Fine Structure Effect in Electron Impact Ionization

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Spin resolved (e,2e) experiments provide an extremely sensitive test of theories of electron impact ionization and many-body Coulomb effects. We present here results for (e,2e) collisions with xenon which show the first experimental evidence of the fine structure effect in electron impact ionization, analogous to the well known effect in electron impact excitation of atoms by polarized electrons. Comparison with distorted-wave Born-approximation calculations shows the sensitivity of the results to details of the target atom wave functions as well as the treatment of relativistic effects.

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Our understanding of such diverse fields as the physics and chemistry of the upper atmosphere, plasma formation, gas discharge, and laser physics requires an understanding of the process of electron impact ionization. Detailed information concerning this process is provided by kinematically complete $(e,2e)$ measurements, in which the energies and momenta of all reaction participants and products are determined. Over the past two decades the $(e,2e)$ technique has played a central role in uncovering details concerning both the ionization mechanisms [1,2] and the electronic structure of atoms and molecules [3,4], and more recently of condensed matter [5]. Following the trend towards improved state selectivity, numerous electron scattering experiments are now being performed using spin polarized targets and/or electron beams to probe the spin dependent aspects of scattering [6,7]. To date, however, only a handful of $(e,2e)$ experiments have been performed using spin resolved techniques.

There are two mechanisms which give rise to spin dependent scattering in the ionization of atomic targets, namely, exchange and the spin-orbit effect (Mott scattering). Exchange occurs both between incident and target electrons (including capture), enabling mutual transfer of polarization, and between the continuum electron pair emerging after the collision. In contrast, the spin-orbit interaction is a relativistic effect which becomes significant for the scattering of electrons from heavy targets [7,8], producing spin flips for the continuum electrons under conditions where conservation of total spin for the electron-atom system no longer holds.

In the first ever spin polarized $(e,2e)$ ionization experiment, Baum *et al.* [9] investigated the competing processes of direct and exchange scattering by scattering a low energy (54.4 eV) polarized electron beam from a beam of polarized lithium atoms. Performing their experiment with an extremely light target they were able to investigate the scattering process under conditions where spin-orbit interaction of the continuum electrons in the atomic and ionic fields is negligible. In contrast, the Tübingen group [10] recently measured spin asymmetries in the $(e,2e)$ scattering cross section for the ionization of K-shell electrons in unpolarized silver atoms by high energy 300 keV polarized electrons. In this case, the spin asymmetries result from the spin-orbit interaction of the continuum electrons.

The question of what spin effects are present in low energy ionization of an unpolarized target by polarized electrons remains open. For heavier atoms, such as xenon, strong effects are observed in low energy elastic scattering and excitation [7,8], and it might be reasonable to assume some observable effects could also be seen in ionization. Hanne [11], for instance, proposed that spin dependent effects might still be observed even if the effects of spin-orbit interaction are negligible, for the case when the final fine structure levels of the residual ion are resolved. He postulated that spin asymmetries could arise due to the effects of collisionally induced orientation of the residual ion core and from exchange between the core and final state continuum electrons. This effect is directly analogous to the fine structure effect [7,12] in the electron impact excitation of an atom to a state of nonzero orbital angular momentum in which the spin polarization of the scattered electrons differs from that of the primary electrons inducing the excitation when transitions to the individual fine structure levels are considered. When the fine structure levels of the excited state are unresolved no difference in the spin polarization of the scattered electrons from the incident electrons is observed. This effect in excitation results from an interplay between the processes of collisionally induced orientation of the target atom and exchange between the incident and target electrons.

The aim of the present work was to see if spin effects played a significant role at low to medium energies on a medium sized atomic target and to seek experimental verification of any possible fine structure effect. Xenon was

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chosen as the target atom due to the large energy separation between $5p^5\,{}^2P_{1/2}$ and ${}^2P_{3/2}$ ion ground states with ionization energies of 13.44 and 12.13 eV, respectively, ensuring that the fine structure levels of the residual ion could be resolved. Recent calculations for the $(e,2e)$ reaction on xenon have shown that large spin effects may indeed be expected at low impact energies for ionization of the outer filled 5*p* valence shell [13]. Preliminary reports on progress towards $(e,2e)$ measurements on xenon with polarized electrons have previously been reported by our group [14] and the Münster group [15].

