Addendum to "Theory of angular distribution and spin polarization of photoelectrons"

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More convenient formulas are given for the angular distribution and spin polarization of photoelectrons including all multipole transitions.

The angular distribution and spin polarization of photoelectrons including all multipole transitions have been given in Eqs. (4.20)–(4.23) of Ref. 1. They can be cast in more convenient forms as

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

where the angular distribution function is

$$F(\theta,\phi)=1+\sum_{l\geqslant 1}\beta_{0l}d^l_{00}+(S_X\cos2\phi+S_Y\sin2\phi)\sum_{l\geqslant 2}\beta_{1l}d^l_{20}\ , \tag{2}$$

and

$$P_x(\theta,\phi)F(\theta,\phi)=S_Z\sum_{l\geqslant 1}\xi_{3l}d^l_{01}+(S_X\sin2\phi-S_Y\cos2\phi)\sum_{l\geqslant 2}(\xi_{2l}d^l_{21}+\eta_{2l}d^l_{2-1})\ , \tag{3}$$

$$P_y(\theta,\phi)F(\theta,\phi)=\sum_{l\geqslant 1}\eta_{0l}d^l_{01}+(S_X\cos2\phi+S_Y\sin2\phi)\sum_{l\geqslant 2}(\xi_{2l}d^l_{21}-\eta_{2l}d^l_{2-1})\ , \tag{4}$$

$$P_z(\theta,\phi)F(\theta,\phi)=S_Z\sum_{l\geqslant 0}\zeta_{3l}d^l_{00}+(S_X\sin2\phi-S_Y\cos2\phi)\sum_{l\geqslant 2}\zeta_{2l}d^l_{20}\ . \tag{5}$$

Here $d^l_{mn}(\theta)$ are the standard d functions of the rotation matrices, and $d^l_{00}(\theta)=P_l(\cos\theta)$, the Legendre polynomial. The formulas (1)–(5) are similar to those for the fluorescence radiation[2] and the Auger electron[3] in the deexcitation of the residual ion. Besides the total cross section σ there are, in general, eight kinds of dynamical parameters: β_{0l}, β_{1l}, ξ_{2l}, ξ_{3l}, η_{0l}, η_{2l}, ζ_{2l}, and ζ_{3l}. We note that maximum information on the photoelectron from unpolarized target can be obtained at any azimuthal orientation ϕ. Therefore it is sufficient to consider the angular distribution and spin polarization at $\phi=0$. The total cross section σ is given explicitly as

$$\sigma=\frac{4\pi^4c}{\omega[J_0]^2}\bar{\sigma}\ , \tag{6}$$

where

$$\bar{\sigma}=\sum_{jJ\kappa_\alpha}[D^2_\alpha(Ej)+D^2_\alpha(Mj)]\ . \tag{7}$$

The reduced-matrix elements $D_\alpha(Ej)$ and $D_\alpha(Mj)$ are for the electric 2^j-pole transition and the magnetic 2^j-pole transition, respectively. They are defined through the following relations:

$$i^{-l_\alpha}\exp(i\sigma_{\kappa_\alpha})\left\langle\alpha^-J\left\|\sum_{i=1}^{N}\vec{\alpha}_i\cdot\vec{A}^{(Ej)}(\vec{r}_i)\right\|J_0\right\rangle=i^{j-1}\exp(i\sigma_\alpha)D_\alpha(Ej)\ , \tag{8}$$

$$i^{-l_\alpha}\exp(i\sigma_{\kappa_\alpha})\left\langle\alpha^-J\left\|\sum_{i=1}^{N}\vec{\alpha}_i\cdot\vec{A}^{(Mj)}(\vec{r}_i)\right\|J_0\right\rangle=i^{j-1}\exp(i\sigma_\alpha)D_\alpha(Mj)\ , \tag{9}$$

where $\vec{A}^{(Ej)}$ and $\vec{A}^{(Mj)}$ are the normalized electric and magnetic multipole potentials,[1] respectively. The total channel phase shift σ_α is also defined through relations (8) and (9). We note that $D_\alpha(Ej)$, $D_\alpha(Mj)$, and σ_α are real quantities by definition. In this connection, the reduced-matrix element $D(\kappa_\alpha)$ for the electric dipole transition defined in Ref. 1 is related to $D_\alpha(E1)$ as

$$D(\kappa_\alpha)=-\frac{i}{\sqrt{2}}e^{i\sigma_\alpha}D_\alpha(E1)\ . \tag{10}$$

We shall use a more convenient normalization of the continuum wave function. Corresponding modification along with corrections for misprints in Ref. 1 are given in Appendix A.

