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Charge transfer in keV proton collision with atomic oxygen: Differential and total cross sections

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Abstract. Classical Trajectory Monte Carlo method (CTMC) with the modal interaction potential [1] has been used to simulate the differential, total and partial capture cross sections in proton-oxygen atom collisions in the energy range of 0.5–200 keV. An interesting feature of the calculated differential cross sections (DCS) curve below the scattering angle 0.1° is the presence of oscillations showing asymmetry in angular positions. The oscillations in the partial cross sections are explained in terms of swapping effect. The DCS and total cross sections are found to be in good agreement with the experimental as well as other theoretical results.

PACS. 34.70.+e Charge transfer – 34.10.+x General theories and models of atomic and molecular collisions and interactions

1 Introduction

The cross sections for different processes occurring in collision of protons with atomic oxygen are of fundamental physical interest and play an important role in a wide range of phenomena occurring in different atmospheres. Above few hundred kilometers of earth in the outer atmosphere, atomic oxygen has much higher density than, for example, N_2 and O_2 and therefore, cross sections involving proton – oxygen reactions have a particular geophysical importance. In addition to the proton component of the solar wind, which has an average energy of about 1 keV, much more energetic protons are produced in the solar flares [2]. As the behavior of the auroral protons depends critically on the magnitude of these cross sections, investigation of charge transfer collisions involving proton and oxygen atoms provide a better understanding of the proton aurora in the earth's upper atmosphere. Though the oxygen being less attractive target because of the presence of four electrons in its $2p$ and two electrons in $2s$ level that make the theory prohibitively complex, many attempts have been made to calculate the cross sections for different processes [1,3–6]. Experimental research [7–13] groups have studied the capture processes in proton-oxygen atom collision and have determined total capture cross sections for a wide range of energies. Little efforts have however, been made to determine the DCS particularly, in the region of very low scattering angles.

Studies of angular differential scattering at keV energies at very small angles (below 0.1°) are particularly, motivated by the highly forward peaked character of the cross sections, location of the classical rainbow angle within the range, and containing information that permit evaluation of the calculated or proposed interactions potentials. In order to explain the observed results of Lindsay et al. [8] in this paper we give more emphasis on the calculation of DCS and its analysis at the scattering angles below 0.1°.

The Classical Trajectory Monte Carlo (CTMC) method is a well tested method to simulate inelastic ion-atom collisions at intermediate energies [14–19]. In it, the results of the evolution of an ensemble of the corresponding quantum system are examined statistically for understanding the capture and ionization processes. It has been widely used particularly, for ion – one-valence-electron targets by several workers [14–20]. We have also used it not only for single electron but for two valence electron targets [20] as well and reported fairly good agreements of simulated data with other available experimental and theoretical results. In the present work, CTMC method with modified interaction potential [1] has been used to calculate the angular differential as well as total electron capture cross sections for H^+ collisions with oxygen atoms. Our emphasis, as mentioned above, is primarily on understanding the nature of the differential cross sections at very small angles.

2 Theory

The theoretical treatment of CTMC method has been given in detail by Abrines and Percival [21] and Olson and Salop [17] and therefore, only brief outline would be given here. The CTMC procedure is basically a treatment of three-body problem viz.; the projectile ion, active electron and the target core in the three dimensional frame work.

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The details of the CTMC method used in the present calculation can be found in our earlier work published [20] recently. An analytical model interaction potential has been used to describe the interaction between target ionic core and the field electron ($e^- + O^+$) as given by Hamre et al. [1] viz.;

$$V(r) = -\frac{1}{r}\left(7e^{-\alpha r} + 1\right) \tag{1}$$

with $\alpha = 1.96$. This interaction potential has been shown to approximate the Hartree potential of the ground state configuration. This model potential has been shown [1] to have the correct asymptotic behavior at large as well as small values of 'r'.

