Role of the postcollision interaction in electron-impact ionization of argon and krypton

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There has been impressive progress in the theoretical treatment of electron collisions with atoms in the last decade. As a result, the fundamental collision problems of electron-hydrogen or electron-helium scattering are now understood fairly well. For heavier atoms, an accurate treatment of atomic ionization remains more elusive than atomic excitation due to the final-state three-body Coulomb problem. For higher impact energies, the first-order distorted-wave Born approximation is typically in reasonable agreement with fully differential cross sections (FDCS) for ionization. However, FDCS measurements are starting to be reported for lower incident electron energies and here agreement between experiment and theory is not good. In this paper we examine the importance of exchange distortion and the final-state electron-electron interaction on these collision processes.

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I. INTRODUCTION

Fully differential cross section (FDCS) measurements have been made for ionization of hydrogen and helium for almost three decades (reviews of this work have been given by Weigold and McCarthy [1], McCarthy and Weigold [2], Weigold [3], Lahmam-Bennani [4], Walters, Zhang, and Whelan [5], Whelan *et al.* [6], Coplan, Moore, and Doering [7], and Jones and Madison [8]). The first-order distorted-wave Born approximation (DWBA) has been successful for incident electrons with energies of about 200 eV or greater (Madison, Calhoun, and Shelton [9]). For energies in the 50–200 eV range, the DWBA breaks down primarily due to the neglect of the final-state electron-electron interaction [normally called post collision interaction (PCI)]. If PCI is properly included in the final-state wave function, much improved agreement with experiment is found (Brauner, Briggs, and Klar [10], Berakdar and Briggs [11], and Jones and Madison [8]).

There has been fewer studies on electron-impact ionization of heavier atoms. Heavier atoms are of interest since multiple electron interactions could potentially introduce new physical effects that would not be seen for lighter atoms. For example, screening of the nucleus provided by the passive electrons or the possible exchange between an active electron and a passive electron might have an important impact on the ionization results. Additionally, for atoms with multiple shells, it is of interest to examine ionization of both the inner and outer shells to see if there are important differences. In this paper, we will examine ionization of the inner s shells for argon and krypton.

For ionization of heavier inert gases, similar to ionization of hydrogen and helium, the DWBA normally yields relatively good agreement with the experimental data particularly for energies higher than about 100 eV (Ehrhardt *et al.* [12], Zhang *et al.* [13,14], Bell, Gibson, and Lohmann [15], Cavanagh and Lohmann [16], Brion *et al.* [17], Cavanagh *et al.* [18], and Taouil *et al.* [19]). However, Haynes and Lohmann [20–22] and Haynes *et al.* [23] have recently reported FDCS results for ionization of the $3s$ and $3p$ shells of argon and ionization of the $4s$ shell of krypton for lower energy incident electrons. In those works, very poor agreement was found with the DWBA calculations of Madison and Lang [24], McCarthy [25], and Biava *et al.* [26]. For ionization of the $3s$ shell of argon in the coplanar asymmetric case, the DWBA calculations predicted incorrect positions for the peaks, incorrect shapes and incorrect ratios of binary to recoil peaks. The DWBA recoil peaks were larger than the binary peaks and apparently significantly larger than the experimental measurements. The experimental binary and recoil peaks were shifted away from the DWBA in the direction that would be expected if there were a strong final-state repulsion between the ejected and ionized electrons. Since PCI is not included in the DWBA except through first-order perturbation theory, it was thought that this might account for some of the discrepancy between experiment and theory. However, one of the standard methods for including PCI, which has been relatively successful, is to approximate PCI using the Gamov factor (Whelan *et al.* [27]) and it was found that the Gamov factor produced much smaller shifts in the peaks than the observed differences between experiment and theory.

An even more severe test of theory is normally presented by the symmetric collisions in which both final-state electrons have the same energy and are observed at the same scattering angles on opposite sides of the beam direction in the scattering plane. Measurements of this type have been made on the $2s$ and $2p$ shells of neon (Rioual *et al.* [28,29]), the $3s$ shell of argon (Haynes and Lohmann [21]), the $3p$ shell of argon (Bell, Gibson and Lohmann [15] and Rouvellou *et al.* [30]) and the $4s$ shell of krypton (Haynes *et al.* [23]). DWBA calculations including PCI using the Gamov factor were performed for neon and argon (Rioual *et al.* [28], Rouvellou *et al.* [29], and Haynes and Lohmann [21]) and it was found that this effect led to a small improvement in the overall agreement with experimental data, but significant discrepancies between theory and experiment were found particularly for incident energies below 100 eV.