The angular-distribution and spin-polarization parameters are given explicitly as

$$\beta_{0l} = \sum_{\alpha'\alpha} G_{l0}(\pi_{l+} uc + \pi_{l-} vs) \ , \tag{11}$$

$$\beta_{1l} = \sum_{\alpha'\alpha} G_{l2}(\pi_{l+} pc + \pi_{l-} qs) \ , \tag{12}$$

$$\xi_{2l} = \frac{1}{2} \sum_{\alpha'\alpha} H_{l2}(qc - ps) \ , \tag{13}$$

$$\xi_{3l} = \sum_{\alpha'\alpha} H_{l0}(\pi_{l-} uc + \pi_{l+} vs) \ , \tag{14}$$

$$\eta_{0l} = \sum_{\alpha'\alpha} H_{l0}(\pi_{l-} vc - \pi_{l+} us) \ , \tag{15}$$

$$\eta_{2l} = (-)^{l+1} \frac{1}{2} \sum_{\alpha'\alpha} H_{l2}(qc + ps) \ , \tag{16}$$

$$\zeta_{2l} = - \sum_{\alpha'\alpha} G_{l2}(\pi_{l+} qc - \pi_{l-} ps) \ , \tag{17}$$

$$\zeta_{3l} = - \sum_{\alpha'\alpha} G_{l0}(\pi_{l-} uc + \pi_{l+} vs) \ . \tag{18}$$

In Eqs. (11)–(18) we have used the notations

$$\sum_{\alpha'\alpha} \equiv \sum_{j'J'\kappa'_\alpha} \sum_{jJ\kappa_\alpha} \ , \tag{19}$$

$$c \equiv \cos(\sigma_{\alpha'} - \sigma_\alpha) \ , \tag{20}$$

$$s \equiv \sin(\sigma_{\alpha'} - \sigma_\alpha) \ , \tag{21}$$

$$\begin{aligned} u \equiv\ & \pi_{k+}(-)^{k/2}(E'E + M'M) \\ & + \pi_{k-}(-)^{(k+1)/2}(E'M - M'E) \ , \end{aligned} \tag{22}$$

$$\begin{aligned} v \equiv\ & \pi_{k-}(-)^{(k+1)/2}(E'E + M'M) \\ & - \pi_{k+}(-)^{k/2}(E'M - M'E) \ , \end{aligned} \tag{23}$$

$$\begin{aligned} p \equiv\ & \pi_{k+}(-)^{k/2}(E'E - M'M) \\ & - \pi_{k-}(-)^{(k+1)/2}(E'M + M'E) \ , \end{aligned} \tag{24}$$

$$\begin{aligned} q \equiv\ & \pi_{k-}(-)^{(k+1)/2}(E'E - M'M) \\ & + \pi_{k+}(-)^{k/2}(E'M + M'E) \ , \end{aligned} \tag{25}$$

$$\pi_{l}\pm = \begin{cases} l \text{ even} \\ l \text{ odd} \ , \end{cases} \tag{26}$$

$$E \equiv D_\alpha(Ej) \ , \tag{27}$$

$$M \equiv D_\alpha(Mj) \ , \tag{28}$$

$$k = j' - j \ . \tag{29}$$

The coupling coefficients G_{lm} and H_{lm} in Eqs. (11)–(18) are defined as

$$G_{lm} = K_l \begin{pmatrix} j'_\alpha & j_\alpha & l \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix} \begin{pmatrix} j' & j & l \\ -1 & 1-m & m \end{pmatrix} \ , \tag{30}$$

$$H_{lm} = K_l (-)^{j'_\alpha + l'_\alpha + 1/2} \begin{pmatrix} j'_\alpha & j_\alpha & l \\ -\frac{1}{2} & -\frac{1}{2} & 1 \end{pmatrix} \begin{pmatrix} j' & j & l \\ -1 & 1-m & m \end{pmatrix} \ , \tag{31}$$

where

$$\begin{aligned} K_l = \ & \bar{\sigma}^{-1} (-)^{J_0 - J_\alpha + 1/2} [jJj_\alpha][j'J'j'_\alpha][l]^2 \\ & \times \begin{Bmatrix} J & J' & l \\ j'_\alpha & j_\alpha & J_\alpha \end{Bmatrix} \begin{Bmatrix} J & J' & l \\ j' & j & J_0 \end{Bmatrix} \ , \end{aligned} \tag{32}$$

with the notation $[j] \equiv (2j+1)^{1/2}$, etc.

