Classical analysis of angular differential and total cross sections for charge transfer and ionization in He-like systems-helium atom collisions

M.K. Pandey*, Y.-C. Lin, Y.K. Ho

Institute of Atomic and Molecular Sciences, Academia Sinica, P.O. Box 23-166, Taipei 106, Taiwan, ROC

A classical approach is used to determine the angular differential and total cross sections for charge transfer and ionization in He-like systems (Li\(^{+}\), Be\(^{2+}\), B\(^{3+}\), C\(^{4+}\), N\(^{5+}\), O\(^{6+}\)) and helium atom collisions. It is found that the classical approach, i.e., classical trajectory Monte Carlo method (CTMC), gives adequate results for charge transfer and ionization in He-like systems and helium atom collisions. A model potential has been used for interactions of the active electrons with the projectile and target ion. We also observed sudden increase in the ionization cross sections at lower velocities, and it is explained in terms of quasi-molecular formation and multiple interactions. The behavior of angular differential cross sections calculated at very small scattering angle (<0.1°) in all systems shows a forward peak followed by an asymptotic fall with oscillatory structure at higher angles. These oscillations were classically interpreted in terms of swapping. The calculated cross sections are found in reasonable agreement with the available experimental and theoretical results.

© 2016 The Physical Society of the Republic of China (Taiwan). Published by Elsevier B.V. All rights reserved.

1. Introduction

During the last four to five decades, studies on single-electron capture and ionization for impact of multiple charge ion and neutral atom have been carried out by many theoretical as well as experimental groups [1−29]. This is because of great importance not only in basic atomic collision physics but also in such diverse fields as fusion plasmas [30], stellar atmospheres [31], controlled-thermonuclear-fusion research, developments of x-ray laser device and astrophysics [32,33]. Considerable efforts have been devoted to understand the interaction between the highly charged solar wind minor ions and the atomic molecular constituents of atmospheres which produces X-ray emission [33−36]. In the study of radiotherapy, electron capture and ionization phenomena are found during damaging the DNA of cancerous tissue [37,38]. Particularly, charge transfer and ionization process in He-like systems (Li\(^{+}\), Be\(^{2+}\), B\(^{3+}\), C\(^{4+}\), N\(^{5+}\), O\(^{6+}\)) and helium atom collisions play a key role in plasma application [39−43].

Among others, the helium atom is an interesting target atom, because its electronic structure is simple enough to treat theoretically and it can be easily prepared as a target atom in collision experiments. On the other hand, the collision induced
by multi-charge ions and helium atoms, in which two target electrons are involved in the collision system, is more complex than one electron target and therefore it would be interesting to investigate the single electron capture processes. In the low and intermediate energy range, many experiments [18–28] of electron capture process in collision of various ions with helium have been carried out. Recently, we have reported [1,2] the cross sections for single electron charge transfer and ionization in collisions of various charge states of He-like system (Li\(^{+}\), Be\(^{2+}\), B\(^{3+}\), C\(^{4+}\), N\(^{5+}\), O\(^{6+}\)) and hydrogen atom and in a wide energy range and found the calculated results are in good agreement with experimental data as well as with other calculations. Presently, we extend these calculations to a helium target. It is well known, that only one electron is added in helium compared to hydrogen, but the calculations become much more complex due to the interaction between the two electrons.

In the present work, we investigate the charge transfer and ionization processes in collision of helium-like system A\(^{q+}\) (Li\(^{+}\), Be\(^{2+}\), B\(^{3+}\), C\(^{4+}\), N\(^{5+}\), O\(^{6+}\)) and helium atom in the energies range from 1 to 500 keV/u.

\[
A^{q+} + \text{He} \rightarrow A^{(q-1)+} + \text{He}^+ \text{(Charge transfer)} \tag{1}
\]

\[
A^{q+} + \text{He} \rightarrow A^{q+} + \text{He}^+ + e^- \text{(Ionization)} \tag{2}
\]

For the above reaction, helium-like system A\(^{q+}\) and He atom, model potential has been used for interactions of the active electrons with the projectile and target ion [44]. This model potential suggested by Schweizer et al. [44] representing the e-A\(^{q+}\) interaction in the form,

\[
V_{A^{q+}e}(r) = -\frac{1}{r} \left( \hat{Z} + (Z - \hat{Z}) \exp(-ar) + br \exp(-cr) \right). \tag{3}
\]

The concept of model potential \(V_{A^{q+}e}(r)\), to make frozen core of ion, \(r\) being the radial co-ordinate, is to simulate the multi-electron core interaction with the valence electron by an analytic modification of the Coulomb potential. The potential parameters \(\hat{Z}, Z, a, b,\) and \(c\) are tabled in Table 1.

