CALCULATION OF CHARGE-CHANGING CROSS SECTIONS OF IONS OR ATOMS COLLIDING WITH FAST IONS USING THE CLASSICAL TRAJECTORY METHOD *

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Abstract

Evaluation of ion-atom charge-changing cross sections is needed for many accelerator applications. A classical trajectory Monte Carlo simulation has been used to calculate ionization and charge exchange cross sections. For benchmarking purposes, an extensive study has been performed, first for the simple case of hydrogen and helium targets in collisions with various ions. Despite the fact that the simulation only accounts for classical mechanics, the calculations are comparable to experimental results for projectile velocities in the region corresponding to the vicinity of the maximum cross section.

INTRODUCTION

Ion–atom ionizing collisions play an important role in many applications such as heavy ion inertial fusion [1], collisional and radiative processes in the Earth's upper atmosphere, ion beam lifetimes in accelerators, atomic spectroscopy, and ion stopping in matter, and are of considerable interest in atomic physics [2]. The recent resurgence of interest in charged particle beam transport in background plasma is brought about by the recognition that plasma can be used as a magnetic lens [3]. To estimate the ionization and stripping rates of fast ions propagating through gas or plasma, the values of ion–atom ionization cross-sections are necessary. In contrast to the electron and proton ionization cross-sections, where experimental data or theoretical calculations exist for practically any ion and atom, the knowledge of ionization cross sections by fast complex ions and atoms is far from complete. When experimental data and theoretical calculations are not available, approximate formulae are frequently used [2]. For the interaction of complex projectile and target atoms or ions, Classical Trajectory Monte Carlo (CTMC) simulations can be utilized [4]. Though frequently used, we have not found a detailed study of the validity of the CTMC method. The validity of the classical trajectory approximation has been studied by comparing the results of simulations with available experimental data and the full quantum-mechanical calculations in Ref. [2]. Additionally, a theoretical criterion has been developed for validity of the classical trajectory approximation [5]. The range of validity of the Born approximation and quasiclassical approximation can be estimated by evaluating the action $S(\rho,vt)=\int_{-\infty}^{\infty}\Phi_p[r(\rho,vt)]dt$ along the trajectory $r(\rho,vt)=[\rho^2+(vt)^2]^{1/2}$. Here, $\Phi_p(r)$ is the projectile atomic potential and ρ is the impact parameter, and v is the projectile velocity. When $S(\rho,v)>\hbar$, we can apply classical mechanics [2], whereas the Born approximation fails. At higher velocities when $S(\rho,v)<\hbar$, quantum-mechanical effects become more significant and the CTMC results agree less with the experimental values of cross sections, whereas the Born approximation is valid. Also at very low velocities, $S(\rho,v)>>\hbar$, the probability of charge exchange transitions in classical mechanics may be significantly less than that due to classically forbidden transitions, which can be described in quantum mechanics using quasiclassical approximations, see e.g., Ref. [2] for more details. Therefore, the CTMC method can be generally applied in the narrow range $S(\rho,v)\sim\hbar$. To further investigate the region of validity, an extensive study has been performed for the simple case of hydrogen and helium targets in collisions with various ions.

DESCRIPTION OF CTMC METHOD

Application of the CTMC method consists of computation of the electron trajectory in an atom when another ion or atom is passing by at a certain impact parameter. For calculating the total cross section it is only necessary to determine the outcome of the collision, i.e., the electron velocity and distances to the target and projectile nuclei at large enough times, when one of the distances is sufficiently large. There are three possible outcomes: the electron remains close to one of the nuclei or it moves far away from both of them. If the electron kinetic energy (in the proper reference frame) is smaller than the attractive potential of the target or projectile, the electron is assumed to be trapped by the nucleus. If the electron remains near the target, no ionization or charge exchange events has occurred. If the electron is trapped by the projectile nucleus, the exchange event have occurred. If none of these events has happened, ionization takes place. The results have to be averaged over all possible initial electron positions and impact parameters. To have a steady-state distribution, the electron velocity distribution function (EVDF) should be a function of the constants of motion: the total energy, which is equal to the binding energy $E_{ln}=-I_{nl}$ determined by the ionization potential I_{nl}, and the total orbital momentum l. In classical mechanics, the EVDF of an electron orbital n,l is given by the micro-canonical ensemble distribution

