Fully differential ionization cross sections in fast ion-atom collisions

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Abstract. Fully differential cross sections for helium ionization by fast ion collisions are analyzed. The emitted-electron angular distributions for fixed momentum transfer and electron energies are described theoretically and compared to the experiment. The effect of uncertainties in the determination of the momentum is considered within the theoretical model. The cross sections are found to be extremely sensitive to the inclusion of the uncertainties. Important quantitative and qualitative modifications of the calculated cross sections are obtained by including small uncertainties in the determination of the momentum transferred by the projectile to the target.

1. Introduction
The study of atomic single ionization by fast ion impact has rapidly expanded during the last few years due to the addition of experimental capabilities to determine the projectile deflection. In particular, fully differential cross sections (FDCS) have recently become feasible in ion-atom collisions. The comparison of this novel data with theoretical models should lead to new insights on the dynamics governing the atomic ionization process [1]. However, serious discrepancies between quantum mechanically calculated Continuum Distorted Wave (CDW) fully differential cross sections and measurements were found and extensively discussed in the literature [2–7].

In order to attempt to understand the sources for the serious discrepancies with the experiment, theoretical work analyzed several variables that could modify the result. These efforts include the investigation of the sensitivity of the cross sections to different forms for the interaction potential between the projectile and He nucleus [3, 4], several 4-body effects that incorporate the possibility of simultaneous excitation of the receding He$^+$ ion [7–9], the loss of flux due to helium double ionization [3, 8], and also the sensitivity of the cross sections to various forms for the initial and final wavefunctions [3, 10].

One of the most puzzling examples of this situation constitutes the single ionization of helium by 100 MeV u$^{-1}$ C$^{6+}$. For this system the theory qualitatively agrees with the experiment for electrons emitted in the scattering plane but differs both quantitatively and qualitatively in the plane perpendicular to it [6]. For the same collision partners but at a smaller incident energy of 2 MeV u$^{-1}$ were also found discrepancies between theory and experiment [5, 11].

In a series of publications we have analyzed other possible sources for the observed differences between measurement and calculations of FDCS on different systems, including collisions of C$^{6+}$

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and Au$^{53+}$ with helium [12–14]. In a first approach, by using Classical Trajectory Monte Carlo calculations we averaged the data over bins as those employed in the experiment to collect the data [1, 3, 8, 15, 16]. As a second step we included this same information in the quantum-mechanical calculations [9]. These studies showed that the inclusion of the bins modify the data by 100% and larger. Finally, the inclusion of other uncertainties, which included those due to the initial distribution of the atoms showed that the magnitude of fully differential cross sections may change by an order of magnitude and the shapes are completely modified [9, 12–14].

2. Definition of the problem
We study ionization processes in collisions of fast, heavy, multiply-charged carbon ions with helium. In particular we are interested in the evaluation of the fully differential cross sections (FDCS) $d\sigma/dQ_\perp dE_e d\Omega_e$, where $E_e$ and $\Omega_e$ are the ionized electron energy and solid angle and $Q_\perp$ is the perpendicular component of the momentum transferred to the atom by the projectile $Q = M_P v - K$. Here $M_P$, $v$ and $K$ are the projectile’s mass, initial velocity and final momentum, respectively. Since the final projectile momentum is very close to the initial ($Q \ll K$), the scattering angle is related to the magnitude of the perpendicular momentum transfer by $Q_\perp \approx M_P v \theta$, and the corresponding cross sections are approximately proportional to each other

$$d\sigma \approx \frac{1}{(M_P v)^2} \frac{d\sigma}{dQ_\perp dE_e d\Omega_e}.$$  

The quantum-mechanical calculation of the cross sections is performed through the expressions (atomic units are used)

$$\frac{d\sigma}{dQ_\perp dE_e d\Omega_e} = (2\pi)^4 \frac{k|t_{if}|^2}{v^2}, \quad t_{if} = \langle \Psi_f^- | V_f | \Psi_i \rangle, \quad (1)$$

where $t_{if}$ is the transition matrix element between the initial and final states $\Psi_i$ and $\Psi_f$.

2.1. Theoretical model
The final state employed for the calculation of the transition matrix element is the Continuum Distorted Wave (CDW) wavefunction, given by

$$\Psi_f^\pm (r, R) = \frac{e^{i(k_T \cdot r_T + K_T \cdot R_T)}}{(2\pi)^3} D_T^\pm(k_T, r_T) D_N^\pm(k_N, r_N) D_P^\pm(k_P, r_P). \quad (2)$$

Here $r_\alpha, k_\alpha$ are the relative two-body coordinate and momentum of a pair of particles, as shown in figure 1. $R_\alpha$, $K_\alpha$ are the position and the momentum of the remaining particle relative to the pair [17]. As a result of the collision, the ionized electron acquires momentum $k$ in the laboratory frame.