The core-core and projectile-electron interactions are however, taken as pure Coulomb potential. Hamilton's equations of motion for this three body system are solved numerically with the model interaction potential in the three dimensional Cartesian coordinate system. Six random numbers [20] are used to initialized each trajectory and determine the impact parameter, and the plane and eccentricity of the electron's orbit about the target nucleus. Kepler's equation has been used to locate the electron in the orbit.

The cross section for a single electron capture is determined using the formula [22],

$$\sigma_{cap} = \left(\frac{N_{cap}}{N}\right)\pi b_{max}^2. \tag{2}$$

Cartesian coordinates (which are known all through the collision time) of the colliding partners after the collision have been used to determine the centre of mass scattering angle. The angular differential cross sections for the single electron capture were computed using the formula [20,23],

$$\frac{d\sigma_{cap}}{d\Omega} = \frac{2\pi\, b_{max} \sum_j b_j^{(i)}}{N\Delta\Omega}, \tag{3}$$

and the standard deviation for the cross section is calculated as

$$\Delta\sigma_{cap} = \sigma_{cap}\left(\frac{N - N_{cap}}{N N_{cap}}\right)^{1/2}. \tag{4}$$

N is the total number of trajectories calculated for an impact parameter less than or equal to b_{max}, N_{cap} is the number of trajectories that satisfy the criteria for capture, $b_j^{(i)}$ is the impact parameter for which the criteria for capture is fulfilled and $\Delta\Omega$ is the emission solid angle interval of the captured electron. The statistical error limit, to a good approximation, can be written as $\Delta\sigma_{cap} \approx \sigma_{cap}/N_{cap}^{1/2}$. This implies that in order to reduce the error in the calculation one has to take a large number of trajectories. For the results presented here more than 5×10^5 trajectories were computed to obtain good statistics (<3%) for the differential cross section.

In the final product the quantum states corresponding to the negative energy of the electron with respect to the projectile are fixed. Following the procedure of Becker and Mackellar [24] where one defines a classical number n_c corresponding to the binding energy E_0 of the electron relative to the proton as

$$E_0 = -(1/2n_c^2). \tag{5}$$

The value of n_c is then related to the quantum number n of the final state using the condition

$$[(n-1/2)(n-1)n]^{1/3} \leqslant n_c < [(n+1/2)(n+1)n]^{1/3}. \tag{6}$$

From the normalized classical angular momentum $l_c = (n/n_c)(\mathbf{r}\times\mathbf{k})$, where $\mathbf{r}$ and $\mathbf{k}$ are referred to as the position and momentum vectors of the projectile ionic core, an orbital quantum number l of the final state is obtained as

$$l \leqslant l_c \leqslant l + 1.$$

Once the capture states are characterized by these quantum numbers, the probability of capture in a specified state of the hydrogen is calculated.

The one-electron probabilities have been used in the evaluation of the independent-particle multi-electron probabilities [1]. Given a capture probability to be P for the first electron transfer, the probability for the 2nd electron to be transferred is $(1-P)P$. Following this procedure the total probability for the one electron to be transferred out of N equivalent electrons becomes $1-(1-P)^N$. In the present case however, with four electrons in the p-orbit and two electrons in s-orbit, the $N = 6$ electron available for transition is really divided into two groups of two equivalent electrons in $2s$ and four equivalent electrons in $2p$ level or, in general, two groups with M and N independent particles. The above transfer probability then modifies as [1]

$$\begin{aligned} P_T &= [1-(1-P_a)^N] + (1-P_a)^N \\ &\quad \times [P_b + P_b(1-P_b) + ... + P_b(1-P_b)^{M-1}] \\ &= 1 - (1-P_a)^N(1-P_b)^M. \end{aligned} \tag{7}$$

This means that for neutralization of protons from both $2s$ and $2p$ shells of oxygen we obtain the total probability as,

$$P_T = 1 - (1-P_{2s})^2(1-P_{2p})^4. \tag{8}$$

The cross sections are then obtained by integrating over impact parameter the probabilities in equation (8).