Brauner, Briggs, and Klar [10] demonstrated that the proper way to include PCI in a calculation is to include the Coulomb interaction directly into the final-state wave function. Including the Coulomb interaction in the final-state wave function means that the PCI Coulomb repulsion is contained to infinite order in perturbation theory in the final

state. They demonstrated, for electron-hydrogen scattering, that this Coulomb distortion factor greatly improved agreement between experiment and theory for incident energy electrons less than about 250 eV. For hydrogen scattering, the final-state wave function was chosen to be a product of a Coulomb wave for the projectile, a Coulomb wave for the ejected electron, and the Coulomb distortion factor for the final-state PCI (this wave function is called the $3C$ wave function). For heavier atoms, one would not expect a $3C$ wave function to be accurate since a Coulomb wave of some effective charge will not accurately represent the final-state wave function for a continuum electron in the field of an ion. A much better generalization of the $3C$ wave function for heavier targets would consist of distorted waves for both final-state electrons in the field of the ion plus the Coulomb distortion factor for PCI (we call this wave function 3DW). We investigate the importance of PCI for ionization of heavy targets using a wave function of this type in this work.

A second effect that could cause the DWBA calculations to fail for low-energy incident electrons is electron exchange. Electron exchange enters a calculation in two different ways. The first is through the exchange amplitude in which the role of the projectile and ejected electron is reversed. Typically, theories include the calculation of both the direct and exchange amplitudes and this is not the concern for this paper. The second effect of exchange occurs in the calculation of the continuum electron wave function. In the standard distorted-wave treatment, the continuum wave function is found by solving the Schrödinger equation for some effective static potential representing the atom or ion. This static potential does not take into account the fact that the projectile electron can potentially exchange with any of the atomic electrons. This is the type of exchange that will be examined in this paper and we call this effect exchange distortion.

The importance of this exchange distortion has been known for several years now. It first became apparent through the investigation of $(e,2e)$ processes for spin-polarized electrons. Investigations of spin effects have been performed for inert gases (Duemmler, Hanne and Kessler [31], Guo *et al.* [32], Dorn *et al.* [33], Granitza *et al.* [34], and Mette *et al.* [35]) and alkali atoms (Baum *et al.* [36]). When the experiment and the theory were compared for the inert gases, it was found that the standard first-order DWBA was in good accord with the spin-asymmetry measurements in some cases, but not others. It was subsequently determined that the discrepancy between experiment and theory lay not in relativistic effects, as one might assume, but rather in an inadequate treatment of exchange distortion (Madison *et al.* [37–39], and Mazevet, McCarthy, and Weigold [40–41]). Whereas a proper treatment of exchange distortion would consist of a Hartree-Fock treatment for the projectile electron wave function, Biava *et al.* [26,42] showed that a local potential approximation could be accurately used for ionization of *s* shells, but not *p* shells. We study ionization of *s* shells here, so the local potential approximation of Biava *et al.* [26] is used to study the importance of exchange distortion in this work.

II. THEORY

The exact transition amplitude for ionization is given by

$$T_{fi}=\langle \Psi_f|H-H_0|\Phi_i\rangle, \tag{1}$$

where H is the full Hamiltonian for the system, H_0 is an approximate initial-state Hamiltonian and the wave functions in the T matrix are eigenfunctions of the two Hamiltonians

$$H|\Psi_f\rangle=E|\Psi_f\rangle, \tag{2}$$

$$H_0|\Phi_i\rangle=E|\Phi_i\rangle. \tag{3}$$

In terms of the physics contained in the T matrix, any interaction, which is included in the calculation of the initial-and final-state wave functions, is contained to all orders of perturbation theory for that channel, while any interactions contained in the operator $(H-H_0)$ are contained to first order in perturbation theory. To evaluate the T matrix, one must choose H_0 and approximate Ψ_f.

