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Spin-Orbit Coupling Effects in Parameters that Describe Electron-Photon Coincidence Experiments

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Parameters are introduced to characterize the electron-photon coincidence rate for atoms where spin-orbit interaction is present in the radiating target state. It is shown that two of these parameters (called Δ and ϵ) obey rigorous selection rules which require that they go to $\pi/2$ at 0° and 180° electron scattering angles in the presence of spin-orbit coupling while their limit in the LS-coupled case is 0. Numerical results are presented.

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In recent years, application of electron-photon coincidence technique[1-6] to the study of inelastic scattering of electrons by atoms has resulted in valuable new information about the collision physics. The angular correlation parameters which are extracted from these measurements provide a stringent test of the theoretical models used to describe electron-impact excitation processes.[7] However, most cases studied to date have been atoms that are well described by an LS-coupling scheme (such as He[1-6]) where two parameters, λ and χ, have been used to characterize the coincidence rate. For heavier atoms the introduction of spin-orbit interaction breaks the planar symmetry in the scattering amplitudes valid in the LS-coupling scheme and introduces explicit spin summations through the spin dependence of the scattering amplitudes due to the unpolarized nature of the incident electrons. As a consequence new parameters have to be introduced to describe the coincidence rate. In this Letter we use the approach of Fano and Macek[8] (a generalization of the earlier treatment of Macek and Jaecks[9]) to show that the spin-orbit interaction in the target atom produces effects in these parameters that can be readily observed experimentally at electron scattering angles (ϑ_e, with respect to the incident beam) close to 0° and 180°, in the excitation of an electronic state with angular momentum $J=1$ from a $J=0$ ground state.

In general the presence of spin-orbit interaction in the excited state of the target prohibits the reduction of the four independent Fano-Macek source parameters to two parameters (λ, χ), as is possible in the LS-coupled case.[1-6] We propose a new four-parameter description of the source parameters which makes the spin-orbit effect in the target more transparent.[10] The advantage is that two of these parameters obey rigorous selection rules which require that they go to $\pi/2$ at $\vartheta_e = 0°$ and 180° in the presence of spin-orbit coupling, while their limit in the LS-coupled case is zero. This behavior has not yet been observed experimentally since the few available measurements for heavier atoms have assumed planar symmetry for the scattering amplitudes. We present below numerical results for excitation of Ar,[11,12] to illustrate the detailed behavior of these parameters.

A brief derivation of the new parameters is as follows. The Fano-Macek source parameters can be written as for a $J=1$ state

$$O_{1-}{}^{\rm col} = -(2)^{1/2}\,{\rm Im}\langle a(0)a(1)\rangle/(\sigma_0+2\sigma_1), \qquad (1a)$$

$$A_0{}^{\rm col} = [\langle a(1)a(1)\rangle - \langle a(0)a(0)\rangle]/(\sigma_0+2\sigma_1), \qquad (1b)$$

$$A_{1+}{}^{\rm col} = (2)^{1/2}\,{\rm Re}\langle a(0)a(1)\rangle/(\sigma_0+2\sigma_1), \qquad (1c)$$

$$A_{2+}{}^{\rm col} = \langle a(-1)a(1)\rangle/(\sigma_0+2\sigma_1), \qquad (1d)$$

where

$$\langle a(M_J)a(M_J')\rangle = \tfrac{1}{2}\sum_{m_{s1},\,m_{s2}}[a^*(M_J)]_{m_{s1}m_{s2}}[a(M_J')]_{m_{s1}m_{s2}}, \qquad (2)$$

and $[a(M_J)]_{m_{s1}m_{s2}}$ refers to the scattering amplitude for the excitation of the M_J magnetic sublevel with incident-electron spin component m_{s1} and the scattered-electron spin component m_{s2}. In Eqs. (1a)–(1d), $\sigma_{M_J}=\langle a(M_J)a(M_J)\rangle$ refers to the magnetic sublevel excitation cross section. Introducing the parameters

