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Classical Trajectory Monte Carlo Simulations for Charge Transfer Processes

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Abstract

I have calculated electron transfer cross sections for slow, highly charged ion-atomic hydrogen collisions by using the classical trajectory Monte Carlo method. Similar calculations for alkaline metal targets are also carried out using a simple one-electron model. I compare the results to predictions by the extended classical over barrier model and available experimental data. The calculated cross sections are in good agreements with data. A simple scaling formula for the cross sections of electron transfer collisions between slow ions and hydrogenic targets is proposed.

Keywords:

charge exchange, electron transfer, electron capture, cross section, classical trajectory Monte Carlo simulation, CTMC

1. Introduction

Charge transfer cross sections in slow, highly charged ion-atomic hydrogen collisions are important for studying the physics of edge and diverter plasmas, and charge exchange diagnostics. However, it is difficult to measure the absolute cross sections with high accuracy due to the experimental difficulties in preparing ground state pure atomic hydrogen targets and determining the absolute target density. Furthermore, it has been known that the well-established scaling law for charge transfer cross sections [1], which is based on the extended classical over barrier model (ECBM) [2,3], cannot be adopted for atomic hydrogen and alkaline metal targets that have only one valence electron. Therefore, I have constructed a simulation code based on the classical trajectory Monte Carlo (CTMC) method to calculate charge transfer cross sections from atomic hydrogen and alkaline metal atoms. It is noted that both of the two classical treatments of the ECBM and CTMC are not adequate for low charge state ($q \leq 5$, where q is the initial charge state of incident ion) ion-atom collisions because quantum features appear strongly originated from the discreteness of the energy levels of both of the collision partners in such collision systems [2,4]. I also note that since inner electrons in alkaline metal targets are deeply bounded to core nuclear, the contribution of inner electrons to electron transfer processes is negligibly small, and one electron transfer process is dominant [1-3].

2. Classical trajectory Monte Carlo method

The basic concept of the present CTMC code is similar to that developed by Olson and coworkers [5,6]. The CTMC method is pure classical, but no approximation is required. It has been successfully applied to investigate ion-atom collisions. In the present code, the coupled equations of motion are numerically solved for three-body, three-dimensional system by using the traditional fourth-order Runge-Kutta method with variable step size [7]. The three charged particles involved in collisions, incident ion, target core and electron are treated as point charges. The target core is initially fixed at the origin. The incident ion starts from $x_{i0} = -10q$ au and approaches the target along the x-axis. The impact parameter is given by the Monte Carlo way. The initial conditions of the target electron are also determined with the Monte Carlo technique. I use two classical models to represent one-electron hydrogenic systems. One is the simplest Bohr's atom model and the other is some sophisticated microcanonical ensemble model (MEM) argued by Abrines and Percival [8,9] and Olson and Salop [5]. The latter describes the spherically symmetric hydrogen atom by a microcanonical ensemble of elliptic Kepler's orbits. In the Bohr's model, the orbital radius and momentum of target electron are consistent with the expectation values of probability distributions of quantum position and momentum respectively. On the other hand, the MEM well reproduces the momentum distribution obtained from quantum theory, whereas there are some differences between the spatial

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distributions predicted by the classical MEM and quantum theory. I compare the results obtained with the two models in the next chapter. Once the trajectories are calculated, complete collision information can be extracted from the results. In order to obtain cross sections with the statistical uncertainties less than ±2%, about one to two million trajectory calculations are needed, and it takes typically 1–5 hours with a DEC alpha workstation.

3. Results and discussion

I have calculated total electron transfer cross sections in highly charged ion-atomic hydrogen collisions at the collision velocity of 0.1 au. For incident ions, highly charged I^{q+} (q = 5–53), and bare Os^{76+} and U^{92+} ions are considered to study the initial charge dependence of cross sections. In addition to atomic hydrogen, I have carried out the calculations for alkaline metal targets (Na, K, Rb and Cs), which can be assumed to be quasihydrogenic, at the collision energy of 1.5q keV to study ionization energy dependence of cross sections. Since the NICE group has measured electron transfer cross sections in 1.5q keV I^{q+}-alkaline metal targets [10,11], then direct comparisons are possible. In such slow ion-atom collisions, it has been well known both experimentally and theoretically that the energy dependence of charge transfer cross section is very weak and that the value is almost constant [4,12]. I have calculated electron transfer cross sections at different collision velocities for Rb target to verify it. The results are listed in Table 1. The differences between them are very small, less than 2%, as expected. In addition to the energy dependence, I have studied model dependence with two classical model atoms, the Bohr's atom model and MEM. Figure 1 shows the comparison of the cross sections obtained with the two model atoms. It is found that the difference is not significant whereas the cross sections calculated with the MEM are somewhat smaller than those by Bohr's model. I believe that the MEM is more realistic and suitable because it reproduces well the momentum distribution of target electron. Therefore, I use the MEM throughout the calculations below.

