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Interaction of positronium with helium atoms – the classical treatment of the 5-body collision system*

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Abstract. The interaction between positronium and a helium atom is studied using the 5-body classical trajectory Monte Carlo method. We present the total cross sections for the dominant channels, namely for single ionization of the target, and ionization of the projectile, resulting from pure ionization and also from electron transfer (capture or loss) processes for 1–5.7 a.u. incident velocities of the positronium atom. Our results were compared with the calculated data using hydrogen projectiles having the same velocities as well as with the experimental data in collisions between H and He [R.D. DuBois, Á. Kövér, Phys. Rev. A **40**, 3605 (1989)]. We analyze the similarities and deviations for ionization of helium atoms by positronium and hydrogen projectile impact.

1 Introduction

Understanding the ionization process during atomic collisions is fundamental both from the experimental and theoretical points of view. Ionization by positron impact has also been extensively studied in recent decades [1–11]. In most cases noble gas atoms were used as the target. For designing new experiments, such as production of antimatter, ionization cross sections for many other atoms are also necessary. Recently, improvements in experimental techniques have enabled the determination of inner shell ionization cross sections by positron impact [12–14].

During the last two decades more and more studies also became available for positronium impact [15–31]. Experimental measurements also exist for Ps fragmentation by noble gas atoms and small molecules [15–22]. Starrett et al. [23] calculated the Ps fragmentation in the inert gases from He to Xe using the impulse approximation and the first Born approximation. They also took into account the fragmentation of excited Ps [24]. Ionization of atomic hydrogen [25] and noble gas atoms [26–31]were also studied theoretically. Coupled-state calculations were presented for Ps + He scattering in the energy range between 0 and 40 eV by Blackwood et al. [27]. They have shown that the ionization of the Ps is the main process at the higher energies. At low energies they found serious conflict between different experiments and also between the different theoretical approximations.

The theoretical treatment of the problem is extremely difficult because it requires accounting for the many-body character of the collision system. This behavior is even more significant for light particle impact where the projectile trajectory cannot be approximated by a straight-line trajectory, as is done for heavy projectile impact. Therefore, the success of different approaches strongly depends on their ability to describe the many-body character of the collision. The classical trajectory Monte Carlo (CTMC) method has been quite successful in dealing with both ionization and capture processes in ion atom collisions [32–34]. It was also shown that the CTMC method can be applied to light projectile impact as well [3,4,35–37]. It is a non-perturbative method. All interactions between the colliding partners can be taken into account exactly during the collision.

In this work the collision between positronium and helium atoms is studied using the 5-body CTMC method. Our results are compared with calculations using hydrogen projectiles having the same velocities as well as with the experimental data for collisions between H and He [38]. We compare and analyze the similarities and deviations in the ionization of helium atoms by positronium and hydrogen projectile impact.

2 Theory

In our model the projectile contains two particles (electron and positron) and they represent the ground state positronium with binding energy of 0.25 a.u. The target

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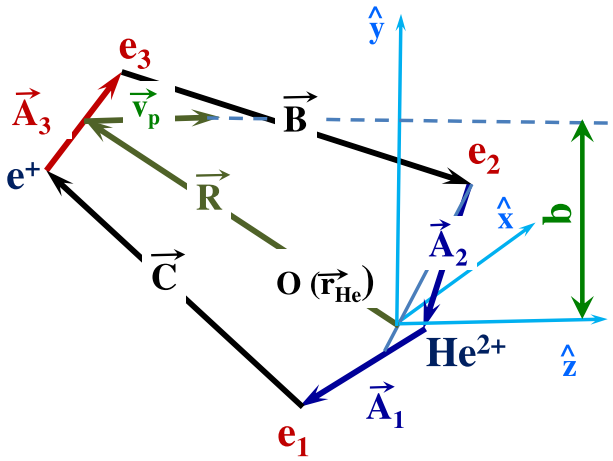

Fig. 1. (Color online) The relative position vectors of the particles involved in 5-body collisions.

contains three particles, the helium core and two electrons. The binding energies of the target electrons to the target core are 0.903 a.u. and 2 a.u. according to the first and second ionization energy of helium. The five particles are characterized by their masses and the interaction potentials between them. Figure 1 shows the relative position vectors of the particles involved in 5-body collisions. The center of mass of helium is positioned at the origin with the positronium center a distance $\boldsymbol{R}$ and impact parameter b away. Vectors $\boldsymbol{A}$ are the positions of the electrons bound to the helium nucleus and the separation of the electron and positron in positronium while vectors $\boldsymbol{B}$ and $\boldsymbol{C}$ are the interaction distances between the positronium and the bound target electrons.

