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CDW-EIS theoretical calculations of projectile deflection for single ionization in highly charged ion–atom collisions

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Abstract

We present continuum distorted wave-eikonal initial state (CDW-EIS) theoretical calculations for the projectile deflection in single ionization of helium by heavy-ion impact as a function of ionized electron energies. These calculations account for the helium passive electron shielding in the internuclear interaction improving standard CDW-EIS theory. The results are compared with recent experimental results by impact of 100 MeV/amu C^{6+} and 3.6 MeV/amu Au^{53+}. For highly charged projectiles there is a poor quantitative agreement between theory and experiment. However, this refined calculation does share some qualitative features with the data. In particular the variation of the effective charge of the residual He^{+} ion from $Z_{\rm eff} = 1$ to $Z_{\rm eff} = 2$ when going from small to large projectile scattering angles is able to represent a shoulder observed in the double differential cross sections. Important qualitative differences are observed at the level of triple differential cross sections.

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1. Introduction

The scattering of the projectile in ion–atom collisions has been experimentally investigated for excitation and electron capture processes during the past two decades. Let us mention for instance, the remarkable observation of Thomas' peak in charge exchange collisions by Horsdal-Pedersen et al. [1] in 1983. On the other hand, experimental studies of ionization processes measuring cross sections differential in the projectile scattering angle have been available only a few years ago [2–4]. The theoretical descriptions [5,6] did include both the projectile-active electron and the internuclear interaction in order to get a correct description of the projectile deflection. In particular, the well-established continuum distorted wave-eikonal initial state (CDW-EIS) theory [7,8] was improved to account for both interactions and compared with the available projectile scattering measurements in helium single ionization by proton impact [10]. In a work by Schulz et al. [9], double differential cross sections for the same system were systematically measured as a function of the projectile energy loss and scattering angle in a lower energy range

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(50–150 keV). Again the CDW-EIS accounting for the internuclear interaction reproduces well the main features [11].

However, it is only recently that multiply differential cross sections have been measured for highly charged ion helium ionization [12,13]. Both double and triple differential cross sections have been measured in the perturbative regimen for C^{6+} impact and in a strongly non-perturbative regime for Au^{53+} ion impact. These measurements represent the state of the art in the field. On the other hand, all the theoretical efforts to reproduce the experimental data have employed an effective three-body problem [14,15]. For instance in [15] the authors use a C3 approximation focusing on the interaction of the residual ion with the active electron, which is described by a Hartree–Fock potential. However, for highly charged ion impact efforts should be addressed to describe interactions involving the projectile.

The aim of the present work is to compare these recent experimental data with a CDW-EIS calculation accounting for the final-state interactions among the three collision partners (active electron, projectile and residual ionic target). The projectile-residual target interaction is considered by using the concept of effective Coulomb charge. The theory is briefly reviewed in the following section. Since we are particularly interested in the projectile angular distribution, much care has been taken in the calculation to get a proper description of the effective internuclear interaction.

2. General theory

Let us consider the effective three-body problem: the ionization of the active electron bounded to its ionic core by the collision of a projectile of charge Z_P and impact energy E_P. The interaction potential of the ionic core will be taken to be a Coulomb one with an effective charge Z_{eff}. The outcome of this collision process is completely described by the final-state momenta of the ejected electron and the scattered projectile. Among these six momentum components, only five are linearly independent, the other one being determined from energy conservation. For describing this final-state we arbitrarily choose the electron energy E_e, its solid angle $\mathbf{\Omega}_e$ and $\boldsymbol{q}_\perp$, the perpendicular component of the momentum $M_P\mathbf{v} - \mathbf{K}$ transferred in the collision, where M_P, $\mathbf{v}$ and $\mathbf{K}$ are the projectile's mass, initial velocity and final momentum. The corresponding triple differential cross section TDCS in the laboratory coordinate system reads (atomic units are used throughout)

$$\frac{d^3\sigma}{d\mathbf{q}_\perp d\Omega_e dE_e} = \frac{k_e q_\perp}{2\pi v^2} |T(\mathbf{q}_\perp)|^2. \quad (1)$$

Here $T(\mathbf{q}_\perp)$ is the corresponding transition matrix element and k_e the module of the electron momentum. For small projectile scattering angles $q_\perp \approx M_P v_P \theta_P$, with θ_P the projectile scattering angle.

