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Theoretical investigations on the projectile coherence effects in fully differential ionization cross sections*

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Abstract. We propose a theoretical investigation method for testing the effect of the projectile beam coherence on single ionization processes in light atoms. The method is carried out in the framework of a first-order approximation, and the results are tested for single ionization of helium produced by fast charged projectiles. Based on the same ionization amplitudes fully differential cross section calculations are performed for coherent and incoherent projectile beams. Projectile coherence effects are investigated through these fully differential cross sections and the interference effects are evidenced through cross section ratios. The obtained results are compared to the available experimental data. By these calculations we confirm that projectile coherence effects may have important role in these ionization processes.

1 Introduction

Fully differential cross sections (FDCS) give us the most complete information about an ionization process. After the development of the reaction microscopes [1] a great interest has been focused on measuring and calculating this quantity for different ionization processes. Regarding this topic, one of the most discussed processes is the ionization of helium by fast charged projectiles [2–6]. Despite of the existence of many theoretical descriptions, significant discrepancies between measured and calculated FDCS values have been reported. It was thought that partly the projectile-target nucleus scattering [5,7] and partly the experimental uncertainties [8,9] are responsible for these discrepancies.

In the last few years, the effect of the projectile beam coherence on ionization processes has been experimentally studied. In this sense, the first experiment has been performed in case of molecular H_2 target [10]. Later, qualitative differences in case of ionization of helium by fast charged projectiles depending on the projectile beam coherence have been reported [11], as well. FDCS for ionization of He by 3 MeV proton impact have been measured, with projectile beam of a coherence length larger than typical atomic scales. Compared to the incoherent 100 MeV/u C^{6+} projectile beam pronounced differences have been observed.

In the present work we propose a theoretical investigation method for testing the effect of the projectile beam coherence on single ionization processes by calculating FDCS with quantum mechanical and impact parameter approximations. The main idea is to use in both cases the same ionization amplitudes, calculated in first order impact parameter approximation. The calculated coherent and incoherent cross sections for ionization of He by 100 MeV/u C^{6+} projectile beam are compared to the existing coherent and incoherent measurements in different electron ejection planes. The interference effects in the coherent projectile beam are evidenced by analyzing the coherent and incoherent FDCS ratios, as well.

In the following section the proposed method is presented by describing the calculation of ionization amplitudes, and the calculations of the incoherent and coherent FDCSs by impact parameter and quantum mechanical methods, respectively. The third section presents our results for the ionization of He by 100 MeV/u C^{6+} projectiles in comparison to existing experimental data. The final conclusions are drawn in the last section of the paper.

2 Theoretical model

The proposed method for theoretical investigation of projectile coherence effects consists of two parts. First, ionization amplitudes are calculated by a suitable method, and second, using the ionization amplitudes coherent and incoherent cross sections are calculated. These coherent and incoherent cross sections are also compared through their ratio, which emphasizes the interference effects [11].

In the following, these steps are discussed in detail in case of ionization of helium by 100 MeV/u C^{6+} projectile

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beam. The amplitudes are calculated in the framework of the first-order, semiclassical approximation.

In these calculations standard spherical coordinates are used. The coordinate system is determined by the directions of the projectile momentum $\mathbf{p}_0$ and the momentum transfer $\mathbf{q}$. Namely, the polar angle θ is measured relative to the projectile beam direction and the azimuthal angle $\phi = 90°$ coincide with the direction of the transverse component of $\mathbf{q}$. Accordingly, the so-called scattering plane is spanned by $\mathbf{p}_0$ and $\mathbf{q}$, characterized by $\phi = \pi/2$ or $3\pi/2$. Further, the azimuthal plane is perpendicular to the projectile beam and it is characterized by $\theta = \pi/2$. Finally, the plane perpendicular to the momentum transfer is given by $\phi = 0$ or π.

