Three-Body Coulomb Problem Probed by Mapping the Bethe Surface in Ionizing Ion-Atom Collisions

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The three-body Coulomb problem has been explored in kinematically complete experiments on single ionization of helium by 100 MeV/u C^{6+} and 3.6 MeV/u Au^{53+} impact. Low-energy electron emission ($E_e < 150$ eV) as a function of the projectile deflection ϑ_p (momentum transfer), i.e., the Bethe surface [15], has been mapped with $\Delta\vartheta_p \pm 25$ nanoradian resolution at extremely large perturbations (3.6 MeV/u Au^{53+}) where single ionization occurs at impact parameters of typically 10 times the He K-shell radius. The experimental data are not in agreement with state-of-the-art continuum distorted wave–eikonal initial state theory.

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The electromagnetic interaction, driving essentially all atomic and molecular processes, is the most precisely known fundamental interaction in physics and the basis of quantum electrodynamics. At the same time, however, the most simple dynamical situation, i.e., the time-evolution three pointlike particles mutually interacting nonrelativistically via the Coulomb force remained one of the most fundamental and lively debated problems in atomic physics (the three-particle Coulomb problem). While the Schrödinger equation for two particles is solvable in closed form, only approximate solutions were known for three or more particles until recently and many state-of-the-art theoretical approaches are often inadequate.

Ionization of atoms by charged particle impact is probably one of the most demanding realizations of the three-particle Coulomb problem because it requires a correct description of the three-particle continuum state even at asymptotically large distances according to the infinite range of the Coulomb potential. For projectiles with small charge Q at high velocities v_p (i.e., at small perturbation $Q/v_p < 1$ in atomic units), it is well established that single ionization is reasonably well described within the first Born approximation. Since the projectile is fast the final state is an effective two-particle system consisting of the target nucleus and the typically slowly emerging electron.

Theoretical difficulties arise when the perturbation approaches or even exceeds unity $Q/v_p > 1$, i.e., for highly charged ions at moderate velocities or for low-energy singly charged projectiles. Then, the strong final state interaction between the outgoing projectile, the ionized electron, and the target nucleus represents a true three-particle system, resulting in significant modifications of the collision dynamics and the requirement of much more sophisticated theoretical treatments.

For the latter case, namely, low-energy electron impact ionization of atomic hydrogen, only one absolutely normalized kinematically complete experimental data set has been reported in literature [1]. Until recently, when a mathematically consistent, extremely time-consuming solution of the three-body Coulomb problem for the $e^- +$ H system was presented [2–4], all theoretical approximate solutions failed to describe the experimental data in some detail.

In this Letter we present the second extreme realization of the three-body Coulomb problem, namely, for highly charged ion impact (Au^{53+}) at moderate velocities (12 a.u.) reaching a perturbation strength of $Q/v_p = 4.4$, never obtained before in kinematically complete experiments. With these projectiles, single ionization occurs at typical impact parameters of 10 a.u., i.e., at more than 10 times the charge radius of the target electron cloud. It is evident that in such a situation the projectile simultaneously interacts with both the target electron and the target nucleus. Ionizing collisions lead to projectile deflections in the nanoradian regime (a few meter deflection on a distance from the earth to the moon) most sensitively depending on the details of the tree-particle Coulomb interaction. State-of-the-art continuum distorted wave approximations, without taking into account the interaction between the two nuclei, which have been demonstrated to accurately describe doubly differential electron emission spectra in such situations [5,6], are shown to completely fail in describing the three-particle momentum exchange. This is surprising because it was generally accepted that the nuclear interaction is important only at small impact parameters or, if noticeable at all at larger impact parameters, adds only a small correction to the data. It is even more surprising that real three-particle theories including the internuclear interaction

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are still in striking disagreement with the experimental data.

In order to substantiate these results, a reference experiment was performed in the perturbative regime at $Q/v_p = 0.1$ for 100 MeV/u C^{6+} impact recording identical data, i.e., differential cross sections for low-energy electron emission as a function of the projectile scattering angle. In this regime, Schulz *et al.* [7] have previously reported doubly differential cross sections as a function of the projectile energy loss and scattering angle for proton impact at lower energies. Systematic deviations between experiment and theory were found only at large scattering angles corresponding to close collisions and, consequently, were attributed to the missing internuclear interaction in the calculation. Its inclusion resulted in considerably improved agreement [8]. A similar conclusion, namely, that the interaction with the target nucleus has to be included in close collisions at large scattering angles beyond the maximum projectile-free electron deflection angle $\vartheta_p > \vartheta_{p\text{-}e} = m_e/M_p$ (m_e, M_p: electron and projectile mass, respectively), was drawn from single differential ionization cross sections as a function of ϑ_p, measured for light projectiles (protons and deuterons) at intermediate and high energies (see, for example, [9,10]). Only recently, Weber *et al.* [11] found that the inclusion of the nuclear interaction is important to describe their measured transverse recoil-ion momentum distribution in ionizing proton collisions, especially at large transverse momenta. Moreover, a theoretical study demonstrated that the momentum distribution of the emitted electrons themselves is not sensitive at all on the internuclear interaction and can be switched off in the corresponding calculations [12].

