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Probing Scattering Wave Functions Close to the Nucleus

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Recently, three-dimensional imaging of the ejected electrons following 100 MeV/amu C^{6+} single ionization of helium led to the observation of a new structure not predicted by theory [M. Schulz *et al.*, Nature (London) **422**, 48 (2003)]. Instead of the usual "recoil lobe" centered on the momentum-transfer axis, a ring-shaped structure centered on the beam axis was observed. New measurements at 2 MeV/amu exhibit a similar structure, which is now predicted by theory. We argue that the same theory failed at 100 MeV/amu because the faster projectiles probe distances much closer to the nucleus, where our multiple-scattering model is expected to break down.

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Three-dimensional imaging of the ejected electrons following 100 MeV/amu C^{6+} single ionization of helium with fully resolved kinematics revealed an extraordinary ring-shaped structure that appears to be centered on the beam axis [1]. At this high energy, which corresponds to an impact speed of about 60 a.u., one would normally expect even the first-Born approximation (FBA) to be reasonably accurate, since the magnitude of the momentum $\mathbf{q}$ transferred to the target was fairly small ($|\mathbf{q}| = 0.75$ a.u.). However, the FBA could never predict a ring structure centered on the beam axis since FBA cross sections are cylindrically symmetric about $\mathbf{q}$. Moreover, even a multiple-scattering model using a three-body final-state wave function consisting of a product of exact wave functions for each two-body subsystem, which we label three-body distorted wave (3DW), failed to reproduce any sign of the observed structure.

The complete three-dimensional fully differential cross section (FDCS) for 100 MeV/amu C^{6+} ionization of helium reported in [1] is shown in Fig. 1. The bottom part shows the experimental data and the top part the theoretical results using a 3DW-FBA approach (3DW final state, FBA initial state). The scattering plane is determined by the incident momentum $\mathbf{p}_0$ and $\mathbf{q}$. The large lobe on the right in Fig. 1 is called the binary peak since the electrons have a momentum close to $\mathbf{q}$ which would correspond to a classical collision between the projectile and a free electron at rest. The smaller lobe on the left is called the recoil peak because the momentum transfer is predominantly picked up by the recoil ion. This peak has been interpreted as resulting from a double scattering process in which the electron is initially moving in the $+\mathbf{q}$ direction and then backscatters from the target ion.

While the calculation is in excellent agreement with the data in the scattering plane [2,3], surprising discrepancies were found outside the scattering plane. The theoretical results are nearly cylindrically symmetric about $\mathbf{q}$ as the FBA would predict. The experiment, on the other hand, shows a strong breaking of this symmetry in that the recoil lobe in the calculation emerges as a "recoil ring" centered on $\mathbf{p}_0$ in the experimental data.

Such a disagreement has not been observed for electron-impact ionization results. It is therefore quite possible that the heavy-projectile cross sections contain some new physical effects that were not seen in decades of electron work. Schulz *et al.* [1] speculated that the ring-shaped structure centered on $\mathbf{p}_0$ in the experimental data might result from a double projectile-scattering process. The first collision is with the electron and would determine the fate of the electron. The second collision is with the ion and would determine the definition of the scattering plane which could easily rotate about $\mathbf{p}_0$.

