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Spin asymmetry in weakly relativistic $(e,2e)$ collisions

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Two geometries are chosen to make predictions and to test the Coulomb-Born approximation against the distorted-wave Born approximation and experiment, the symmetric coplanar constant Θ_{12} geometry for *K*-shell ionization of Ag and the asymmetric coplanar geometry for *L*-subshell ionization of U. Even for the heaviest target, good agreement is found as long as the two electrons emerge on opposite sides of the beam axis.

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I. INTRODUCTION

Inner-shell ionization of atoms by electron impact is one of the basic processes in atomic-collision physics. The coincident detection and spectroscopy of the two outgoing electrons, together with the determination of the bound electron's initial state provides a complete analysis of the three-body collision kinematics [1]. In order to achieve the same goal in heavy-ion collision experiments, not only a very complex detection system is needed (the COLTRIMS detector [2]), but one usually has to deal with a large variety of emitted particles due to the strong perturber field, which inhibits an accurate study of a pure three-body process. Moreover, if in the $(e,2e)$ experiments the projectile electron is polarized, fine-structure effects become accessible. Hence, a comparison of theory with experiment, both for the triply differential cross sections and for the spin asymmetry provides an optimal test of the underlying theoretical models.

During the last two decades, series of absolute measurements on *K*- and *L*-shell ionization of targets from copper to uranium by relativistic polarized and unpolarized electrons with impact energies up to 500 keV were performed by Nakel and his Tübingen collaborators (for a review, see Ref. [1]). The first quantum-mechanical theory able to explain quantitatively the early data on angular and energy distribution of the emitted electrons was the (semirelativistic) Coulomb-Born approximation (CBA) [3]. This theory is a first-order approximation in the electron-electron interaction, which allows for relativistic kinematics and which includes the Coulomb field in all electronic states by means of semirelativistic Coulomb states. Polarization effects and postcollisional electron-electron correlation are disregarded since they are immaterial for the relativistic incoming and outgoing electrons under consideration.

An improvement of the CBA was provided by the fully relativistic Coulomb-Born theory (RCBA [4]), which employs exact relativistic Coulomb functions for the electronic states, as well as by the relativistic distorted-wave Born approximation (RDWBA [5]), where the target potential is taken from a self-consistent relativistic Kohn-Sham local-density approximation and its bound and scattering eigenstates are generated numerically. RDWBA turned out to be very successful in reproducing the measured angular distribution of the ejected electrons [1].

Deviation between CBA and RDWBA can be used as an indicator for situations where a fully relativistic representation of the electronic wave functions is mandatory in contrast to situations where a correct account of relativistic kinematics is sufficient. This is possible because the other two deficiencies of the CBA as compared with the RDWBA, the nonorthogonality between the bound and continuum states as well as the neglect of screening the target nuclear field by the passive electrons beyond Slater screening, were found to be immaterial for inner-shell ionization of the heavy targets under consideration [4,6].

This work concentrates on the comparison between CBA, RDWBA, and experiment in the case of weakly relativistic target states, that is, *L*-shell ionization of very heavy atoms and *K*-shell ionization of atoms with intermediate nuclear charge. Atomic units ($\hbar=m=e=1$) are used unless otherwise indicated.

II. COULOMB-BORN APPROXIMATION

In a first-order theory such as the CBA, the electron emission is mediated by one single electron-electron interaction V_{ee}. Using the Fourier representation of V_{ee} in its relativistic form, the transition amplitude for ejecting an electron from the initial state $\phi_i^{(\sigma_i)}$ into the final state $\phi_{\boldsymbol{\kappa}_f}^{(\sigma_f)}$ while simultaneously scattering the projectile electron from $\psi_{\mathbf{k}_i}^{(s_i)}$ into $\psi_{\mathbf{k}_f}^{(s_f)}$ is given by [7]

