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Singly differential electron emission cross sections for ionization of helium by protons

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Abstract

Angular differential cross sections are calculated for electrons emitted in proton–helium collisions within the framework of the time-dependent coupled channel-method. The channel wave functions are constructed from Slater functions and Coulomb wave packets. As projectiles we consider protons with energies between 0.3 and 1.5 MeV. We compare our results with experimental data and other theoretical calculations using the first Born approximation, different distorted wave models and classical trajectory Monte Carlo simulations.

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1. Introduction

In this work we extend our one-center coupled-channel (CC) method to calculate angular differential cross-section of the electrons ejected in single ionization of helium by proton impact. We compare our CC calculations with experimental data [1] and other theories. According to our knowledge, there are no angular differential cross section calculations available for ionization of atoms by impact with multiply charged ion projectile using this method until now. Our CC method was previously successfully used to calculate single- and double-ionization total cross sections of helium in heavy ion collisions [2,3], and later for photo-ionization of helium with short intense XUV laser pulses [4].

As basis set for the channels we use configuration interaction (CI) wave functions built up from

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Slater-like orbitals to describe the helium bound states and regular Coulomb wave packets to have a discrete representation of the single and double electron continuum. The projectile is considered as a point charge without inner structure and moves on a straight-line which is sometimes referred to as semiclassical approximation. For projectile–electron interaction the time-dependent Coulomb potential is used. With the help of the density operator we calculate the angular distribution of the electron emission probability. The integration of the probability distribution over the impact parameter gives us the angular differential cross sections, the new aspect in this work. Atomic units are used throughout the paper unless otherwise mentioned.

2. Theory

2.1. Coupled-channel method

The coupled-channel method has been widely used in various fields of atomic collision physics with the recognition that it is one of the most reliable and powerful theoretical approaches. Our single-center coupled-channel code has been introduced in detail in previous works [2,3] and we give here only a brief summary. The time dependent wave function is represented by the expansion

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,t)=\sum_{j=1}^{N}a_j(t)\Phi_j(\mathbf{r}_1,\mathbf{r}_2)\mathrm{e}^{-\mathrm{i}E_jt}, \tag{1}$$

where $\Phi_j(\mathbf{r}_1,\mathbf{r}_2)$ are the eigenfunctions of the unperturbed helium Hamiltonian, determined through a diagonalization procedure. This configuration interaction (CI) wavefunction $\Phi_j(\mathbf{r}_1,\mathbf{r}_2)$ is in our calculations a finite linear combination of symmetrized products of single particle wave functions built up from Slater-like orbitals and Coulomb wave packets. The wave packets are constructed by an integral over the regular radial Coulomb wave function in a well-defined finite energy interval. The method of calculating the wave packets and matrix elements is described in [2]. The width and the number of the packets included in the basis cannot be fixed a priori and depend strongly on the properties of the collision system. Inserting Eq. (1) into the time-dependent Schrödinger equation leads to a system of first-order differential equations for the expansion coefficients

$$\frac{\mathrm{d}a_k(\mathbf{b},t)}{\mathrm{d}t}=-\mathrm{i}\sum_{j=1}^{N}V_{kj}(\mathbf{b},t)\mathrm{e}^{\mathrm{i}(E_k-E_j)t}a_j(t)\quad(k=1,\ldots,N), \tag{2}$$

where $a_k(\mathbf{b},t)$ are the impact parameter ($\mathbf{b}$) dependent state amplitudes and $V_{kj}(\mathbf{b},t)$ are the coupling matrix elements containing all the information about the collision process. E_k and E_j stand for the energy of the final and initial state, respectively. As initial condition we consider that only the ground state ($j=1$) is populated. To determine the total cross section we integrate over all impact parameters,

$$\sigma_k=2\pi\int|a_k(\mathbf{b},t\to\infty)|^2\mathrm{d}^2b. \tag{3}$$

In order to separate the excitation, double-ionization and single-ionization cross sections from each other, we use a Feshbach projection method [2,3].