3 Results and discussion

The calculated differential cross sections for single electron capture to H^+ ion from the oxygen atoms at 0.5, 1.5, 5, and 20 keV projectile energies at the angles below $\sim 0.1^\circ$ are shown in Figures 1–4, respectively. The cross sections are found to be in agreement with the experimental results of Lindsay et al. [8]. This agreement further improves with the increase in the incident energy. At

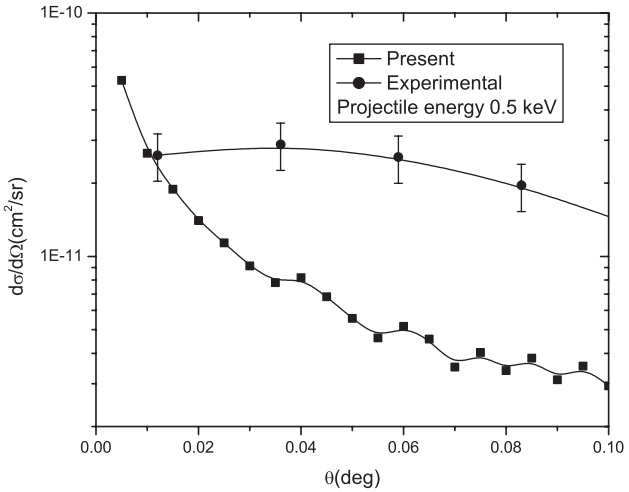

Fig. 1. Differential cross sections for charge-transfer scattering of H^+ + O at projectile energy 0.5 keV.

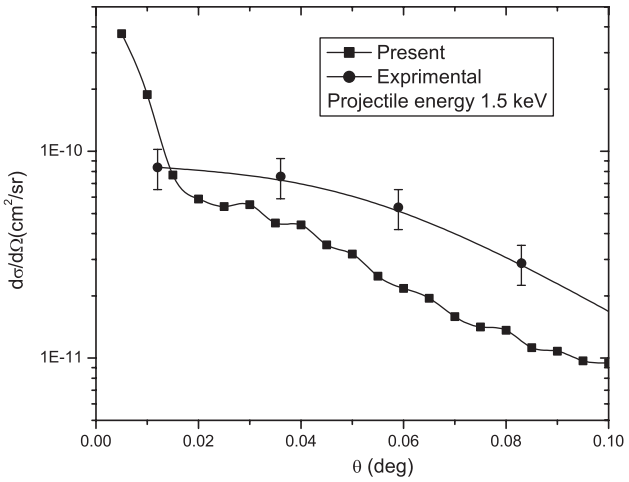

Fig. 2. Differential cross sections for charge-transfer scattering of H^+ + O at projectile energy 1.5 keV.

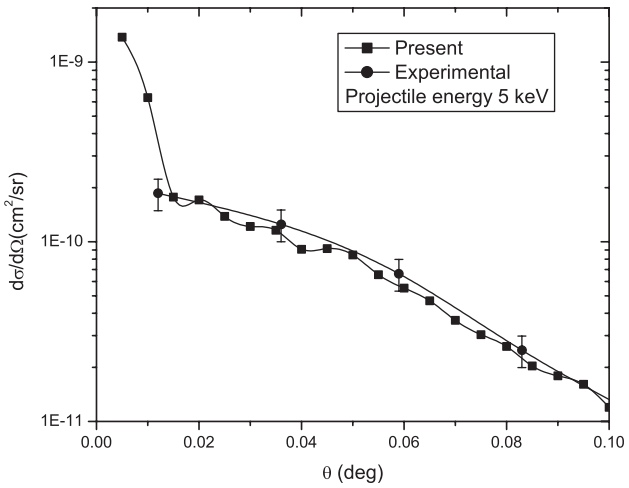

Fig. 3. Differential cross sections for charge-transfer scattering of H^+ + O at projectile energy 5 keV.

