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# Semiclassical fully differential ionization cross sections of helium with negatively charged fast projectiles

**Research Article**

Ferenc Járai-Szabó*, Ladislau Nagy

*Faculty of Physics, Babes-Bolyai University,*
*RO-400084 Cluj-Napoca, str. Kogalniceanu nr. 1, Romania*

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**Abstract:** Fully differential cross sections are calculated for the ionization of helium by negatively charged fast projectiles using a semiclassical model developed previously for the ionization of atoms by positive projectiles. The method is tested in the case of 1 keV electron and 500 keV antiproton projectiles. The semiclassical results show reasonable agreement with the experiments and other theories. The origin of the obtained structures has been investigated by a partial wave analysis.

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**Keywords:** fully differential cross section • ionization • semiclassical approximation



## 1. Introduction

In impact ionization of atoms, differential cross sections for production of secondary electrons ejected during ionization are of immense importance in different fields such as radiation physics, quantum chemistry, atmospheric and plasma physics. From the purely theoretical point of view, it is of great importance for understanding many-body problems, for understanding the different interactions, mechanisms and correlations between participant particles. Nowadays, after the development of the so-called reaction microscopes [1], interest is focused on the in-detail analysis of the electron ejection from atomic or molecular targets [2–4]. These analyzes may be performed by measuring and calculating fully differential ionization cross sections which give us the most complete information about an ionization process describing the entire energy and angular distribution of the ionized electron, residual ion and projectile.

On the experimental side, a few years ago the group of Schulz reported interesting data for the complete electron emission pattern in single ionization of helium by the impact of fast $C^{6+}$ ions [5, 6]. Then, Dürr et al. reported absolute measurements of fully differential cross section (FDCS) for single ionization of helium by 1 keV [7] electron impact. In both cases the projectile velocity is high enough and the collision may be considered to be a fast one. Besides the kinematic conditions, the main difference between these experiments is the sign of the projectile's charge.

On the other hand, many theoretical models have been applied to explain FDCS measurements of single ionization of helium by fast $C^{6+}$ ion [8–10] and electron [11] impact. Moreover, in the last years the theoreticians' attention

*E-mail: ferenc.jarai@phys.ubbcluj.ro

has been directed to negatively charged antiproton projectiles [12]. Here, the results are mostly compared with first-order Born calculations.

Regarding our present work, three theoretical approximations have to be noted: (1) the perturbative first-order Born approximation [13], where only the first term of the Born series is taken into account; (2) the eikonal-type Glauber approximation (GA) [14], which is supposed to be more complete than the Born approximation and is used since 1969 to study a wide variety of atomic collision processes and (3) the nonperturbative convergent close-coupling model (CCC) [15], which is based on a close-coupling expansion of the multielectron wavefunction.

Previously, based on the semiclassical impact-parameter method, we have constructed a theoretical model to calculate the FDCS for single ionization of light atoms. The method was tested in the case of positive projectiles in comparison to the experiments of Schulz et al. [5, 6] and good agreement was achieved in the scattering plane, while in the perpendicular plane a structure similar to that observed experimentally was obtained [16, 17].

The objective of the present work is to apply the semiclassical impact-parameter method to analyze the FDCS for the single ionization of helium by negatively charged fast projectile impact in both the scattering and the perpendicular planes. The results of the semiclassical model will be compared with available experimental and other theoretical data. A partial wave analysis for different ejection directions is also performed. Our main goal is to explore the capability of the semiclassical impact-parameter method for calculating FDCS in case of negative projectiles, too.

## 2. The semiclassical model

The semiclassical model for calculating fully differential ionization cross sections is described in detail in our previous works [16, 17]. In this approximation, the projectile is treated separately and it moves along a classical trajectory. This implies that only the electron system needs to be described by a time-dependent Schrödinger equation, while the projectile follows classical laws throughout.