In summary, from all the results in the perturbative regime, it was generally accepted that the nucleus-nucleus interaction is definitely not needed for the accurate prediction of emitted electron spectra and that it only significantly affects the three-body dynamics at scattering angles beyond the maximum projectile-free electron deflection angle.

The experiments were performed at the Universal Accelerator (UNILAC) of GSI (Gesellschaft für Schwerionenforschung) and at GANIL in Caen (France) using a multielectron recoil-ion momentum spectrometer. Details about the operating principle and the resolution of the spectrometer have been reported previously [13]. Briefly, a collimated (0.5 mm diam) and charge state selected beam of 3.6 MeV/u Au^{53+} and 100 MeV/u C^{6+} ions, respectively, is crossed with a supersonic beam (2.8 mm diameter) of He. Electrons and target ions produced in the collision region are extracted into opposite directions by a weak (1–3 V/cm) electric field acting over 22 cm along the ion-beam (longitudinal) direction. An additional solenoidal magnetic field of 20.5 G confines the electron transverse motion. In this way all electrons with transverse energies below 150 eV and all recoil ions are projected onto position sensitive multihit detectors. The recoil-ion charge state and the full momentum vector of both, recoil-ion and electron, are calculated from their measured absolute flight times and their positions on the detectors. The outgoing projectile is charge state analyzed after the collision chamber and detected by a fast scintillator in coincidence with the target fragments.

The transverse momentum transfer of the projectile is calculated event by event from the transverse momenta of the ejected electron and the recoil ion $\mathbf{q}_\perp = (\mathbf{p}_{e\perp} + \mathbf{p}_{r\perp})$ making use of momentum conservation. It is related to the projectile scattering angle by $\vartheta_p = q_\perp/(M_p v_p)$. In this way projectile scattering angles as small as 50 nrad became accessible for the first time. The total momentum transfer for fast and heavy projectiles is given by $\mathbf{q} = \mathbf{q}_\perp + q_{\min} \cdot \hat{v}_p$, where $\hat{v}_p$ is the unit vector along the initial projectile velocity with $\hat{v}_p \cdot \mathbf{q}_\perp = 0$. The quantity $q_{\min} = (I + E_e)/v_p$ is the minimum momentum transfer (corresponding to zero degree scattering) required to overcome the initial binding energy I of the electron and to promote it into a continuum state with energy E_e. For the present projectiles and for soft electron emission ($E_e <$ 150 eV) the longitudinal momentum transfer is very small, $q_{\min} < 0.5$ a.u., and it can be deduced with high accuracy directly from the measured electron energy. The uncertainty in the determination of $q_\perp$ is related to the achieved transverse momentum resolution for the recoil ion and the electron of $\Delta p_{r\perp} = 0.15$ a.u. and $\Delta p_{e\perp} =$ 0.1 a.u., respectively. This results in an estimated resolution of $\Delta q_\perp < 0.2$ a.u. for the transverse momentum transfer. The electron energy resolution is $\Delta E_e = 1$ eV at $E_e = 10$ eV and $\Delta E_e = 5$ eV at $E_e = 130$ eV. The efficiency of the spectrometer is constant over the whole energy range and the determination of relative cross sections is limited by statistical errors only. The sum of all recorded events is normalized to the measured total He single ionization cross sections [14] of $\sigma_{6+} = 1.2 \times 10^{-17}$ cm^2 and $\sigma_{53+} = 8.0 \times 10^{-15}$ cm^2 for 100 MeV/u C^{6+} and 3.6 MeV/u Au^{53+} projectiles, respectively.

In Fig. 1 the doubly differential cross section (DDCS) $d^2\sigma/(dq_\perp dE_e)$ for single ionization of He by 100 MeV/u C^{6+} ions is plotted as a function of the projectile transverse momentum transfer $q_\perp$ and for specified electron energies E_e. A value of $q_\perp = 1$ a.u. corresponds to a projectile deflection angle of only 750 nrad. For each set of DDCS for fixed E_e the longitudinal momentum transfer $q_{\min} = (I + E_e)/v_p < 0.1$ a.u. is constant but varies slightly with E_e. Thus, the total momentum received by the target atom is pointing essentially in the direction perpendicular to the ion beam. For small $E_e <$ 50 eV, i.e., for more than 60% of the total ionization cross section, "photonlike" dipole transitions dominate at small momentum transfers close to the minimum momentum transfer in the Bethe-Born limit [15]. Only with increasing electron energy more violent encounters start to contribute significantly. The DDCSs exhibit a peak at a transverse momentum transfer equal to the momentum of the ejected electron $q_\perp \cong \sqrt{2E_e}$ (arrows in Fig. 1) clearly