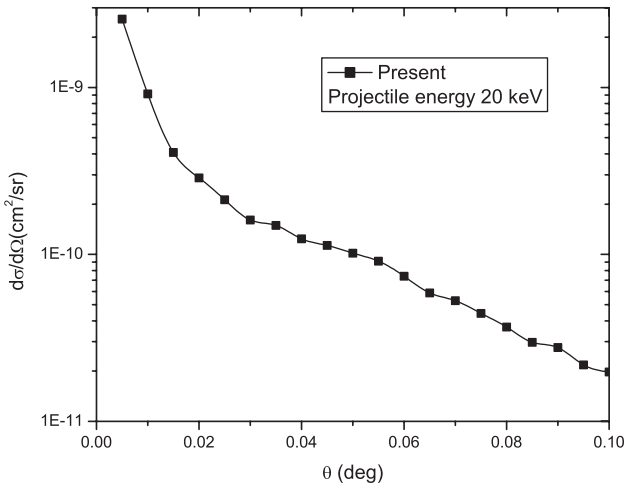

Fig. 4. Differential cross sections for charge-transfer scattering of H^+ + O at projectile energy 20 keV.

5 keV energy, for example, the present data are in excellent agreement with observed ones [8]. These DCS are forward peaked at all the energies and become somewhat oscillatory in nature at higher angles. The magnitude of the cross sections increases in forward direction with increase in energy as shown in Figure 5. The amplitude of the oscillations reduces both with the increase in angle as well as the incident energy. The *p*-orbital electrons distribution being asymmetric in space, the electron capture from these *p*-orbits may give rise to these oscillations in the capture cross sections curve. The experimentally measured DCS, however, does not show any oscillation in its magnitude. A likely reason could be the lack of sensitivity and resolution of the detector in their experimental set up capable of resolving these oscillations. Further, they used a microwave discharge to get the target atoms, which contained approximately 74% molecular oxygen, 24% atomic oxygen, 1.5% water vapor, and 0.5% molecular nitrogen and carbon dioxide along with their excited species. The

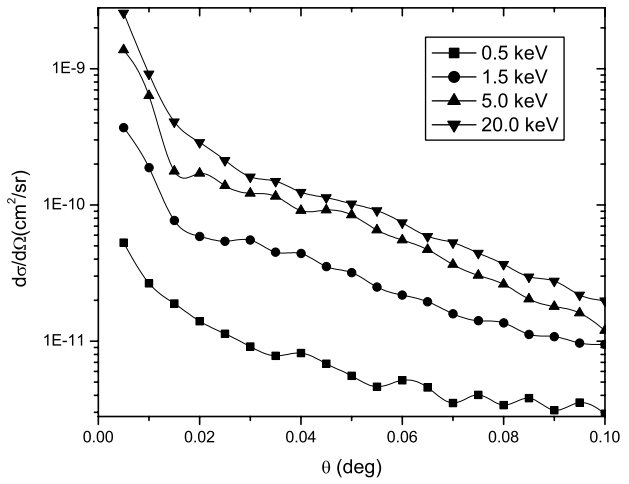

Fig. 5. Differential cross sections for charge-transfer scattering of H^+ + O at projectile energy 0.5, 1.5, 5, and 20 keV.

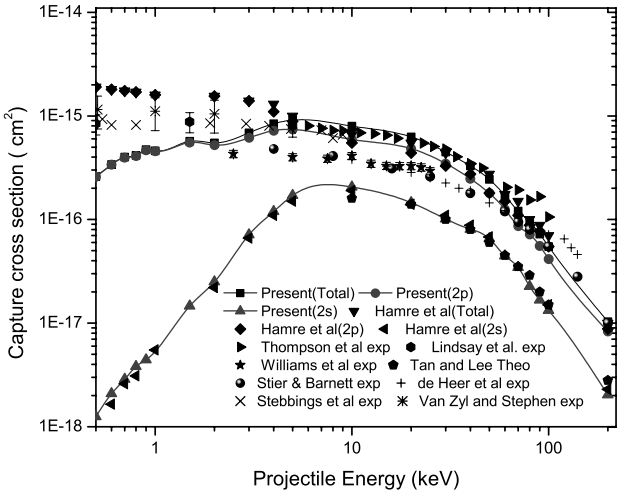

Fig. 6. Capture cross sections for the H^+ + O collision.

