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Semiclassical description of kinematically complete experiments

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Abstract

Based on the semiclassical impact parameter method, a theoretical model is constructed to calculate fully differential cross sections for single ionization of helium by impact with fast C^{6+} ions. A good agreement with the experiment is achieved in the scattering plane, while in the perpendicular plane a structure similar to that observed experimentally is obtained. The contribution of different partial waves to the cross section is also investigated.

The most complete information about ionization processes in atomic collisions is provided by fully differential cross sections. These quantities describe the entire energy and angular distribution of the ionized electron, residual ion and projectile.

Recently, interesting data for the complete electron emission pattern in single ionization of helium by the impact of C^{6+} ions for certain momentum transfers have been reported [1, 2]. The three-dimensional images were generated using experimentally measured fully differential cross section values. These experiments were performed on a cold-target-recoil-ion-momentum spectrometer (COLTRIMS) apparatus. The results show the characteristic double-lobe structure with a binary peak and a smaller recoil peak.

Several theoretical calculations exist [3–5], which are able to reproduce the experimental data in the scattering plane (determined by the momentum of the scattered projectile and the momentum transfer vectors). Right after the publication of the first experimental results of fully differential cross section measurements for ionization by fast ion impact, an intense debate arose concerning the discrepancy between experiment and theoretical calculations (mainly performed using the CDW-EIS method) in the plane perpendicular to the momentum transfer. Here, the theoretical results are essentially isotropic and do not show the observed peak structures perpendicular to the beam direction. Some authors have suggested that it may be important to include in the calculations the internuclear interaction [6]. On the other hand, very recently, the importance of taking into account the uncertainties of the experimental measurements and to perform a convolution of the theoretical results on the experimental resolution [7] was proved. At the same time, it was suggested that all aspects of the experimental resolution may be included in the theories by the use of a quantum-theory-based

Monte Carlo event generator [8]. In this paper, the authors conclude that the structures observed in the perpendicular plane may be explained only partly by the experimental uncertainties.

In the present work, a theoretical model is constructed to calculate fully differential cross sections for single ionization of helium by the impact of fast C^{6+} ions. The constructed model is based on the first-order semiclassical impact parameter approximation. The aim of this work is to explore how the semiclassical impact parameter approximation may be used to calculate fully differential cross sections. The main problem is to assign a value of the impact parameter for a given momentum transfer and electron energy and ejection angle. A partial wave analysis for different ejection directions is also performed.

In order to study the ionization process of helium produced by fast charged projectiles, first the ionization amplitudes have to be calculated. In the semiclassical approximation, the projectile is treated separately and it moves along a classical trajectory. This implies that only the electronic system needs to be described by a time-dependent Schrödinger equation, while the projectile follows the classical laws of motion. Using the first-order perturbation theory, the transition amplitude may be written as

$$a^{(1)} = -\mathrm{i} \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(E_f - E_i)t} \langle f | V_1(t) + V_2(t) | i \rangle, \tag{1}$$

where i and f represent the initial and final electronic states of the target system, respectively. E_i and E_f are the energies of the corresponding (unperturbed) states of the system, while $V_1(t)$ and $V_2(t)$ denote time-dependent interactions between the projectile and the electrons.

The initial state of the dielectronic system is described by a Hartree–Fock wavefunction [9], while the final state is described by a symmetric combination of a hydrogenic and a continuum wavefunction

$$\begin{aligned} |i\rangle &= \big|i_b^{(1)}\big\rangle \big|i_b^{(2)}\big\rangle \\ |f\rangle &= \tfrac{1}{\sqrt{2}} \big(\big|f_b^{(1)}\big\rangle \big|f_c^{(2)}\big\rangle + \big|f_c^{(1)}\big\rangle \big|f_b^{(2)}\big\rangle \big). \end{aligned} \tag{2}$$

Here indexes b and c represent the bound and continuum states, respectively, while the indexes (1) and (2) are the labels of electrons. The continuum wavefunction is calculated in the mean field of the final He^+ ion.

