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Total and angular differential cross sections of electrons emitted in collision between antiprotons and helium atoms

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Abstract

We present total and angular differential single-ionization cross sections for antiproton–helium collisions in the energy range of 1–1000 keV within the framework of time-dependent coupled-channel-, a continuum distorted wave eikonal initial state and classical trajectory Monte Carlo methods. The results are compared with other theoretical results and experimental data.

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1. Introduction

The investigation of the low energy antiproton–helium collision is a challenging task both from theoretical and experimental points of view. In the last decade, a large number of non-perturbative studies have been performed to explain experimental single- and double-ionization total cross sections (Andersen et al., 1990; Hvelplund et al., 1994). The forced impulse method (FIM) (Ford and Reading, 1994) presents one of the most successful approaches to explaining proton– and antiproton–helium collisions. An improved version of the FIM is the multi-cut forced impulse (MFIM) method (Reading et al., 1997). The multi-electron hidden crossing (MEHC) theory is also used to study the single ionization of He in an antiproton impact (Bent et al., 1998). The time-dependent density functional theory (TDDFT) is another powerful method to describe non-perturbative many-electron ionization processes, even in the low keV/amu impact energy range (Lüdde et al., 1998; Keim et al., 2003; Tong et al., 2002).

Recently, a fully correlated three-dimensional Cartesian lattice calculation approach has been applied to study the ionization of the He atom in antiproton collisions (Schulz and Krstic, 2003). The widely used B-spline basis is a further useful tool to investigate ionization problems because of its ability to represent the electron continuum channels more accurately in comparison to other conventional bases (Sahoo et al., 2004).

On the level of independent particle models, calculations have been performed using the classical trajectory Monte Carlo (CTMC) method (Schultz, 1989; Cohen, 2004). The Coulomb distorted wave eikonal initial state (CDW-EIS) method (Fainstein et al., 1987) presented astonishingly good agreement with experimental data below 100 keV antiproton impact energies and induced a debate about the validity of CDW-EIS. Unfortunately, there are no experimental data available in the low keV energy range to clarify the validity range of the various approaches.

The aim of this paper is twofold. First, we apply our time-dependent coupled-channel (CC) method to calculate single-ionization total cross sections. Second, we compare our CC, to CDW-EIS and CTMC approach calculating angular differential ionization cross sections. Atomic units are used throughout the paper unless otherwise mentioned.

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2. Theoretical models

2.1. Coupled-channel model

The CC 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 two-electron CC method is introduced in detail in our previous works (Barna et al., 2003, 2005) and we give here only a brief summary. The time-dependent wavefunction is represented by the expansion

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

where $\Phi_j(\mathbf{r}_1, \mathbf{r}_2)$ are the eigenfunctions of the unperturbed helium Hamiltonian, determined through a diagonalization procedure. Our configuration interaction (CI) wavefunction $\Phi_j(\mathbf{r}_1, \mathbf{r}_2)$ is a finite linear combination of symmetrized single particle wavefunctions built up from Slater-like orbitals and Coulomb wave packets. The wave packets are constructed by an integral over the regular radial Coulomb wavefunction in a well-defined finite energy interval. Inserting Eq. (1) into the time-dependent Schrödinger equation leads to a system of first-order differential equations for the expansion coefficients

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

where $a_k(t)$ are the impact parameter (**b**) dependent state amplitudes and $V_{kj}(t)$ 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 states, respectively. The antiproton is assumed to move on a straight line which is sometimes referred to as semiclassical approximation. Below 10 keV impact energy, however, Coulomb hyperbolas are used. For antiproton–electron interaction the time-dependent Coulomb potential is used. As initial condition we consider that only the ground state ($k = 1$) is populated. To determine the total cross section we integrate over all impact parameters. In order to separate the excitation, double-ionization and single-ionization cross sections from each other, we use a Feschbach projection method.

One can calculate the angular differential ionization cross sections from the final-state electron density, which is determined from the time-dependent wavefunction after the collision as the expectation value of the reduced one-particle density operator.