$$\lambda = \sigma_0/(\sigma_0+2\sigma_1), \qquad (3a)$$

$$\cos\Delta = |\langle a(0)a(1)\rangle|/(\sigma_0\sigma_1)^{1/2}, \qquad (3b)$$

$$\cos\bar{\chi} = {\rm Re}\langle a(0)a(1)\rangle/|\langle a(0)a(1)\rangle|, \qquad (3c)$$

$$\cos\epsilon = -\langle a(-1)a(1)\rangle/\sigma_1, \qquad (3d)$$

one obtains

$$O_{1-}{}^{\rm col} = -[\lambda(1-\lambda)]^{1/2}\sin\bar{\chi}\cos\Delta, \qquad (4a)$$

$$A_0{}^{\rm col} = \tfrac{1}{2}(1-3\lambda), \qquad (4b)$$

$$A_{1+}{}^{\rm col} = [\lambda(1-\lambda)]^{1/2}\cos\bar{\chi}\cos\Delta, \qquad (4c)$$

$$A_{2+}{}^{\rm col} = \tfrac{1}{2}(\lambda-1)\cos\epsilon. \qquad (4d)$$

It should be noted that under LS-coupling conditions because of the spin factorization $[a(M)]_{m_{s1}m_{s2}} = a(M)\delta_{m_{s1}m_{s2}}$ and planar symmetry[9] $a(-M)=(-1)^M \times a(M)$, from Eqs. (3b) and (3c) it follows that $\cos\Delta=\cos\epsilon=1$; i.e., $\Delta=\epsilon=0$ at any angle. In experiments where $O_{1-}{}^{\rm col}$ is not measured (i.e., circularly polarized correlation is not determined) the number of parameters can be further reduced by defining $\cos\chi=\cos\bar{\chi}\cos\Delta$, to obtain a description for χ which is identical with that of Malcolm and McConkey.[11]

Substituting the above parametrization into Eq. (18) of Fano and Macek,[8-13] and the resulting formulas into Eq. (14) of the same work we obtain for the electron-photon coincidence rate in terms of the four new parameters,

$$\begin{aligned} I = \tfrac{1}{3}CS\Big(&1+\tfrac{1}{2}(1-3\lambda)\tfrac{1}{2}(3\cos^2\vartheta-1)+[\lambda(1-\lambda)]^{1/2}\cos\bar{\chi}\cos\Delta\tfrac{3}{2}\sin 2\vartheta\cos\varphi+\tfrac{1}{2}(\lambda-1)\cos\epsilon\tfrac{3}{2}\sin^2\vartheta\cos 2\varphi \\ &-3\{\tfrac{1}{2}(1-3\lambda)\tfrac{1}{2}\sin^2\vartheta\cos 2\psi+[\lambda(1-\lambda)]^{1/2}\cos\bar{\chi}\cos\Delta(\sin\vartheta\sin\varphi\sin 2\psi+\sin\vartheta\cos\vartheta\cos\varphi\cos 2\psi) \\ &+\tfrac{1}{2}(\lambda-1)\cos\epsilon[\tfrac{1}{2}(1+\cos^2\vartheta)\cos 2\varphi\cos 2\psi-\cos\vartheta\sin 2\varphi\sin 2\psi\}\cos 2\beta \\ &-3[\lambda(1-\lambda)]^{1/2}\sin\bar{\chi}\cos\Delta\sin\vartheta\sin\varphi\sin 2\beta\Big). \end{aligned}$$

β, ϑ, φ, and ψ are defined in Ref. 9 as well as the constant C which includes the light frequency and the detector–source–atom distance and S. The specialized form of this coincidence rate for angular correlation and polarization correlation experiments has been discussed earlier.[14]