With the use of the above-described wavefunctions, the ionization probability amplitude depending on the momentum transfer vector, ejected electron energy and ejection angles is reduced to a 1-electron amplitude

$$a^{(1)} = -\frac{\mathrm{i}\sqrt{2}}{v} \langle f_b | i_b \rangle \int_{-\infty}^{+\infty} \mathrm{d}z\, \mathrm{e}^{\mathrm{i}\frac{E_f - E_i}{v} z} \langle f_c | V_1(t) | i_b \rangle. \tag{3}$$

This amplitude is calculated expanding the final continuum-state wavefunctions into partial waves. In this way, amplitudes for transitions to ionized states with different angular momenta $\big(a_{l_f m_f}^{(1)}\big)$ are obtained.

The fully differential cross sections relative to the momentum transfer value, ejected electron energy and electron ejection angles are obtained by the relation

$$\frac{\mathrm{d}^5\sigma}{\mathrm{d}E\, \mathrm{d}\theta\, \mathrm{d}\phi\, \mathrm{d}q\, \mathrm{d}\phi_q} = B \left| \sum_{l_f, m_f} a_{l_f m_f}^{(1)}(\mathbf{B}) \right|^2 \left| \frac{\mathrm{d}B}{\mathrm{d}q} \right|, \tag{4}$$

where $\mathbf{B}$ is the impact parameter vector and l_f and m_f are quantum numbers of the partial waves describing the ejected electron.

In order to assign an impact parameter to a momentum transfer as a first approach, the projectile deviation angle is calculated using the Rutherford scattering formula, as if we had

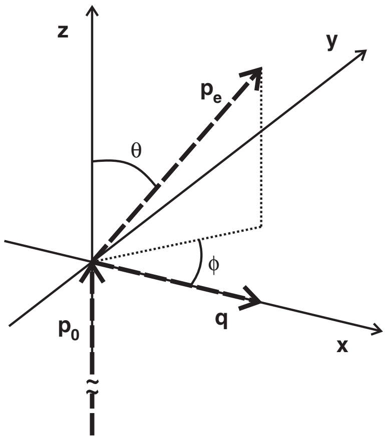

Figure 1. Sketch of the coordinate system used.

only elastic scattering. Assuming that the momentum transfer modifies only the direction of the projectile's momentum vector and applying some approximations valid for small projectile deviations, the impact parameter corresponding to a certain momentum transfer will be

$$B = \frac{2Z_{\text{proj}}Z_{\text{targ}}}{v_p q}, \tag{5}$$

where Z_{proj} is the charge of the projectile, Z_{targ} is the effective charge of the target seen by the projectile, v_p is the projectile velocity and q denotes the momentum transfer. This means that to a certain value of the momentum transfer is assigned a value of the impact parameter regardless of the ejection angle of the electron.

We have applied the model outlined above for the ionization of helium induced by 100 MeV u^{-1} C^{6+} projectiles.

In these calculations, the used coordinate system is sketched in figure 1. The initial projectile direction is along the z-axis and the momentum transfer vector $\mathbf{q}$ points nearly in the x-direction. Standard spherical coordinates are used with the azimuthal angle θ measured relative to the projectile beam direction and with the polar angle ϕ measured in the xy plane relative to the x-axis.

We calculate fully differential ionization cross sections for an ejected electron energy of $E_e = 6.5$ eV and a momentum transfer of $q = 0.75$ au. Calculating the impact parameter value with expression (5) we get $B = 0.253/0.506$, depending on the effective value of the target's charge ($Z_{\text{target}} = 1/2$).

Figure 2 shows theoretical cross section values in two different cuts from the 3D theoretical data. The curves show single ionization cross section values as a function of the electron ejection angle θ. The top panel shows the scattering plane characterized by $\phi = 0$ or π. The bottom panel shows the plane perpendicular to the momentum transfer with $\phi = \pi/2$ or $3\pi/2$. From figure 2, it is immediately observable that the curves representing impact parameter values in the range $B = 0.253/0.506$ are in disagreement with the experimental results in both planes. This means that the simple model describing the projectile motion as a simple Rutherford scattering is not quite a valid description.