One of the most successful approximations for calculating atomic ionization by electron impact has been the first-order distorted-wave Born approximation [9,24–26]. In the standard DWBA the initial-state Hamiltonian is chosen to be

$$H_0=H_{\rm atom}+T_p+U_i, \tag{4}$$

where $H_{\rm atom}$ is the Hamiltonian for the atom with eigenfunction $\psi_{\rm atom}$, T_p is the kinetic energy operator for the projectile, and U_i is an initial-state distorting potential. The distorting potential consists of the nuclear term plus a spherically symmetric approximation for the interaction between the projectile electron and the atomic electrons obtained from the Hartree-Fock charge density of the atom. The initial-state distorted wave χ_i is an eigenfunction obtained from the initial-state distorting potential

$$(T_p+U_i)\chi_i=\varepsilon_i\chi_i, \tag{5}$$

where ε_i is the energy of the incoming projectile. In the DWBA, the exact final-state wave function is approximated as a product of wave functions for each of the final three particles:

$$\Psi_f\approx\chi_{\rm proj}\chi_{\rm eject}\psi_{\rm ion}. \tag{6}$$

Here $\psi_{\rm ion}$ is the final-state wave function for the ion and the final-state distorted waves $\chi_{\rm proj}(\chi_{\rm eject})$ are obtained from a final-state distorting potential $U_{\rm ion}$:

$$(T_p+U_{\rm ion})\chi_a=\varepsilon_a\chi_a, \tag{7}$$

where "a" is a generic label for either the projectile or ejected electron. The final-state distorting potential $U_{\rm ion}$ consists of the nuclear term plus a spherically symmetric approximation for the interaction between the continuum electron and the atomic electrons obtained from the Hartree-Fock charge density of the ion. As a result, the DWBA T matrix is given by

$$T_{fi}^{DW}=\langle \chi_{\rm proj}\chi_{\rm eject}\psi_{\rm ion}|V_i-U_i|\psi_{\rm atom}\chi_i\rangle. \tag{8}$$

Here V_i is the initial-state interaction between the projectile and the atom. We will label results obtained from Eq. (8) as DW. The physical effects contained in the DW T matrix are the following. For the final state, the Coulomb interaction between the projectile and a screened nuclear charge is contained to all orders of perturbation theory and the Coulomb interaction between the ejected electron and a screened nuclear charge is contained to all orders of perturbation theory. For the initial state, the Coulomb interaction between the projectile and a screened nuclear charge for a neutral atom is contained to all orders of perturbation theory. The interactions contained in $(V_i - U_i)$ are the nonspherical part of the projectile-atomic-electron(s) interaction (the nuclear terms cancel and the spherically symmetric part of the electron-electron interaction cancel), so the nonspherical part of the initial-state projectile-electron interaction is contained to first order only.

The DWBA has been highly successful for calculating the FDCS for ionization by higher-energy electrons. However, as the energy of the electron is decreased, the DWBA starts to fail and one source of this failure is an inadequate treatment of the projectile-electron interaction. Brauner, Briggs, and Klar [10] demonstrated that good agreement with experiment for electron-hydrogen scattering could be achieved for lower incident electron energies by including the final-state projectile-electron interaction in the approximation for the final-state wave function. In the Brauner, Briggs, and Klar [10] approach, the exact final state is approximated as

$$\Psi_f \approx CW_{\text{proj}} C W_{\text{eject}} C_{\text{proj-eject}}, \tag{9}$$

where CW is a Coulomb wave for a nuclear charge of unity and C is the Coulomb distortion factor, which contains the effects of the final-state Coulomb interaction between the projectile and the ejected electron (PCI). The wave function (9) is called the $3C$ wave function. For heavier atoms, a $3C$ approach would not be appropriate since heavy ions cannot be reasonably represented as a point charge even if effective charges are used. For this case, a generalization of the $3C$ to the distorted-wave approach is required. The DWBA equivalent of the $3C$ wave function for the final-state wave function would be

$$\Psi_f \approx \chi_{\text{proj}} \chi_{\text{eject}} C_{\text{proj-eject}} \Psi_{\text{ion}}. \tag{10}$$

Asymptotically this wave function would be a phase-shifted $3C$ wave function. We will call the wave function (10) 3DW. One of the attractive features of this wave function is that it is an exact asymptotic solution of the three-body problem. The distorted-wave T matrix with the final-state wave function (10) is given by

$$T_{fi}^{3DW} = \langle \chi_{\text{proj}} \chi_{\text{eject}} C_{\text{proj-eject}} \psi_{\text{ion}} | V - U_i | \psi_{\text{atom}} \chi_i \rangle. \tag{11}$$

The physics contained in 3DW is the following. The final-state Coulomb interaction between the projectile and a screened nuclear charge, the Coulomb interaction between the ejected electron and a screened nuclear charge, and the Coulomb interaction between the projectile and the ejected electron are contained to all orders of perturbation theory. For the initial state, the Coulomb interaction between the projectile and a screened nuclear charge for a neutral atom is contained to all orders of perturbation theory. Similar to the DWBA, the only interaction contained only to first order in the 3DW is the initial-state nonspherical projectile-atomic-electron interaction.