One can determine the electron final-state density from the time dependent wave function after the collision ($t\to\infty$) as the expectation value of the density operator $\hat{\rho}=\sum_{i=1,2}\delta(\mathbf{r}-\mathbf{r}_i)$ for a fixed impact parameter

$$\rho_{\mathbf{b}}(\mathbf{r})=\left\langle\Psi(\mathbf{r}_1,\mathbf{r}_2,t\to\infty)\left|\sum_{i=1,2}\delta(\mathbf{r}-\mathbf{r}_i)\right|\Psi(\mathbf{r}_1,\mathbf{r}_2,t\to\infty)\right\rangle. \tag{4}$$

In order to extract the angular distribution of the ionized electron two additional operations are needed:

(1) We project the wave function Ψ onto the single-ionization continuum $|\Psi_{\mathrm{ion}}\rangle=(1-\widehat{P}_{\mathrm{b}}-\widehat{P}_{\mathrm{di}})|\Psi\rangle$ where $\widehat{P}_{\mathrm{b}}$ is the projector onto the bound state subspace and $\widehat{P}_{\mathrm{di}}$ is the projector onto double-ionized states.

(2) The radial and the azimuthal coordinates have to be integrated over to get the polar angle distribution of the ionized electrons:

$$P_{\mathbf{b}}(\theta) = \frac{1}{2\pi}\int_0^{2\pi}\int_0^{\infty}\langle \Psi_{\text{ion}}|\sum_{i=1,2}\delta(\mathbf{r}-\mathbf{r}_i)|\Psi_{\text{ion}}\rangle r^2\,\mathrm{d}r\,\mathrm{d}\varphi$$
$$= \frac{1}{\pi}\int_0^{2\pi}\int_0^{\infty}\int_{\mathbf{r}_1}|\Psi_{\text{ion}}(r,\theta,\varphi;\mathbf{r}_1)|^2 d^3r_1 r^2\,\mathrm{d}r\,\mathrm{d}\varphi. \quad (5)$$

The angular differential cross section is obtained by integrating $P_{\mathbf{b}}(\theta)$ over the impact parameter. A more detailed description of the method can be found in [5].

2.2. The CDW and CDW-EIS method

Despite of the well-known limitations, continuum distorted wave (CDW) theories provide an adequate framework to treat the electron emission from atomic targets under energetic heavy ion impact [6]. The CDW [7] and its hybrid version, the continuum distorted wave with eikonal initial states (CDW-EIS) [8] model, have been studied in detail. In the CDW approximation the initial and final states of the target are distorted by continuum Coulomb wave factors so that the full wavefunction satisfies the correct boundary conditions [7]. The ionization process is sensitive to this feature as the emitted electron evolves in the combined Coulomb fields of the projectile and the residual target-ion. However, the CDW model is known to overestimate the experimental data at intermediate energies, due to the lack of normalization of the initial state [8]. This failure is corrected in the CDW-EIS approximation by using Eikonal distortions for the initial state at the expense of neglecting higher order terms in the projectile fields. These models were extended within the frame of the independent electron model to multi-electronic targets [9] and generalized recently by introducing a more appropriate representation of the bound and continuum target states [10,11].

2.3. The CTMC method

In the present CTMC approach, Newton's classical non-relativistic equations of motion for a three-body system are solved numerically for a statistically large number of trajectories [12–14]. The three particles in our model were chosen as follows: the projectile, an atomic electron and the helium ion (He^+). The target potential of the helium is represented by a central model potential developed by Garvey et al. [15] which is based on Hartree–Fock calculations. The initial conditions are selected as described by Reinhold and Falcon [16] for non-Coulombic systems. The initial state of the target is characterized by a microcanonical ensemble which is constrained to an initial binding energy of 0.903 a.u. The equations of motion were integrated with the standard Runge–Kutta method. The angular differential cross sections for single-ionization were computed with the formula

$$\frac{\mathrm{d}\sigma_{\text{i}}}{\mathrm{d}\Omega} = \frac{2\pi b_{\max}\sum_j b_j^{(\text{i})}}{N\Delta\Omega}. \quad (6)$$

The standard deviation for a cross section is given by

$$\Delta\sigma_{\text{i}} = \sigma_{\text{i}}\left(\frac{N-N_{\text{el}}}{NN_{\text{i}}}\right)^{1/2}. \quad (7)$$

In Eqs. (6) and (7) N is the total number of trajectories calculated for impact parameters less than $b_{\max}$, N_{i} is the number of trajectories that satisfy the criteria for ionization, $b_j^{(\text{i})}$ is the impact parameter where the criteria for ionization are fulfilled, and $\Delta\Omega$ is the emission solid angle interval of the ionized electron.

