. Crasemann (Academic, New York, 1975), pp. 159–199.

[8] J. H. Hubbell, At. Data 3, 241 (1971).

[9] J. H. Scofield, Lawrence Livermore Lab. Rep. No. UCRL-51326 (NBS, Springfield, Virginia, 1973).

[10] L. J. Kieffer, *Bibliography of Low Energy Electron and Photon Cross Section Data*, NBS Special Publication 426 (U.S. Government Printing Office, Washington, D.C., 1976).

[11]V. W. Hughes *et al.*, Phys. Rev. A 5, 195 (1972).
[12]M. J. Alguard *et al.*, in *Proceedings of the IXth International Conference on High Energy Accelerators* (SLAC, Stanford, Cal., 1974), p. 309.
[13]J. Kessler, *Polarized Electrons* (Springer, Berlin, 1976).
[14]M. S. Lubell, in *Atomic Physics, Vol. 5*, edited by R. Marrus, M. Prior, and H. Sugart (Plenum, New York, 1977), pp. 325–373.
[15]W. B. Atwood *et al.*, Phys. Rev. D 18, 2223 (1978).
[16]C. Y. Prescott *et al.*, Phys. Lett. 77B, 347 (1978).
[17]U. Fano, Phys. Rev. 178, 131 (1969); 184, 250 (1969).
[18]B. Brehm, Z. Phys. 242, 195 (1971).
[19]V. L. Jacobs, J. Phys. B 5, 2257 (1972).
[20](a) N. A. Cherepkov, Zh. Eksp. Teor. Fiz. 65, 933 (1973) [Sov. Phys.-JETP 38, 463 (1974)]; (b) J. Phys. B 12, 1279 (1979).
[21]C. M. Lee, Phys. Rev. A 10, 1598 (1974).
[22]K.-C. Chou, Zh. Eksp. Teor. Fiz. 36, 909 (1959) [Sov. Phys.-JETP 9, 642 (1959)].
[23]M. Jacob and G. C. Wick, Ann. Phys. (N.Y.) 7, 404 (1959).
[24]K.-N. Huang, Phys. Lett. A (in press).
[25]G. G. Stokes, Trans. Cambridge Philos. Soc. 9, 399 (1852).
[26]U. Fano, Rev. Mod. Phys. 29, 74 (1957).
[27]M. Born and E. Wolf, *Principles of Optics* (Pergamon, New York, 1959), p. 554
[28]A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, N. J., 1957).
[29]G. Breit and H. A. Bethe, Phys. Rev 93, 888 (1954).
[30]M. E. Rose, *Elementary Theory of Angular Momentum* (Wiley, New York, 1957).
[31]U. Fano and G. Racah, *Irreducible Tensorial Sets* (Academic, New York, 1959).
[32]I. P. Grant, J. Phys. B 7, 1458 (1974).
[33]W. R. Johnson and C. D. Lin, Phys. Rev. A 20, 964 (1979).
[34]K.-N. Huang, Rev. Mod. Phys. 51, 215 (1979).
[35]E. P. Wigner, *Group Theory* (Academic, New York, 1959).
[36]C. N. Yang, Phys. Rev. 74, 764 (1948).
[37]J. W. Cooper and R. N. Zare, in *Lectures in Theoretical Physics*, edited by S. Geltman, K. T. Mahanthappa, and W. E. Britten (Gordon and Breach, New York, 1969), Vol. 11c, p. 317
[38]J. W. Cooper and S. T. Manson, Phys. Rev. 177, 157 (1969).
[39]M. Peshkin, Adv. Chem. Phys. 18, 1 (1970).
[40]J. A. R. Samson, J. Opt. Soc. Am. 59, 356 (1969); Philos. Trans. R. Soc. London A 268, 141 (1970).
[41]V. Schmidt, Phys. Lett. 45A, 63 (1973).
[42]J. A. R. Samson and A. F. Starace, J. Phys. B 8, 1806 (1975).
[43]T. E. H. Walker and J. T. Waber, J. Phys. B 7, 674 (1974).
[44]W. R. Johnson and K. T. Cheng, Phys. Rev. A 20, 978 (1979).
[45]W. R. Johnson and K. T. Cheng, J. Phys. B 12, 863 (1979); W. R. Johnson and C. M. Lee (unpublished).
[46]J. J. Chang, J. Phys. B 10, 3195 (1977).
[47]K.-N. Huang, Bull. Am. Phys. Soc. 24, 1181 (1979).
[48]U. Fano and J. W. Cooper, Rev Mod. Phys. 40, 441 (1968).
[49]K.-N. Huang and A. F. Starace, Phys. Rev. A 21, 697 (1980).
[50]K.-N. Huang, W. R. Johnson, and K. T. Cheng, Phys. Rev Lett. 43, 1658 (1979).
[51]K. T. Cheng, K.-N. Huang, and W. R. Johnson, J. Phys. B (in press).
[52]K.-N. Huang, W. R. Johnson, and K. T. Cheng (unpublished).
[53]U. Heinzmann, G. Schönhense, and J. Kessler, Phys. Rev. Lett 42, 1603 (1979).
[54]U. Heinzmann, G. Schönhense, and J. Kessler (unpublished).
[55]K.-N. Huang, Phys. Lett. A 63, 262 (1977); J. Phys. B 11, 787 (1978); Phys. Rev. A 18, 1119 (1978).