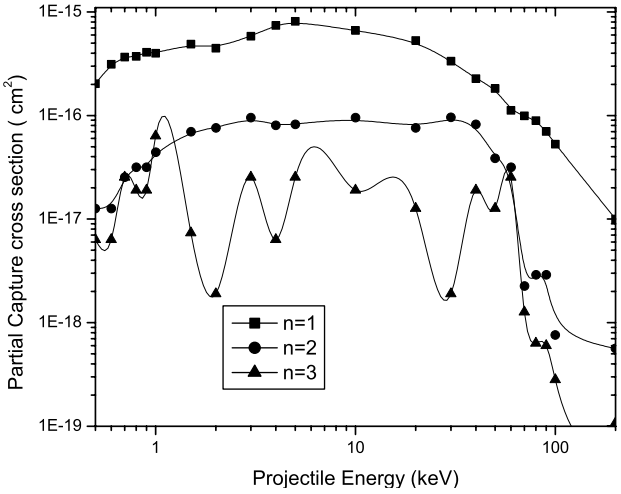

Fig. 7. Partial capture cross sections for the H^+ + O collision for $n = 1$, 2 and 3 shells of hydrogen atoms.

presence of all these in the target chamber with oxygen atoms may also cause the suppression of these oscillations in the cross sections. No other experimental or theoretical data except that of Lindsay et al., exists with which to compare our CTMC differential cross sections to settle this controversy.

Figure 6 shows the variation of the total capture cross sections in the energy range of 0.5–200 keV. The CTMC cross sections are compared with different experimental results (Thompson et al. [9], Lindsay et al. [8], Williams et al. [13], Stier et al. [10], de Heer et al. [11], Stebbings et al. [7] and Van Zyl and Stephen [12]) as well as the calculations of Tan and Lee [5], and Hamre et al. [1]. The AOCC data of Hamre et al. for single electron capture from $2p$, $2s$ and combined shells are found to be in excellent agreement with our results above 2 keV energy. Though the $2s$-partial cross sections are in very good agreement in the entire energy range, the total cross sections deviate from each other below about 2 keV of energy. The experimental results of Thompson et al. and of Stebbings et al. in the energy range of 6–100 keV and 0.5–10 keV, respectively are also in very good agreement with the present CTMC cross sections. The measurements of Williams et al. [13] reported in the energy range 2.5–25 keV, are particularly, in large deviation with the present data. A slight deviation of the present CTMC cross sections, from that of the results of Stebbings et al. is noticed below 2 keV energy. The results reported by Lindsay et al. at 0.5, 1.5, 5.0 keV were obtained by integration of the measured differential cross sections for electron capture over the angular range of 0.01°–2.26°. In their experiment the presence of so many atomic and molecular species along with the target O atoms is very likely to complicate the extraction process of these cross sections from the observed signal. Nevertheless, their results can be seen to be in good accord with the measurements of Stebbings et al. The measured as well as calculated cross sections of Tan and Lee in the entire energy range are lower as compared to the present results. However, their results match with our cross sections for the $2s$ subshell.

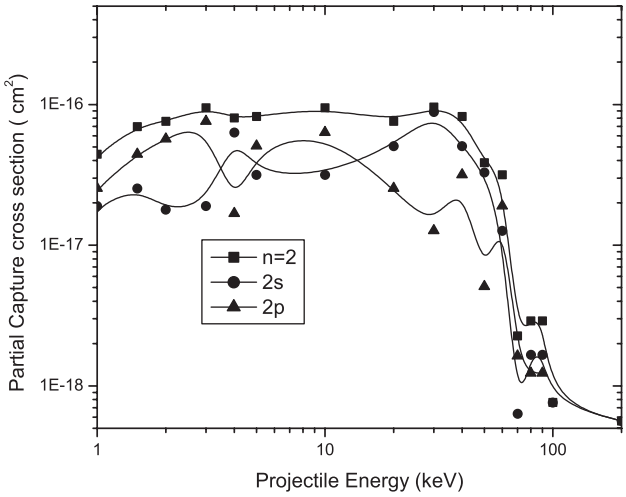

Fig. 8. Partial capture cross sections for the H^+ + O collision for $n = 2$, $2p$ and $2s$ shell of hydrogen atoms.