3. Results and discussion

We calculate the angular differential cross section for electrons emitted in single-ionization processes for the p^+ + He system at energies between 300 keV and 1.5 MeV. We present our CC results together with experimental data [1] and calculations of other theories such as the Continuum Distorted Wave (CDW) [7], Continuum Distorted Wave Eikonal Initial State (CDW-EIS) [10] , first Born approximation (FBA) and Classical Trajectory Monte Carlo (CTMC) [14].

Table 1 presents the experimental total cross sections compared with our calculations. The experimental data include contributions from both single- and double-ionization processes. However, for the present collision system contributions from

Table 1
Angle-integrated single-ionization total cross sections (in units of 10^{-17} cm^2) for proton–helium collision

Energy (MeV)	Exp.	CC	CTMC	1. Born	CDW-EIS
0.3	7.14[a]	3.11	4.83	5.50	5.54
	5.29[b]	3.11	4.83	5.50	5.54
	7.16[c]	3.11	4.83	5.50	5.54
0.5	4.46[a]	3.71	3.27	3.82	3.84
1.0	1.94[a]	1.82	1.79	2.24	2.24
1.5	1.66[a]	1.60	1.20	1.61	1.61

Different experimental data for 300 keV collision energy, (a), from Rudd (b), from Toburen and (c), from Stolterfoht are taken from [1].
Note that the difference between CDW-EIS and CDW data is less than 3% and not listed here.

the double-ionization channels are less than 5% and thus negligible. In cases where double-ionization would be more prominent the second electron would contribute to the forward scattering in the case of a two-step process and would be isotropically distributed in the case of a shake-off.

Fig. 1 displays the angular differential cross sections for the collision energy of 300 keV. Our CC calculation underestimates the experimental data by a factor of 2 at small scattering angles ($\theta \leqslant 50°$). This effect is due to the fact that we have only a single-center model. At this projectile energy the projectile-centered continuum states have a non-negligible contribution to target ionization.

In Fig. 2 we present the results for 500 keV proton impact. At low scattering angles no experimental data are available. The CC calculation and the first Born approximation give the lowest cross section near 0°. At about 60° all the quantum mechanical models, except for the CC calculation, display a maximum. The CDW and CDW-EIS models explain this phenomenon within the framework of a binary encounter (BE) collision. Our CC calculation yields an approximative constant value for the cross section between the scattering angles 30° and 70°. For angles larger than 70°, the CC curve slightly underestimates the experimental data. Above 80° all quantum mechanical models

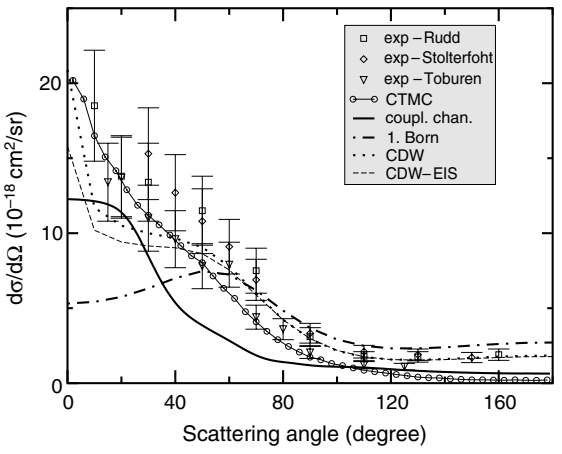

Fig. 1. Angular differential cross sections for electrons emitted in 300 keV proton–helium collisions. Open squares, diamonds and triangles are experimental data, hollow circles: CTMC, solid line: coupled-channel, dot-dashed line: first order Born approximation, dotted line: CDW, thin dashed: CDW-EIS.