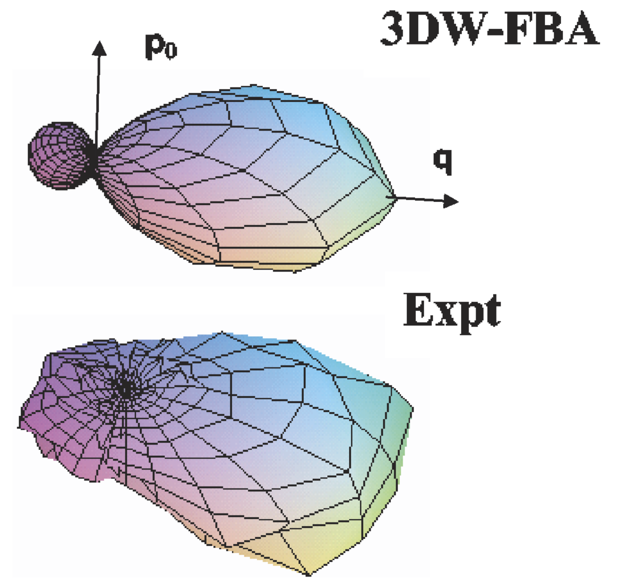

FIG. 1 (color online). Comparison of theory and experiment (Expt) for single ionization of helium by 100 MeV/amu C^{6+} ions. The fully differential cross section is shown. The momentum of the incident projectile is $\mathbf{p}_0$ and the momentum transfer is $\mathbf{q}$. The energy of the ejected electron is 6.5 eV and $|\mathbf{q}| = 0.75$ a.u. The 3DW-FBA model is discussed in the text.

Consequently, a recoil peak could become a recoil ring similar to the observed experimental cross section. If this is the correct explanation for the observed structure, then one would think that the 3DW-FBA would reproduce it, since this model includes the final-state projectile-ion interaction to all orders of perturbation theory and has been quite successful for much slower projectiles.

Here we report new measurements and calculations at 2 MeV/amu. We again observe a ring-shaped structure in the experimental data instead of the usual recoil lobe. Much to our surprise, however, our 3DW-FBA model now predicts a ring-shaped structure similar to the data. This unexpected discovery presents a dilemma. Why does theory predict the shape of the experimental data better at low energy than at high energy? This behavior is counterintuitive with all of our experience with scattering theory. Here, we offer a possible explanation. We provide plausibility arguments that the 100 MeV/amu projectiles are penetrating very close to the nucleus, leading to short distances ($\sim\frac{1}{2}a_0$) between all three collision fragments in order to eject electrons out of the scattering plane. At 2 MeV/amu, on the other hand, it can be argued that the same process involves quite larger impact parameters ($\sim 2a_0$), where the 3DW-FBA would be expected to be more reliable.

The multiple-scattering model that has been used so far is the 3DW-FBA [1,2], which takes into account all two-particle interactions in the final state to infinite order in perturbation theory. An even better approach would be the three-body distorted wave–eikonal initial state (3DW-EIS), which takes into account all two-particle interactions in the initial state as well. A version of the 3DW-EIS called the CDW-EIS (continuum distorted wave–eikonal initial state), which neglects the projectile-ion interaction, has been very successfully used for many years in heavy-ion–impact collisions for studies of doubly differential cross sections in which the deflection of the projectile is not measured [4]. For cases like this, it is appropriate to neglect the projectile-ion interaction and assume an undisturbed straight-line trajectory for the projectile ([5–7] and references therein). This approach is not appropriate for the present case where the deflection of the projectile is measured. For this case a full quantum-mechanical approach is needed. Jones and Madison [8] reported a fully quantal CDW-EIS approach for electron-impact ionization and here we adapt that method to heavy-ion collisions.

The exact T matrix is given by [8]

$$T_{fi} = \langle \chi_f^- | V_i | \beta_i \rangle + \langle \chi_f^- | W_f^\dagger | (\Psi_i^+ - \beta_i) \rangle. \tag{1}$$

Here χ_f^- is an approximation to the exact final-state wave function and W_f is the corresponding perturbation. Ψ_i^+ is the exact scattering wave function developed from the initial asymptotic state β_i, where

$$\beta_i = \psi_{\rm PW}(\mathbf{r}_a)\psi_{1s}(\mathbf{r}_b). \tag{2}$$

Here ψ_{1s} is a Hartree-Fock wave function for the ground state of helium and $\psi_{\rm PW}$ is a plane wave for the projectile. The corresponding initial-state interaction potential is given by

$$V_i = \frac{Z_P}{r_a} - \frac{Z_P}{r_{ab}}, \tag{3}$$

where, following [2], we are approximating the initial-state interaction with the ion as if it were a unit point charge. For the final state χ_f^- we use a product of wave functions for each two-particle subsystem,