Here we treat ionization of heavier atoms as a three-body problem. In the following section, we will examine ionization of the $3s$ shell of argon and the $4s$ shell of krypton. For these cases, the three particles are two electrons and an ion with a s shell vacancy. Consequently, we approximate the initial-state interaction as

$$V_i = -\frac{1}{r_{ab}} + U_{\text{ion}}. \tag{12}$$

Here $-1/r_{ab}$ represents the interaction between the projectile electron and the active atomic electron, and U_{ion} is the interaction between the projectile electron and the rest of the atomic electrons and the nucleus. The initial-state distorting potential is given by

$$U_i = U_{ns} + U_{\text{ion}}, \tag{13}$$

where U_{ns} is the spherically symmetric interaction potential for the active ns electron. As a result,

$$V_i - U_i = -\frac{1}{r_{ab}} - U_{ns}. \tag{14}$$

We evaluate the direct term in the T matrix only. Neglecting the exchange T matrix is justified by the fact that, for the asymmetric cases we will examine in the following section, there is a large energy difference between the two final-state electrons such that DWBA results both with and without the exchange T matrix are almost the same. For the symmetric cases, the direct and exchange amplitudes are identical; so one gets the same answer with direct only as one gets with direct and exchange.

Exchange enters theoretical calculations in two different ways. One is through the exchange T matrix mentioned above. The second place exchange enters lies in the calculation of the continuum wave functions. Equations (5) and (7) for the distorted waves treat the electron charge cloud as a static potential. Such a static potential neglects the fact that a continuum electron is indistinguishable from the atomic electrons. A proper continuum wave function should take this into account. One of the standard methods for treating all the electrons on an equal footing is the Hartree-Fock approximation (HF). In the HF method, Eq. (5) for the initial projectile wave function is replaced by

$$(T_p + U_i - \varepsilon_i)\chi_i^+(\mathbf{r}) = \int V_{ex}(\mathbf{r}, \mathbf{r}')\chi_i^+(\mathbf{r}')d\mathbf{r}', \tag{15}$$

where V_{ex} is the nonlocal exchange potential that takes into account the effect of all the other electrons in the system. Due to the difficulties involved in obtaining solutions to the integrodifferential equation (15), it is desirable to make simplifying approximations. The standard approximation is to

assume that the nonlocal exchange potential V_{ex} can be replaced by a local approximation (Hara [43], Furness and McCarthy [44], Riley and Truhlar [45,46], Vanderpoorten [47], and Bransden *et al.* [48]):

$$(T_0+U_i-\varepsilon_i)\chi_i^+(\mathbf{r})=U_{ex}(r)\chi_i^+(\mathbf{r}). \quad (16)$$

A commonly used expression for the local potential is the semiclassical exchange approximation of Riley and Truhlar [45,46], which is given by

$$U_{ex}=-\tfrac{1}{2}[(\varepsilon_i-U_i)-\sqrt{(\varepsilon_i-U_i)^2-(-)^s 2\rho(r)}], \quad (17)$$

where S is either zero (singlet) or one (triplet) and ρ is the radial charge density. For the final channel, Eqs. (16) and (17) are replaced with equivalent expressions for the final-state ion. Biava *et al.* [26,42] showed that, with a proper choice for the radial charge density ρ, the local potential approximation is an accurate approximation for the full HF solution for Eq. (15) for ionization of s states, but not p states. Since this paper is concerned with ionization of s states, we use the local potential approximation of Biava *et al.* [26] to examine the effects of exchange. We label results obtained including electron exchange in the calculation of the distorted waves with EX and we call this effect exchange distortion, since adding the exchange potential to Eq. (16) has the effect of providing an additional part to the potential used in calculating the distorted waves.