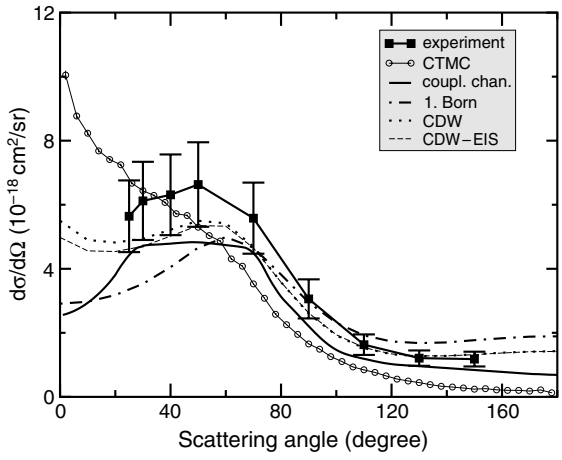

Fig. 2. Angular differential cross sections for electrons emitted in 500 keV proton–helium collisions. Full squares: experiment, hollow circles: CTMC, solid line: coupled-channel, dot-dashed line: first order Born approximation, dotted line: CDW, thin dashed: CDW-EIS.

are in satisfactory agreement with the experimental data, while the CTMC underestimates the cross sections by 30%.

Fig. 3 shows the calculations and the experimental data for 1 MeV proton energy. At small angles the CDW, CDW-EIS and the FBA underestimate the experimental data by a factor of 1.5. The CC method gives a better result at this energy, but the theoretical curve has a smaller peak than the experimental one and is shifted to the forward direction. The CDW, CDW-EIS and the FBA have a BE peak again at 70°, while the experimental curve has its maximum at about 60°. The experimental distribution at this energy is shifted forward compared with the theoretical FBA predictions which may imply the presence of a very weak two-center effect. It is interesting that in this case the CDW models also underestimate the two-center effect and the post-collision interaction contribution.

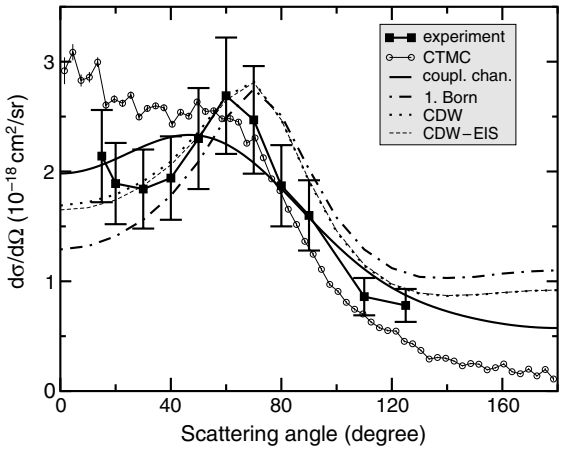

Fig. 3. The same as Fig. 2 but for 1 MeV proton energy.

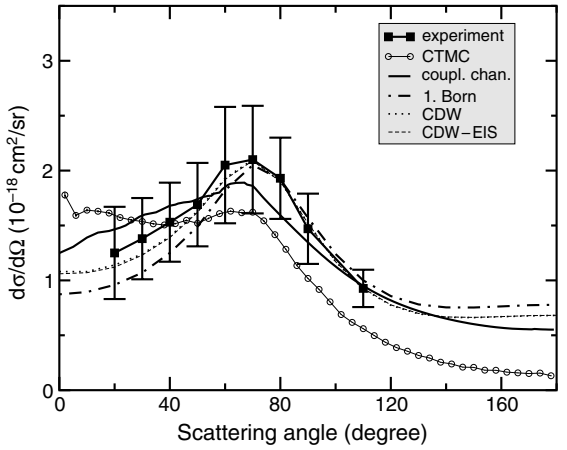

Fig. 4. The same as Fig. 2 but for 1.5 MeV proton energy.

Fig. 4 presents the calculations and the experimental data for 1.5 MeV impact energy. All the quantum mechanical results agree with the experimental data. The CTMC systematically underestimates the cross sections by a factor of about 3 at large angles due to the lack of non-classical dipole emission channels [17].

4. Summary

The coupled-channel method has been used to calculate the angular differential cross sections of single-ionized electrons emitted in proton–helium collisions. The choice of the collision systems was dictated by the available experimental data. Our results for 0.3, 0.5, 1 and 1.5 MeV proton impact energies have been compared with results from different other theoretical methods. The angular differential cross sections calculated with the coupled-channel method are in reasonable agreement with the experimental data. Further work is in progress to calculate single differential cross sections of helium in antiproton collisions.

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