Spin-Resolved $(e, 2e)$ Coincidences for Heavy Rare-Gas Targets

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It has been well established that the Coulomb force alone can produce spin-dependent effects for electron-impact excitation of heavy rare-gas atoms if the incident electrons are spin polarized and the final J state of the atom is resolved. This effect has become known as the fine-structure effect. Here we demonstrate that the same type of effect may be expected for electron-impact ionization.

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The dynamics of electron-impact ionization of atomic targets in $(e, 2e)$ coincidence experiments has focused much interest on understanding the final-state correlations of this three-body problem where two continuum electrons are emitted after scattering from a positively charged core [1]. Although there have been numerous studies of the $(e, 2e)$ problem, only little attention has been paid to spin effects in these collisions [2,3]. For the case of atomic excitation, on the other hand, it has been shown in experimental [4] and theoretical [5–7] investigations that a spin up-down asymmetry exists for electron-impact excitation of the bound states of rare-gas atoms with a np^6 configuration in the ground state. The question was raised whether the mechanism that produces these asymmetries will also be important in $(e, 2e)$ electron-impact ionization studies of the heavier rare gases [8].

A simple picture shown in Fig. 1 illustrates the mechanism that produces spin up-down asymmetries in electron-impact excitation of heavy rare-gas atoms. In the excitation, a vacancy is produced in the closed p^6 shell, e.g., a $np^6 \to np^5(n+1)l$ transition. It is well established that the Coulomb interaction may produce an oriented ionic $np^5\,{}^2P$ core; i.e., the cross sections for exciting the $m_l = \pm 1$ magnetic sublevels of the ionic ${}^2P$ core are different for a quantization axis perpendicular to the scattering plane [9]. This orbital orientation effects a spin orientation of the ionic core, if its final J state is resolved, since, e.g., in the ${}^2P_{1/2}$ configuration the projections of spin $\langle \mathbf{s}_c \rangle$ and orbital angular momentum $\langle \mathbf{l}_c \rangle$ are opposite. Let us, for the sake of simplicity, assume that in a collision the ${}^2P_{1/2}$ core is completely orientated, say with $m_l = +1$. The spin of this state is therefore down, which means that the spin $\langle \mathbf{s}_e \rangle$ of the excited $(n+1)l$ electron is up, because in the initial np^6 configuration the spins compensated each other. It is obvious that in such a situation a spin up-down asymmetry may be observed since both direct and exchange scattering are possible for an incident spin-up electron while only direct scattering is possible for an incident spin-down electron.

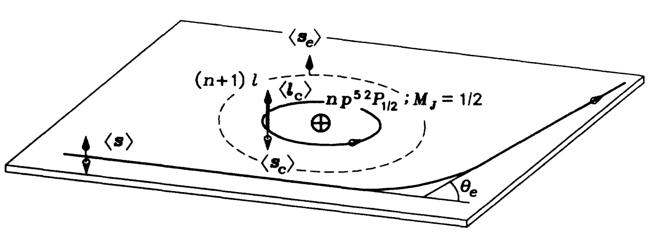

FIG. 1. Simple picture of spin effects in $np^5\,({}^2P_{1/2})\,(n+1)l$ excitation of heavy rare gases.

The purpose of this paper is to demonstrate that the same mechanism applies to ionization processes, where the excited electron is ejected into the continuum. The prediction that spin up-down asymmetries may be observed in $(e, 2e)$ coincidence studies [8] has stimulated very recent experimental [10,11] and the present theoretical investigation. From an experimental point of view, $(e, 2e)$ studies with xenon and krypton targets are of particular interest, since their fine-structure splittings of 1.31 eV and 0.67 eV, respectively, can be resolved without major difficulties.