The ionization probability amplitudes for the ionization of helium produced by fast projectiles are calculated using first-order time-dependent perturbation theory. The initial state of the dielectronic He($1s^2$) system is described by Hartree-Fock wavefunction [18], while the final state of the $He^+(1s)$ system is described by a symmetric combination of a hydrogenic and a continuum wavefunction calculated in the mean field of the final $He^+$ ion. Therefore, the ionization probability amplitude is reduced to a one-electron amplitude

$$a^{(1)} = -\frac{i\sqrt{2}}{v}\langle f_b|i_b\rangle \int_{-\infty}^{+\infty} dz\, e^{i\frac{E_f-E_i}{v}z}\langle f_c|V|i_b\rangle, \qquad (1)$$

where $i$ and $f$ represent the target system's initial and final electronic states, while the indices $b$ and $c$ represent bound and continuum states. Similarly, $E_i$ and $E_f$ are the energies of the corresponding (unperturbed) states of the system and $V$ denotes the time-dependent Coulomb interaction between the projectile and the active electron. By the $z = vt$ relation, the time dependence of this potential is converted to a $z$-coordinate dependence. The projectile velocity is denoted by $v$ and the integral is calculated along its classical trajectory over the $z$ axis considered to be a straight line. It has to be noted that this approximation is valid only for fast projectiles where the projectile scattering angles are very small.

This amplitude is calculated expanding the final continuum-state wavefunctions into partial waves. As a result, the amplitudes for transitions to ionized states with different angular momenta $\left(a^{(1)}_{l_f m_f}\right)$ are obtained.

The fully differential cross section for the electron ejected into the energy range $[E, E+dE]$ and into the solid angle $d\Omega_e$ and the projectile scattered into the solid angle $d\Omega_p$ can be expressed as

$$\frac{d^3\sigma}{dE\; d\Omega_e\; d\Omega_p} = \frac{B}{\sin\theta_p}\left|\frac{dB}{d\theta_e}\right|\left|\sum_{l_f,m_f} a^{(1)}_{l_f m_f}(\mathbf{B})\right|^2, \qquad (2)$$

where $\mathbf{B}$ is the impact-parameter vector, $l_f$ and $m_f$ are quantum numbers of the partial waves describing the ejected electron and $\theta_e$ is the projectile scattering angle. The second part of the calculations consists in assigning impact-parameter values to a certain momentum transfer. As described in [17] this task may be completed in two successive steps.

First, the projectile scattering angle is calculated by the use of the transverse momentum balance [1]. 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.

Second, impact-parameter values are assigned to projectile scattering angles. Accordingly, the projectile scattering will be treated as a classical potential scattering problem in the field of the target helium system [13]. Therefore, the scattering angle may be calculated as

$$\theta_p = \pi - 2B\int_{r_0}^{\infty}\frac{dr}{r^2}\left(1-\frac{U(r)}{E_p}-\frac{B^2}{r^2}\right)^{-\frac{1}{2}}, \qquad (3)$$

where $r_0$ is the distance of closest approach defined by

$$\left(1 - \frac{U(r)}{E_p} - \frac{B^2}{r^2}\right) = 0$$

and $U(r)$ is the scattering potential. The simplest way to include the effect of the electrons around the target nucleus is to consider the potential to be a product of the Coulomb potential and the Bohr-type screening function [19]

$$U(r) = \frac{Z_{\text{proj}} Z_{\text{target}}}{r} e^{-\frac{r}{a}}. \qquad (4)$$

Using this potential the integral (3) may be calculated numerically. Here it has to be noted that this part of the model includes the charge sign dependence of the FDCS through the scattering potential $U(r)$ while the ionization amplitudes do not depend on it.

## 3. Results and discussion

In order to test the validity of the results of our semiclassical model for the ionization of helium by negative projectiles, calculated FDCS for fast electron and antiproton projectile impact are compared with available experimental and other theoretical data [7, 11, 12]. Then, a partial wave analysis for different ejection planes is also performed.

In the paper of Dürr et al. [7] absolute measurements of FDCS for single ionization of helium by 1 keV electron impact have been reported. These cross sections have been measured using the "reaction microscope", which covers a large fraction of the emission angles for emitted low-energy electrons and a wide range of projectile scattering angles. The experimental data available is for an ejected electron energy of $E = 10$ eV and for momentum transfers of 0.5, 0.75 and 1.0 a.u. The authors compare their experimental results with predictions from several state-of-the-art theoretical calculations. Other authors [11] have reported theoretical results based on the Glauber approximation for this scattering process. In the scattering plane, the results are in good agreement with the experimental data. In the perpendicular plane, the results for small momentum transfers are in close agreement with experiment magnitude-wise. For larger momentum transfers substantial discrepancies are observed.