$$\begin{aligned} W_{s_f\sigma_f s_i\sigma_i}(\mathbf{k}_f,\boldsymbol{\kappa}_f) = \int \frac{d\mathbf{q}}{q^2-q_0^2-i\epsilon}\{ &\langle \psi_{\mathbf{k}_f}^{(s_f)}|e^{-i\mathbf{q}\cdot\mathbf{r}_1}|\psi_{\mathbf{k}_i}^{(s_i)}\rangle \\ &\times\langle \phi_{\boldsymbol{\kappa}_f}^{(\sigma_f)}|e^{i\mathbf{q}\cdot\mathbf{r}_2}|\phi_i^{(\sigma_i)}\rangle \\ &-\langle \psi_{\mathbf{k}_f}^{(s_f)}|e^{-i\mathbf{q}\cdot\mathbf{r}_1}\boldsymbol{\alpha}_1|\psi_{\mathbf{k}_i}^{(s_i)}\rangle \\ &\times\langle \phi_{\boldsymbol{\kappa}_f}^{(\sigma_f)}|e^{i\mathbf{q}\cdot\mathbf{r}_2}\boldsymbol{\alpha}_2|\phi_i^{(\sigma_i)}\rangle\}, \end{aligned} \tag{2.1}$$

where the spatial coordinates of the scattered and of the ejected electron are denoted by $\mathbf{r}_1$ and $\mathbf{r}_2$, respectively, $\mathbf{k}_i$, $\mathbf{k}_f$, and $\boldsymbol{\kappa}_f$ are the momenta of the unbound electronic states, and $\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2$ are the Dirac matrices of the two electrons originating from the relativistic current-current interaction. With E_{k_i} and E_{k_f} the total (relativistic) energy of the projectile electron in its initial and final state, respectively, one has

$q_0=(E_{k_i}-E_{k_f})/c$. The spin projections of the electronic states are denoted by s_i, σ_i, s_f, and σ_f. In the representation of the wave function in terms of Dirac spinors, the polarization direction of a free electron is along its momentum. If the incident electron is polarized in a given spatial direction, a spin rotation has to be performed. For transversely polarized electrons, as in the experiments discussed below, the amplitude for ionization by spin-up ($s_i=+$) and spin-down ($s_i=-$) electrons is obtained from Eq. (2.1) by means of the following rotation [7]:

$$V_{s_f\sigma_f+\sigma_i}(\mathbf{k}_f,\boldsymbol{\kappa}_f):=\frac{1}{2}\{(1+i)W_{s_f\sigma_f+\sigma_i}(\mathbf{k}_f,\boldsymbol{\kappa}_f)+(1-i)W_{s_f\sigma_f-\sigma_i}(\mathbf{k}_f,\boldsymbol{\kappa}_f)\},$$

$$V_{s_f\sigma_f-\sigma_i}(\mathbf{k}_f,\boldsymbol{\kappa}_f):=\frac{1}{2}\{-(1+i)W_{s_f\sigma_f+\sigma_i}(\mathbf{k}_f,\boldsymbol{\kappa}_f)+(1-i)W_{s_f\sigma_f-\sigma_i}(\mathbf{k}_f,\boldsymbol{\kappa}_f)\}. \quad (2.2)$$

The triply differential cross section for detecting the two electrons with momenta $\mathbf{k}_f$ and $\boldsymbol{\kappa}_f$ in the solid angles $d\Omega_{k_f}$ and $d\Omega_{\kappa_f}$, respectively, is for initially polarized electrons given by

$$\frac{d^3\sigma(\pm)}{dE_{\kappa_f}d\Omega_{k_f}d\Omega_{\kappa_f}}=\frac{2N_i}{c^6k_i}\kappa_f E_{\kappa_f}k_f E_{k_f}E_{k_i}\times\sum_{|m_i|}\sum_{s_f\sigma_f\sigma_i}|V_{s_f\sigma_f\pm\sigma_i}(\mathbf{k}_f,\boldsymbol{\kappa}_f)-V_{\sigma_f s_f\pm\sigma_i}(\boldsymbol{\kappa}_f,\mathbf{k}_f)|^2. \quad (2.3)$$

The number of electrons in the initial subshell with total angular momentum $\pm m_i$ is denoted by N_i. The last term in Eq. (2.3) is the exchange contribution, obtained from the direct term by means of interchanging s_f with σ_f and $\mathbf{k}_f$ with $\boldsymbol{\kappa}_f$. The sum runs over the unobserved spin quantum numbers.