2.1 Ionization amplitudes

The ionization of helium by fast charged projectiles is described in the framework of the first-order, impact parameter approximation [5]. According to this model the projectile is treated separately, and only the target electron system is described by time-dependent Schrödinger equation. Then, ionization probability amplitudes are calculated using the first-order time dependent perturbation theory. In these calculations the initial state of the two-electron system is described by a Hartree-Fock wavefunction [12]. The final state is described by a symmetric combination of a hydrogen-type and a continuum radial wavefunction, which is calculated in the mean field of the final He^+ ion. Therefore, the ionization probability amplitude is reduced to a one-electron amplitude

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

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 interaction between projectile and active electron. The projectile velocity is denoted by v and the integral is calculated through classical trajectory along z axis considered to be a straight line, and characterized by the impact parameter vector $\mathbf{B}$.

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

2.2 Cross sections

In calculating FDCS for ionization of helium by fast charged projectiles two ways are arising.

On one hand, the *impact parameter approximation* [5,13] can be used. According to this approximation, the FDCS relative to the perpendicular momentum transfer value $\mathbf{q}_\perp$, ejected electron energy E and electron ejection solid angle Ω are obtained by the relation

$$\frac{d^3\sigma_{\rm inc}}{dE\, d\Omega\, d\mathbf{q}_\perp} = B\left|\frac{dB}{d\theta}\right|\left|\sum_{l_f,m_f} a^{(1)}_{l_f,m_f}(\mathbf{B})\right|^2, \quad (2)$$

where θ denotes the polar angle of the ejected electron.

In order to calculate the ionization FDCS (2) impact parameter values to a certain momentum transfer have to be asigned. This task may be completed in two successive steps.

First, the projectile scattering angle is calculated according to the transverse momentum balance [1], which states that the momentum transfer is the sum of the transverse components of electrons and residual ions momenta. Moreover, if we suppose that the momentum transfer is modifying only the direction of the projectile momentum vector (valid for fast projectiles), we get the projectile scattering angle

$$\theta_{\rm proj} = \frac{\sqrt{p^2\sin^2\theta + q^2 - 2pq\sin\theta\cos\left(\phi - \frac{\pi}{2}\right)}}{p_0}, \quad (3)$$

where p and p_0 denotes the moduli of the ejected electron and projectile momentum, respectively. In this case the momentum transfer $\mathbf{q}$ is practically perpendicular to the projectile momentum, and coincides with $\mathbf{q}_\perp$. This calculation assumes that in case of electrons ejected into binary peak region the most of the momentum transfer is taken by the electron. However, in case of the recoil peak region most of the momentum transfer is taken by the target nucleus.

Second, impact parameter values B to projectile scattering angles $\theta_{\rm proj}$ have to be assigned. In order to achieve this goal, the projectile scattering is treated as a classical potential scattering problem in the field of the target helium system [14]. 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 [15]. Using this potential, the projectile scattering angles as a function of the impact parameter value can be calculated numerically. The technical details of this calculations are discussed in detail in reference [13].

By the above described impact parameter method each particle from the projectile beam is characterized by a single impact parameter value. Therefore, no coherence exists between different impact parameters.

On the other hand, the ionization FDCS can be calculated by a method used in *quantum scattering theory*, as well. According to this approach [16], the scattering matrix element is calculated by the inverse Fourier transform

$$R(\mathbf{q}_\perp) = \frac{1}{2\pi}\sum_{l_f m_f}\int d\mathbf{B}\, e^{i\mathbf{B}\mathbf{q}_\perp} B^{2i\frac{Z_p Z_t}{v}} a^{(1)}_{l_f m_f}(\mathbf{B}), \quad (4)$$

where $B^{2i\frac{Z_p Z_t}{v}}$ is a phase factor representing the internuclear potential. The FDCSs are then obtained as