The calculated electron transfer cross sections are listed in Table I and plotted in Fig. 2. The figure shows clearly that the electron transfer cross section σ_H can be scaled as,

$$\sigma_H = 4.6qP^{-2} \quad (1)$$

where q is the initial charge of projectile and P is the ionization potential of target electron, and both σ_H and q are expressed in the atomic units. I show the comparison between the scaling formula and absolute experimental cross sections measured by the NICE group for 1.5q keV $I^{6\text{-}30+}$-Na, Rb and Cs collisions in Fig. 3. The experimental uncertainties have been estimated to be about 25–35%. Experimental data for highly charged A^{q+}-H collisions ($q \geq 5$) reported by some another groups are also plotted in the figure [13-19]. The experimental cross sections are found to be well reproduced by the scaling relation deduced from the present CTMC calculations. Of course, the scaling relation can be also determined from the available data and it is expressed as $\sigma_H^{Exp} = 4.7qP^{-2}$ that agrees well with eq. (1).

Similar qP^{-2} scaling has been seen for multielectron targets such as rear gas atoms, but the coefficient is about 2.7 times larger [1],

$$\sigma_m = 4\pi qP^{-2}. \quad (2)$$

The scaling law for multielectron targets is based on the ECBM by Niehaus [2] and proposed by Kimura *et al.* [1], and has been confirmed to reproduce data well. Incident highly charged ion is frequently called 'absorbing sphere'. In the absorbing sphere picture, it is considered that once target enters inside the sphere with a critical radius around projectile, target electrons are absorbed into the projectile with the probability of almost unity due to the strong Coulomb field generated by the incident ion. If the closet approaching distance between projectile and target core is longer than the critical radius, no electron is transferred. Following the ECBM and Kimura's paper, the critical radius r_m is approximated to be $r_m = 2\sqrt{q}P^{-1}$ for highly charged ion-atom collisions, and then the cross section is deduced geometrically as $\sigma_m = \pi r_m^2$. I examine the validity of the absorbing sphere picture. The

Table 1 Electron transfer cross sections in au calculated with the CTMC method for $I^{5+\text{–}53+}$, Os^{76+}, U^{92+}-quasihydrogenic targets.

q	H[1)]	Na[2)]	K[2)]	Rb[1)]	Rb[2)]	Cs[2)]
5	7.34×10^1	5.30×10^2	7.55×10^2	8.82×10^2	8.85×10^2	9.42×10^2
10	1.66×10^2	1.18×10^3	1.66×10^3	1.94×10^3	1.99×10^3	2.07×10^3
20	3.35×10^2	2.48×10^3	3.49×10^3	4.04×10^3	4.07×10^3	4.37×10^3
30	5.11×10^2	3.86×10^3	5.40×10^3	6.19×10^3	6.14×10^3	6.70×10^3
40	6.70×10^2	5.12×10^3	7.22×10^3	8.17×10^3	8.32×10^3	8.80×10^3
53	8.47×10^2	6.68×10^3	9.38×10^3	1.09×10^4	1.10×10^4	1.17×10^4
76	1.17×10^3	9.59×10^3	1.34×10^4	1.56×10^4	1.58×10^4	1.67×10^4
92	1.36×10^3	1.16×10^4	1.63×10^4	1.87×10^4	1.89×10^4	2.02×10^4

1) Collision velocity of 0.1 au.
2) Collision energy of 1.5q keV.

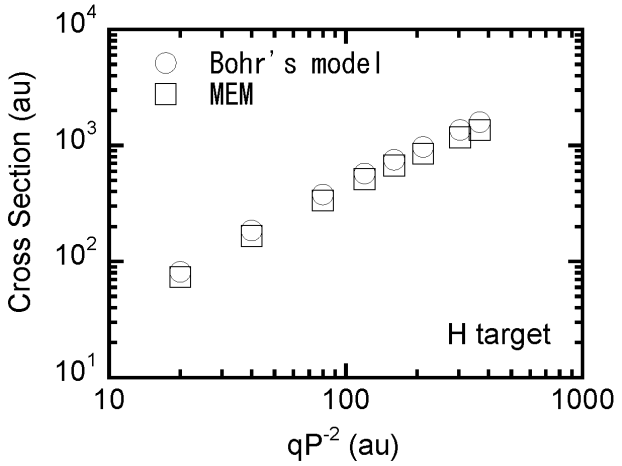

Fig. 1 Comparison of electron transfer cross sections calculated with Bohr's atom model and microcanonical ensemble model for I^{5-53+}-H collisions.