Other calculations with higher impact parameter values have also been performed. One of these results corresponding to an impact parameter of 2.2 au is drawn with a solid line. In the scattering plane one can observe the presence of the characteristic double-lobe structure with

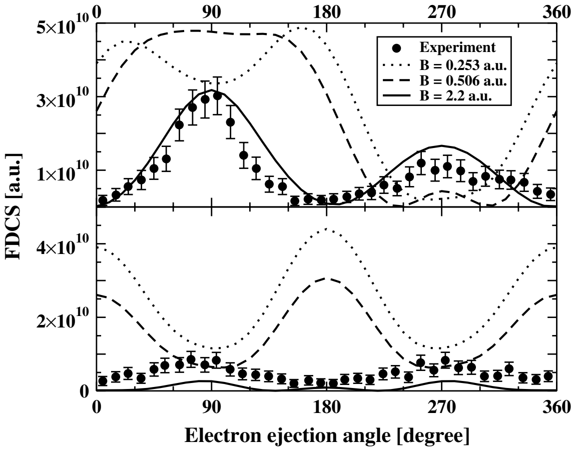

Figure 2. Fully differential cross sections in the scattering (top) and perpendicular (bottom) planes, calculated using the Rutherford-type model using different impact parameters in comparison with experiments [7] for ionization of helium by 100 MeV u^{-1} C^{6+} projectile. The ejected electron energy is $E_e = 6.5$ eV and the momentum transfer is $q = 0.75$ au.

the binary peak at $\theta = 90^\circ$ and the recoil peak at $\theta = 270^\circ$, in agreement with experiments. The agreement is worse in the case of a recoil peak having larger theoretical cross section values than the experimental ones. This difference in the recoil peak region becomes more accentuated in the case of larger momentum transfers.

Our attempt to use the simplest Rutherford formula to describe the projectile scattering and obtain a correct impact parameter failed. In contrast with the elastic scattering, there is no direct correspondence between the momentum transfer and the impact parameter [10]; the impact parameter also depends on the ejected electron energy and angle.

We have investigated several models for obtaining the impact parameter. Results in good agreement with the experimental data have been obtained for those, which suppose a larger impact parameter for the binary peak (where most of the momentum transfer is taken by the electron) and a smaller impact parameter for the recoil peak (where most of the momentum transfer is taken by the target nucleus).

A simple calculation is sketched in this sense by the use of the transverse momentum balance [10], meaning that the momentum transfer q is the sum of the transverse components of the momenta of the electron and the residual ion. This vectorial relation may be written in a scalar form as

$$p_{T\perp}^2 = p_{e\perp}^2 + q^2 - 2p_{e\perp}q\cos\phi, \tag{6}$$

where $p_{T\perp}$ is the transverse momentum taken by the residual ion and $p_{e\perp}$ is the transverse momentum of the ionized electron ($p_{e\perp} = p_e \sin\theta$). Further, we assume that the impact parameter is related to the momentum transfer to the residual ion and take into account the projectile–electron interaction separately. Under these conditions, the impact parameter is obtained as

$$B = \frac{2Z_{\rm proj}Z_{\rm targ}}{v_p\sqrt{p_{e\perp}^2 + q^2 - 2p_{e\perp}q\cos\phi}}. \tag{7}$$

In the case of a binary peak, one has to deal with $\phi = 0$ while in the case of a recoil peak the value of the angle ϕ is 180°. This means that higher impact parameters have to be used