The double differential cross sections are obtained by integrating the TDCS over the electron emission angles. We remark that the dependence on the projectile azimuthal angle vanishes by symmetry. As far as we are interested in the magnitudes related to the projectile scattering angle the interaction between the projectile and the ionic core must be accounted for. The internuclear interaction may be included by means of an integral transformation [11]. The "static" core potential which distorts the projectile trajectory [16] is assumed to be given by a pure Coulomb interaction between the projectile and target residual ion. To account for the screening of the target nucleus charge by the passive electron the target ion is considered to have an effective charge Z_{eff}. For helium we choose two different approaches. First, a fixed effective charge given by

$$Z^*_{eff} = 1.35 \quad (2)$$

arising from the binding energy of the active electron is used. Secondly, a scattering angle dependent effective charge accounting for the screening by the passive electron (within the first Born approximation) given by

$$Z_{eff}(q_\perp) = Z_T - 16\frac{(Z_T - 5/16)^4}{[4(Z_T - 5/16)^2 + q_\perp^2]^2} \quad (3)$$

is employed. Here, the passive electron is in a 1s state of the hydrogenic atom with target variational charge $Z_T - 5/16$ being $Z_T = 2$ for helium.

For the transition matrix element we employ the CDW-EIS approximation, introduced by Crothers and McCann [7] for the ionization collision. While the initial scattering state is distorted by an eikonal phase factor accounting for the active electron-projectile Coulomb interaction, the final-state incorporates the interaction of the emitted electron with both the projectile and the residual target ion, by a product of the individual Coulomb continuum wave functions ψ^-_{eP} and $\psi^-_{eHe^+}$, respectively.

An independent electron description of the two-electron target atom is employed. The initial bound state is described by a Hartree–Fock wave function, and the final-state by a hydrogenic wave function with the effective charge Z_{eff}. The presence of two-electrons in the target is taken into account by multiplying the corresponding single-ionization cross section by a factor two. We remark that this procedure is valid whenever the double ionization process is small. The integral transformation yielding the proper transition matrix element which includes the projectile – ionic core interactions is numerically performed as described in [10].

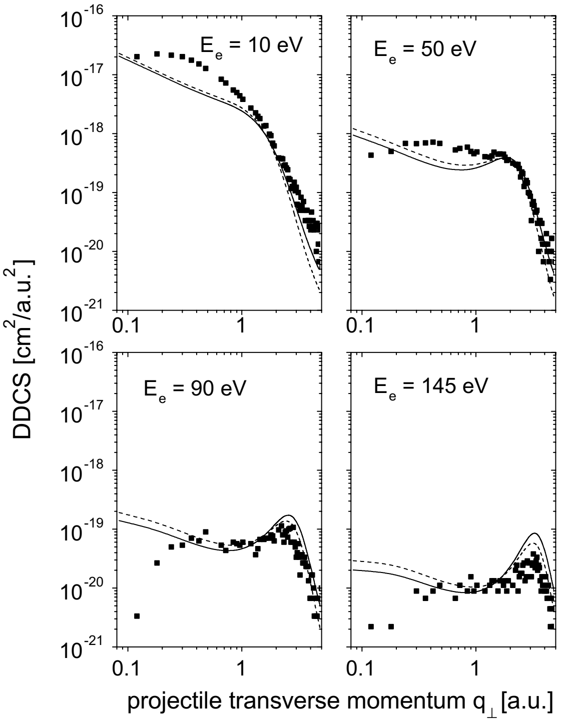

Fig. 1. Double differential cross sections DDCS as a function of the transverse projectile momentum transfer for fixed electron energies for single ionization of He by 100 MeV amu^{-1} C^{6+} impact. Symbols, experimental data from [12]. Solid (dashed) lines, CDW-EIS with ionic Coulomb effective charges $Z_{eff}(q_\perp)$ (Z^*_{eff}).

3. Results

Two sets of reference experiments on helium single ionization have been recently reported, one of them in the perturbative regime at $Z_P/v = 0.1$ corresponding to 100 MeV/amu C^{6+} impact and the other one in the non-perturbative regime at $Z_P/v = 4.4$ for 3.6 MeV Au^{53+} impact [12,13]. The comparison of the present CDW-EIS with these experiments by considering first the DDCS and then the most detailed TDCS is examined.

3.1. Double differential cross sections

In Fig. 1, the doubly differential cross sections (DDCS) $d^2\sigma/(dq_\perp dE_e)$ for single ionization of He by 100 MeV/amu C^{6+} ions are displayed as a function of the projectile transverse momentum transfer $q_\perp$ and for specific electron energies E_e. The data show a clear transition from the distant ionizing collision (photon like) for low electron energy towards the binary encounter one for higher electron energies. In fact, for the latter the DDCS exhibit a characteristic peak at a transverse momentum transfer equal to the momentum of the ejected electron $q_\perp \sim \sqrt{2E_e}$. Our results using the shielded effective charge $Z_{eff}(q_\perp)$ (solid lines) and the fixed Z^*_{eff} (dashed lines) are close each other and also in a reasonably good agreement with the experimental data. In particular the binary peak is clearly reproduced, although some quantitative departures are observed for small $q_\perp$.