Only a brief description of the $(e,2e)$ technique and the apparatus is given here, with the details to be published elsewhere [16]. In the present experiment a 147 eV beam of polarized electrons was crossed with an effusive beam of xenon atoms. The polarized electron beam was generated by photoemission from a GaAs crystal irradiated with circularly polarized light from a GaAlAs laser. After electrostatic deflection through 90°, the extracted electrons are transversely polarized with respect to the reaction plane (Fig. 1). Spin flip of the electron beam is effected by reversing the helicity of the laser light incident upon the GaAs photocathode through rotation of a quarter wave plate. The beam polarization was measured to be 0.24 ± 0.01 in a Mott polarimeter. This value was checked by measuring the Sherman function for elastic electron-xenon scattering at an incident beam energy of 50 eV. The excellent agreement found with measurements of Müller and Kessler [8] provided a consistency check for the magnitude of beam polarization vector and its sign of projection along the quantization axis perpendicular to the collision plane.

Scattered electrons were energy and momentum analyzed in two hemispherical electrostatic analyzers. One analyzer was adjusted to measure electrons scattered to the left through a fixed angle of 28° relative to the incident beam direction, and within a 6 eV energy band centered at 100 eV (the Bethe-Ridge kinematics). The second analyzer measured an identical width energy band of mean energy 35 eV, the scattering angle θ_s to the right of the incident electrons being scanned in the experiment. The apparatus was configured for coplanar scattering geometry (Fig. 1). Each analyzer incorporated channel plate electron multipliers and position sensitive detectors at its exit plane. Fast timing pulses from the channel plates were used to identify coincident electron pairs after correction for time of flight variations through the analyzers. A coincidence energy resolution of 0.6 eV was achieved at typical count rates between 1.0 and 0.1 Hz.

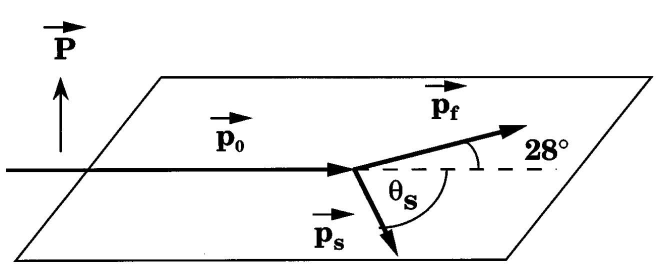

FIG. 1. Kinematics for the present coplanar asymmetric $(e,2e)$ experiments on xenon. $\mathbf{p}_0$, $\mathbf{p}_f$, and $\mathbf{p}_s$ correspond to momenta for the incident electron and the faster and slower emitted electrons, respectively; θ_s to the scattering angle varied in the experiment; and **P** to the polarization of the incident electron beam, directed orthogonally to the reaction plane. The primary beam energy is 147 eV, with fast scattered electrons of average energy 100 eV detected to the left at an angle of 28° relative to the primary beam direction.

The $(e,2e)$ spin asymmetry is defined by the relation

$$A_J = \frac{\sigma_J^\uparrow - \sigma_J^\downarrow}{\sigma_J^\uparrow + \sigma_J^\downarrow},$$

where $\sigma_J^\uparrow$ and $\sigma_J^\downarrow$ are, respectively, the $(e,2e)$ differential cross sections to the final ion state of angular momentum J for incident electrons with spin up and spin down perpendicular to the scattering plane. Experimentally, A_J is determined from the relation

$$A_J = \frac{1}{P}\frac{N_J^\uparrow - N_J^\downarrow}{N_J^\uparrow + N_J^\downarrow},$$

where P is the component of electron beam polarization perpendicular to the scattering plane and $N_J^\uparrow$ and $N_J^\downarrow$ are the measured $(e,2e)$ count rates for the final state J for incident spin up and spin down electrons, respectively.