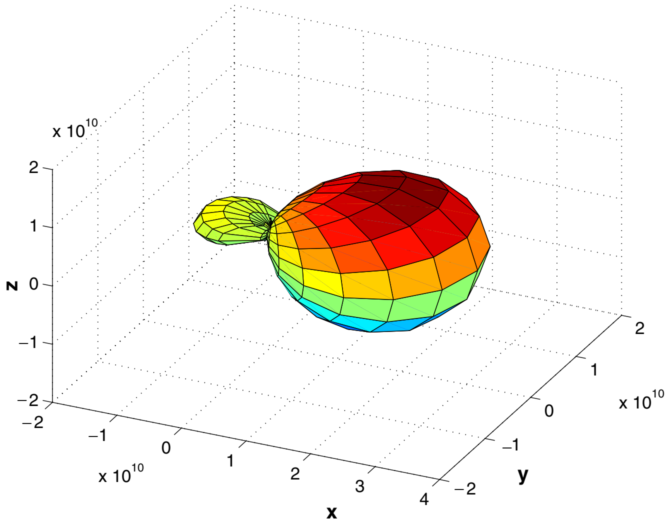

Figure 3. Theoretically obtained 3D image of the electron emission pattern for single ionization of helium produced by 100 MeV u^{-1} C^{6+} projectile impact. The ejected electron energy is $E_e =$ 6.5 eV and the momentum transfer $q = 0.75$ au.

(This figure is in colour only in the electronic version)

in the case of a binary peak than of a recoil peak. The numerical calculations show higher impact parameter values than the previously investigated simple case. In the case of an ejected electron energy of $E_e = 6.5$ eV and a momentum transfer of $q = 0.75$ au using an effective charge of $Z_{\text{target}} = 1$, impact parameters of 4.3 and 0.176 au may be obtained for binary and recoil peaks, respectively.

The two sketched possibilities are two extreme descriptions. The Rutherford model treats the residual ion and the electron as one system on which the projectile is scattered. The second model treats separately the electron and the residual ion. However, the reality may stand between these descriptions, while prior to the ionization process the target is one single system and after the ionization the ionized electron and the recoil ion interact separately with the projectile.

In order to find the correct combination of the two extremes and to determine the impact parameter values for the binary and recoil peak regions, an empirical method is used. Cross section values for binary and recoil peaks are considered as a function of the impact parameter value, and the best impact parameter values for binary and the recoil peak regions are selected based on the experimental data available in the scattering plane. The transition between these impact parameter values is realized smoothly in the $0 < \theta < 50^\circ$ and $130^\circ < \theta < 180^\circ$, $90^\circ < \phi < 270^\circ$ transition regions.

In the case of electron ejection energy $E_e = 6.5$ eV and momentum transfer $q = 0.75$ au, the experimental results in the scattering plane show cross sections of 3×10^{10} au and 1.1×10^{10} au for binary peak and recoil peak, respectively. In order to obtain these values, impact parameters of 2.2 and 0.7 au are chosen for the binary peak and for the recoil peak regions, respectively.

Figure 3 shows the theoretically obtained 3D image of the electron emission pattern for the studied case. The results are obtained using the previously determined impact

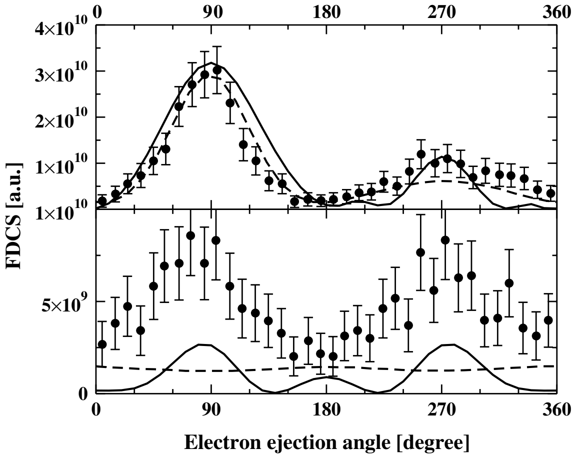

Figure 4. Theoretical results in scattering (top) and perpendicular (bottom) planes compared with experiments [7] for the same case as in figure 3. The solid curve shows the present theory while the dashed line is obtained by the CDW model [7].

parameter values. On the image, one can observe the presence of the characteristic double-lobe structure towards the x-axis with the binary peak at $\theta = 90^\circ, \phi = 0^\circ$ and the recoil peak at $\theta = 90^\circ, \phi = 180^\circ$. Now, by using this semi-empirical model, the magnitude of the recoil peak is smaller in agreement with experiments.