$$\chi_f^- = \psi_{\rm CW}(\mathbf{r}_a)\psi_{\rm DW}(\mathbf{r}_b)C(\mathbf{r}_{ab}), \tag{4}$$

where $\psi_{\rm CW}$ is a Coulomb wave for the final state of the projectile in the field of a unit point charge, $\psi_{\rm DW}$ is a numerical distorted wave for the ejected electron calculated using the Hartree-Fock potential for a helium ion, and $C(\mathbf{r}_{ab})$ is the Coulomb distortion between the projectile and the ejected electron. For the case of hydrogen ionization, χ_f^- would be a product of three Coulomb waves, so it is frequently called the 3C wave function (we used this notation in [2]). However, we have learned that it is crucially important to use a distorted wave calculated in the static Hartree-Fock potential of the ion for the ejected electron (as opposed to a Coulomb wave for some effective charge), so 3DW is perhaps more appropriate. The final-state perturbation W_f involves ratios of confluent hypergeometric functions and is given in Jones and Madison [9].

The first term in the T matrix (1) is the 3DW-FBA approximation of Madison *et al.* [2] (which was called 3C-HF in that paper). The T matrix (1) is exact (i.e., it contains no approximations). Consequently, in the 3DW-FBA, one approximates the exact initial-state wave function Ψ_i^+ as the asymptotic form β_i such that the second term vanishes. The second term in Eq. (1) represents higher-order terms in a perturbation series with the leading term being 3DW-FBA. It is clear that these higher-order terms result from approximating the exact initial state as something better than β_i. Here we make the eikonal approximation

$$\Psi_i^+ \approx \tilde{\psi}_{\rm CW}(\mathbf{r}_a)\psi_{1s}(\mathbf{r}_b)\tilde{C}(\mathbf{r}_{ab}). \tag{5}$$

Crothers and McCann [10], following the work of Crothers [11], showed that the asymptotic form of the Coulomb distortion (denoted by a "tilde") should be used in order to have a properly normalized wave function. We label results obtained with the eikonal initial-state wave function as 3DW-EIS.

Finally, we should mention the difference between the present work and the CDW-EIS calculations that have been performed for heavy ions for a couple of decades. The CDW-EIS calculations are based upon rewriting the T matrix of Eq. (1) as

$$T_{fi} = \langle \chi_f^- | W_f^\dagger | \Psi_i^+ \rangle + \langle \chi_f^- | V_i - W_f^\dagger | \beta_i \rangle. \tag{6}$$

To make the calculation more tractable, an approximation is normally made in which the projectile trajectory is assumed to be a straight line and this assumption is valid for double differential cross sections but not FDCS. Next, it is always assumed that the second term in Eq. (6) can be neglected which would be valid if the operators were Hermitian in that matrix element. However, they will not be Hermitian for the chosen final-state wave function. In summary, (i) all of the CDW-EIS calculations in the 1990s for less differential cross sections used a classical straight-line trajectory for the projectile while we use a full quantum-mechanical treatment, (ii) we use Hartree-Fock wave functions for the bound and continuum states of the active electron, (iii) all previous CDW-EIS calculations evaluate only the first term of Eq. (6) whereas we evaluate both terms, and (iv) we make no approximations in the evaluation of the T matrix other than those discussed above.

In Fig. 2, experimental and theoretical results are compared for 2 MeV/amu C^{6+} ionization of helium. Here, the ejected-electron energy is 1 eV and $q = 1.5$ a.u. In the figure, the FBA results correspond to approximating the final state as $\chi_f^- = \psi_{\mathrm{PW}}(\mathbf{r}_a)\psi_{\mathrm{DW}}(\mathbf{r}_b)$ and neglecting the projectile-ion interaction in V_i. The PCI (postcollision interaction) results correspond to approximating the final state as $\chi_f^- = \psi_{\mathrm{PW}}(\mathbf{r}_a)\psi_{\mathrm{DW}}(\mathbf{r}_b) \times C(\mathbf{r}_{ab})$ plus ignoring the projectile-ion term in V_i. We found that PCI changed the magnitude of the FDCS considerably but did not change the shape. The difference between the PCI calculation and the 3DW-FBA lies in the initial- and the final-state interaction between the projectile and ion (i.e., the final-state plane wave for the projectile is changed to a Coulomb wave and the initial-state projectile-ion interaction is included in V_i).