The one-half of the capture cross section for O_2 target measured by de Heer et al. are in good agreement with the present results. The magnitude of the capture cross section is maximum at 5 keV incident energy after which it decreases rapidly.

The calculated results of partial capture cross sections for $n = 1$, 2, and 3 shells of hydrogen atom are given in Figure 7. The energy defect ΔE primarily governs the process of capture and accordingly, it can be seen from Figure 7 that the capture cross section to the $n = 1$ level is maximum throughout the whole energy range. In case of $n = 3$, there are oscillations in the cross section variation with energy. The partial cross section for $n = 2$, $2s$ and $2p$ shells of hydrogen atom are shown in Figure 8. An interesting feature viz.; oscillatory structure, has been observed in the partial cross sections curve. This kind of oscillatory structure has also been observed by several researchers in the partial capture cross sections [15, 26,27] and distinct models have been proposed towards

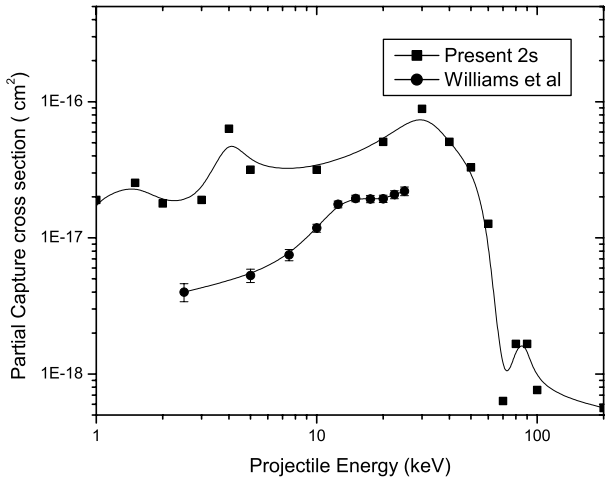

Fig. 9. Partial capture cross sections for the H^+ + O collision for 2*s* shell of hydrogen atoms with experimental result of Williams et al.

its explanation. However, the identification of any explicit mechanism responsible for the observed structure is yet to crystallize. Alternatively, these structures could well be collective coherence phenomenon involving many states and, thus, could be explained, at least qualitatively by classical models [28]. A classical analog of this process has been proposed by MacAdam et al. [25] in which a transient molecular ion formation and the partially resolved contributions of one-, tree- and higher-odd swap processes have been ascertained to cause these oscillations in case of ion-Rydberg atom collisions. The classical picture of quasi-molecular-ion formation has been illustrated by Ovchinnikov and Solov'ev [29] wherein they have shown to exist a specific topology corresponding to a specific range of internuclear distance for the classically allowed motion of an electron under the influence of both the target and projectile nuclei. These oscillations disappear in the total capture cross sections due to the averaging. The cross sections for capture to 2*s* states are compared with the experimental results of Williams et al. (see Fig. 9). There is large deviation in magnitude but nature of variation is more or less similar for both the results. It is to be noted that Thompson et al. [9] have already reported about the gross error in the method used by Williams et al.

4 Conclusions

The CTMC method along with the model interaction potential has been shown to be applicable even for the targets like O atom that contains four valence electrons in it. The reported differential cross sections are in fairly good agreement with the observed ones. The oscillations in the differential cross sections near the forward direction caused by the asymmetry in the *p*-electron distribution are reported for the first time. Also, oscillations in the partial capture cross sections corresponding to $n = 3$ level reported presently is altogether a new feature.

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