In Fig. 2, the same DDCS but for He ionization by 3.6 MeV/amu Au^{53+} impact, i.e., in the non-perturbative regime are shown. The curve corresponding to the shielded case seems to have a similar two-bend structure as the experimental data for the higher electron energies. On the quantitative aspect important differences are observed

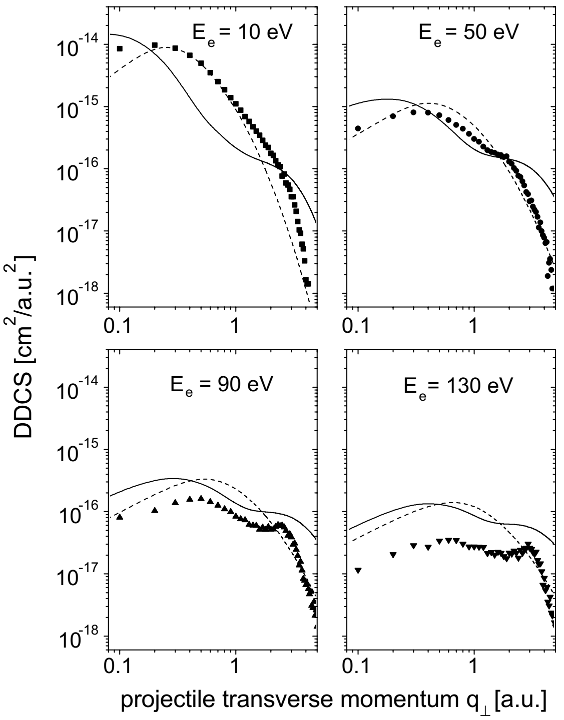

Fig. 2. As in Fig. 1 for single ionization of He by 3.6 MeV amu^{-1} Au^{53+} impact. Symbols, experimental data from [12]. Solid and dashed lines as in Fig. 1.

between present calculations and the experimental data.

In our theory, the double bend structure arises from changes in projectile-He^+ interactions from an effective charge $Z_{\rm eff}(q_\perp) = 1$ for full-screening by the passive electron at distant collisions (small $q_\perp$) to $Z_{\rm eff}(q_\perp) = 2$ for the non-screening case (close collisions).

3.2. Triple differential cross sections

We would like now to compare our theoretical CDW-EIS calculations with recent complete experiments reporting triple differential cross sections (TDSC) $d^3\sigma/(d\Omega_P d\Omega_e dE_e)$ for single ionization of He by 3.6 MeV/amu Au^{53+} and 100 MeV/amu C^{6+} ion impact [13]. In both cases the electrons emitted into the scattering plane for fixed electron energy and fixed magnitude of the momentum transferred as a function of the polar electron emission angle are considered.

In Fig. 3 the results for the non-perturbative He ionization by Au^{53+} impact are presented. Two fixed electron energies are considered, $E_e = 17.5$ eV (top) and $E_e = 55$ eV (bottom) and momentum transfer of (left to right) 0.65, 1.0 and 1.5 au. The theoretical results are normalized to be represented in the same scale. Relative normalization factors range from 1.3 for the largest $q_\perp$ up to 7 for the lower one. This fact evidences that at this more detailed level important quantitative differences arise from relatively small changes in the effective charge used. In addition, some qualitative differences can be appreciated for the small projectile momentum transfer considered. For instance, a double loop structure appears in the CDW-EIS results using the $Z_{\rm eff}(q_\perp)$ in apparent agreement with the data. However, the theoretical results do not follow the trend of the experiments that exhibit a prominent binary peak (electrons emitted along the projectile transfer momentum) for the larger q values. On the contrary, in the CDW-EIS results the electrons have opposite transverse momentum component to that of the projectiles, while keeping the sign for the parallel component. This behavior may not be attributed to the recoil peak.