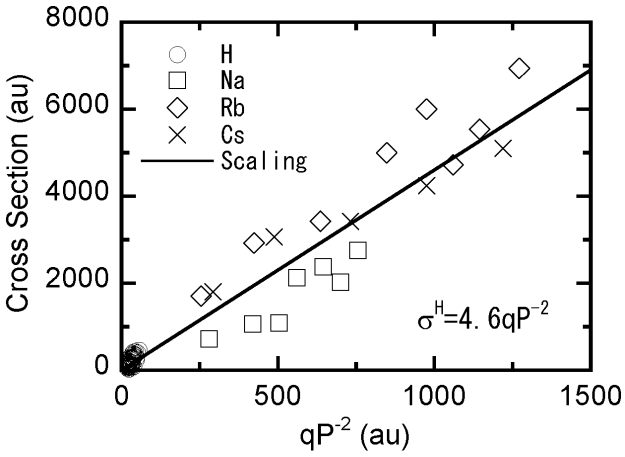

Fig. 3 Comparison between the scaling formulae obtained from the CTMC calculations and experimental data. The uncertainties of the data are estimated to be about ±25–35%.

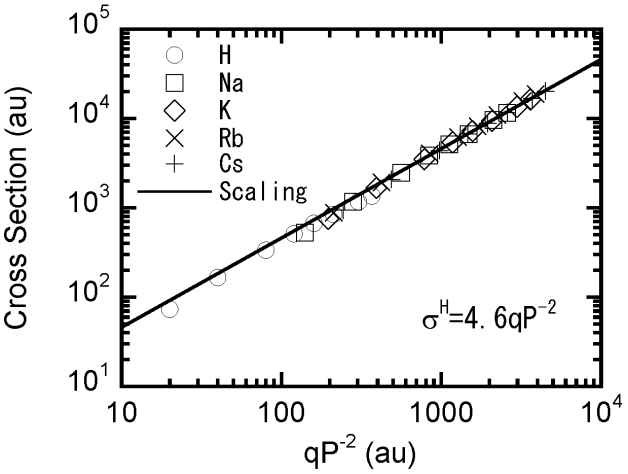

Fig. 2 CTMC cross sections for electron transfer processes. The solid line shows the scaling relation determined from the CTCM results, $\sigma^H = 4.6qP^{-2}$.

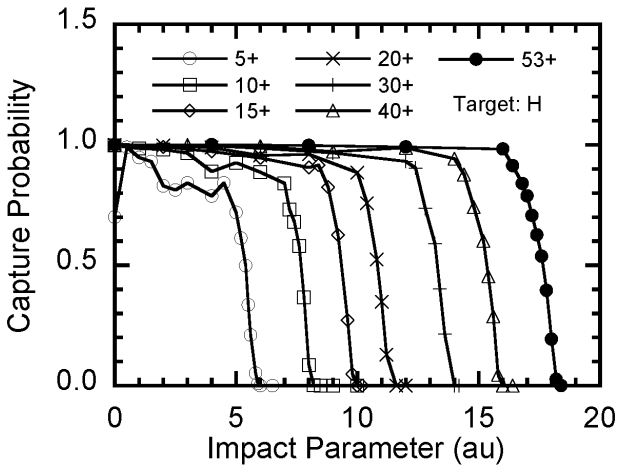

Fig. 4 Impact parameter dependence of the capture probability for I^{5-53+}-H collisions at the collision velocity of 0.1 au. From a critical radius, the capture probability falls rapidly. The sphere of the critical radius is called *'absorbing sphere'*.

closet approaching distance can be approximated by the impact parameter in ion-atom collisions. Fig. 4 shows the impact parameter dependence of electron transfer probability. As expected from the absorbing sphere model, the electron transfer probability is almost unity within a critical impact parameter and the probability decreases rapidly from the critical value. However the critical radius is found to be smaller and approximated by $r_H : 1.2\sqrt{q}P^{-1}$. This is the reason why the coefficient of the scaling law of σ_H is smaller than that for σ_m. The ECBM may be a good picture qualitatively but not valid quantitatively for the electron transfer collisions between highly charged ions and guasihydrogenic. There are a few candidates for the explanation about the reason why the ECBM fails in the description of ion-hydrogenic atom collisions. In the ECBM, no dynamical effect is taken into account and the critical radius is estimated by the static initial two parameters, initial charge q and ionization energy P. However, the ionization potential of target electron changes dynamically and drastically during the collision due to the Coulomb field of the incident ion. Especially, since atomic hydrogen has only one electron, no cancellation mechanism against the Coulomb field, such as dynamical screening effects by core electrons, can be expected in the pure three-body Coulomb systems. In the case of multielectron targets, since many electrons surround the target nuclear, then the screening effects may be able to reduce the dynamical changes in ionization potential of outer electrons. In order to further improve the ECBM, such dynamical effects need to be incorporated into the model by some ways. Important knowledge may be obtained from the collision dynamics

analysis using the CTMC calculations.

4. Summary

By using the CTMC code developed for three-dimensional three-body Coulomb systems, I have calculated electron transfer cross sections for the collisions of I^{5-53+}, Os^{76+} and U^{92+} with H, Na, K, Rb and Sc at low collision velocities. It has been found that the calculated cross sections agree well experimental data, and the cross section can be scaled as $\sigma_H = 4.6qP^{-2}$ for highly charged ion-hydrogen and alkaline metal collisions.

Acknowledgements

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