Figures 2(a) and 2(b) show experimentally and theoretically determined asymmetries for ionization to the $5p^5\,{}^2P_{1/2}$ and ${}^2P_{3/2}$ residual ion states of xenon, respectively. Figure 2(c) shows results for the sum $(A_{1/2} + 2A_{3/2})/3$ which for a "pure" (in the nonrelativistic limit) fine structure effect should be zero. In Fig. 2(d) branching ratios are presented for ionization to the ${}^2P_{1/2}$ and ${}^2P_{3/2}$ ion states by unpolarized incident electrons. These results are compared with calculations performed within a distorted-wave Born-approximation (DWBA) formalism [17]. In our theoretical approach, a semirelativistic DWBA calculation with Dirac-Fock wave functions is performed. The distorted waves are calculated in the static exchange potential of the target or ion, as appropriate, with the addition of the Thomas spin-orbit term. The asymmetry parameter is expressed using the density matrix formalism to take into account both the contribution of the fine structure effect and the spin-orbit interactions for the continuum electrons. To demonstrate the degree of the sensitivity of calculation on the description of the target and on the spin-orbit potential, we present for comparison results from a second calculation where Hartree-Fock wave functions replace the Dirac-Fock wave functions and the Thomas spin-orbit term in the potential is omitted. In this nonrelativistic calculation, the effects of the 1.3 eV fine structure splitting on the ionization cross sections are allowed for by adjusting the energy of the slow outgoing electron by 1.3 eV between calculations for the ${}^2P_{1/2}$ and ${}^2P_{3/2}$ transitions.