The distortion factors $D_\alpha^\pm$ in (2) are related to the two-body continuum eigenstates $\psi_{\alpha}^\pm(r_\alpha)$ by

$$\psi_{\alpha}^\pm(r_\alpha) = \frac{e^{iK_\alpha \cdot r_\alpha}}{(2\pi)^{3/2}} D_\alpha^\pm, \quad \left[ -\frac{\nabla^2}{2m_\alpha} + V_\alpha - \frac{k_\alpha^2}{2m_\alpha} \right] \psi_{\alpha}^\pm(r_\alpha) = 0.$$  

where $m_\alpha$ is the two-body reduced-mass.

In the case of Coulomb interactions, this final state reduces to the C3 wavefunction and the distortion factors have closed forms [18, 19].

The final distortion potential $V_f$ in the transition matrix element (1) can be written for the CDW wavefunction (2) as

$$V_f = \frac{\langle k_P k_N \rangle}{M_P} - \frac{\langle k_T k_N \rangle}{M_T} - \frac{k_T k_P}{M_T} \quad \frac{\nabla D_j^\mp(k_j, r_j)}{D_j^\mp(k_j, r_j)}.$$  

2
where $M_P$ and $M_T$ are the masses of the projectile and target-nucleus, respectively. The above expression is valid for any relation of masses between the fragments [3, 17].

In atomic collisions, the target nucleus is much heavier than the electron and the distortion potential may be simplified by neglecting the term proportional to $1/M_T$. This expression has been recently employed in electron-atom collisions [20]. For ion impact, where the projectile mass may also be approximated as infinitely heavy, only the last term contributes and the usual CDW result is recovered [21].

In this work, the two-body target-electron wavefunction in both the initial and final states are obtained as numerical solutions of the same Hamiltonian with a Hartree-Fock model potential [22] (for details see also [3] and references therein). Moreover, the use of full expressions (1-3) ensures that the internuclear interaction is taken into account on the same level that the projectile-electron and target-electron interactions.

2.2. Inclusion of momentum uncertainties

Due to the strong dependence of the cross sections with the momentum transfer $Q$ the observed FDCS are very sensitive to small uncertainties that are always present in the experiment [12–14]. Thus, in order to compare the experimental data with the theoretical results, we must convolve the calculations with the uncertainties in the determination of the electron and recoil momenta. In order to simplify this procedure we assume that the uncertainties in the determination of the electron momentum is small compared to the uncertainty in the determination of the recoil [2, 23] and employ an overall uncertainty for the momentum transfer.

The inclusion of the uncertainties has been carried out by integrating the cross sections weighted by Gaussian distributions in two dimensions perpendicular to the initial velocity. Thus, the observed cross section for a nominal momentum transfer $Q_0$ is obtained from:

$$
\frac{d\sigma}{dQ_0 dE_e d\Omega_e} = \int \frac{d\sigma}{dQ dE_e d\Omega_e} p_x (Q_x - Q_{0x}) p_y (Q_y - Q_{0y}) dQ_x dQ_y,
$$

$$
p_i(Q_i) dQ_i = \frac{1}{\sqrt{2\pi \sigma_i^2}} \exp(-Q_i^2 / 2\sigma_i^2) dQ_i.
$$
Since the \( x, y \) axis for the uncertainties \( \sigma_x \) and \( \sigma_y \) are fixed in laboratory but the cross sections depend only on the relative azimuthal angle \( \varphi_{kQ} \), an additional convolution on the azimuthal angle \( \varphi_{Q_0} \) of the momentum transfer \( Q_0 \) must be performed. This last integration is unnecessary when \( \sigma_x = \sigma_y \) because in this case the Gaussian weight is isotropic.

3. Comparison between theory and experiment
At very high projectile energy 100 MeV \( u^{-1} \) \( (v \approx 58.7 \text{ a.u.}) \) the cross sections in the scattering plane present a two maxima structure familiar from previous electron-atom and ion-atom studies. The larger maximum located at approximately the direction of the momentum transfer \( Q \) is called “binary-peak”, and is associated with a projectile-electron collision, with no important participation of the recoil ion. The second maximum, located in the direction of \(-Q\) corresponds to the recoil-peak [See for instance 24].

**Figure 2.** Helium ionization CDW fully differential cross sections for collision with 100 MeV \( u^{-1} \) \( C^6^+ \). CDW approximation (---); theory with convolution on uncertainties with \( \sigma_x = \sigma_y = 0.23 \) (- - -); The experimental data (●) are from reference [6]. Additionally, Results for \( \sigma_x = 0.17 \) and \( \sigma_y = 0.26 \), corresponding to the conditions of the experiment (see [25]), have been plotted in the perpendicular plane (---).

**Figure 3.** FDCS for ionization in 100 MeV \( u^{-1} \) \( C^6^+ \) + He collisions. The electron energy is \( E_e = 6.5 \text{ eV} \) and the momentum transfer \( Q_\perp = 0.75 \text{ a.u.} \). Right: experimental data. Left: CDW calculations after convolution on momentum transfer uncertainties.