In recent years, charge transfer processes (1) and ionization processes (2) have been subject to many theoretical studies using various methods to describe their dynamics. Recently, Baowei Ding [29] have done charge transfer and ionization calculations using classical method in the frame of independent-electron model in the energy range of 20–2500 keV/u for various ions (\(q = 2–6\)) with helium atom collisions. Tergiman et al. [45] have used semiclassical approach for the N\(^{4+}\) + He and B\(^{3+}\) + He/H\(_2\) collision in the energies range below 1–100 keV/u. The semiclassical molecular orbital close-coupling (MOCC) method has been used by Gargaud et al. [46], Hansen et al. [47], in the energy region from 1 to 100 keV/u. Alejandro et al. [5] have done the calculations within the framework of the perturbed stationary-state (PSS) approach for B\(^{3+}\) + He collision. However, classical approach for these studies has not been reported and therefore in the present work, we perform such calculations. The rest of this paper is organized as follows. In the next section, we describe the brief outline of theoretical method used in the cross section calculations. The calculated results of cross sections for charge transfer and ionization are presented in section III. Finally, conclusions are presented in section IV.

2. Theory

In this study, we employed the classical trajectory Monte Carlo (CTMC) method developed by Abrines and Percival [48,49], and Olson and Salop [50] to calculate the charge transfer and ionization cross sections for ion-atom collisions. This method is well known (for details see the references [48–54]) and has been proven successfully in previous applications [50–56]. Thus we present only the essential details here.

The classical trajectory Monte Carlo (CTMC) method is basically a treatment of the three body problem i.e., the projectile ion, active electron and the target core, in a three dimensional framework. To determine the trajectories of these three partners, the Hamilton’s equations of motion are established and solved numerically for several thousands of classical trajectories which are finally tested for the occurrence of capture and ionization processes. In order to evaluate the integrals, their limits have been generated randomly based on the Monte Carlo technique. In the CTMC method quantum wavefunctions are replaced with a random sampling of the initial coordinates from statistical distributions. In this present study, we used the microcanonical distribution for picking up the initial momentum and coordinates out of a uniform distribution and it is

<table>
<thead>
<tr>
<th>Ion</th>
<th>(Z)</th>
<th>(Z_{a})</th>
<th>(a)</th>
<th>(b)</th>
<th>(c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li</td>
<td>3</td>
<td>1</td>
<td>3.395</td>
<td>3.212</td>
<td>3.207</td>
</tr>
<tr>
<td>Be</td>
<td>4</td>
<td>2</td>
<td>4.733</td>
<td>4.804</td>
<td>4.817</td>
</tr>
<tr>
<td>B</td>
<td>5</td>
<td>3</td>
<td>6.152</td>
<td>6.290</td>
<td>6.300</td>
</tr>
<tr>
<td>C</td>
<td>6</td>
<td>4</td>
<td>7.655</td>
<td>7.654</td>
<td>7.674</td>
</tr>
<tr>
<td>N</td>
<td>7</td>
<td>5</td>
<td>9.100</td>
<td>9.109</td>
<td>9.108</td>
</tr>
<tr>
<td>O</td>
<td>8</td>
<td>6</td>
<td>10.467</td>
<td>10.449</td>
<td>10.552</td>
</tr>
</tbody>
</table>
subject to the condition that the total energy retains its quantum mechanical value. This provides a statistical momentum distribution that is equal to the quantum mechanical one. The initial conditions of the projectile are specified by its relative velocity $v_p$, impact parameter ‘$b’ and the position with respect to the center of mass of the target core and the electron. Also we used B-spline-based configuration interaction approach [1,2] to determine the initial electronic binding energies with the model potential. The position of the target electron with respect to the target core and its momentum distribution is obtained by solving the Kepler’s equation. The cross sections for the event $q$ (capture or ionization in the present case) is determined using the formula

$$\sigma_q = \left( \frac{N_q}{N_f} \right) \pi b_{\text{max}}^2$$

(4)

where, $N_f$ is the total number of trajectories calculated with impact parameter “$b$” lying in the range $0 \leq b \leq b_{\text{max}}$, and $N_q$ is the number of trajectories that satisfy the criteria for a specified event $q$ to take place.