III. RESULTS

A. Effect of PCI

Very recently, Haynes and Lohmann [20,21] have measured FDCS for electron-impact ionization of the inner $3s$ shell of argon in both the coplanar asymmetric and coplanar symmetric geometry. In Fig. 1, the coplanar asymmetric results are compared with the first-order DWBA including exchange distortion in the calculation of the distorted waves (DW-EX) and the present results including both PCI and exchange distortion (3DW-EX). For argon, the DW-EX results are the same as the DWFM (distorted wave Furness-McCarthy) results of Biava *et al.* [26], although normalized differently. Note that the only difference between these two calculations is the inclusion of the projectile-ejected-electron Coulomb interaction in the final-state wave function. (Of course, numerically this is a huge difference—DW-EX results take seconds to generate, while 3DW-EX results take days.) For Fig. 1, the energy of the incident electron is 113.5 eV and the faster final-state electron is observed at 345° (or −15°) in the coordinate system we are using. The energy of the slower final-state electron is indicated in the figure and the horizontal axis is the observation angle for the slower electron measured clockwise from the beam direction when viewed from above the scattering plane. The experimental data are not absolute, so we have normalized the experiment and DW-EX to the 3DW-EX at the first peak located near 70° (normally referred to as the binary peak). The second peak at large scattering angles is called the recoil peak since it is associated with a double scattering process.

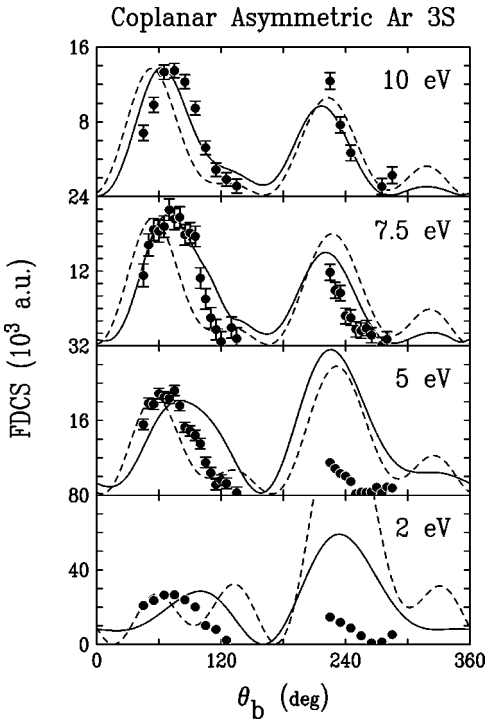

FIG. 1. Fully differential cross section for electron impact ionization of the $3s$ shell of argon in coplanar asymmetric geometry. The atomic units are $a_0^2/(sr^2\ H)$. The incident electron has an energy of 113.5 eV and the faster final-state electron is detected at an angle of 345° (−15°). The energy of the ejected electron is shown on each part of the figure and the horizontal axis is the angle of observation for the ejected electron measured clockwise relative to the beam direction as viewed from above. The solid curve is the 3DW-EX calculation and the dashed curve is DW-EX.

The repulsive effect of PCI would logically increase the angular separation between the two final-state electrons. As a result, one would expect the binary peak to be shifted to larger scattering angles and the recoil peak to smaller angles. One would also guess that the binary peak would be shifted by a larger amount than the recoil peak since the angle between the electrons is around 85° for the binary peak and around 120° for the recoil peak. These qualitative shifts are observed in Fig. 1. For the two higher energies of the ejected electron, 3DW-EX is in noticeably better agreement with experiment. For the lower energies, the shift in the binary peak is too large as compared to the data and the data appears to have a much smaller recoil peak than predicted by the theory. On the other hand, the size and location of the experimental recoil peak is not clear due to the problems associated with making measurements near the backward direction.

The coplanar symmetric measurements of Haynes and Lohmann [20,21] for ionization of the $3s$ shell of argon are compared with the present theoretical results in Fig. 2. For this case, both final-state electrons have the same energy noted in the figure and both electrons are measured at the same scattering angle on opposite sides of the beam direction in the scattering plane. In this geometry, the cross section for zero-degree scattering should be zero since two equal energy electrons would not both come out in the forward direction.