In order to analyse in detail the obtained results, cross section values for a scattering plane and a perpendicular plane are plotted separately in figure 4. The results obtained by the present theory may be compared in absolute value to experimental data and CDW calculations. The top panel shows fully differential cross sections in a scattering plane. The semi-empirical model gives good agreement with experimental data of Schulz *et al* [1]. In contrast to the previous calculations using a single value for the impact parameter, a smaller magnitude for the recoil peak has been obtained. However, we have to note that the shape of the binary peak is slightly wider than the experimental one.

Better results in the case of a perpendicular plane have also been obtained (bottom panel of figure 4). The curve shows the same behaviour as the experimental data with strong maxima at $\theta = 80^\circ$ and $\theta = 280^\circ$. A third smaller maximum is also obtained in the direction of $\theta = 180^\circ$. Here, we have to note that a better agreement in shape has been obtained than the isotrope results of the CDW model. However, the magnitude of the cross section is smaller than the experimental one in the perpendicular plane. The recently reported inclusion of the experimental momentum uncertainties [7] should also improve the agreement between theory and experiments by increasing the cross sections in the perpendicular plane. Our result is consistent with the conclusions of Dürr *et al* [8] that the experimental uncertainties are responsible partly only for the structure observed in the perpendicular plane; half of the value of the maxima may be due to some real physical effect.

Another analysis has also been performed in order to clarify which type of transitions are responsible for the obtained structures. Cross sections corresponding to different terms of the multipole expansion series are shown in figure 5.

Let us first discuss the results in the scattering plane depicted in the top panel. The main contribution to the cross section (solid line) has the $l = 1$ dipole term. Moreover, this term gives a large contribution in the case of a recoil peak, which is reduced by the destructive interferences with the monopole term ($l = 0$) which has contribution only in the recoil

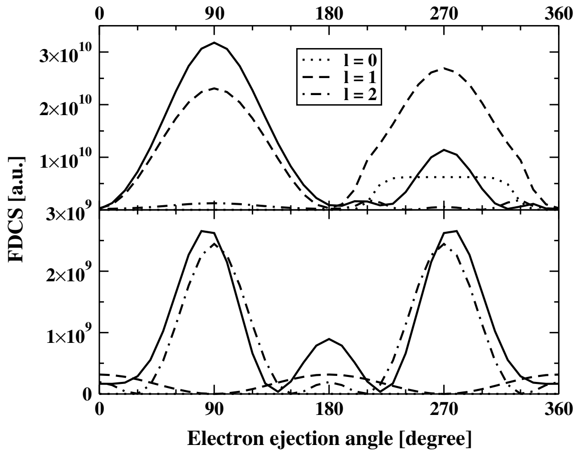

Figure 5. Multipole contributions to the ionization cross sections in scattering (top) and perpendicular (bottom) planes for ejected electron energy $E_e = 6.5$ eV and momentum transfer $q = 0.75$ au in comparison with the FDCS values of the present theory (solid line). Cross sections for different transition mechanisms are drawn separately (see text).

peak region calculated with a smaller impact parameter. Terms with $l \geqslant 2$ have negligible contribution to the fully differential cross section values in the scattering plane.

In contrast, in the case of a perpendicular plane (bottom panel of figure 5) the main contributing term is the $l = 2$ quadrupole term from the multipole expansion of the perturbation potential. This term is responsible for the shape of the electron emission pattern in this plane. The corresponding contribution has maxima at $\theta = 90^\circ$ and $\theta = 270^\circ$. These maxima are shifted to 80° and 280° due to the interferences with other multipole terms. This shifting is also detectable in the experimental results. The monopole term practically has no contribution to the cross sections in this plane. A constructive interference occurs at $\theta = 180^\circ$ being responsible for the additional maximum occurring in the theoretical results. Terms with $l \geqslant 3$ have negligible contribution to the fully differential cross section values in the perpendicular plane, too.