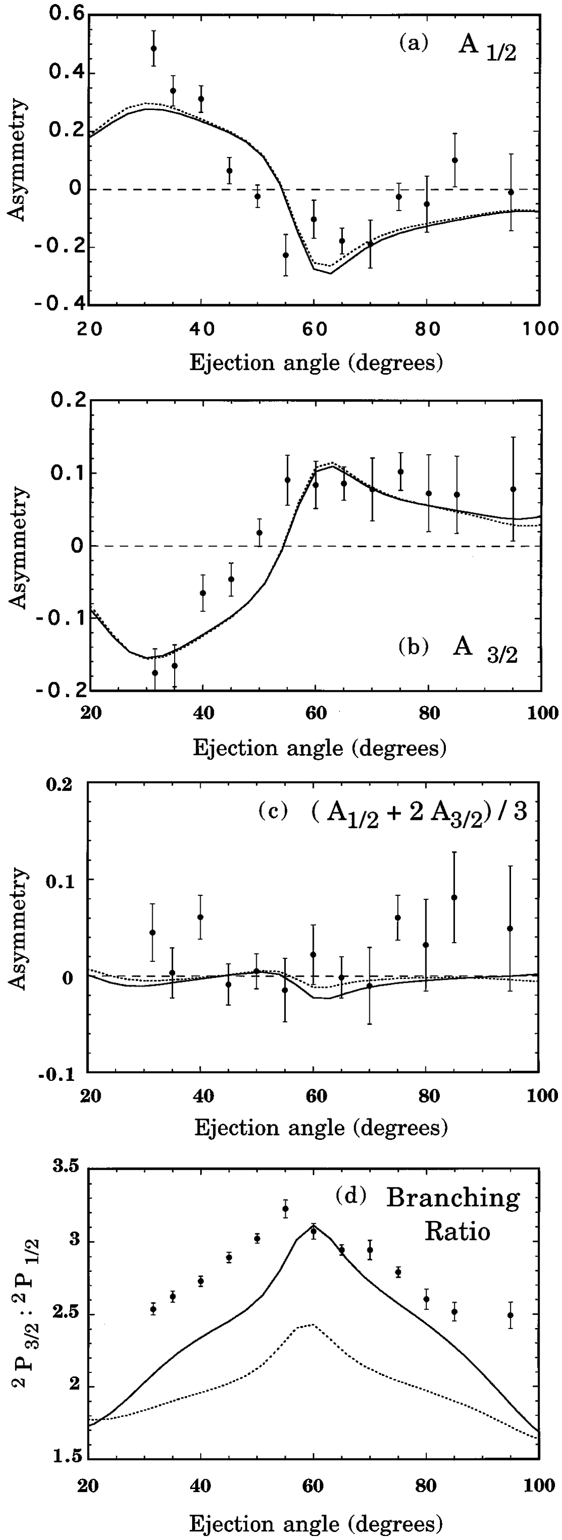

FIG. 2. Results for spin resolved $(e, 2e)$ collisions on xenon as a function of the scattering angle θ_s of the slow outgoing electrons of median energy 35 eV. (a) and (b) show spin asymmetries corresponding to the ${}^2P_{1/2}$ and ${}^2P_{3/2}$ final ion states, respectively. In (c) the quantity $(2A_{3/2} + A_{1/2})/3$ is presented. (d) presents the ${}^2P_{3/2}$:${}^2P_{1/2}$ branching ratios for an unpolarized incident electron beam. The DWBA calculations: semirelativistic with Dirac-Fock target wave function (solid line) and nonrelativistic with Hartree-Fock target wave function (dotted line).

The data in Figs. 2(a) and 2(b) clearly establish the existence of significant spin up/spin down asymmetries in the ionization of the closed shell xenon target when the fine structure levels of the final ion state are resolved. Under the present kinematics, the asymmetry is both large and highly angular dependent. Our theories show reasonable agreement with the experimentally derived data over the full angular range, predicting well both the magnitude and sign of the asymmetries. A small angular shift between the theoretical and experimental results is, however, evident. The calculated asymmetries are insensitive to the details of the target description and to the spin-orbit potential, whilst the strong variations in their magnitudes with ejection angle show their sensitive dependence on the details of the ionization dynamics. It is interesting to note that the ejection angle for which theory predicts both asymmetries to change sign corresponds exactly to the condition where the residual ion recoil momentum is zero. This corresponds to the high symmetry kinematical condition in which the summed momentum of the two final state continuum electrons is parallel to and equals the momentum of the incident electron.

The pure fine structure effect is characterized by nonzero values of the asymmetry parameters ($A_{1/2}$ and $A_{3/2}$) but a zero asymmetry if the fine structure states are degenerate (and hence not resolved). In the nonrelativistic limit where the energies and nonspin part of the wave functions are the same for the ${}^2P_{3/2}$ and ${}^2P_{1/2}$ ion states, the asymmetry parameters for a pure fine structure effect must be related by

$$A_{1/2} + 2A_{3/2} = 0,$$

where the factor of 2 is due to the relative statistical weighting of the two states. Figure 2(c) shows the quantity $(2A_{3/2} + A_{1/2})/3$ plotted as a function of scattering angle for the slow outgoing electron. Given the errors the measurement of this quantity is indeed consistent with zero, although some evidence for a small nonzero asymmetry contribution is present at the larger angles. This could reflect the effect of spin-orbit interaction of the continuum electrons and/or the process of capture under the present experimental conditions. The DWBA calculations predict extremely small values for this summed asymmetry parameter consistent with the results of our measurement. Thus both measurements and calculations agree that the observed ${}^2P_{3/2}$ and ${}^2P_{1/2}$ asymmetries are almost entirely due to the fine structure effect.

In contrast to the asymmetries [Figs. 2(a) and 2(b)], the influence of relativistic effects in the target wave function plays a dominant role in determining the branching ratio. This can be seen in Fig. 2(d) which shows the calculated branching ratios compared with the measured ones obtained by averaging the ionization cross sections for transitions to the individual ${}^2P_{1/2}$ and ${}^2P_{3/2}$ ion states over the spin direction of the incident electron. Agreement between experiment and theory incorporating a Dirac-Fock description of the target and ionic wave functions is again reasonable whilst the calculation employing a Hartree-Fock description fails completely to describe the experimental results.

The present work shows that the use of polarized electrons in $(e, 2e)$ collisions provides a powerful tool for unraveling competing spin and nonspin dependent effects in the ionization process, some effects being clearly dependent upon the dynamics of the reaction mechanism, and others, such as branching ratios on the details of the target wave function. Further experiments of the type described in this paper are now being performed over an extended kinematic range to further increase our understanding of fundamental processes involved in electron impact ionization.

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