We have calculated spin up-down asymmetries

$$A_J = \frac{\sigma_J(\uparrow) - \sigma_J(\downarrow)}{\sigma_J(\uparrow) + \sigma_J(\downarrow)} \tag{1}$$

for ionization of xenon in a coordinate system with the z axis perpendicular to the scattering plane, where the cross sections for spin-up $(\uparrow)$ or spin-down $(\downarrow)$ incident electrons with energy E_0 are given by [12]

$$\sigma_{1/2}(\uparrow) = \frac{(2\pi)^4}{E_0}\frac{2}{3}\left(|f_{-1}|^2 + |g_{-1}|^2 + |f_{+1} - g_{+1}|^2\right), \tag{2a}$$

$$\sigma_{1/2}(\downarrow) = \frac{(2\pi)^4}{E_0}\frac{2}{3}\left(|f_{+1}|^2 + |g_{+1}|^2 + |f_{-1} - g_{-1}|^2\right), \tag{2b}$$

$$\sigma_{3/2}(\uparrow) = \frac{(2\pi)^4}{E_0}\Big(|f_{+1}|^2 + |g_{+1}|^2 + \frac{1}{3}|f_{+1} - g_{+1}|^2 + \frac{1}{3}|f_{-1}|^2 + \frac{1}{3}|g_{-1}|^2 + |f_{-1} - g_{-1}|^2\Big), \tag{2c}$$

$$\sigma_{3/2}(\downarrow) = \frac{(2\pi)^4}{E_0}\Big(|f_{-1}|^2 + |g_{-1}|^2 + \frac{1}{3}|f_{-1} - g_{-1}|^2 + \frac{1}{3}|f_{+1}|^2 + \frac{1}{3}|g_{+1}|^2 + |f_{+1} - g_{+1}|^2\Big). \tag{2d}$$

Here f_{m_l} is the direct amplitude and g_{m_l} is the exchange

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amplitude. Although not explicitly indicated in Eq. (2), the amplitudes depend on the final J state of the ion (in the present work this is due only to the difference in ionization energies for the two J states). The capture amplitude h_{m_l} (exchange with the core electron) is not included in Eq. (2) since it vanishes in the model used here. For equal-energy final-state electrons leaving the ion in opposite directions (the case considered here) it can be shown that $\sigma_J(\downarrow,\theta) = \sigma_J(\uparrow, \pi-\theta)$, where θ is the angle that the interelectronic axis makes relative to the incident beam direction.

The calculations were carried out using the improved version [13] of the DWBA (distorted-wave Born approximation) model of Jones, Madison, and Srivastava [14]. In this model the direct and exchange amplitudes are given by

$$f_{m_l} = \left\langle \chi_1^-(1)\chi_2^-(2) \left| \frac{1}{r_{12}} \right| \phi_{np,-m_l}(2)\chi_0^+(1) \right\rangle, \quad (3a)$$

$$g_{m_l} = \left\langle \chi_2^-(1)\chi_1^-(2) \left| \frac{1}{r_{12}} \right| \phi_{np,-m_l}(2)\chi_0^+(1) \right\rangle, \quad (3b)$$

where $\phi_{np,-m_l}$ is a Hartree-Fock orbital [15] for the active electron that is removed from the atom, which has the quantum number $-m_l$ for the projection of the orbital angular momentum since this projection and that of the ion ($+m_l$) cancel. To obtain the distorted waves χ_j, $j = 0, 1, 2$, we solve the equations

$$\left(-\frac{1}{2}\nabla^2 + U_j\right)\chi_j = E_j\chi_j \quad (4)$$

and then orthogonalize each χ_j to $\phi_{np,-m_l}$. Here

$$U_j = z_j U_{\text{ion}} + (1 - z_j) U_{\text{atom}} \quad (5)$$

plus the Furness-McCarthy exchange potential [16], where $U_{\text{atom(ion)}}$ is the static potential for the atom (ion), $z_0 = 0$ and

$$z_1 = z_2 = 1 - \frac{1}{2\sin(\theta_{12}/2)}, \quad (6)$$

where θ_{12} is the angle between the two final-state electrons (see Ref. [13]).