It is seen that the projectile-ion interaction completely changes the shape of the distribution and brings it into significantly improved qualitative agreement with the experimental data. Unlike the theoretical high-energy results in Fig. 1 and the FBA results of Fig. 2, the "recoil peak" is no longer cylindrically symmetric about $\mathbf{q}$. Instead, it "flattened" in the plane perpendicular to $\mathbf{p}_0$; i.e., it is broader in this plane than it is in the scattering plane consistent with the speculation of Schulz *et al.* [1]. These results represent an indirect verification of the mechanism suggested in Ref. [1], where the shape of the recoil peak results from a double scattering process in which the projectile-ion collision would change the scattering plane with the net effect of changing the recoil peak into a recoil ring. Although the classical ideas for collisions cannot be checked in a fully quantal calculation, the fact that turning on the projectile-ion interaction produced a recoil ring is compelling evidence to the validity of these ideas. Adding the eikonal initial state (3DW-EIS) introduces the asymptotic initial-state projectile-ion and projectile-electron interactions which further improved agreement between experiment and theory.

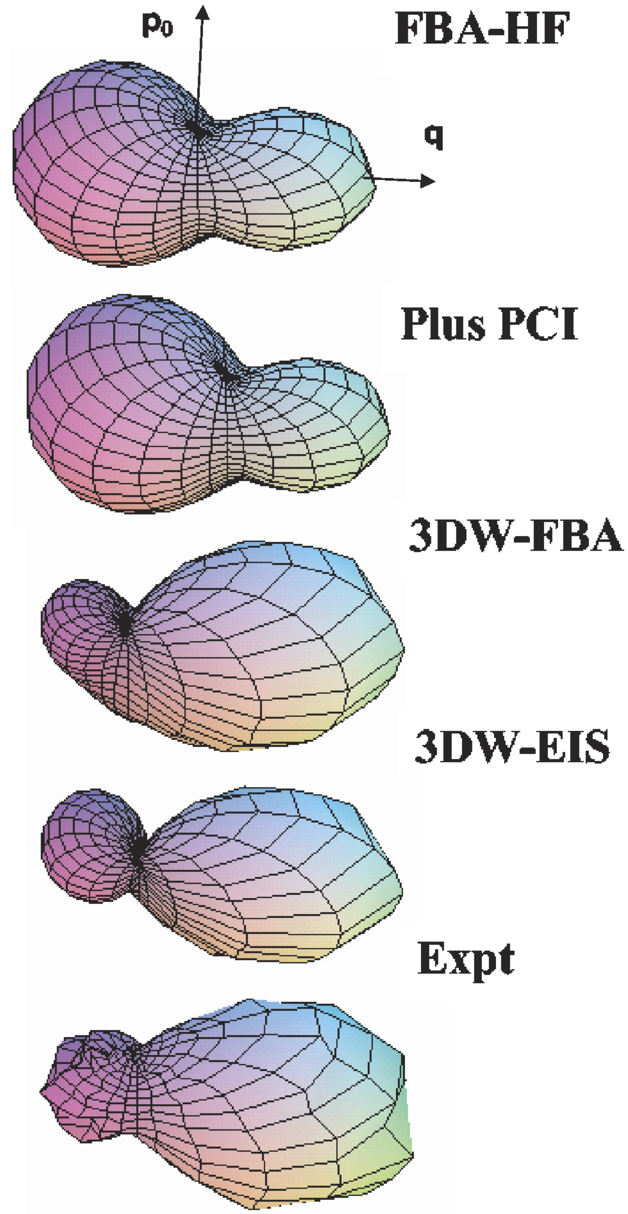

FIG. 2 (color online). Same as Fig. 1 for 2 MeV/amu collision energy, 1 eV electron energy, and $|\mathbf{q}| = 1.5$ a.u. The FBA, PCI, 3DW-FBA, and 3DW-EIS models are discussed in the text.