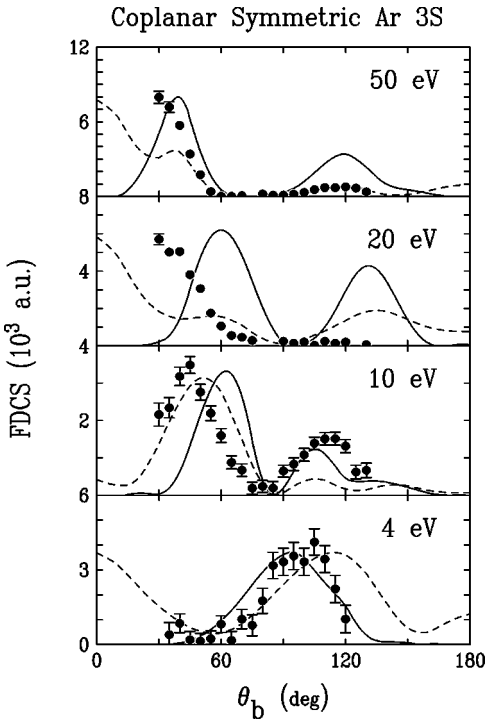

FIG. 2. Fully differential cross section for electron impact ionization of the 3*s* shell of argon in coplanar symmetric geometry. Both the ejected and projectile electrons have the same energy, which is indicated on each part of the figure and both electrons are observed at the same angle (horizontal axis) on opposite sides of the beam direction in the scattering plane. The solid curve is the 3DW-EX calculation and the dashed curve is DW-EX.

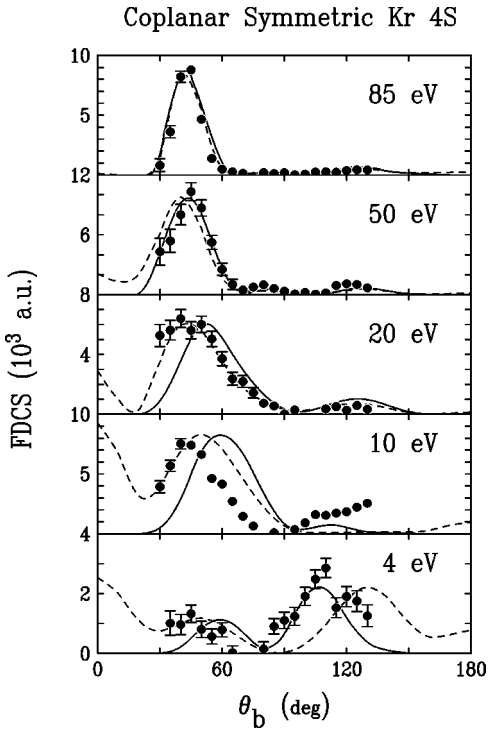

FIG. 3. Fully differential cross section for electron impact ionization of the 4*s* shell of krypton in coplanar symmetric geometry. Both the ejected and projectile electrons have the same energy, which is indicated on each part of the figure and both electrons are observed at the same angle (horizontal axis) on opposite sides of the beam direction in the scattering plane. The solid curve is the 3DW-EX calculation and the dashed curve is DW-EX.

The 3DW-EX cross sections for zero degrees are very small as would be expected. The DW-EX results, on the other hand, are frequently very large at zero degrees. In the DW calculation, the electron-electron repulsion is contained only to first order in the initial-state interaction potential and it is clear from the figure that the higher-order PCI terms in the final channel are very important. Using the same logic as above, one would expect PCI to shift the small angle peak to larger angles and the large angle peak to smaller angles. While this behavior is generally observed, the binary peak is shifted to a significantly larger angle than was found in the data. PCI also tends to significantly increase the recoil peak. For the higher energies, the 3DW-EX recoil peaks are significantly larger than the experimentally observed ones. However, as the energy is lowered, the experimental recoil peaks get relatively larger and it is interesting (and surprising) that the best agreement with experiment is found at the lowest energy.

Haynes *et al.* [23] have recently reported coplanar symmetric results for ionization of the inner 4*s* shell of krypton and Fig. 3 contains a comparison of the present results with those data. For this case, the highest measured energy was 85 eV and at this energy there is very little difference between DW-EX and 3DW-EX, and both calculations are in good agreement with experiment. The krypton results are qualitatively similar to the argon results except that, overall, agreement with experiment is better for krypton. For example, at 50 eV, the 3DW-EX small angle peak shift yields a very good agreement with experiment, while the corresponding argon case is not nearly as satisfactory. Also, the krypton recoil peak is not enhanced for high energies; so there is much better agreement in this angular range. Similar to argon, the binary peak for the intermediate energies appear to be shifted too much as compared to data and there is much better than expected agreement between experiment and theory for the lowest energy.