Let $N_q$ denote the number of event that are detected in the solid angle. The differential cross sections for the ionization were computed using the formula.

$$\frac{d\sigma_q}{d\Omega} = \frac{N_q}{N_f \Delta \Omega} \pi b_{\text{max}}^2$$

(5)

The standard deviation for the reactive cross section is given by

$$\delta \sigma_q = \left(\frac{\sigma_q}{N_q} \right)^{1/2}.$$  

(6)

For the statistical error within a good approximation can be expressed as $\delta q = \sigma_q / N_q^{1/2}$. This shows that in order to reduce the error in the calculation one has to take a large number of trajectories. Also, if the value of $b_{\text{max}}$ is increased, $N_f$ must also be increased to achieve the same value of the standard error. Therefore, the interest of efficiency $b_{\text{max}}$ should be chosen to be as small as possible. In the present study, more than $5 \times 10^5$ trajectories were computed to obtain good statistics (<3%).н

In order to calculate single electron capture or ionization cross sections in collision of ion and two electrons helium atom, the one-electron probabilities have been used in evaluation of the independent-particle multi-electron probabilities [57]. Let $P$ be the given capture probability for the 1st electron and $(1 - P)^N$ will be the probability for the 2nd electron to be captured. Therefore, the total probability for one electron to be captured of the $N$ equivalent electrons becomes $1 - (1 - P)^N$. In the present case, two electrons in the s-orbital and hence the total probability for two electron to be capture is given by $1 - (1 - P)^2$.

3. Results and discussion

3.1. Charge exchange cross section

Fig. 1a shows the variations of total charge exchange cross sections in $O^{6+} + \text{He}$ collision for the present calculation in the energy range from 1 to 500 keV/u. In the same figure, the experimental data of Crandall et al. [8] at 49.2 keV, and Gardner et al. [6] at 48 keV are shown for comparison. It can be observed that the present CTMC calculation compares quite well with experimental data of Crandall et al. [8]. The present results lie higher than the experimental data of Gardner et al. [6], but our results are quite close to the experimental data of Gardner et al. [6]. For other energies, there are no other data or calculations to compare with our results.

In Fig. 1b, we show the variations of total charge exchange cross sections in $N^{3+} + \text{He}$ collision for the present calculations in the energy range from 1 to 500 keV/u. The results of present CTMC calculations are compared with the experimental data of Crandall et al. [7] in the energy range 10–50 keV, and Gardner et al. [6] at 40 keV and Hoekstra et al. [58] in the energy range 1–6 keV. It can be observed that, while the present CTMC calculations compare quite well with experimental data of Hoekstra et al. [58], they do not agree too well with experimental data of Crandall et al. [8] in the energy range 10–50 keV, and Gardner et al. [6] at 40 keV.

In Fig. 1c, we show the variations of total charge exchange cross sections in $C^{4+} + \text{He}$ collision for the present CTMC calculations in the energy range from 1 to 500 keV/u. In the same figure, the present CTMC calculations are compared with experimental data of Crandall et al. [8] in the energies range 20–80 keV. Gardner et al. [6] at 32 keV, Hoekstra et al. [58] in the energy range 1–6 keV and Zwally et al. [9] at 32 keV. It has been observed that the agreement between the present calculations and the experimental data is not too well, but the present values are close to those in Hoekstra et al. [58] and Zwally et al. [9] at 1 and 32 keV/u respectively. The most easily postulated reason for this discrepancy is that underestimating many factors in the experiment.