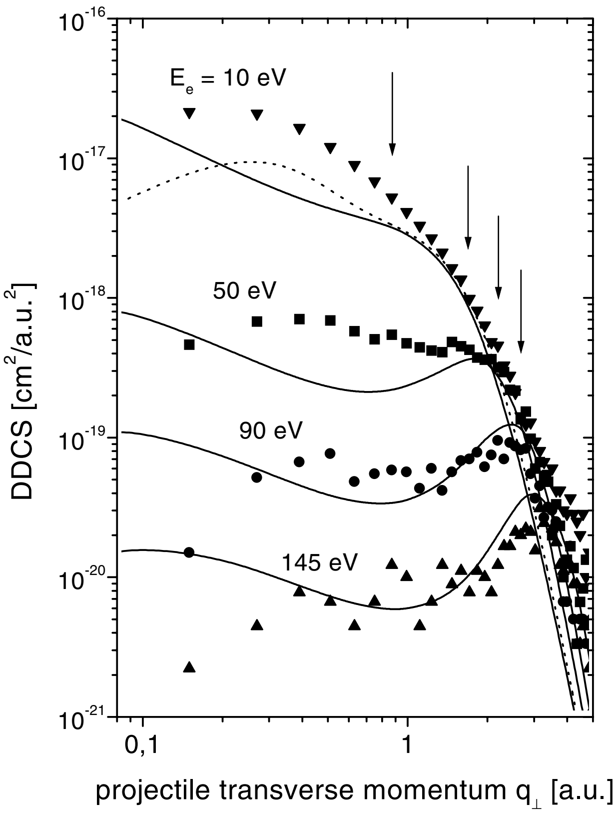

FIG. 1. The doubly differential cross section DDCS $= d^2\sigma/(dq_\perp dE_e)$ as function of the projectile transverse momentum transfer for specified and fixed electron energies for pure single ionization of He by 100 MeV/u C^{6+} impact ($Q/v_p = 0.1$). Solid lines: theoretical first Born results. Dotted line: convolution of theoretical DDCS for $E_e = 10$ eV with the experimental resolution of $\Delta q_\perp = 0.2$ a.u.

demonstrating the increasing importance of binary collisions between the electron and the projectile. According to momentum conservation it is evident that under these conditions the target ion stays practically at rest while the electron is ejected in the transverse direction. This is the so-called Bethe ridge.

The experimental data are compared with theoretical results obtained within standard first Born and CDW-EIS (continuum distorted wave–eikonal initial state) calculations [16], where an effective one-electron description is used to model the He initial state. The presence of two electrons in the target is taken into account by multiplying the corresponding single ionization cross section by a factor of 2. The initial and final electronic states are described by a hydrogenic wave function with an effective charge of $Z_T = 1.34$ for the target.

The total cross section as well as electron emission spectra are fairly well reproduced by both theories, first Born and CDW-EIS, which, as expected for a small perturbation of $Q/v_p = 0.1$, yield identical results. Though there is reasonable overall agreement between the experimental data presented here and theory in magnitude and shape (solid lines in Fig. 1), distinct deviations are observed at small momentum transfers. These might be due to both the quite crude approximation for the He ground state and the experimental $q_\perp$ resolution which causes a smoothing of the experimental DDCS at very small momentum transfers (see dotted line in Fig. 1). Convolution of theory with the experimental resolution was performed only for $E_e = 10$ eV; other curves are affected in a similar way. At small $q_\perp$ systematic discrepancies to the first Born approximation have also been observed for 50 to 150 keV protons [7] which were found to be due to the missing "postcollision interaction" (PCI) between the emerging projectile and the ionized electron. However, at the very large projectile energies studied here PCI is expected to be of minor importance and, in addition, is accounted for in the CDW-EIS results.

