## On the observation of the fine structure effect in non-relativistic (e, 2e) processes

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**Abstract.** The spin asymmetry arising in an (e, 2e) process using spin-polarized incoming electrons with non-relativistic energies is shown to be dominated by the fine structure effect if a suitable kinematical regime is chosen. Calculations in the distorted wave Born approximation (DWBA) for both the triple differential cross-section and the spin asymmetry are presented for the inner shell ionization of argon. This process would provide an accessible target for existing experimental set-ups.

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## 1 Introduction

In an (e, 2e) process an electron is fired at a target, ionizes it and the two outgoing electrons are detected in coincidence with their energies and angles resolved. This is a kinematically complete experiment. Ideally one would like to determine the spins of the target, incident and scattered electrons and thus perform a truly quantum mechanically complete experiment. This goal is beyond present experimental capabilities. However, experiments have been performed with spin polarized incident electrons [1,5,8,16]. This allows one to define an asymmetry parameter

$$A = \frac{\mathrm{d}\sigma(+) - \mathrm{d}\sigma(-)}{\mathrm{d}\sigma(+) + \mathrm{d}\sigma(-)},\tag{1}$$

where  $d\sigma(+)$  denotes the triple differential cross-section (TDCS) measured for 'spin up' and  $d\sigma(-)$  the one for 'spin down' states of the incident electron. In this paper it will be assumed that all the electrons remain in the scattering plane and that the incident electrons are polarized perpendicular to this plane. It has been predicted [8] that even if we are working in an kinematic regime where all spin dependent forces on the continuum electrons are negligible it should be possible to observe a spin up-down asymmetry provided that a target fine structure may be

experimentally resolved. In fact, in the absence of all other contributions to the spin asymmetry, it can be shown [9] that for p target electrons

$$A(p_{1/2}) = -2A(p_{3/2}), (2)$$

where the bound electron has been specified by its angular momentum (p) and its  $m_i$  quantum number.

However, it has been shown theoretically [14,15] that in previous experiments which measured the spin asymmetries in fine-structure split p states [5,6,8,9] exchange distortion is the dominant contribution. This is particular true when considering the interaction of the slow outgoing electron and the residual ion. A similar effect was noted [18] when considering the spin asymmetry studies on Li(2s) [1] where no relativistic target effects could be present. Indeed, Lechner et al. [13] used a sophisticated density functional treatment of exchange in looking at spin asymmetries in the outer shell of xenon rather than the cruder Furness-McCarthy potential used in earlier calculations and came to the conclusion that the apparent relativistic effects seen in [6] were exclusively a result of the choice of exchange potential used.

The spin asymmetry for the  $2p_{3/2}$  state of uranium at relativistic energies has been measured [2] using a transversely polarized beam of electrons of energy 300 keV. Agreement with the relativistic distorted wave approximation (rDWBA) predictions [12] is extremely good.

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Fig. 1. Spin asymmetries for the electron impact ionization of hydrogen-like uranium with the bound electron residing in either the  $2p_{1/2}$  (solid line) or  $2p_{3/2}$  (dashed line) state in coplanar asymmetric geometry. The fast outgoing electron is detected so that the Bethe-ridge condition is fulfilled. For uranium this point is given by  $\theta_1 = -27.4^{\circ}$  and  $\theta_2 = 50.0^{\circ}$ . The angles  $\theta_1$  and  $\theta_2$  correspond to the angles formed between the z-axis and the momentum vector of the fast and slow outgoing electron respectively.

Unfortunately it was not possible experimentally to resolve the  $2p_{1/2}$  state and thus to confirm the rDWBA predictions in this case. The fully relativistic calculation contains no exchange in the calculation of the distorted waves but does include the effect of Mott scattering from the nucleus. The rDWBA asymmetries show something of the character of the fine structure but the relationship between  $A(p_{1/2})$  and  $A(p_{3/2})$  is far more complex than equation (2) would suggest. In Figure 1 we illustrate this by showing the spin asymmetry calculated in the rDWBA for a uranium ion target as given in [11].

The objective of this paper is to give guidance to the ongoing experimental program (see [18] and references therein) by delineating a kinematical set-up and target where the fine structure effect is not swamped by competing processes. Consequently, we are looking for a regime where the outgoing electrons are sufficiently fast that exchange distortion may be neglected and yet where relativistic multiple scattering effects can be ignored.