The spin asymmetry A is defined as the relative cross section difference between impinging spin-up and spin-down electrons

$$A:=\frac{d^3\sigma(+)/dE_{\kappa_f}d\Omega_{k_f}d\Omega_{\kappa_f}-d^3\sigma(-)/dE_{\kappa_f}d\Omega_{k_f}d\Omega_{\kappa_f}}{d^3\sigma(+)/dE_{\kappa_f}d\Omega_{k_f}d\Omega_{\kappa_f}+d^3\sigma(-)/dE_{\kappa_f}d\Omega_{k_f}d\Omega_{\kappa_f}}. \quad (2.4)$$

In the Coulomb-Born approximation, semirelativistic Darwin wave functions are used for the bound states $\phi_i^{(\sigma_i)}$, while every continuum state is represented by a product of nonrelativistic Coulomb wave and free Dirac spinor [3].

III. RESULTS

The symmetric coplanar constant Θ_{12} geometry was suggested by Whelan and co-workers [8]. In this geometry, the two outgoing electrons have equal energy and are emitted in-plane with the beam axis while the angle Θ_{12} between them is kept fixed. Hence, for a given Θ_{12}, their emission angles ϑ_{k_f} and ϑ_{κ_f} are related by $\vartheta_{\kappa_f}=\vartheta_{k_f}+\Theta_{12}$. This geometry is particularly sensitive to the electron-nucleus interaction in initial and final channels, and both binary region (where the two electrons are detected on opposite sides of the beam axis) and recoil region (where both electrons are emitted to the same side of the beam axis) can be studied within a quite narrow range of ϑ_{κ_f} [1].

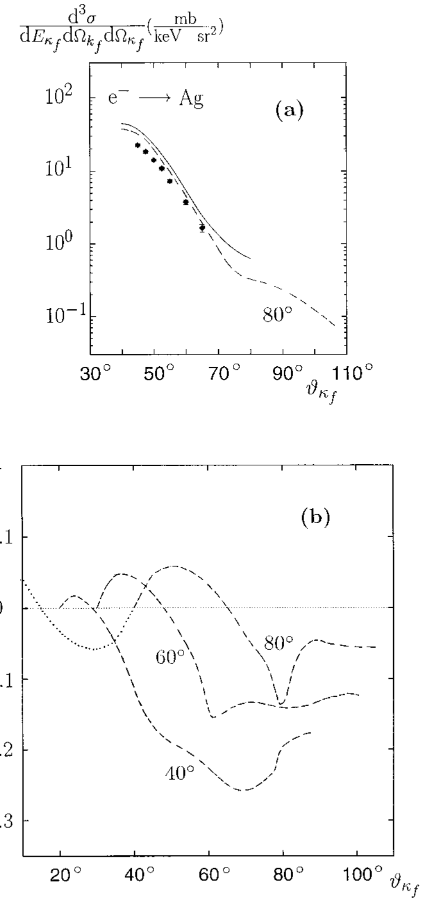

FIG. 1. *K*-shell ionization cross section of Ag by 300 keV electrons in symmetric coplanar constant Θ_{12} geometry ($E_{k_f}=E_{\kappa_f}=137.25$ keV) with $\Theta_{12}=80°$ (a), and corresponding spin asymmetry A for $\Theta_{12}=40°$, 60°, and 80° in the case of electrons polarized perpendicular to the collision plane (b). Theory: ——, RDWBA from Ast (taken from Ref. [9]); – – –, CBA. The experimental data, ⧫, are from Nakel's group [9].

In Fig. 1(a), the dependence of the *K*-shell ionization cross section of Ag on ϑ_{κ_f} [calculated from the mean value of the two expressions given by Eq. (2.3)] is displayed for an opening angle Θ_{12} of 80°. The cross section is only shown for $\vartheta_{\kappa_f}\geq\frac{1}{2}\Theta_{12}$ because of the symmetry with respect to $\vartheta_{\kappa_f}=|\vartheta_{k_f}|=\frac{1}{2}\Theta_{12}$. In the angular range corresponding to the binary region ($\Theta_{12}/2\leq\vartheta_{\kappa_f}\leq\Theta_{12}$, which implies $-\frac{1}{2}\Theta_{12}\leq\vartheta_{k_f}\leq 0$), the CBA results are close to those from RDWBA, both theories reproducing the experimental trend. This is also true for $\Theta_{12}=40°$ and 60° (not shown). For