Using the semiclassical model presented above, we have performed calculations for this scattering process. The projectile energy is $E_p = 1$ keV, the momentum transfer is $q = 0.5$ a.u. and the ejected electron energy is $E = 10$ eV. For this kinematic situation impact parameters of 0.7 a.u. and 0.31 a.u. are assigned which correspond to 0.0417 rad and 0.1583 rad binary and recoil scattering angles.

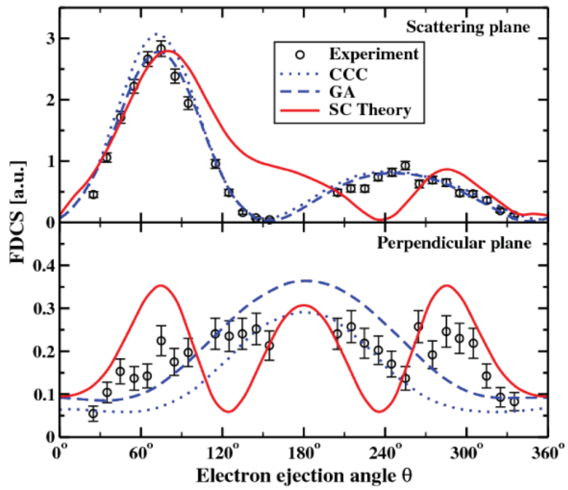


**Figure 1.** FDCS for ionization of helium by 1 keV electron impact as a function of the ejected electron angle in scattering (top) and perpendicular (bottom) planes for the ejected electron energy of $E_e = 10$ eV and the momentum transfer $q = 0.5$ a.u. Experimental results of Dürr et al. [7] are represented by circles, CCC results [7] are represented by dotted curves, dashed curves show GA calculation results [11] and the present semiclassical results are drawn with continuous lines.

In order to analyze in detail the obtained results, cross section values for scattering plane (top) and perpendicular plane (bottom) are plotted separately on Figure 1.

In the scattering plane determined by the momentum of the scattered projectile and the momentum transfer vectors, the semiclassical model reproduces well the double-peak structure of the electron ejection pattern with a binary peak (where most of the momentum transfer is taken by the electron) and a smaller recoil peak (where most of the momentum transfer is taken by the target nucleus). In absolute value, the magnitudes of these peaks are in agreement with the experimental data, however a small shift of about 5° of the binary peak and a grater shift of about 20° of the recoil peak may be detected. One may also observe, that the semiclassical binary peak is slightly wider than the experimental one.

In the perpendicular plane, the magnitude of the theoretical FDCS is the same as in the experiments, but the structure shows some discrepancies. While the theory produces three maxima at 72°, 180° and 288°, in the experimental data the central maximum is missing (probably only because of the dead angle of the detector), and the positions of the other two maxima is not clear.

Compared to other theoretical results included in Fig. 1, like CCC calculations [7] or the recent GA calculation with post-collision interactions included [11], the present semiclassical results show worst agreement with the experiments in the scattering plane. This may be understood by taking into account that the present calculations have been made by an approximation which separates the behavior of the projectile and the target atomic system. However, in the perpendicular plane the predicted structure differs from those predicted by other theories, which lead only to one maximum at 180°, because we reproduce the experimentally observed maxima at 75° and 285°. In this plane the present results are closer to the experimental observations.

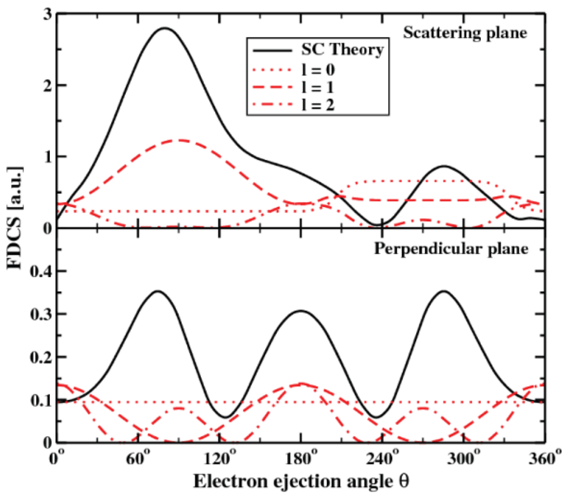


**Figure 2.** Multipole contributions to the ionization cross sections in scattering (top) and perpendicular (bottom) planes for the same case as Fig. 1 in comparison with the FDCS values of the present theory (solid line). Cross sections for different transition mechanisms are drawn separately (see text).