In the present case, all interactions among the particles are the pure Coulomb interactions except the interaction between the two target electrons. To avoid spontaneous autoionization this interaction is completely neglected during the calculations. The initial conditions of the individual collisions are chosen at sufficiently large internuclear separations such that the interaction between the projectile and the target constituents is negligible. The initial states of the target and the projectile are characterized by a micro-canonical ensemble constrained to the binding energies.

In the present CTMC approach, Newton's classical nonrelativistic equations of motions for a three-body system are solved [32–34]. Newton's equations are written as:

$$m_i \frac{\mathrm{d}^2 \boldsymbol{r}_\mathrm{i}}{\mathrm{d}t^2} = \sum_{j=1, i\neq j}^{5} \alpha_{ij} Z_i Z_j \frac{\boldsymbol{r}_i - \boldsymbol{r}_j}{|\boldsymbol{r}_i - \boldsymbol{r}_j|^3}, \quad (i = 1, \ldots, 5) \quad (1)$$

where m_i, $\boldsymbol{r}_i$ and Z_i denote the mass, position vector, and the charge of the ith particle, respectively. The α_{ij} are the switching parameters of the corresponding interactions defining the strength of the interaction among the particles. The value of α_{ij} is set equal to 1 when the interaction between the ith and jth particles is on and equal 0 when the interaction is off. Thus in our case $\alpha(e_1^-, e_2^-) = 0$ ensures that we switch off the interaction between the two target electrons and mimic the independent electron approach in the helium atom.

Then, Newton's classical non-relativistic equations of motions for a five-body system are solved numerically for a statistically large number of trajectories for given initial conditions until the converged final states are reached. Eighteen different classical final states were distinguished. Large numbers of classical trajectories were computed to calculate the total cross sections for the dominant channels, namely single ionization of the target, and ionization of the projectile, resulting from pure ionization and also from electron transfer (capture or loss) processes for 1–5.7 a.u. incident velocities of the positronium atom. Large numbers of trials were required because the total cross sections are composed of the cross sections for many partial levels. Then the total ionization cross section was computed with the following formulas:

$$\sigma = \frac{2\pi b_{\max}}{T_N} \sum_{j=1}^{T_N^{(c)}} b_j^{(c)}. \quad (2)$$

The statistical uncertainty of the cross section is given by:

$$\Delta\sigma = \sigma \left[\frac{T_N - T_N^{(c)}}{T_N T_N^{(c)}} \right]^{1/2}. \quad (3)$$

In equations (2) and (3) T_N is the total number of trajectories calculated for impact parameters less than $b_{\max}$, $T_N^{(c)}$ is the number of trajectories that satisfy the criteria for the investigated final channel, and $b_j^{(c)}$ is the actual impact parameter for the trajectory corresponding to the investigated final channel.

3 Results and discussion

To study the collision between positronium and helium atoms we have performed a classical simulation with an ensemble of 5×10^6 primary trajectories. The calculations are based on the five-body model.

Although we distinguish 18 different classical exit channels during the calculations in this work we focus on the investigation of the major channels. Naturally, at first, let us begin with the net target single ionization channel:

$$\mathrm{Ps} + \mathrm{He}(1's^2) \rightarrow \mathrm{Ps} + \mathrm{He}^+ + \mathrm{e}^-. \quad (4)$$

In this case as a result of the collision between positronium and helium atom asymptotically we detect positronium, a single charged helium ion and one electron. Classically, however this channel is a sum of two channels. We can call the first one the *one electron target loss* channel. This channel originates from a one step process. Due to the fact that classically the particle motions are deterministic and the electrons in the helium atom are distinguishable we can define this channel as:

$$(\mathrm{e}^+, \mathrm{e}_3^-) + \mathrm{He}(\mathrm{e}_1^-, \mathrm{e}_2^-) \rightarrow (\mathrm{e}^+, \mathrm{e}_3^-) + \mathrm{He}^+(\mathrm{e}_1^-) + \mathrm{e}_2^-, \quad (5)$$