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$$f_{n,l}(\mathbf{v}_e,\mathbf{r}) = C_{n,l}\delta\left[\frac{mv_e^2}{2} + \Phi_{n,l}(r) - E_{nl}\right]\delta(l - |\mathbf{v}_e \times \mathbf{r}|),$$

where $\Phi_{n,l}(r)$ is the atomic potential describing the interaction of the atomic electron with the nucleus and the rest of the electrons and $C_{n,l}$ is a normalization constant. We use spherical coordinates $d^3\mathbf{r} = r^2 \sin\theta dr d\theta d\phi$. The velocity vector has two components: one is directed along the radius vector $\mathbf{v}_r$, and the rotational velocity $\mathbf{v}_\beta$, is rotated in the plane perpendicular to $\mathbf{v}_r$ by an angle α For a spherically symmetric model of an atom, the rotation velocity v_β, is determined by angular momentum conservation $l = v_\beta r$; and the radial electron velocity is determined from energy conservation $v_r^2 + (l/r)^2 = -2I_{n,l} - 2\Phi_{n,l}(r)$. The difficult part of the calculation is to obtain the direction of the rotational velocity. The initial position of an electron is

$$\mathbf{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = r \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix}.$$

The velocity is given by

$$\mathbf{v} = \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = \begin{pmatrix} v_r \sin\theta\cos\varphi + v_\beta(\cos\varphi\cos\theta\cos\alpha - \sin\varphi\sin\alpha) \\ v_r \sin\theta\sin\varphi + v_\beta(\sin\varphi\cos\theta\cos\alpha + \cos\varphi\sin\alpha) \\ v_r\cos\theta - v_\beta\sin\theta\cos\alpha \end{pmatrix}.$$

There are two methods in which we can assign values to the initial conditions. We can use a stochastic method where the initial conditions are chosen randomly. In general, weights in the probability calculation have to be used before summing up the outcomes for cross section calculations, because if one picks values of the angles and radius randomly, this doesn't correspond to a uniform distribution of points on the surface of the sphere in phase- space, i.e, to the micro-canonical ensemble. Therefore, instead of initializing the variable radius, we use the phase of motion in the radial direction, or the time of flight $\Omega_r(r) = 2\pi\tau/T = \pm 2\pi\int_{r_-}^{r} dr/v_r(r)T$, where $T = 2\int_{r_-}^{r_+} dr/v_r(r)$ is the period of radial motion, and $r_\pm$ are the distances of minimum and maximum approaches. It can be shown that the uniform distribution in $\Omega_r(r)$ is equivalent to the microcanonical ensemble.

Using this approach, the ionization cross section is given by

$$\sigma = \frac{2\pi\rho_{\max}\Sigma_{i,j,k,m,s}\rho_i c_{i,j,k,m,s}}{N_t}, \qquad (1)$$

where ρ_i is the impact parameter, $\rho_{\max}$ is the maximum impact parameter used in the simulations, and *i, j, k, m, s* are indexes labeling the simulation in impact parameter, radius, and three spherical angels; $N_t = N_i N_j N_k N_m N_s$ is the total number of trajectories that are simulated, and $c_{i,j,k,m,s} = 1$, if the ionization event takes place, and $c_{i,j,k,m,s} = 0$ otherwise.

COMPARISON OF CTMC CALCULATIONS AND EXPERIMENTAL DATA

Using a classical trajectory simulation, we calculated the ionization and charge exchange cross sections for collisions of various ion projectiles on hydrogen and helium targets. Figures 1-4 show the charge-changing cross sections (ionization or charge exchange) for fully or partially stripped ions colliding with an atomic hydrogen. Atomic units are used in all figures. The experimental data are taken from Ref. [6].

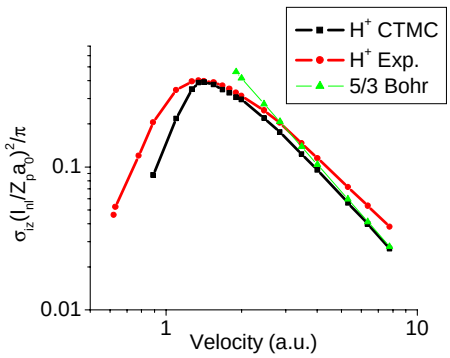

Figure 1. Normalized ionization cross section for proton collisions with atomic hydrogen.

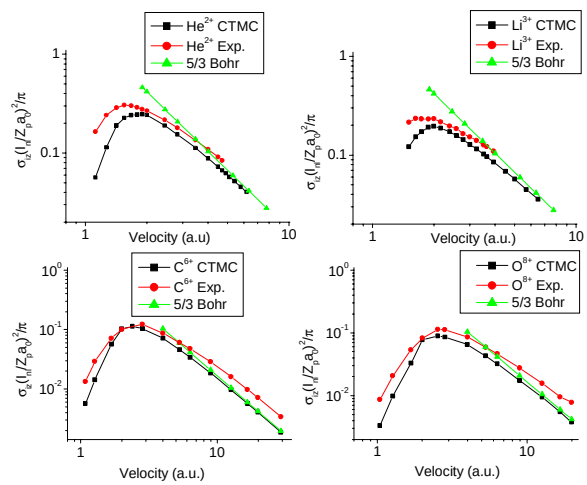

Figure 2. Normalized ionization cross sections for fully stripped ions colliding with atomic hydrogen.