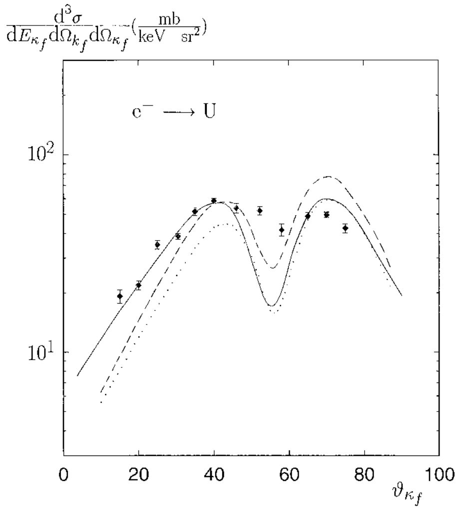

FIG. 2. $2p_{3/2}$-subshell ionization cross section of U by 300 keV electrons in coplanar asymmetric geometry with $E_{k_f}=210$ keV and $\vartheta_{k_f}=-26°$. Theory: ——, RDWBA (taken from Ref. [10]); – – –, CBA; · · · ·, CBA without spin flip. The experimental data, ♦, are from Kull [10].

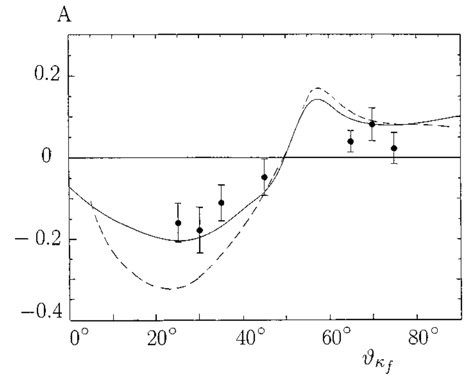

FIG. 3. Spin asymmetry for $2p_{3/2}$-subshell ionization of U by 300 keV electrons polarized perpendicular to the collision plane. The parameters are $E_{k_f}=210$ keV and $\vartheta_{k_f}=-24.8°$. Theory: ——, RDWBA (taken from Ref. [11]); – – –, CBA. The experimental data, ●, are from Besch *et al.* [11].

larger angles ϑ_{κ_f}, CBA underestimates RDWBA by a factor of 2.

Figure 1(b) predicts the corresponding spin asymmetry for the three angles, which is caused by the spin-orbit interaction of the relativistic continuum electrons in the strong field of the target nucleus. While for $E_{k_f}=E_{\kappa_f}$, the cross section is symmetric with respect to $\vartheta_{\kappa_f}=\frac{1}{2}\Theta_{12}$, the spin asymmetry is antisymmetric (shown for $\Theta_{12}=80°$ as dotted line) since the interchange of ϑ_{κ_f} and $-\vartheta_{k_f}$ corresponds to a 180° rotation around the beam axis such that $d^3\sigma(+)$ turns into $d^3\sigma(-)$ leading to a sign reversal in Eq. (2.4). The extension of the binary regime with increasing Θ_{12} is readily seen from the broadening of the angular region associated with a small, positive A. The recoil region, $\vartheta_{\kappa_f}>\Theta_{12}$, is characterized by a large, negative spin asymmetry, indicating the importance of relativistic wave function effects. These effects increase when the separation between the two outgoing electrons gets smaller.

In the asymmetric coplanar geometry, the fast electron is emitted at a small fixed angle ϑ_{k_f} relative to the electron beam, and the slow electron is detected in this scattering plane. Figure 2 shows the $2p_{3/2}$-subshell ionization cross section for uranium in that geometry. Results for the Bethe-ridge angle $\vartheta_{k_f}=-26°$ (corresponding to zero momentum transfer to the target nucleus) are given where measurements of absolute cross sections were made recently. The dip in the binary region resulting from the node of the initial *p*-state wave function in momentum space is quite prominent in the calculations. Taken into consideration that the experimental filling of this dip is likely to be due to multiple-scattering effects caused by the thick uranium targets that were used [10], both theories provide a satisfactory description of the measurements with respect to the peak intensities and shapes. Included in Fig. 2 are the CBA results without spin flip. In contrast to *K*-shell ionization of Ag, where spin flip is negligible in the binary peak region, there is a considerable reduction of the $2p_{3/2}$ ionization cross section when spin-flip transitions are disregarded.