The variations of total charge exchange cross sections in $B^{3+} + \text{He}$ collision for the present CTMC calculations in the energy range from 1 to 500 keV/u are shown in Fig. 1d. In the same figure, the present CTMC calculations are compared with the experimental data of Zwally et al. [9] at 24 keV, Crandall et al. [8] in the energy range 20–80 keV, Gardner et al. [6] at 24 keV to 80, Gargaud et al. [7] in the energy range 1–10 keV. We have also compared our results with the theoretical calculation based on semi-classical molecular-state expansion method by Kimura et al. [3] in the energy range 1–50 keV, Lopez-Castillo et al. [5]
in the energy range 1–60 calculated within the framework of the perturbed-state approach and with the result of Hansen [4] based on semiclassical two-center close-coupling expansions in the energy range 1–100 keV. We found that our computed CTMC results are in excellent agreement with the experimental results of Zwally et al. [9], Crandall et al. [8] and Gargaud et al. [7]. However, our results do not fare well with those by Gardner et al. below 30 keV/u, but the nature of variations of cross

Fig. 1. a. The total charge transfer cross sections for O$^{6+}$ + He collision. b. The total charge transfer cross sections for N$^{5+}$ + He collision. c. The total charge transfer cross sections for C$^{4+}$ + He collision. d. The total charge transfer cross sections for B$^{3+}$ + He collision. e. The total charge transfer cross sections for Be$^{2+}$ + He collision. f. The total charge transfer cross sections for Li$^+$ + He collision.
sections is the same. It has already reported by Kimura et al. that the cross sections measured by Gardner et al. [6] are smaller and it appears that they might have an experimental problem. Our calculated results are in very good agreement with the calculated results of Kimura et al. [3] at all energy ranges except at 50 keV/u. The results of Lopez-Castillo et al. [5] and Hansen [4] appears to agree reasonably well with our results except for few energy points, but the nature of variation of cross sections are the same.

In Fig. 1e–f, we show the variations of total charge exchange cross sections in Be\(^{2+}\) + He, and Li\(^+\) + He collisions, respectively for the present CTMC calculations in the energy range from 1 to 500 keV/u. The behaviors of all the system are the same as those for the B\(^{3+}\) + He, C\(^{4+}\) + He, N\(^{5+}\) + He and O\(^{6+}\) + He collisions.

Fig. 2 shows the comparative study of variations of total charge exchange cross sections in O\(^{6+}\) + He, N\(^{5+}\) + He, C\(^{4+}\) + He, B\(^{3+}\) + He, Be\(^{2+}\) + He, and Li\(^+\) + He collisions for the present CTMC calculations in the energy range from 1 to 500 keV/u. The behaviors of variation cross sections for all the systems are almost the same. From this figure we found that the capture cross section is a function of the projectile charge. It is also noticed that the magnitude of cross sections increases with increasing projectile charge in the whole energy range, and hence in the case of O\(^{6+}\) + He, it reaches a maximum for the capture cross sections. The magnitude of cross sections is decreasing as we go from O\(^{6+}\) + He to Li\(^+\) + He in the whole energy range.

3.2. Ionization cross sections

Fig. 3 shows the variations of ionization cross sections in C\(^{4+}\) + He collision for the present calculation in the energy range from 1 to 100 keV/u. There are no other data to compare with our results except one calculated data by Wood et al. [59] for C\(^{4+}\) + He at 100 keV/u. However, we notice that the behaviors of ionization cross sections are similar to our previous calculations for O\(^{6+}\) + H, N\(^{5+}\) + H, C\(^{4+}\) + H, B\(^{3+}\) + H, Be\(^{2+}\) + H, and Li\(^+\) + H collision [1] and O\(^{8+}\)He collision [2] results. Further, we don’t have any experimental data or calculated results to compare and therefore, we hope that the present work will stimulate experimentalists for further work in this direction.