In order to clarify which type of transitions are responsible for the obtained structures, a partial wave analysis has been performed. Cross sections corresponding to different terms of the multipole expansion series are shown in Figure 2. The top panel of the figure shows the situation in the scattering plane. Here, 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 ($l = 0$). 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 Fig. 2) all $l \leqslant 2$ terms are responsible for the shape of the electron emission pattern. Here, the $l = 2$ term produces the three maxima at $\theta = 90°$, 180° and 270°. Two of them are shifted to 75° and 285° approximately, due to the interferences with other multipole terms. Terms with $l \geqslant 3$ have negligible contribution to the FDCS values in the perpendicular plane, too.

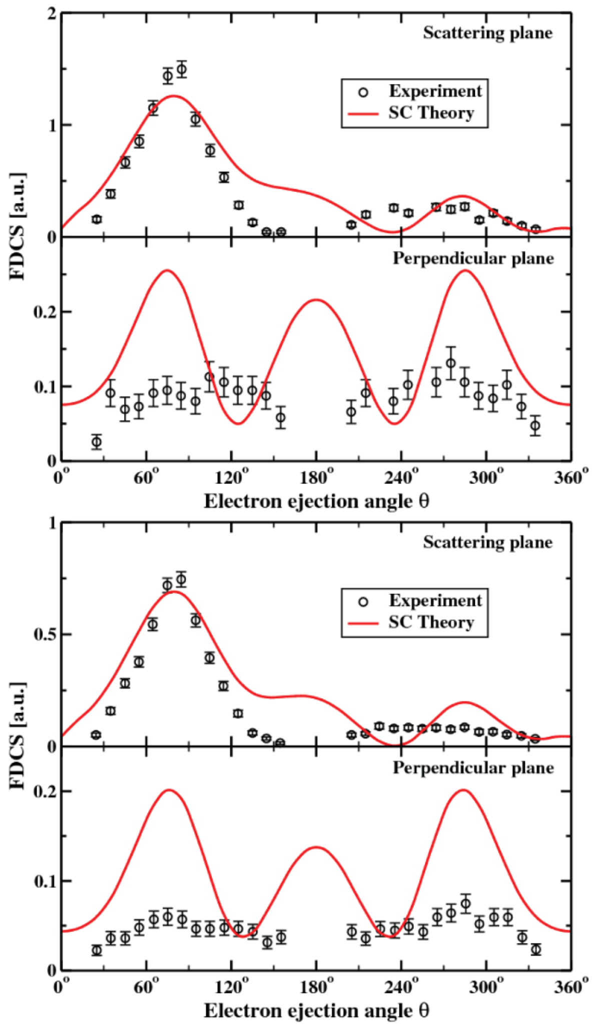


**Figure 3.** Same as Fig. 1 but for the momentum transfer $q = 0.75$ a.u. (top) and $q = 1.0$ a.u. (bottom), respectively. The ejected electron energy is $E_e = 10$ eV in both cases.

In Figure 3 semiclassical FDCS results are shown for momentum transfers of $q = 0.75$ a.u. and $q = 1.0$ a.u., respectively. The ejected electron energy remains the same as in previous case. In the scattering planes, the semiclassical model describes well the collision processes with higher momentum transfers. As in the previous case, the magnitudes of binary and recoil peaks are in agreement with the experiments. In contrast, in the perpendicular plane, as the momentum transfer grows, the semiclassical FDCS becomes systematically greater than the measured ones.