## 2 Prediction

Consider an (e, 2e) measurement on  $\operatorname{Ar}(2p)$  in coplanar asymmetric geometry for an impact energy of  $E_0 =$ 1949 eV, ejected energy of  $E_2 = 500$  eV and a scattering angle for the fast electron of  $\theta_1 = 30^\circ$ . This is exactly the kinematical arrangement of experiments reported earlier [18]. The kinematics are chosen to include the Bethe ridge point,  $\mathbf{k}_0 = \mathbf{k}_1 + \mathbf{k}_2$ , where  $\mathbf{k}_0$  is the momentum of the incident,  $\mathbf{k}_1$ ,  $\mathbf{k}_2$  the fast and slow electrons respectively. We will first use a non relativistic distorted wave



Fig. 2. TDCS for electron impact ionization of  $\operatorname{Ar}(2p)$  for an incident energy of  $E_0 = 1949$  eV. The slow outgoing electron has an energy  $E_2 = 500$  eV. The geometrical arrangement is coplanar asymmetric with a detection angle of  $\theta_1 =$  $30.0^{\circ}$  for the fast scattered electron. The solid line is the rDWBA calculation where we have summed over the  $2p_{1/2}$  and the  $2p_{3/2}$  sublevels, the dashed a non-relativistic DWBA calculation with a static exchange potential. Clearly these are almost indistinguishable. The dotted line is a DWBA calculation with a Furness-McCarthy local exchange potential for the slow outgoing electron and the dashed-dotted line represents a DWBA calculation with a local exchange approximation for all continuum electrons.

approximation to calculate the triple differential crosssection given by

$$\frac{\mathrm{d}^3 \sigma}{\mathrm{d}\Omega_1 \,\mathrm{d}\Omega_2 \,\mathrm{d}E} = 2(2\pi)^4 \frac{k_1 k_2}{k_0} \\ \times \sum_m \left( |f_{nlm}|^2 + |g_{nlm}|^2 - \mathrm{Re}(f^*_{nlm}g_{nlm}) \right), \quad (3)$$

where  $f_{nlm}$  is the direct and  $g_{nlm}$  the exchange amplitude as presented previously [10]. Here a direct  $f_{nlm}$  and an exchange  $g_{nlm}$  amplitude are included because the electrons are indistinguishable in their final state. Furthermore, exchange distortion is included in our calculations by using distorted waves for the incoming and fast outgoing electrons. The wavefunctions for the incoming and fast outgoing electrons are calculated in the static exchange potential of the atom and the wavefunction for the slow electron in the static exchange potential of the ion. We are concerned that these exchange effects in the calculation of the distorted waves should not be too large. In Figure 2 we show the DWBA calculated with all the elastic exchange potentials included, with no exchange potentials included and with only the exchange potential for the slow electron included. The effect of exchange distortion is clearly small.

Similar to the calculations presented in [15] we use a Furness-McCarthy local exchange approximation: this is really quite a simple treatment of exchange and it might be argued that will give us a serious error. The form of the exchange potential to be used in the calculation of the static



Fig. 3. Spin asymmetries for the electron impact ionization of argon with the bound electron residing in either the  $2p_{1/2}$  (solid line) or  $2p_{3/2}$  (dashed line) state in coplanar asymmetric geometry. The fast outgoing electron is detected under an angle of  $\theta_1 = 30.0^{\circ}$  so that the Bethe-ridge condition is fulfilled. This point is given by  $\theta_2 = 50.0^{\circ}$ .

exchange problem is not unambiguously defined [3,4,17]. Here we use a spin singlet Furness-McCarthy potential. It has been found that for our choice of kinematics the effect of using a triplet form is negligible. In the DWBA we expand the distorted waves corresponding to the elastic scattered electrons in partial waves. In the argon calculation we used 55 partial waves for the slow outgoing electron; exchange contributes only to the first few. Although the Furness-McCarthy approach is not highly accurate or indeed unambiguously defined, it does give a correct order of magnitude estimate for the exchange effects.

In Figure 2 we also show the result of calculating the triple differential cross-section with the rDWBA code. The rDWBA can be viewed as a fully relativistic generalization of the DWBA where the Dirac equation is solved for the static scattering and includes the full photon propagator. The Ar(2p) target wavefunctions were generated using the Oxford Dirac Fock program [7]. Agreement between the fully relativistic and non-relativistic calculations of cross-sections is very good.

We may thus conclude that for our choice of kinematics, Mott scattering effects will be small and that exchange distortion will not be strong. This is thus an ideal experimental arrangement to look for the fine structure effect. In Figure 3 we plot the spin asymmetry calculated in the rDWBA code. Equation (2) is close to being exactly satisfied. We recommend this arrangement to our experimental colleagues. CTW is grateful to the DFG and would like to thank Professor R.M. Dreizler for his splendid hospitality at Institut für Theoretische Physik, Universität Frankfurt am Main and for more than a decade of useful discussions. This work was supported by the EPSRC under grants GR/L81277 and GR/M01785 (CTW, HRJW). DHM gratefully acknowledges the support of the NFS under grant PHY-0070872. MK gratefully acknowledges financial support from the *Gottlieb-Daimler* und Karl-Benz Stiftung, Germany.

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