The ionization cross sections for O\(^{6+}\) + He, N\(^{5+}\) + He, C\(^{4+}\) + He, B\(^{3+}\) + He, Be\(^{2+}\) + He, and Li\(^+\) + He collision are shown in Fig. 4. The nature of variations of cross sections is the same in all the above systems. The main differences are the magnitudes of the cross sections which are different in all the systems throughout the energy range and the energy points from where unusual raise of ionization cross sections are started (i.e., for O\(^{6+}\) + He it is around ~30 keV/u, for Li\(^+\) + He it is around ~20 keV/u). In the energy range below ~20 keV/u and above ~100 keV/u, we observe that the cross sections are more enhanced with highly charged target systems. But, in the energy range 20 keV/u–100 keV/u, the trend is reversed, i.e., the cross sections are enhanced more with low charge target systems. Same feature was also observed for O\(^{6+}\) + H, N\(^{5+}\) + H, C\(^{4+}\) + H, B\(^{3+}\) + H, Be\(^{2+}\) + H, and Li\(^+\) + H collisions as in our previous study [1]. The only difference between both systems is the energy point and range.

Here, we have noticed the most interesting aspects of the ionization cross sections are its unusual raise at low energy. This intriguing aspect of the ionization cross sections was also observed for O\(^{6+}\) + H, N\(^{5+}\) + H, C\(^{4+}\) + H, B\(^{3+}\) + H, Be\(^{2+}\) + H, and Li\(^+\) + H collision in our previous study [1]. Another important point observed from this figure is the unusual rising point in cross sections depends on the collision system (i.e., the dip point of the cross section is shifting towards lower energies as the charge of the projectile decreases). Homan [60] has been observed such behavior the first time, but he did not put forth any
reason for its occurrence and reported it was an unexpected feature. Further, Perumal et al. [55,56] has observed the same behavior in collision of Na$^+$ and Ar$^+$ ions colliding with a variety of states in selected Na Rydberg atom targets and reported that the multiple interactions of the active electron with the projectile enhance ionization. Recently [1,2,61], we have also found this type of behavior in O$^{6+}$ + He, N$^{5+}$ + He, C$^{4+}$ + He, B$^{3+}$ + He, Be$^{2+}$ + He, and Li$^+$ + He collisions and O$^{8+}$ + H collision system and we reported that this is only due to the multiple interactions of the active electron with the projectile. In the present study also, we have found the same reason for unusual raise in ionization cross sections at low energy, i.e., multiple interactions of the active electron with the projectile would enhance the ionization probability in lower energies. Basically during collision processes the active electron, after suffering multiple interactions between two cores, may end up either in an excited state of the ion or in an excited state of the helium, or may move away from the cores and leave them ionized.

3.3. Differential cross sections

Angular differential cross sections (DCS) in ion-atom provide detail information about the interaction between two collision partners. Very little effort has been made towards the understanding of DCS for capture and ionization [62–72].
Studies of angular differential scattering at keV/u energies at very small angles (below 1°) are particularly motivated by the highly forward peaked character of the cross sections, formation of the classical rainbow angle within the range, and containing information that permits to analysis the proposed interactions potentials. Also, observation of the Fraunhofer diffraction pattern in this angular range is one of the most fascinating processes that need attention.

Fig. 5. a. Shows the variation of charge transfer differential cross sections for O\(^{6+}\) + He atoms collision at projectile energies of 1, 10, 50 & 100 keV/u. b. Shows the variation of charge transfer differential cross sections for N\(^{5+}\) + He atoms collision at projectile energies of 1, 10, 50 & 100 keV/u. c. Shows the variation of charge transfer differential cross sections for C\(^{4+}\) + He atoms collision at projectile energies of 1, 10, 50 & 100 keV/u. d. Shows the variation of charge transfer differential cross sections for B\(^{3+}\) + He atoms collision at projectile energies of 1, 10, 50 & 100 keV/u. e. Shows the variation of charge transfer differential cross sections for Be\(^{2+}\) + He atoms collision at projectile energies of 1, 10, 50 & 100 keV/u. f. Shows the variation of charge transfer differential cross sections for Li\(^{+}\) + He atoms collision at projectile energies of 1, 10, 50 & 100 keV/u.
Fig. 5a–f shows the variation of charge transfer differential cross sections at projectile energies of 1, 10, 50 & 100 keV/u for helium-like systems ($\text{Li}^+$, $\text{Be}^{2+}$, $\text{B}^{3+}$, $\text{C}^{4+}$, $\text{N}^{5+}$, $\text{O}^{6+}$) and helium atoms collision at projectile energies of 1 keV/u. b. Shows the variation of charge transfer differential cross sections for helium-like systems ($\text{Li}^+$, $\text{Be}^{2+}$, $\text{B}^{3+}$, $\text{C}^{4+}$, $\text{N}^{5+}$, $\text{O}^{6+}$) and helium atoms collision at projectile energies of 10 keV/u. c. Shows the variation of charge transfer differential cross sections for helium-like systems ($\text{Li}^+$, $\text{Be}^{2+}$, $\text{B}^{3+}$, $\text{C}^{4+}$, $\text{N}^{5+}$, $\text{O}^{6+}$) and helium atoms collision at projectile energies of 50 keV/u. d. Shows the variation of charge transfer differential cross sections for helium-like systems ($\text{Li}^+$, $\text{Be}^{2+}$, $\text{B}^{3+}$, $\text{C}^{4+}$, $\text{N}^{5+}$, $\text{O}^{6+}$) and helium atoms collision at projectile energies of 100 keV/u.