It has to be noted that the shoulder structure appearing in the scattering plane around $\theta = 150°$–180° for all momentum transfers may be explained by the partial wave analysis. As one may observe in Fig. 2 the $l = 2$ term has a maximum in this range. The contribution of this term becomes more significant in case of higher momentum transfers producing more visible shoulders in the semiclassical FDCS data.

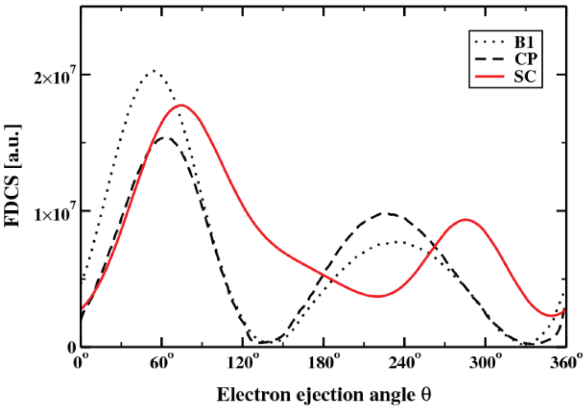


**Figure 4.** FDCS for ionization of helium by 500 keV antiproton impact as a function of the ejected electron angle in scattering plane for the ejected electron energy of $E_e = 5$ eV and the momentum transfer $q = 0.4$ a.u. First Born and CP calculations results of McGovern et al. [12] are represented by dotted and dashed lines respectively, while our semiclassical results are drawn with continuous lines.

In the last years the theoreticians' attention has been directed to negatively charged antiproton projectiles [12]. In order to show the limits of the semiclassical approximation, FDCS for ionization produced by 500 keV antiproton projectiles are calculated and compared with the theoretical data of McGovern et al. [12]. The velocity of this projectile is almost half of the previous electron projectile velocity. Figure 4 shows this comparison only in the scattering plane. In absolute value, the magnitudes of the binary and recoil peaks are accurately reproduced by the semiclassical calculations. However large angular shift of the positions of these maxima compared to the first Born and coupled pseudostate (CP) formalism calculations may be observed.

Our model takes into account explicitly the projectile-target nucleus interaction, but lacks a precise description of the post-collision interactions of the ejected electron with the projectile. As a consequence, in comparison with other theories, our model does not bring improvement in the scattering plane for the presented moderate velocity collisions. As it was shown in our previous paper [16], for high energy collisions our model leads to good results also in this plane. However, also for the present moderate velocity projectiles, we can reproduce the structures observed in the perpendicular plane, unexplained by the other theories. By the present calculations we have shown once again, that the experimentally observed structures in the perpendicular plane may be reproduced theoretically, and are partly caused by the projectile-nucleus interaction.

## 4. Conclusions

The theoretical model based on the first-order semiclassical impact-parameter approximation for calculating fully differential single ionization cross sections of helium, measured by coincidence experiments, has been applied to negatively charged fast projectiles. The method has been tested in the case of 1 keV electron and 500 keV antiproton projectiles. The origin of the obtained structures has been analyzed by means of partial waves and it was concluded that interferences between the multipole expansion terms are important to understand the exact structure of the electron emission patterns.

In case of the faster electron projectiles, except for a small angular shift in the peaks' positions, the obtained scattering plane results show good agreement with the experiments [7] and other theories [7, 11]. At the same time, the scattering plane results obtained for slower antiproton projectiles show larger shifts of the binary and recoil peaks in comparison with other theories [12]. In the perpendicular plane, for small momentum transfers the magnitude of the semiclassical FDCS is the same as in experiments, and the predicted structure seems to be closer to the experiment than that predicted by other theories. The semiclassical theory shows that the projectile-target nucleus scattering included into the model may be partially responsible for the FDCS structures in the perpendicular plane. For higher momentum transfers the discrepancy between experiments and theory grows.

One of the advantages of our semiclassical model relative to other theories is its simplicity and low computer time requirement. Because it does not take into account the post-collision interactions, for the presented moderate velocity collisions our results in the scattering plane do not reproduce exactly the experiments. However, the main advantage of our method is revealed in the perpendicular plane, where the experimentally observed structures are reproduced only by our model.

Therefore, by these calculations it was evidenced that the semiclassical model is able to treat complex many-body problems in the case of negatively charged projectiles, too.

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