We now prove that at both $\vartheta_e=0°$ and $180°$ angles the quantities $\langle a(0)a(1)\rangle=\langle a(1)a(-1)\rangle=0$ but σ_0 and σ_1 are different from 0, thereby showing that $\cos\Delta=\cos\epsilon=0$ [i.e., $\Delta=\epsilon=\pi/2$] at these angles. This is in contrast to the LS-coupled target case for which $\Delta=\epsilon=0$. To prove these results we assume an atom in a $^1S(J=0)$ ground state, neglect the hyperfine interaction, and assume that the nuclear spin (I) and its orientation $\langle\vec{I}\rangle$ remain unchanged during the collision process.[15] In an inelastic collision for which $\vartheta_e=0°$ and $180°$ [the axis of quantization (Z) is coincident with the incoming beam] the component of the total angular momentum of the system (electron + atom) along this axis is conserved. For both the incident and scattered electron, the only component of angular momentum along this axis is that of the spin, for which there are two possible situations, (i) $m_{s1}=m_{s2}$ which requires that the component of the total angular momentum of the atom ($M_F=M_I+M_J$) remain the same (i.e., M_J be conserved since M_I was assumed not to change), (ii) $m_{s1}\neq m_{s2}$ which requires $\Delta M_F=\pm 1$ (or $\Delta M_J=\pm 1$, since $\Delta M_I=0$), depending on the initial spin ($m_{s1}=\pm\frac{1}{2}$) implying $[a(1)]_{1/2,-1/2}\neq 0$ and $[a(-1)]_{-1/2,1/2}\neq 0$. This further implies that $\langle a(0)a(1)\rangle=\langle a(1)a(-1)\rangle=0$ which follows from the definition of these quantities [Eq. (2)] and from the incompatibility of the conditions for $[a(0)]_{m_{s1}m_{s2}}$, $[a(1)]_{m_{s1}m_{s2}}$, and $[a(-1)]_{m_{s1}m_{s2}}$ to be different from zero simultaneously.[16] However, since $[a(1)]_{1/2,-1/2}\neq 0$, then σ_1

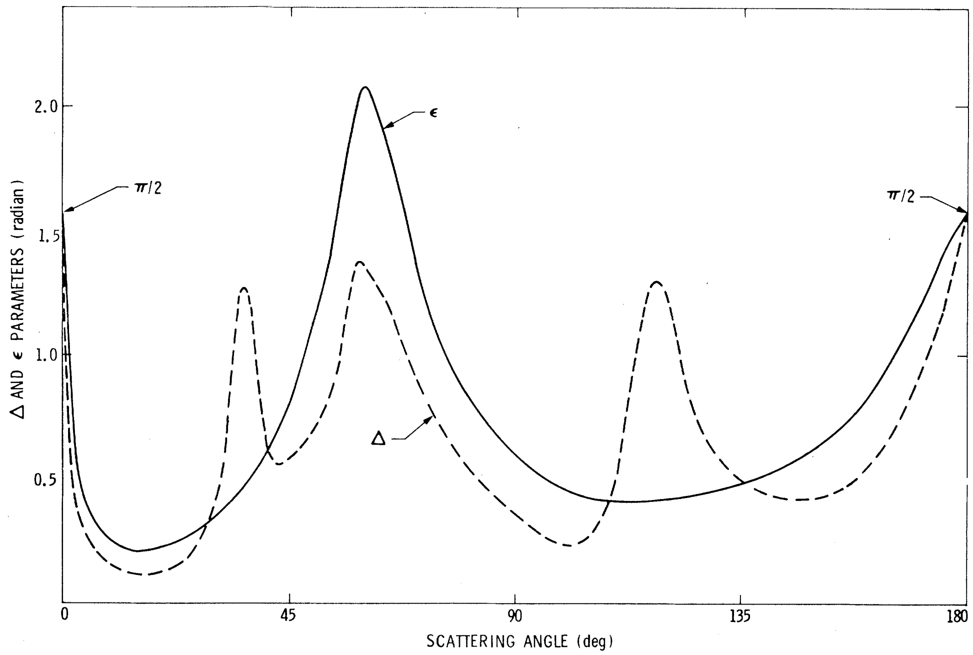

FIG. 1. First-order many-body–theory results for the Δ and ϵ parameters for the excitation of the $4s'[\frac{1}{2}]_1^0$ state of argon by E = 20 eV electrons.