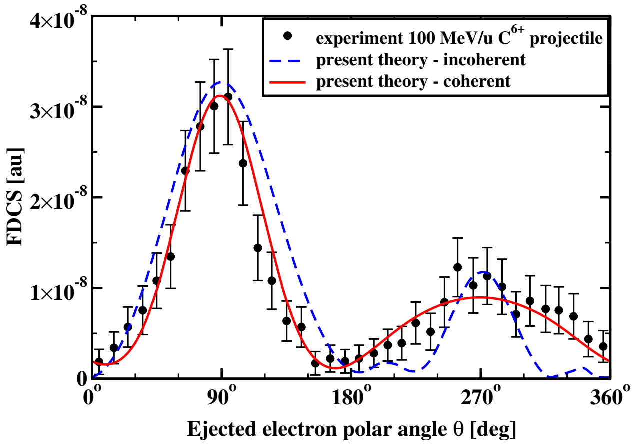

Fig. 1. Experimental [2] and theoretical FDCS for ionization of He by 100 MeV/u C^{6+} impact. The electron is ejected in scattering plane with energy $E_e = 6.5$ eV, and the momentum transfer is $q = 0.75$ a.u.

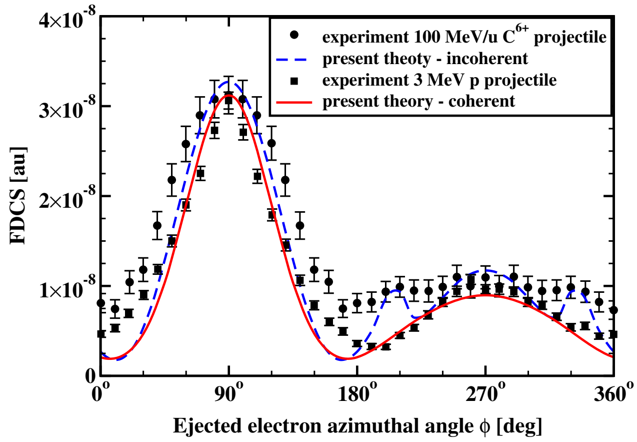

Fig. 2. Comparison of coherent and incoherent FDCS's in azimuthal plane for the same process as in Figure 1. Experimental data for incoherent 100 MeV/u C^{6+} projectile beam is by [2] and for coherent 3 MeV proton projectile beam is from [11].

the square of modulo of the scattering matrix element

$$\frac{d^3\sigma_{\rm coh}}{dE\, d\Omega_e\, d\mathbf{q}_\perp} = p_0\, |R(\mathbf{q}_\perp)|^2 . \qquad (5)$$

By these quantum mechanical calculations the projectile beam is described as a coherent plane wave. Consequently, interference may occur between the ionization obtained for different impact parameters.

3 Results and discussion

The above presented model is used to calculate coherent and incoherent FDCS for ionization of He produced by 100 MeV/u C^{6+} impact, ejected electron energy of $E_e = 6.5$ eV and momentum transfer of $q = 0.75$ a.u. The experimental data [2] for this process in the scattering plane is presented with solid circles in Figure 1. It shows a double-peak structure with a binary-peak at $\theta = \pi/2$, where most of the momentum transfer is taken by the electron, and a recoil peak at $\theta = 3\pi/2$, where most of the momentum transfer is taken by the target nucleus.

According to our model described in the previous section, the incoherent FDCS's are calculated first. For this reason, impact parameter values are assigned to the momentum transfer $q = 0.75$ a.u. Based in equation (3) the projectile scattering angles for this scattering process have values of $\theta_{\rm proj}^{\rm binary} = 4.2073 \times 10^{-8}$ rad and $\theta_{\rm proj}^{\rm recoil} = 1.0337 \times 10^{-6}$ rad for binary and recoil peaks, respectively. As discussed in detail in reference [13], the numerical solution of the classical scattering integral results in impact parameters corresponding to these binary and recoil scattering angles of $B^{\rm binary} = 2.47$ a.u. and $B^{\rm recoil} = 0.68$ a.u.