In Fig. 2(a), results are presented for 15.44 eV incident electrons ionizing xenon with the residual ion being left in the $J = 1/2$ state. The ionization energy of this state is 13.44 eV and the 2 eV excess energy is shared equally between the two final-state electrons. In Fig. 2(b), results are shown for 14.13 eV incident electrons with the residual ion being left in the $J = 3/2$ state. The ionization energy of this state is 12.13 eV and again the 2 eV excess energy is shared equally between the two final-state electrons. In the top part of each figure, triply differential cross section results in the scattering plane are presented for the case in which the angle between the two final-state electrons is fixed at 180° and the angle that one of these

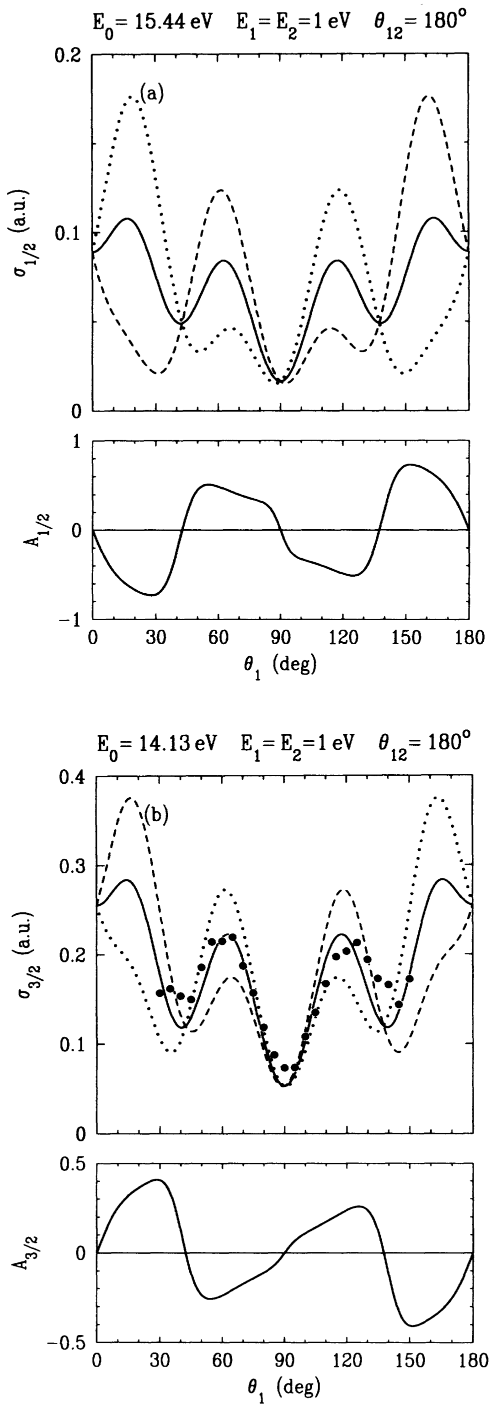

FIG. 2. Spin-resolved cross sections and spin up-down asymmetries for electron-impact ionization of xenon at 2 eV above threshold using the theoretical model discussed in the text. The angle θ_1 is measured counterclockwise from the forward beam direction (to the left). (a) $J = 1/2$ results: dashed line, $\sigma_{1/2}(\uparrow)$; dotted line, $\sigma_{1/2}(\downarrow)$; solid line, statistical average (cross section for unpolarized electrons). (b) $J = 3/2$ results: dashed line, $\sigma_{3/2}(\uparrow)$; dotted line, $\sigma_{3/2}(\downarrow)$; solid line, statistical average (cross section for unpolarized electrons). The solid circles are the relative measurements of Rösel *et al.* [15] for unpolarized electrons.

electrons makes relative to the incident beam direction is varied. Results are presented for unpolarized incident electrons as well as for electrons polarized with spins up and down relative to the scattering plane. For the case of unpolarized electrons, experimental results are available for the $J = 3/2$ case. The present results for $J = 3/2$ are compared with the relative measurements of Rösel *et al.* [17] normalized to our theory at 65°. It is seen that the present theory is in very good agreement with the shape of the experimental data. A qualitatively similar DWBA model is also in good agreement with the shape of these data [18]. For the case of polarized incident electrons, the cross sections are significantly different for spin-up and spin-down electrons.

In the lower part of each figure, the spin up-down asymmetry is shown. The asymmetry is large and very angular dependent. It is important to note that this large asymmetry results only from exchange scattering in a nonrelativistic model. Relativistic effects would be expected to produce additional asymmetries and these effects are not included in the present model. Consequently, it is conceivable that the actual spin up-down asymmetry may be even larger than predicted here. As a result, we would conclude that very large spin effects may be found in $(e, 2e)$ collisions if the incident electrons are spin polarized and the experiment is able to distinguish between the final J states of the residual ion.

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