$\neq 0$ and similarly $\sigma_0 \neq 0$ at $\vartheta_e = 0°$ and 180°. Hence from Eqs. (3b) and (3c) it follows that $\cos\Delta = \cos\epsilon = 0$. If we choose $0 \leq \Delta \leq \pi/2$ and $0 \leq \epsilon \leq \pi$, then $\Delta = \pi/2$ and $\epsilon = \pi/2$ for $\vartheta_e = 0°$ and 180°. Therefore, if one measures just $\cos\chi$ (i.e., $|\chi|$) one will *always* obtain $|\chi| = \pi/2$ at $\vartheta_e = 0°$ and 180° because $\cos\chi = \cos\bar{\chi}\cos\Delta$ and $\cos\Delta = 0$ at these angles. It is important to note here that the quantity $|\chi|$ does not allow a differentiation between LS-coupled and spin-orbit–coupled targets. However, it will be seen in the case of argon that the spin-orbit-coupling effect appears to be strong at small scattering angles and readily observable in $|\chi|$ also.

In order to see the behavior of these new parameters we present numerical results from a first-order many-body theory calculation[17] for the excitation of the $4s'[\frac{1}{2}]_1^0$ $(^1P_1)$ state of argon at E = 20 eV incident energy.[18]

Figure 1 presents results for the Δ and ϵ parameters and shows clearly that both Δ and ϵ rise to the $\pi/2$ value as ϑ_e approaches 0° and 180°. This rise begins at an experimentally accessible angle of 15°. In addition both new parameters show strong structure at intermediate scattering angles. This additional structure is attributed to the minima in σ_0 (in the case of Δ) and σ_1 (in the case of ϵ and Δ) and is analogous to the spin-polarization effect of Kessler[19] that occurs at the minimum of the differential cross section. Figure 2 shows the behavior of $|\chi|$ for small angles as well as the value of $|\chi|$ in the LS coupling

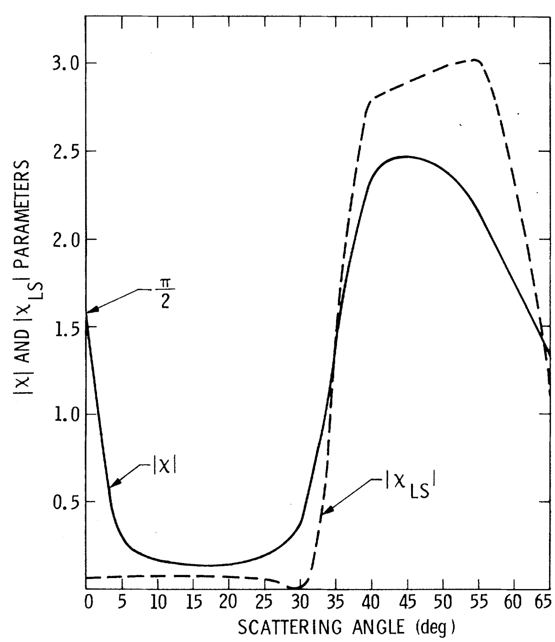

FIG. 2. Same as Fig. 1 except for $|\chi|$ and for $|\chi_{LS}|$ (see text).

scheme: $|\chi_{LS}|$.

Malcolm and McConkey[11] and Pochat *et al.*[12] have recently reported results for $|\chi|$ deduced from coincidence rate data with the assumption $\cos\epsilon = 1$. Even though there is no rigorous selection rule for χ_{LS} at $\vartheta_e = 0°$ a small value is expected since the Born and Glauber approximation which has some limited validity around $\vartheta_e = 0°$ would give $\chi_{LS} \equiv 0$ (identically) for all angles. This tendency is not supported by either of these measurements. Figure 2 indicates that the sudden rise of $|\chi|$ to reach to the $\pi/2$ limit value is due to spin-orbit coupling effect in the excited state and the spin-exchange scattering process as discussed here. These new parameters can be extracted from electron-photon coincidence experiments on targets such as argon and their behavior will provide additional information as to the details of the inelastic electron scattering process.

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