B. Effect of exchange distortion and single-particle term

It is of interest to examine the effect of electron-exchange distortion in the calculation of the projectile wave function, since it is expected that this may be important for lower energy collisions. Another interesting effect lies in the U_{ns} term in the initial-state interaction potential of Eq. (14). The spherically symmetric potential U_{ns} depends only on the radial coordinate of the projectile electron. Since U_{ns} depends only on the coordinates of the projectile, it is often referred to as the single-particle term. For the first order DW calculation of Eq. (8), this single-particle term will vanish if the ejected-electron wave function is orthogonal to the initial bound-state wave function, since the single-particle term contains the overlap between these two wave functions with no interaction in the middle. In most DW calculations, it is either assumed that this orthogonality exists or the ejected-

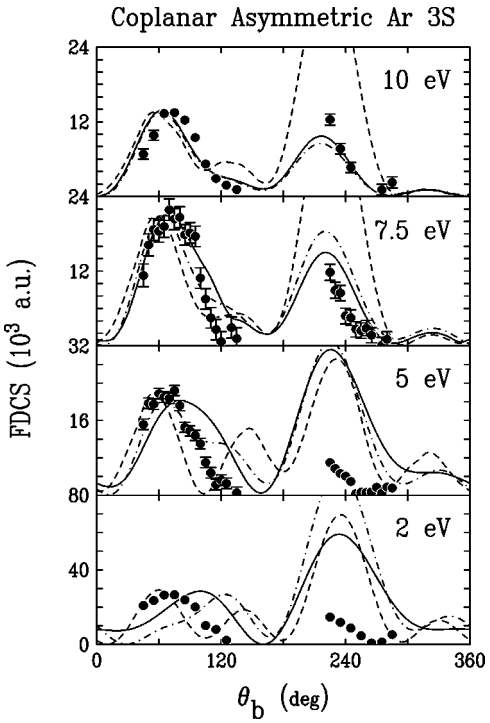

FIG. 4. Fully differential cross section for electron impact ionization of the 3*s* shell of argon in coplanar asymmetric geometry. The incident electron has an energy of 113.5 eV and the faster final-state electron is detected at an angle of 345° (−15°). The energy of the ejected electron is shown on each part of the figure and the horizontal axis is the angle of observation for the ejected electron measured clockwise relative to the beam direction as viewed from above. The solid curve is 3DW-EX, the dashed is 3DW-EX without the single-particle term, and the dashed-dotted is 3DW.

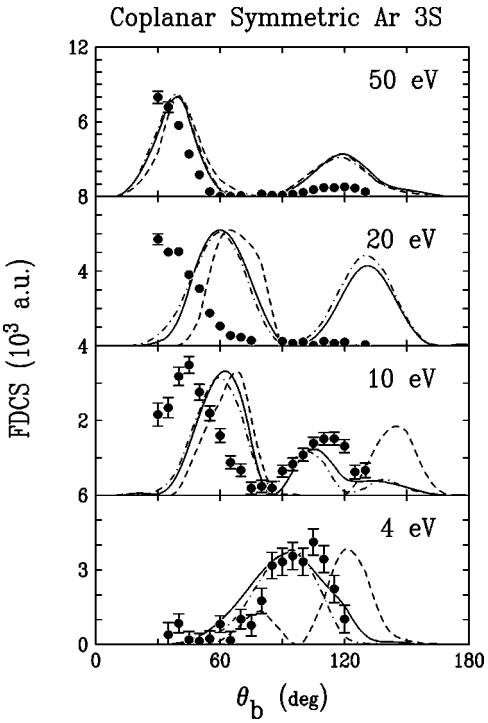

FIG. 5. Fully differential cross section for electron impact ionization of the 3*s* shell of argon in coplanar symmetric geometry. Both the ejected and projectile electrons have the same energy, which is indicated on each part of the figure and both electrons are observed at the same angle (horizontal axis) on opposite sides of the beam direction in the scattering plane. The solid curve is 3DW-EX, the dashed is 3DW-EX without the single-particle term, and the dashed-dotted is 3DW.

electron wave function is forced to be orthogonal to the bound-state wave function so that the term can be ignored. However, in the 3DW matrix element (11), the U_{ns} term will make a contribution even if the ejected-electron and bound-state wave functions are orthogonal due to the Coulomb repulsion factor, which depends on both the projectile and ejected-electron coordinates. Consequently, it is of interest to investigate the importance of this term.

In Figs. 4–6, the effects of exchange distortion are examined by comparing 3DW-EX with 3DW (i.e., the present PCI results both with and without exchange distortion included in the calculation of the distorted waves). Comparing the solid vs dashed-dot curves on Figs. 4–6, it is seen that exchange distortion has little effect for higher energies and becomes more important with decreasing energy as expected. For the higher energies, it could be argued that the small effect of exchange distortion even tended to worsen the agreement between theory and experimental data. For the lower energies, exchange distortion arguably improved agreement with experiment. The most dramatic improvement was found for krypton symmetric scattering at 4 eV where the calculation without exchange distortion had little resemblance to the data. Overall, exchange distortion effects are small and, except for the lowest energies, generally do not tend to improve agreement between experiment and theory.