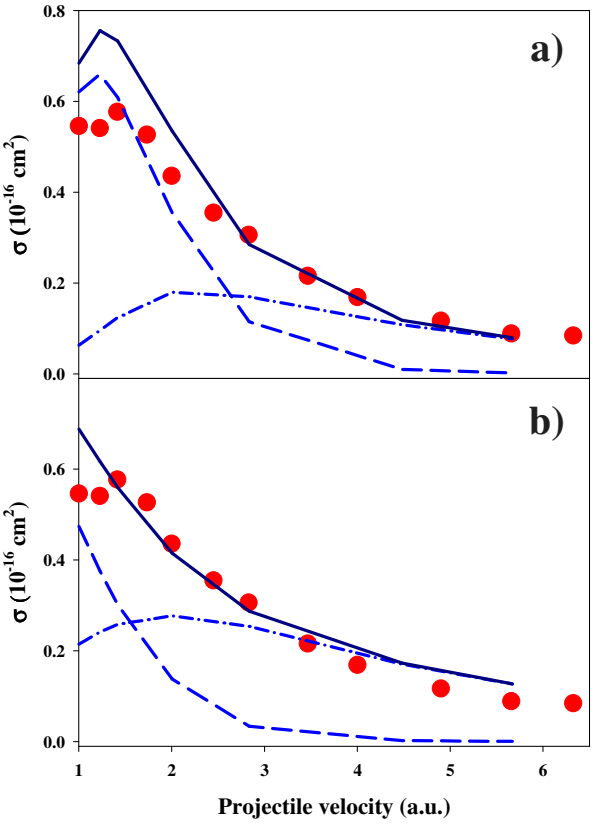

Fig. 2. (Color online) Single electron loss of the target. (a) Ps + He, (b) H + He. Dashed-dotted line: one electron target loss originating from the one step ionization process (P1), dashed line: two step ionization process when the projectile loses one electron and at the same time it captures one electron into its bound state from the target (P2), solid line: sum of channels P1 and P2. Circle: experimental data using hydrogen atom impact from reference [38].

and by

$$(e^+, e_3^-) + He(e_1^-, e_2^-) \rightarrow (e^+, e_3^-) + He^+(e_2^-) + e_1^-. \quad (6)$$

The second possible classical channel producing the same final particles as defined by equation (4) originates from the multi-electron interaction in a two step process. We refer to it as *projectile ionization and at the same time one electron capture of a target electron to the bound state of the projectile*. We can define this channel as:

$$(e^+, e_3^-) + He(e_1^-, e_2^-) \rightarrow (e^+, e_1^-) + He^+(e_2^-) + e_3^-, \quad (7)$$

and by

$$(e^+, e_3^-) + He(e_1^-, e_2^-) \rightarrow (e^+, e_2^-) + He^+(e_1^-) + e_3^-. \quad (8)$$

Figure 2 shows the cross sections of the total single electron loss from the target, when we summed over all final bound states of Ps and He^+, as a function of the projectile velocity. The panel (a) shows the cross sections for Ps + He and the panel (b) shows the cross sections for H + He collisions. The shape of the curves of the partial cross sections is very similar. The absolute total cross sections of the sum of the two sub channels also hardly changes using Ps or H projectiles. However the relative contributions are different for Ps and H. While for H projectile the dominant contribution arises from the one step ionization, for Ps impact the two step process is significant, especially at lower projectile velocities. At high projectile velocities the cross sections are almost independent of the projectile type. The calculated total cross sections are also in good agreement with measurements especially in collisions between H and He.

In the following we focus on the projectile ionization:

$$Ps + He(1s^2) \rightarrow e^+ + e^- + He(1s^2). \quad (9)$$

In this case as a result of the collision between positronium and helium atom asymptotically we detect a helium atom, an electron and a positron. Not surprising, classically this channel is also the sum of two channels. We call the first one *breakup of the projectile* or *the ionization of projectile*. This channel originates from a one step process and we can define as:

$$(e^+, e_3^-) + He(e_1^-, e_2^-) \rightarrow e^+ + e_3^- + He(e_1^-, e_2^-). \quad (10)$$

We can obtain the same the final particles as defined in equation (9) in the following two step processes:

$$(e^+, e_3^-) + He(e_1^-, e_2^-) \rightarrow e^+ + e_2^- + He(e_1^-, e_3^-), \quad (11)$$

and by

$$(e^+, e_3^-) + He(e_1^-, e_2^-) \rightarrow e^+ + e_1^- + He(e_3^-, e_2^-). \quad (12)$$