The failure of the present model is due to the strong projectile-He^+ interaction. The high value of Z_P amplifies the details of the He^+ interaction potential not represented by the effective Coulomb charge concept. To test this conclusion the perturbative case of He ionization by C^{6+} impact is now considered. In Fig. 4, the TDCS for electrons emitted into the scattering plane but for a fixed electron energy of 6.5 eV and a fixed magnitude of the momentum transfer of 0.88 au as a function of the electron emission angle as quoted in [13] are shown. In this case, there is a quite good agreement between both approaches for the effective charges. Further, the prominent binary peak is clearly observed in the data as well as in the CDW-EIS calculations. However, the recoil peak magnitude of the present model is about a half the one shown by the data. In the case of weak projectile-He^+ interaction, a proper description of the electron-He^+ interaction becomes important, and, therefore, a more sophisticated Hartree–Fock

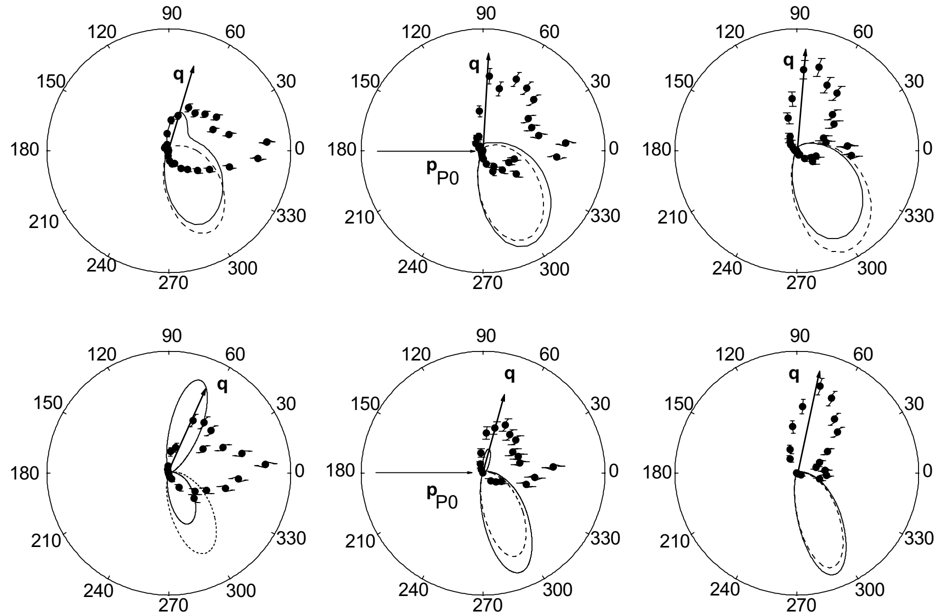

Fig. 3. Triple differential cross sections TDCS for electrons emitted into the scattering plane for fixed magnitude of the momentum transfer as a function of the polar electron emission angle for 3.6 MeV amu^{-1} Au^{53+} + He collisions. The ionized energies are 17.5 eV (top) and 55 eV (bottom) and the momentum transfers are (left to right) 0.65, 1.0 and 1.5 a.u. Data from [13]. Solid (dashed) lines, CDW-EIS with ionic Coulomb effective charges $Z_{\mathrm{eff}}(q_{\perp})$ (Z^{*}_{eff}).

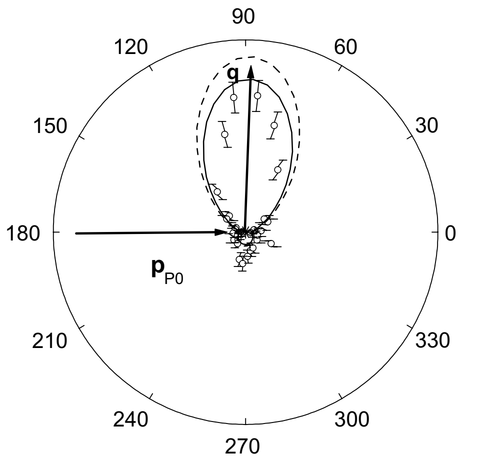

Fig. 4. TDSC for electrons emitted into the scattering plane for a fixed electron energy of 6.5 eV and a fixed magnitude of the momentum transfer of 0.88 a.u. as a function of the polar electron emission angle for 100 MeV amu^{-1} C^{6+} + He. Experiment from [13], theory as in Fig. 3.

model for both bound and continuum states of the active electron is required as stated in [15].

4. Conclusions

In this paper, a theoretical attempt to account for the influence of the non-active electron on projectile scattering related cross sections is presented. This was accomplished by two kinds of effective charges, a fixed one and another one depending on the projectile scattering angle. Although the latter seems to be better, at the DDCS level, on the more detailed TDCS the failure is evident for both approaches when dealing with the non-perturbative case. For the perturbative case the agreement is quite reasonable although the recoil peak is underestimated by both procedures.

We conclude that improvements must come from a full four-body theory, as the projectile-residual target ion interaction is quite important, particularly for the non-perturbative case. Moreover, the new model should provide a correct estimation of single-ionization process even when double-ionization becomes important.

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