The results of the incoherent FDCS calculations are shown with dashed line in Figure 1. The double-peak structure is reproduced well by these calculations, however compared to the experimental data discrepancies are present mostly in the recoil peak region due to the approximations used in description of the projectile scattering process.

As a second step, the coherent calculations are performed. Here, no impact parameter information is needed, while in equation (4) there is an integration over the impact parameter vector. The obtained results are presented with continuous line on Figure 1, which fits almost perfectly the experimental data.

The results become more interesting if we turn our look into the azimuthal plane. These data are shown in Figure 2. Here, two different experimental data are presented. Solid circles represent measurements by [2] for incoherent 100 MeV/u C^{6+} projectile beam. In addition, solid rectangles are scaled experimental results by [11] for coherent 3 MeV proton projectile beam. On theoretical side, again we have coherent (continuous line) and incoherent (dashed line) calculations for the 100 MeV/u C^{6+} projectile beam.

As one can observe in Figure 2, the coherent theoretical data is in great agreement, with the coherent experimental data. Moreover, the incoherent theoretical FDCS are also close to the incoherent measurements. However, due to the incomplete description of the projectile scattering in case of incoherent impact parameter calculations additional small oscillations causing discrepancies in shape exists mostly around azimuthal angles of $\phi = 220°$ and $320°$.

Further, experimental and theoretical data for electron ejected perpendicular to the momentum transfer are compared in Figure 3. Here, the most important feature we have to mention is that the coherent data in this plane is almost isotropic in contrast to the experimental data and incoherent calculations, which shows strong maxima around $\theta = 80°$ and $280°$ polar angles. However, it has to be mentioned that the incoherent calculations are smaller in magnitude than the experimentally measured FDCS's. These results confirm, that up to our theoretical description the projectile coherence effects are partly responsible for the observed FDCS pattern in the perpendicular plane.

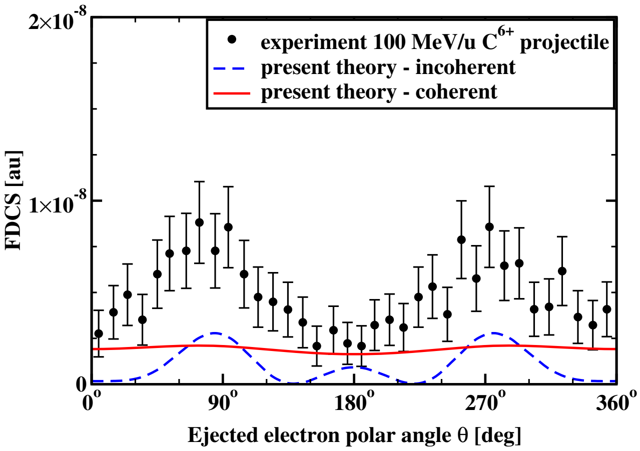

Fig. 3. Comparison of coherent and incoherent FDCS's in perpendicular plane for the same process as in Figure 1.

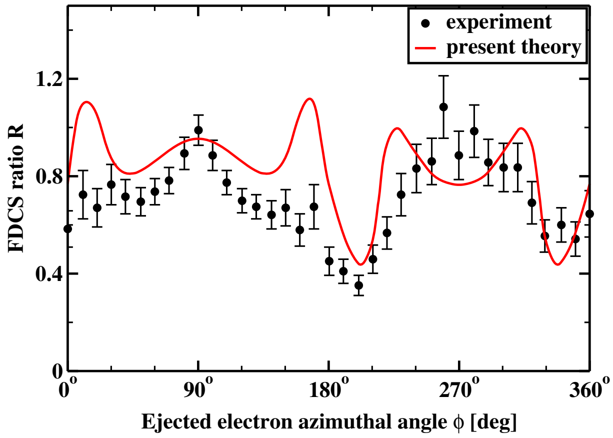

Fig. 4. Coherent to incoherent FDCS ratios in the azimuthal plane. The experimental ratios are taken from [11].