The spin asymmetry resulting from U $2p_{3/2}$-subshell ionization at a slightly smaller angle, $\vartheta_{k_f}=-24.8°$ where experimental data are available and where the cross sections still show the Bethe-ridge dip, is plotted in Fig. 3. In addition to the spin asymmetry due to the spin-orbit interaction of the continuum electrons (which is quite small in the binary region), *p*-subshell ionization contains a large contribution caused by the relativistic fine-structure splitting of the initial bound state [12]. This is confirmed by the measurements that can be explained by the two theories in the whole angular range considered.

IV. CONCLUSION

By investigating triply differential cross sections as well as the spin asymmetry, we have shown that the applicability of the Coulomb-Born approximation can be extended to *L*-shell ionization of the heaviest target accessible to experiment, uranium. As long as the slow electron is ejected into the binary region, CBA and RDWBA give similar results that are in accord with the experimental data. This means that in this situation, relativistic wave function effects are of minor importance. A study of the *L*-shell ionization of Au (at $E_{k_f}=200$ keV and $\vartheta_{k_f}=-10°$) confirms this finding; however, an extension of ϑ_{κ_f} to the recoil regime reveals that, although CBA is able to reproduce the two-peak structure in the triply differential cross section as well as the large asymmetry that is present in experiment and RDWBA [1], it gives a severe underprediction of the peak intensity as well as a shift of the asymmetry maximum to larger ϑ_{κ_f}. This means that even for *L*-shell ionization, the relativistic contraction of the electronic wave functions plays a decisive role in the recoil region. It confirms that large momentum transfers in close collisions are required when the two electrons are ejected into the same hemisphere.

The investigation of the triply differential cross section for an Ag target (and similar calculations for Cu at $E_{k_f}=220$ keV and $\vartheta_{k_f}=-9°$) demonstrates that for the lighter targets, also *K*-shell ionization in the binary regime is well described by using semirelativistic wave functions. In view of the fact that CBA is able to provide a picture of essential features in the whole angular range, we consider the prediction of the asymmetry related to the coplanar constant Θ_{12} geometry to be at least qualitatively correct for the larger angles.

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[1] W. Nakel and C. T. Whelan, Phys. Rep. **315**, 409 (1999).
[2] R. Dörner, V. Mergel, O. Jagutzki, L. Spielberger, J. Ullrich, R. Moshammer, and H. Schmidt-Böcking, Phys. Rep. **330**, 95 (2000).
[3] D. H. Jakubaßa-Amundsen, Z. Phys. D: At., Mol. Clusters **11**, 305 (1989).
[4] L. U. Ancarani, S. Keller, H. Ast, C. T. Whelan, H. R. J. Walters, and R. M. Dreizler, J. Phys. B **31**, 609 (1998).
[5] S. Keller, C. T. Whelan, H. Ast, H. R. J. Walters, and R. M. Dreizler, Phys. Rev. A **50**, 3865 (1994).
[6] D. H. Jakubaßa-Amundsen, Phys. Rev. A **53**, 2359 (1996).
[7] D. H. Jakubaßa-Amundsen, J. Phys. B **28**, 259 (1995).
[8] C. T. Whelan, H. Ast, H. R. J. Walters, S. Keller, and R. M. Dreizler, Phys. Rev. A **53**, 3262 (1996).
[9] T. Kull and W. Nakel, J. Phys. B **32**, L297 (1999).
[10] T. Kull, Ph.D. thesis, University of Tübingen, Germany, 1999; W. Nakel (private communication).
[11] K. H. Besch, M. Sauter, and W. Nakel, Phys. Rev. A **58**, R2638 (1998).
[12] S. Keller, R. M. Dreizler, H. Ast, C. T. Whelan, and H. R. J. Walters, Phys. Rev. A **53**, 2295 (1996).