The spin polarization of the total photoelectron flux including all multipole transitions can also be calculated as

$$P_X = P_Y = 0 \ , \tag{33}$$

$$P_Z = \delta_{31} S_Z \ , \tag{34}$$

where

$$\delta_{31} = \frac{1}{3}(\zeta_{31} - \sqrt{2}\xi_{31}) \ . \tag{35}$$

In the electric dipole approximation only eight parameters survive, i.e., σ, β_{02}, β_{12}, ξ_{22}, ξ_{31}, η_{02}, η_{22}, and ζ_{31}. They reduce to the parameters σ, β, ξ, η, and ζ defined in Eqs. (5.14)–(5.18) of Ref. 1 in the electric dipole approximation:

$$\sigma \to \sigma \ , \tag{36}$$

$$\beta_{02} \to -\frac{1}{2}\beta \ , \tag{37}$$

$$\beta_{12} \to -\sqrt{3/2}\beta \ , \tag{38}$$

$$\xi_{22} \to \eta \ , \tag{39}$$

$$\xi_{31} \to \sqrt{2}\xi \ , \tag{40}$$

$$\eta_{02} \to \sqrt{2/3}\eta \ , \tag{41}$$

$$\eta_{22} \to \eta \ , \tag{42}$$

$$\zeta_{31} \to \zeta \ . \tag{43}$$

Similarly, the total spin-polarization parameters δ_{31} and δ are related as

$$\delta_{31} \to \frac{1}{3}(\zeta - 2\xi) = \delta \ . \tag{44}$$

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APPENDIX

Define the angular momentum eigenstate (D11) of Ref. 1 as the continuum state normalized in the energy scale in atomic units. Corresponding to this definition, we shall make the following modifications along with correctins for misprints in Ref. 1:

(1) Equations (3.1), (3.4), (3.9), (3.10), (3.12), and (3.13): $k_\alpha \rightarrow k_\alpha E_\alpha$ (E_α: total energy of the photoelectron).

(2) Equations (3.9), (3.12), and (3.13): On the right-hand side of these equations, we add a multiplication factor c (the speed of light in atomic units).

(3) Equations (3.15), (3.19), (5.14), and (5.58):

$$\frac{1}{\omega c} \rightarrow \frac{c}{\omega} \ .$$

(4) Equation (3.15):

$$j\mu \rightarrow j_\alpha \mu \ .$$

(5) Equation (4.13):

$$\cos 2\alpha \cos 2\phi \rightarrow \cos 2\alpha \cos 2\bar{\phi} \ .$$

(6) Equation (4.14):

$$\cos 2\alpha \sin 2\phi \rightarrow \cos 2\alpha \sin 2\bar{\phi} \ .$$

(7) Equation (4.16):

$$K_{l\alpha'\alpha} \rightarrow K_{\alpha'\alpha l} \ .$$

(8) Equation (4.20):

$$\begin{pmatrix} j & j' & l \\ 1 & -1 & 0 \end{pmatrix} \rightarrow \begin{pmatrix} j & j' & l \\ -1 & 1 & 0 \end{pmatrix} \ .$$

(9) Equations (4.22) and (4.23):

$$\alpha\alpha' l \rightarrow \alpha' \alpha l \ .$$

(10) Equation (5.5):

$$J \rightarrow \alpha^- J \ .$$

(11) Equation (5.8):

$$\vec{p}_i \rightarrow \vec{p}_i / c \ .$$

(12) Third line after Eq. (5.8):

$$(6\pi^2)^{-1/2} \rightarrow (6\pi^2 c^2)^{-1/2} \ .$$

(13) Equation (5.26):

$$\sin\theta \cos\phi \rightarrow \sin\theta \cos\theta \ .$$

(14) Eighth line after Eq. (A1):

$$-\pi/2 < \alpha < \pi/2 \rightarrow -\pi/4 \leq \alpha \leq \pi/4 \ .$$

(15) Equation (D9):

$$(2\pi)^{-3/2} \rightarrow (2\pi)^{-3/2} [(E + c^2)/2E]^{1/2} \ .$$

(16) Equation (D10):

$$\frac{2l+1}{k(2j+1)} \rightarrow \frac{(2l+1)c^2}{kE(2j+1)} \ .$$

[1]K.-N. Huang, Phys. Rev. A 22, 223 (1980).
[2]K.-N. Huang, Phys. Rev. A 25, 3438 (1982).
[3]K.-N. Huang, Phys. Rev. A 26, 2274 (1982).