Also included in the figures are 3DW-EX calculations including and ignoring the U_{ns} term in the interaction potential of Eq. (14) (solid curves vs dashed curves). For the argon coplanar asymmetric case of Fig. 4, the single-particle term had a huge effect on the ratio of binary to recoil peaks particularly for the higher energies. Although one cannot tell the experimental value for this ratio since the recoil peak is in angular range, which is not experimentally accessible, one would guess that the single-particle term has produced a much more reasonable value for the height of the recoil peak. For the coplanar symmetric cases of both argon and krypton, the single-particle term tended to improve agreement between experiment and theory with the largest effects being observed for the lower energies. For both argon and krypton 4 eV cases, calculations including the single-particle term were in reasonably good agreement with experiment, while those ignoring this term were not.

IV. CONCLUSIONS

We have performed the first distorted-wave calculation for ionization of heavy atoms, which properly included the final-state projectile-electron ejected-electron interaction to all orders of perturbation theory. This was accomplished by representing the final-state three-particle wave function as a product of wave functions for each of the two-particle

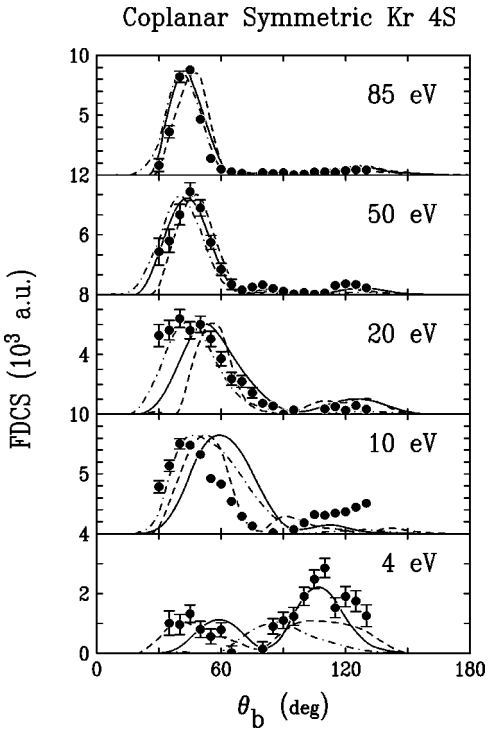

FIG. 6. Fully differential cross section for electron impact ionization of the 4*s* shell of krypton in coplanar symmetric geometry. Both the ejected and projectile electrons have the same energy, which is indicated on each part of the figure and both electrons are observed at the same angle (horizontal axis) on opposite sides of the beam direction in the scattering plane. The solid curve is 3DW-EX, the dashed is 3DW-EX without the single-particle term, and the dashed-dotted is 3DW.

pairs—a distorted wave for the projectile-ion pair, a distorted wave for the ejected-electron–ion pair, and a Coulomb interaction for the projectile-electron–ejected-electron pair. This three-particle wave function is an exact asymptotic solution to the three-body problem.

We examined the effect of the final-state Coulomb interaction between the ejected electron and projectile electron (PCI) for low-energy ionization of argon and krypton. It was found that PCI is very important. Without PCI, the theory predicts unphysical cross sections for small angle symmetric scattering. Overall, the results with PCI were in much better agreement with experiment both in terms of shape and peak location. However, the agreement between experiment and theory is still not as good as one would hope, particularly, for the higher energy argon coplanar symmetric case. Consequently, the present approach is still missing some important physical effects. Since the present calculation contains the final-state interaction between all two-particle pairs to all orders of perturbation theory and the initial-state interactions to first order in perturbation theory, one would guess that higher-order terms in the initial state must also be important. The CDW-EIS (Coulomb distorted wave, Eikonal initial state) approach has higher-order initial-state effects and we are presently working on generalizing the CDW-EIS approach of Jones and Madison [49,50] for hydrogen ionization to heavier atoms.

We also investigated the effect of exchange distortion and the single-particle term in the interaction potential. In general, the effects of exchange distortion were small and arguably did not tend to improve agreement between experiment and theory except for the lowest energy. The only case where exchange distortion produced a significant improvement between experiment and theory was 4 eV krypton scattering. The single-particle term, on the other hand, produced a much larger positive effect. For asymmetric scattering, it produced much reduced recoil peaks for higher energies and better shape and peak positions for symmetric scattering.

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