The next studied case is with the ejected electron energy $E_e = 6.5$ eV and a momentum transfer of $q = 0.88$ au, where the experimental results in the scattering plane show cross sections of 2.36×10^{10} au and 4.2×10^9 au for binary and recoil peaks, respectively. In calculations, impact parameters of 1.7 and 0.6 au are used determined by the above-described semi-empirical method. Cross section values for scattering and perpendicular planes are plotted separately in the left panel of figure 6. The top graph shows fully differential cross sections in the scattering plane. The semi-empirical model gives good agreement with the experimental data [11]. In the case of the perpendicular plane (middle graph), no experimental data were found. However, the structure is similar to the previous case with two maxima and another smaller maximum at 180°. It has to be mentioned that the difference between these two types of maxima is reduced. The bottom graph shows theoretical results in the xy plane perpendicular to the incident beam. The results are in good agreement with the experiments.

The last studied case is with the ejected electron energy $E_e = 17.5$ eV and a momentum transfer of $q = 1.43$ au, where the experimental results in the scattering plane show cross sections of 7.34×10^9 au and 3.71×10^8 au for binary peak and recoil peak regions. In theoretical calculations, impact parameters of 0.8 and 0.4 au are chosen. Here, some discrepancies

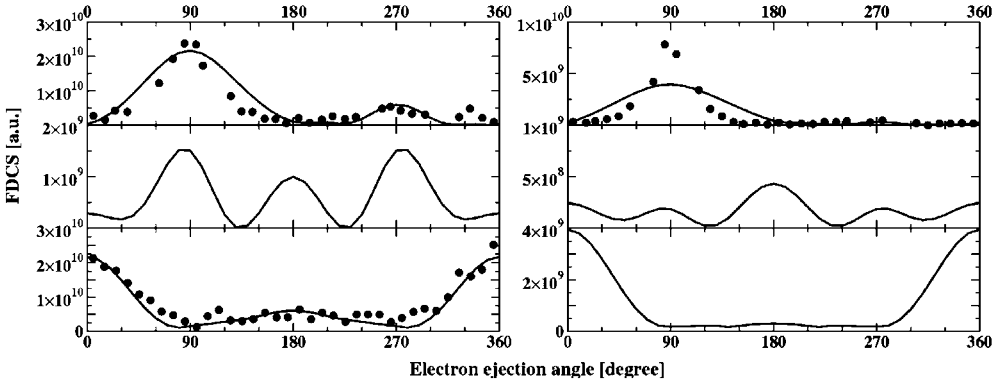

Figure 6. Theoretical FDCS values in the scattering plane (top graphs), in a plane perpendicular to the momentum transfer (middle graphs) and in a plane perpendicular to the beam direction in comparison with experiments [11] for $E_e = 6.5$ eV and $q = 0.88$ au (left panel) and for $E_e = 17.5$ eV and $q = 1.43$ au (right panel).

between theory and experiments can be found in the scattering plane presented in the right panel of figure 6. The theoretical curve for the scattering plane is wider and smaller than the experimental data. In the perpendicular plane, the maximum at 180° became greater than for smaller momentum transfers, and another additional maximum appears at 0°. The model suggests that these maxima occur mainly due to the quadrupole transitions amplified by constructive interferences. According to [8], the experimental uncertainties have no important effect on the structures observed in the experimental data. Our calculations predict in this perpendicular plane a structure similar to the experimental ones [8] but we could not compare them in the absolute scale, because the data are published for this momentum transfer in arbitrary units.

In conclusion, a theoretical model based on the first-order semiclassical impact parameter approximation has been constructed to simulate kinematically complete experiments and was applied for studying single ionization of helium by impact with fast C^{6+} ions. A semi-empirical model was developed, which uses large impact parameters for reproducing the binary peak and smaller impact parameters for the recoil peak. The model well describes the fully differential cross sections for relatively small momentum transfer values. The characteristic structures in the perpendicular plane have also been reproduced; discrepancies with experiments are only in the magnitude of the cross sections. The other part of the cross section values may be explained by the experimental uncertainties. It was found that in the scattering plane the main contribution has the dipole transition term, while in the perpendicular plane the characteristic structure is mainly due to the quadrupole transitions. Another important observation is that interferences between the multipole expansion terms are also important to understand the exact structure of the electron emission patterns. Our semiclassical model includes projectile–nucleus scattering, and we may conclude that this should be important in obtaining the experimentally observed FDCS structures in the perpendicular plane.

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