While the experimental data look astonishingly similar if the perturbation is increased by more than a factor of 40 ($Q/v_p = 4.4$) when preceding to 3.6 MeV/u Au^{53+} projectiles, dramatic disagreement is observed in comparison with the theory in Fig. 2: Standard CDW-EIS theory (dashed lines in Fig. 2), which has been demonstrated to perfectly predict the total ionization cross section as well as doubly differential electron emission spectra up to the largest perturbations studied so far, fails completely over the whole $q_\perp$ regime investigated here, most dramatically, however, at small projectile deflections, where the majority of electrons are found in the experiment. Only binary

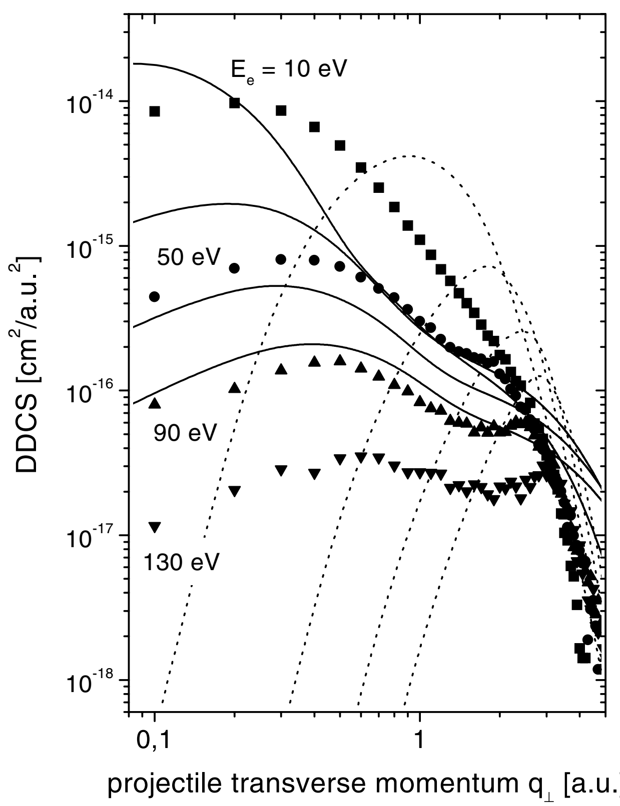

FIG. 2. Same as Fig. 1 for 3.6 MeV/u Au^{53+} impact ($Q/v_p = 4.4$). Solid lines: theoretical CDW-EIS results with screened nucleus-nucleus interaction. Dashed lines: CDW-EIS results without n-n interaction.

encounter electrons (BEE) are represented by this theory. In the light of these results one is forced to conclude that the only plausible reason for the complete failure of standard CDW-EIS to describe the three-particle dynamics at small projectile deflections far below the maximum scattering by a free electron ($\vartheta_{p\text{-}e} = 3\ \mu$rad) lies in the neglect of the internuclear interaction which is usually considered to be of minor importance at such small ϑ_p. Inclusion of this interaction taking into account the screening of the second passive helium electron to derive the static residual target ion potential [17] yields a considerable change of the theoretical prediction (solid lines in Fig. 2). Compared to standard CDW-EIS the pronounced overestimation of BEE emission is removed and most of the cross section appears at small momentum transfers. However, the quantitative agreement with experiment is still rather poor, in particular, at large electron energies where theory strongly overestimates the cross section. We mention that very recent theoretical results [18] for the same collision system disagree with both the present CDW-EIS calculation with screened internuclear potential and experiment.

Intuitively, one might even be surprised that BE electrons are observed at all under such conditions: They indicate the occurrence of close encounters between the projectile and the target electron and at the same time a distant collision (impact parameters of a few atomic units) with the target nucleus, since the projectile deflection is completely balanced by the BEE momentum; i.e., the target ion stays at rest. Any contribution from small impact parameter collisions becomes even more unlikely because those predominantly result in double ionization. However, the unperturbed ground-state electron density at such large distances is negligibly small, prohibiting BEE production at these impact parameters with intensities as observed in the experiment. A possible explanation may be as follows: the attraction of the target electrons by the projectile polarizes the target atom already in the incoming part of the projectile trajectory before the actual ionization process takes place. This leads to a strongly asymmetric electron distribution "pulled" towards the projectile resulting in an increased probability for close projectile-electron encounters.

The great majority of collisions, however, takes place at extremely large impact parameters between the projectile and both the target electron as well as the nucleus. Here, the force on both is of similar magnitude but opposite direction, effectively "ripping apart" the atom with similar but opposite momenta of electron and target nucleus in the final state, and, consequently, with little net effect on the deflection of the passing projectile. It is obvious that under such conditions the projectile scattering angle is determined by a subtle balance of forces between all three particles, strongly influenced by the exact, time-dependent target-electron density distribution in the incoming part of the trajectory.

In summary, the present situation represents an extremely sensitive and challenging realization of the three-body Coulomb problem at large perturbations and large distances serving as a benchmark system for the development and test of theoretical approaches that incorporate the time evolution of three pointlike particles mutually interacting through the nonrelativistic Coulomb force. CDW-EIS fails in the description of the present experimental data, which is remarkable considering the success of this approach in the prediction of total ionization cross sections as well as doubly differential electron spectra.

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