At large velocities the CTMC cross section should approach 5/3 of the Bohr formula [2]:

$$\sigma = \frac{5}{3}\sigma^{Bohr} = \frac{10\pi Z_p^2}{3v^2 I_{nl}}.$$

Similar simulations has been performed for helium and are shown in Fig.5.

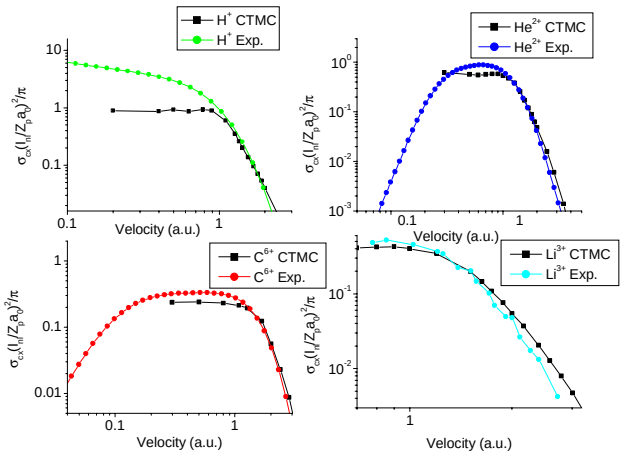

Figure 3. Normalized charge exchange cross sections for collisions of fully stripped ions with atomic hydrogen.

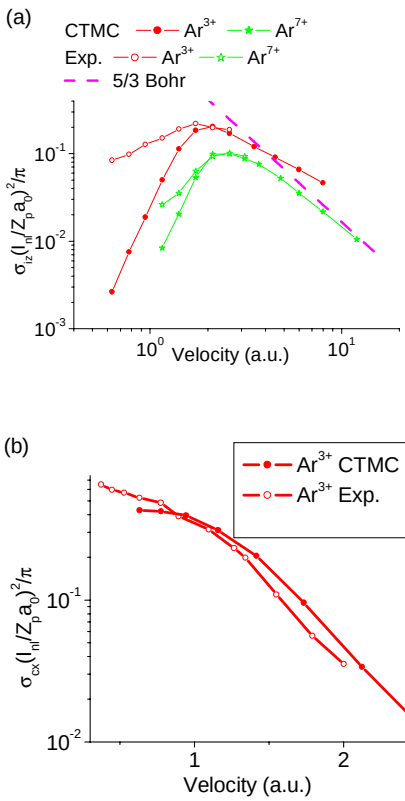

Figure 4. Charge-changing cross sections for collisions of partially stripped argon ions with atomic hydrogen corresponding to: (a) ionization, and (b) charge exchange. The experimental values were taken from Ref. [7].

CONCLUSIONS

As evident from the figures showing comparisons between the simulations and experimental data, the CTMC simulations match the experimental results for projectile velocities between and 1 and 3 a.u, which corresponds to the region near the maximum value of the cross section and $S(\rho, v) \sim \hbar$. The CTMC method can underestimate the value of the cross sections outside this velocity range.

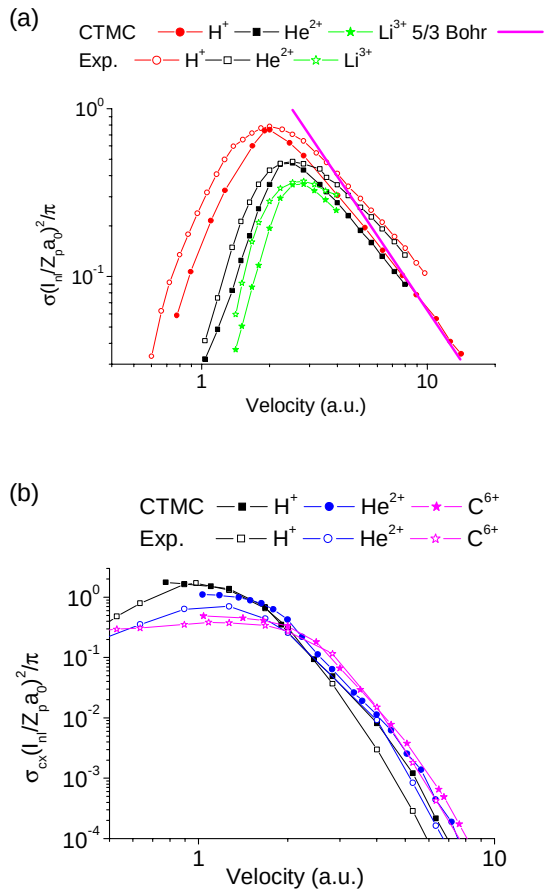

Figure 5. Charge-changing cross sections for fully stripped ions on helium corresponding to: (a) ionization, and (b) charge exchange. The experimental values were taken from Ref. [8].

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