The qualitative reproduction of a recoil ring at the smaller projectile energy leads to a dilemma concerning the relatively poor agreement seen in Fig. 1. We also performed 3DW-EIS calculations for the kinematics of Fig. 1 and the results were almost the same as 3DW-FBA. If the projectile-ion interaction is very important and included in exactly the same way for both 100 and 2 MeV/amu projectiles, why does theory predict a ring-shaped structure at 2 MeV/amu but not at 100 MeV/amu? Normally, one would expect agreement to get better with increasing energy. In the following, we offer a possible explanation for this apparent conflict.

The 3DW final-state wave function is a product of three two-body wave functions. In the case of point charges, it solves the three-body problem when any *two* particles are arbitrarily close together, provided the third particle is infinitely far away from these two [12]. However, the 3DW is not a solution of the three-body problem when all three particles are close together and presumably the error would get greater the closer the particles come together. Consequently, we can imagine a radius r_0 centered on the ion for which the 3DW wave function is good to within some prescribed error for larger distances and increasingly inaccurate for decreasing distances.

In fact, we can loosely quantify these ideas if we attribute the projectile-ion scattering to classical elastic scattering. From momentum conservation, the momentum of the recoil ion is the momentum transfer $\mathbf{q}$ minus the momentum of the ejected electron. If the recoil-ion momentum comes from elastic scattering with the projectile, then classical Rutherford scattering can be used to associate an impact parameter b with a particular recoil-ion momentum. In the scattering plane, Madison *et al.* [2] found good agreement between experiment and theory at the binary peak in two out of three cases at 100 MeV/amu. Performing a simple calculation of the impact parameter for the projectile-ion part of the momentum transfer for the binary peak, one finds good agreement for impact parameters $b = 2a_0$ and $b = 1.3a_0$ but poor agreement for $b = 0.4a_0$. For the out-of-plane part of the recoil ring of Fig. 1, b would be about $0.4a_0$. For the out-of-plane part of the recoil ring of Fig. 2, on the other hand, b would be about $2a_0$. Consequently, in this admittedly simplified model, we see a pattern of good agreement when the impact parameter is greater than about $2a_0$ and poor agreement when the impact parameter is less than about $\frac{1}{2}a_0$. This suggests that the 3DW is reasonably accurate down to surprisingly small distances $\sim a_0$.

In summary, we have presented the first fully quantal 3DW-EIS calculations for atomic ionization by heavy ions including both terms of the exact T matrix and have compared these results with FDCS experimental measurements for 2 MeV/amu C^{6+} ionization of helium. This work demonstrates that the heavy-ion collisions can probe physical effects that have not been observed in electron-impact ionization studies. One of the interesting questions to be examined is whether effects like this recoil ring are also present for electron-impact ionization and have not been seen yet or whether these effects are also present for other types of projectiles. In any event, it appears that the 3DW-EIS approach can be used to either search for or interpret such physical effects as long as the projectile does not penetrate too close to the nucleus.

We conclude that three-dimensional imaging of the ejected electrons following atomic ionization by the impact of very fast heavy ions at fixed $\mathbf{q}$ probes the atomic reaction at both large and small distances simultaneously. Whereas the usual binary and recoil peaks found in the scattering plane for small q result primarily from relatively large impact parameters, the out-of-plane structure discovered by Schulz *et al.* [1] at the same small q is coming from small impact parameters, where the projectile penetrates the atomic "charge cloud" such that all three collision fragments come close together. The multiple-scattering model employed here fails in this case but is in better agreement with experiment for lower energies where the particles do not come so close together. It is now clear that it is very important to test scattering theories outside the scattering plane. For a given $\mathbf{q}$, collisions in the scattering plane tend to probe either just large (for small q) or just small (for large q) distance scales, whereas complete three-dimensional imaging of the reaction probes all distance scales at once. Furthermore, we demonstrated that one has to be cautious in assuming that all aspects of the FDCS are always better described by perturbative approaches with increasing energy.

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