While the CDW calculations agree well with the data in the scattering plane on the left plot of figure 2, particularly at the binary peak, the description of the recoil peak is underestimated by a factor of 2. On the right, the FDCS in the plane perpendicular to the scattering plane that
contains the initial velocity direction \( \varphi_{k,Q} = 90^\circ \), which we will simply refer as perpendicular plane) present serious disagreement between theory and measurements. This lack of agreement is clearly resolved by including the uncertainties into the theory (solid lines). Cross sections for both the scattering (parallel) and perpendicular plane agree well with the theory in shape and magnitude after convolving on momentum transfer uncertainties. This agreement extends to the First Born Approximation (FBA), whose results are nearly indistinguishable from the CDW results [14]. Similar results were also obtained very recently in a First Born Approximation by including a new estimation of the experimental uncertainties [25].

At 2 MeV \( u^{-1} \) collision energy \( (\nu \approx 8.9 \text{ a.u.}) \) the binary peak remains but the recoil peak is broader and less well defined (figure 4). As in the 100 MeV \( u^{-1} \) case, for this energy the theory agrees very well with the experiment only after convolution on the uncertainties.

![Figure 4](image)

**Figure 4.** FDCS for electron emission in the scattering plane for 2 MeV \( u^{-1} \) \( C^{6+} + \text{He} \). CDW approximation (---); CDW with convolution on uncertainties (—) [see also 13]; Experimental data \((\bullet)\) are from [26].

![Figure 5](image)

**Figure 5.** FDCS for ionization in 2 MeV \( u^{-1} \) \( C^{6+} + \text{He} \) collisions. The electron energy is \( E_e = 4 \text{ eV} \) and the momentum transfer \( Q_\perp = 0.65 \text{ a.u.} \). The plot of the right are CDW calculations after convolution on momentum transfer uncertainties.
4. Sensitivity of the cross sections with the parameters

The FDCS $d\sigma/dQ_\perp dE_e d\Omega_e$ depends strongly on the emission energy of the electron and the projectile’s momentum transfer as illustrated in figure 4.

![Figure 4](image)

**Figure 4.** ionization FDCS for 100 MeV u$^{-1}$ in the scattering plane for different momentum transfer values

A broader vision of the dependence of the cross sections with the momentum transfer $Q_\perp$ and the azimuthal angle $\phi$ may be obtained by comparing the electron angular distributions for two different values of $Q_\perp$. Figure 7 shows three-dimensional plots of the FDCS for $Q_\perp = 0.05$ and 1 a.u. Small momentum transfer is associated with relatively soft collisions, characterized by large impact parameters. These collisions, characterized by interactions perpendicular to the projectile’s velocity, produce electron distributions that present a two-lobe structure similar to the observed in photon-impact ionization.

**Figure 5.** Three-dimensional plots of fully differential cross sections for helium ionization by 100 MeV u$^{-1}$ C$^{6+}$. The emitted electrons carry energy $E_e = 6.5$ eV.

5. Effect of the internuclear interaction

The above assertion that for very large projectile energy the FBA gives results that are essentially indistinguishable from more elaborate CDW calculations is valid only for the final-state conditions chosen in the precedent sections. For instance, an obvious kinematic condition where this affirmation is not true corresponds to processes where the momentum transfer $Q$ is appreciably larger than the final electron momentum $k$. In this case the recoil must acquire enough momentum to compensate for the difference between $Q$ and $k$. The impulse given to the target nucleus is partly due to the projectile-recoil interaction, which is not well described.
by the FBA. This is clearly observed in the electron angular distributions in the parallel and perpendicular planes for ionization with large momentum transfer of figure 8. In both cases the FBA appreciably differs from the CDW approximation.

![Graph showing FDCS and FBA comparison](image)

**Figure 8.** Left: FDCS for single ionization of helium by C$_6^{+}$, when the electrons are emitted in the scattering (top) and perpendicular (bottom) planes, as a function of the ejection angle. For high momentum transfer values ($Q = 1.5$ a.u.) the FBA (---) differs from the CDW results (----) at low electron energies, $E_e = 3$ eV. Right: ratio between CDW and FBA cross sections at $\varphi = 0^\circ$.

### 6. Conclusions

We have investigated how the uncertainties in the determination of the momentum transfer affect observed fully differential cross sections. The present investigation demonstrates that FDCS are dramatically modified by the inclusion of small uncertainties in the determination of the final-state momenta. As shown, both experimental resolution and binning parameters strongly modify zero degree in-plane scattering and out-of-plane cross sections, in accord with previous studies [9, 12–14] and very recent studies [25]. The main reason for this extreme sensitivity is the rapid change of the magnitude of the FDCS with the final state variables. Namely, the magnitude of the perpendicular momentum transfer $Q_\perp$ and the azimuthal angle of the electron $\varphi_{k,Q}$.

The convolution of the theoretical results with uncertainties similar to those occurring on present-day nearly-perfect state-of-the-art experiments dramatically modifies not only the magnitude but also the shape of the observed FDCS. Thus, any attempt to compare the measured data with a theory must incorporate an estimation of the uncertainties.

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