2.2. CDW-EIS model

Despite the well-known limitations, continuum distorted wave (CDW) theories provide a useful framework to treat the electron emission from atomic targets under energetic heavy ion impact (Stolterfoht et al., 1997). The CDW (Belkić, 1978) and its hybrid version, the continuum distorted wave with eikonal initial state (CDW-EIS) (Crothers and McCann, 1983) 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. 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. 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 (Fainstein et al., 1988) and generalized by introducing a more appropriate representation of the bound and continuum target states (Gulyás et al., 1995; Gulyás and Fainstein, 1998).

2.3. CTMC model

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 (Abrines and Percival, 1966; Olson and Salop, 1977; Tőkési and Hock, 1996). The three particles in our model are chosen as follows: the projectile, an atomic electron and the helium ion (He^+). The target potential of the helium is represented by a central-field model potential (Garvey et al., 1975) which is based on Hartree–Fock calculations. The initial conditions are selected as for non-Coulombic systems (Reinhold and Falcon, 1986). The initial state of the target is characterized by a micro-canonical ensemble which is constrained to an initial binding energy of 0.903 a.u. The equations of motion are integrated with the standard Runge–Kutta method. The angular differential cross sections for single ionization are computed with the formula

$$\frac{\mathrm{d}\sigma_i}{\mathrm{d}\Omega} = \frac{2\pi b_{\max}\Sigma_j b_j^{(i)}}{N\Delta\Omega}, \tag{3}$$

where N is the total number of trajectories calculated for impact parameters less than $b_{\max}$, $b_j^{(i)}$ 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 first applied our CC method to calculate single-ionization total cross sections inn 1 keV to 1 MeV energy range. The convergence of the basis set was checked with great care. We used 1245 collision channels including different m_l sub-states. Fig. 1 presents our CC results together with experimental data and with other theories

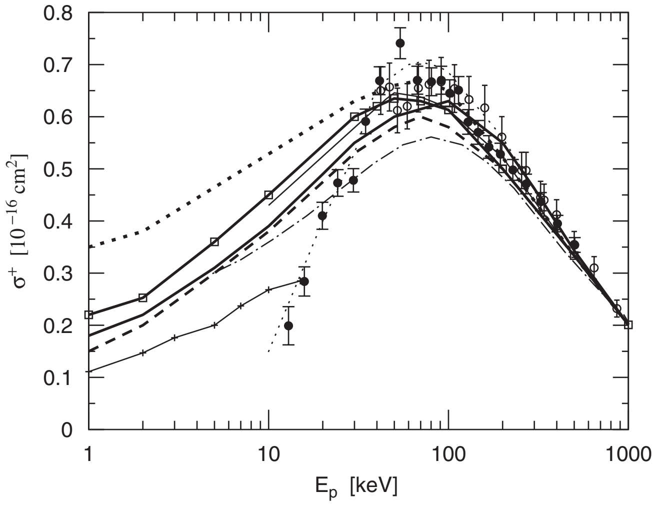

Fig. 1. Total single-ionization cross sections for antiproton–helium collisions. Open circles exp. data (Andersen et al., 1990), solid circles exp. data (Hvelplund et al., 1994), thick solid line our CC results, thick dotted line no resp. BGM, thick dashed line resp. BGM, and connected open squares v_{mod} (Keim et al., 2003), solid thin line multi-cut FIM (Reading et al., 1997), connected plus symbols MEHC (Bent et al., 1998), thin dotted line CDW-EIS (Fainstein et al., 1987), and dash-dotted thin line is from Tong et al. (2002).

(without the claim of completeness). Above an antiproton energy of 100 keV all theoretical and experimental data are in good agreement. Below 100 keV our CC data are lower than the no-response BGM results (Keim et al., 2003) and lie very close to the multi-cut FIM data (Reading et al., 1994) which agrees with our earlier observation (Barna et al., 2003) for proton–helium collisions. We hope that in the near future new experimental total cross sections will be available in the low-energy range which will help us to decide the validity of different models.

Fig. 2 presents our CC angular differential ionization cross sections for 100, 300 and 500 keV antiproton impact, compared to our CDW-EIS and CTMC results. Fig. 2(a) displays our data for 100 keV impact energy. All the three calculations have a minimum at zero scattering angle, which may indicate the existence of the anti-cusp. At about ($\theta = 60°$) both quantum mechanical model display a maximum. The CDW-EIS model explains this phenomenon within the framework of the binary encounter (BE) collision. At large backscattering angles (close to $\theta = 180°$) all three models are in a reasonable agreement.