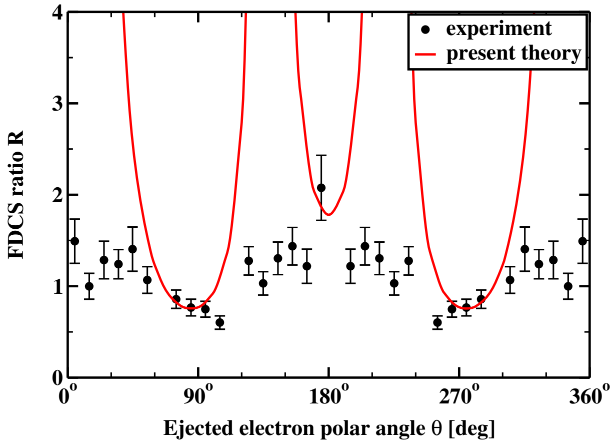

Fig. 5. Coherent to incoherent FDCS ratios in the perpendicular plane. The experimental ratios are taken from [11].

Therefore, our result remains also consistent with the presumptions, that experimental uncertainties are also responsible for the electron ejection structure observed in this plane [3,17].

In addition to these results, the coherent and incoherent cross sections may be compared through the ratio $R = d^3\sigma_{\rm coh}/d^3\sigma_{\rm inc}$. An oscillation trend of this quantity may lend support to the interpretation that the FDCS for the coherent beam are significantly affected by interference effects. This trend has been observed experimentally in case of ionization FDCS's in azimuthal and perpendicular planes [11]. Accordingly, in the framework of our theoretical approach we will focus to these planes and calculate the coherent/incoherent cross section ratios.

The results in azimuthal plane in comparison to the available experimental data [11] are presented in Figure 4. Here it has to be mentioned that in case of experiments, R is defined as the FDCS ratio measured in case of coherent 3 MeV proton and incoherent 100 MeV/u C^{6+} projectile beams. The theoretical FDCS ratios are calculated using the results of coherent and incoherent calculations for 100 MeV/u C^{6+} projectile beams. As one may observe, the theoretical pattern follows the oscillation trend of the experimental data, which confirms the existence of interference effects in the coherent beam. However, there are small additional oscillations in theoretical data which may be caused by the rough approximations used in incoherent, impact parameter calculations.

Finally, the electron ejection plane perpendicular to the momentum transfer is analyzed, as well. Here, the agreement of the theoretically calculated and experimentally measured interference terms are reduced to a small polar angle intervals around $\theta = 80°$, $180°$ and $280°$. This may be explained if we take into account that in other regions the incoherent calculations result in close to zero FDCS values. We think, that the inclusion of the experimental uncertainties [3,17] may increase these cross sections and, accordingly, the ratios may be closer to the experimental ones.

4 Conclusions

In conclusion, we have proposed a theoretical investigation method for testing the effect of the projectile beam coherence on single ionization processes of light atoms. The model consists of calculating FDCSs with quantum mechanical and impact parameter approximations based on the same ionization amplitudes. The calculated coherent and incoherent cross sections for the ionization of He by 100 MeV/u C^{6+} projectile beam have been compared to the available experimental data. The best agreement has been obtained in the azimuthal plane, where coherent and incoherent measurement data are also available. In agreement with the measurements, the comparison of the theoretical FDCS suggested significant differences between the result of coherent and incoherent calculations. These differences, and the existence of interference effects in the coherent beam have been investigated through coherent and incoherent FDCS ratios, as well. In agreement with the experimental findings [11] the results of our theoretical model suggests, that these interferences are present due to the coherent sum of impact parameter-dependent partial wave amplitudes. Based on our theoretical results in the plane perpendicular to the momentum transfer we have concluded that the experimental uncertainties [3,17] may also be partly responsible for the electron ejection structure in this plane.

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