Calculated charge transfer differential cross sections for helium-like systems ($\text{Li}^+$, $\text{Be}^{2+}$, $\text{B}^{3+}$, $\text{C}^{4+}$, $\text{N}^{5+}$, $\text{O}^{6+}$) and helium atoms collision at projectile energies of 1 keV/u, 10 keV/u, 50 keV/u, and 100 keV/u are shown in Fig. 6a–d respectively. It is observed that the magnitude of charge transfer (at all the energies and projectile) peaks in the forwards direction and decreases asymptotically with an increase in the scattering angle, and subsequently becomes oscillatory in nature at higher angles in $\text{B}^{3+}$, $\text{B}^{2+}$, and $\text{Li}^+$ cases.

Moreover, differential cross sections for single electron capture at angles close to the diffraction limit of atom are calculated at different incident energies (1, 10, 50 & 100 keV/u). This is because, in the collision reaction between charge ion and atoms, the interaction region between two particles is replica to a circular aperture, and thus atomic-size Fraunhofer-type diffraction can be observed. Recently, van der Poel et al. [69] and Wang et al. [70] have observed the oscillation pattern in the angular distribution of projectile for $\text{Li}^+$ + $\text{Na}$ and $\text{He}^{2+}$ + $\text{He}$ single electron capture collisions respectively, and explained the structures with Fraunhofer diffraction theory in which the scattering amplitudes (and hence the differential cross sections) for various reaction channels are expressed as a Fraunhofer type integral [71]. However, in the present case, the diffraction pattern of Fraunhofer type due to the annular ring, which is well known in classical optics, does not appear.

The CTMC method, being a classical model, does not support the idea of quantum effects responsible for such structures. The oscillatory structure in the differential cross sections for the helium-like systems appears due to the competition between
the initial and final capture channels. Basically, when an ion approaches to the target, the velocity of project is slowdown and at the same time the active electron have enough time to swaps many times between to core. Hence, classically we can say that these oscillations are analogous to the number of swaps of the active electron experiences between the two cores.

4. Conclusions

In summary, we have studied charge exchange and ionization processes in collision of a He-like system (Li$^+$, Be$^{2+}$, B$^{3+}$, C$^{4+}$, N$^{5+}$, O$^{6+}$) with the helium atom using the CTMC method in the energy range of $1$–$500$ keV/u. Our results are in good agreement with the existing experimental and theoretical predictions. We have observed an interesting feature that shows an increase in the ionization cross sections at lower velocities. A sudden rise in the ionization cross section at low energy has been reported and explained qualitatively through a multiple encounter model. We found that, the peaks of the calculated differential cross sections in all the system are in the forward direction and decreases asymptotically with increase of scattering angle, and subsequently become oscillatory in nature at higher angles, and the amplitude of this oscillations are more enhanced at higher energies. Such oscillatory structure in the differential cross sections for the lighter helium-like systems appears due to the swapping of the electron between the target and projectile core. We believe that such theoretical study will be helpful for experimentalists towards further investigations in this direction.

Acknowledgments

The authors are grateful to the Ministry of Science and Technology of Taiwan, ROC (MOST 104-2811-M-001-097 and MOST 104-2811-M-001-161), for financial support.

References