Fig. 2(b) shows the calculated cross sections for 300 keV antiproton impact. Contrary to the 100 keV collision, both quantum mechanical calculations become much more symmetric around the maximum at about ($\theta = 60°$). A perfect forward–backward symmetry with a maximum at $\theta = 90°$ would mean a pure dipole transition.

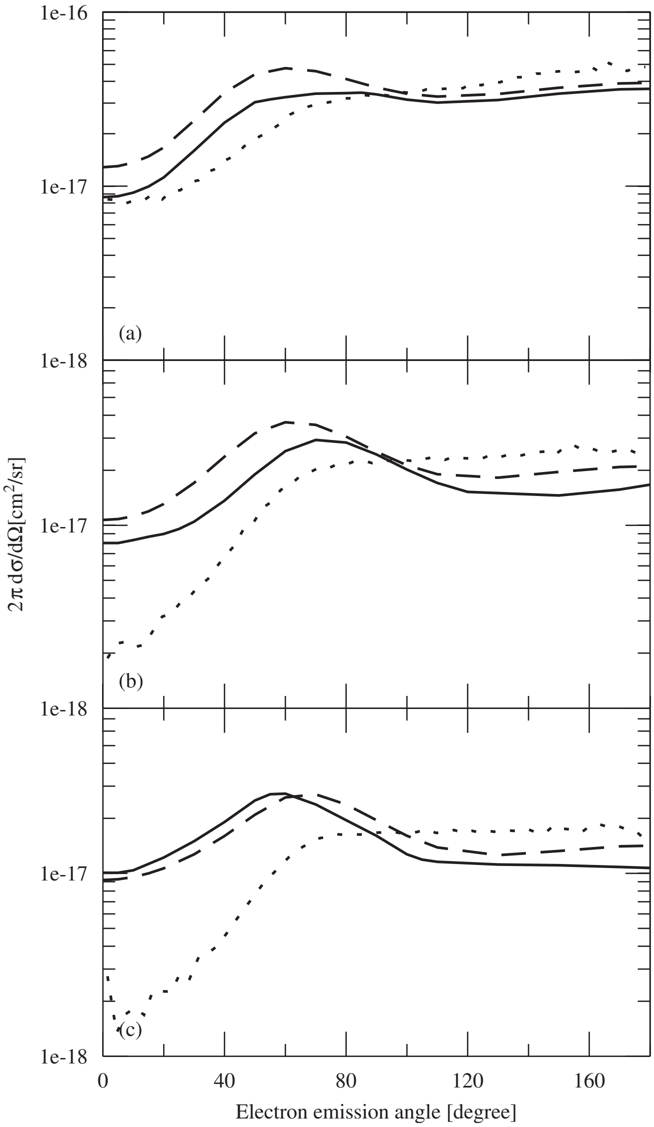

Fig. 2. Angular differential cross sections for electrons emitted in (a) 100 keV, (b) 300 keV and (c) 500 keV antiproton impact energy. Solid line: coupled-channel, dashed line: CDW-EIS, dotted line: CTMC.

Fig. 2(c) presents the calculations for 500 keV impact energy. The two quantum mechanical results are in good agreement which indicates that non-perturbative contributions become small and are treated equally well in both models. The cross sections become more symmetric which means an enhancing dipole contribution. The CTMC systematically underestimates the quantum mechanical cross sections by a factor of about 3 at a small scattering angle, due to the lack of non-classical dipole emission channels (Reinhold and Burgdörfer, 1993).

4. Conclusion

The coupled-channel method has been used to calculate total and angular differential single-ionization cross sections for antiproton–helium collisions. Our total ionization cross section results are comparable to cross sections from different TDDFTs and multi-cut FIM results. The angular differential cross sections calculated with the CC method are in reasonable agreement with the other theoretical models such as CDW-EIS or CTMC. Further work is in progress to calculate double differential ionization cross sections for a more detailed understanding of the anti-cusp region.

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