This channel can be referred to as target single ionization and simultaneously capture of an electron from the projectile into the bound state of the target. Figure 3 shows the cross sections of the total single electron loss from the projectile, when we summed over all final bound states of He, as a function of the projectile velocity. The panel (a) refers to the cross sections for Ps + He and the panel (b) shows the cross sections for H + He collisions. As expected due to differences in the binding energies the projectile ionization is much larger than target ionization both for Ps and H projectiles. For the same reason the projectile ionization is much larger for Ps than for an H projectile. For the Ps projectile the absolute cross sections are about two times higher than for the H projectile. This is primarily due to the binding energy difference. For both projectiles the dominant contribution originates from the one step process. The two step process has minor contributions, although it has some relative importance at lower projectile velocities for H projectile. For Ps projectile impact the two-step process is negligible in the entire range of projectile velocities. At the same time the shape of the total projectile ionization is very similar for Ps and H projectiles. The agreement with the experimental data is not as satisfactory as for the case of the target ionization. This is especially visible at high projectile impact for H projectile. The reason may be due to the importance of the omitted electron-electron interaction.

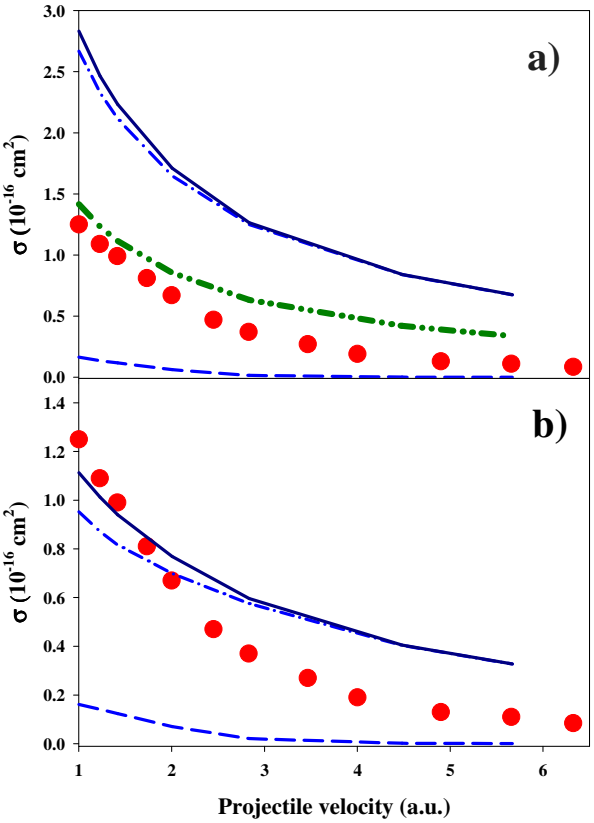

Fig. 3. (Color online) Single electron loss of the projectile. (a) Ps + He, (b) H + He. Dashed-dotted line: one electron projectile loss originating from one step ionization process (P3), dashed line: two step ionization process when the target loses one electron and simultaneously captures one electron from the projectile into the bound state of the target (P4), solid line: sum of channels P3 and P4 (TPI = P3 + P4), dashed-dotted-dotted line: the same as the curve TPI but multiplied by 0.5. Circle: experimental data from reference [38].

4 Conclusion

We presented 5-body Monte Carlo simulation of collisions between Ps and helium atoms. Eighteen different classical final states were distinguished. The total cross sections for the dominant channels, namely the net single ionization of the target, and ionization of the projectile, resulting from pure ionization and also from electron transfer (capture or loss) processes for 1–5.7 a.u. incident velocities of the positronium atom impact were calculated. While the pure ionization channel is a one step, the ionization channel in combination with electron capture and loss is a two-step process. Our results were compared with calculations for hydrogen projectiles having the same velocities as well as with the experimental data in collisions between H and He [38]. We have shown that the projectile velocity dependent cross sections for the two major channels have very similar shapes. The agreement with the experimental results is excellent for the case of target single ionization and less satisfactory for projectile ionization. This is especially visible at high velocities. While for the case of target single ionization the absolute total cross sections are nearly the same for Ps or H projectiles for the case of projectile ionization the cross section is about two times higher for Ps than for H. This fact can be attributed to the difference between the binding energy of Ps and H.

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