Projectile electron loss in collisions of light charged ions with helium*

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We investigate the single-electron loss processes of light charged ions ($Li^{1+,2+}$, $C^{2+,3+,5+}$, and $O^{2+,3+}$) in collisions with helium. To better understand the experimental results, we propose a theoretical model to calculate the cross section of projectile electron loss. In this model, an ionization radius of the incident ion was defined under the classical over-barrier model, and we developed "strings" to explain the processes of projectile electron loss, which is similar with the molecular over-barrier model. Theoretical calculations are in good agreement with the experimental results for the cross section of single-electron loss and the ratio of double-to-single ionization of helium associated with one-electron loss.

Keywords: ion-atom collision, over-barrier model, electron loss

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1. Introduction

The collision systems of multiple charged ions and helium have been widely studied for understanding the many-body dynamics of atoms These studies used the advantage that helium has a simple electron structure. In charged ion-helium collision systems, three processes can occur: (i) direct ionization of helium target, in which the charge state of the projectile is unchanged; (ii) helium electron capture, in this process the charge state of projectile is decreased; (iii) projectile electron loss, which gives an increased charge state of the incident ions. Mostly, research is focused on direct ionization channels and electron capture channels in either experiments or theories. For the channel of projectile electron loss, several experimental and theoretical studies were published,[1–3] but the strong dependences of the charge state and the velocity of projectile were not well understood. When both the target electrons and projectile electrons were ionized, the problem becomes increasingly complex.

Most of the descriptions for electron loss channels are quantum methods. The earliest one was introduced by Bates and Griffing applying the first Born approximation to collisions between two hydrogen atoms.[4] Later, Anholt,[5] McGuire,[6] Dmitriev,[7] and Gillespie[8] researched the dynamics further. Montenegro *et al.* developed the theory of screening and anti-screening in the framework of plan-wave Born approximation (PWBA)[9,10] and provided very good explanations for the projectile electron loss channels. Recently, Montenegro *et al.* extended the PWBA theory to explain all three channels and their result was in good agreement with the experimental measurement in C^{3+} and He^{+} collision with noble gases.[11,12] Other quantum methods were also published, such as the coupled-channel method,[13] sudden approximation,[14] the free-collision model,[15,16] and the independent particle model.[17]

In the classical methods, such as the n-body classical trajectory Monte Carlo (nCTMC) method[18] and the classical over-barrier model (COBM),[19] excellent descriptions have been given for the target ionization channels. Foil *et al.* introduced screening and anti-screening terms into the nCTMC[20] and used it for the projectile electron loss channel. Previously, our group has discussed the calculation of target ionization cross section with and without electron loss based on the COBM.[21–23] Here, we propose to extend the COBM further to explain the process of projectile electron loss with helium electron ionization.

We studied the projectile electron loss in the collision system of $Li^{1+,2+}$, $C^{2+,3+,5+}$, and $O^{2+,3+}$ with helium, and validated the experiment results using the proposed theoretical calculations. Due to the limitation of measurement of the absolute cross section, we measured the ratio of double-to-single ionization of helium associated with projectile electron loss.

2. Theoretical calculation

The channel of projectile one-electron loss in the A^{q+} + He collision system can be divided into three categories: (1) SL0I, single projectile electron loss with no target ionization; (2) SLSI, single projectile electron loss with single helium ionization; and (3) SLDI, single projectile electron loss with double helium ionization

$$A^{q+} + \mathrm{He} \rightarrow A^{(q+1)+} + \mathrm{He} + \mathrm{e}, \quad \text{SL0I},$$
$$A^{q+} + \mathrm{He} \rightarrow A^{(q+1)+} + \mathrm{He}^{1+} + 2\mathrm{e}, \quad \text{SLSI},$$
$$A^{q+} + \mathrm{He} \rightarrow A^{(q+1)+} + \mathrm{He}^{2+} + 3\mathrm{e}, \quad \text{SLDI}.$$

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Theoretically, the projectile could be considered as a hydrogen-like ion ($A^{(q+1)+}$), as shown in Fig. 1. The projectile electron (e) will receive two kinds of forces, one from the projectile core ($A^{(q+1)+}$) and the other from the target (He). To calculate the Columbic force between target and projectile electron, we propose that the target has an effective charge state (Z_T), which will be discussed below.

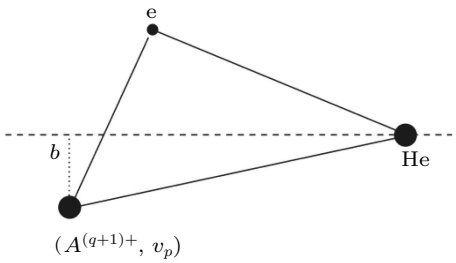


Fig. 1. Sketch of projectile electron loss with impact parameter b in $A^{(q+)}+\mathrm{He}$ collision system.

For the three channels of projectile one-electron loss, three electrons should be considered, the electron of the projectile and the two electrons of helium. These three electrons are ionized in two-center scatter under the independent electron approximation.[10] Electrons have fractions to transfer from one nuclear center to another.

The radius that an electron is able to cross the potential barrier can be written as $R_r = (Z_T + \sqrt{Z_T Z_P})/E_n$, and is named the release radius. In this fomula, Z_T and Z_P are the effective charge states of the target and projectile; E_n is the binding energy of the electron.

For unperturbed trajectories, the fraction of electron transfer at time t is[24]

$$N_\Omega = \frac{\sqrt{Z_P}}{2(\sqrt{Z_P}+Z_T)^2}\left[(\sqrt{Z_P}+Z_T)^2 - Z_P - E_n R\right]. \quad (1)$$

The probability of electron transfer is

$$P(b) = \exp\left(-\int_{-\infty}^{+\infty} \frac{N_\Omega}{T}\,\mathrm{d}t\right). \quad (2)$$

The electron release probability is

$$P_r(b) = 1 - \exp\left(-\int_{-t}^{+t} \frac{N_\Omega}{T}\,\mathrm{d}t\right). \quad (3)$$

The integration time t is defined as $t = \sqrt{R^2 - b^2}/v_p$. Here, R is the internuclear distance and b is the impact parameter, T is the orbital period of electron motion, defined as $T = 2\pi[2(E_n + Z_P/R)]^{-3/2}$ in Ref. [25].

It is possible that the released electrons would be captured by the opposite nuclear center. Bohr and Lindhard pointed out that, for low incident energy, all the released electrons will be captured and the cross section of electron capture is a constant $\sigma_c = \pi R_c^2$.[19] Here, $R_c = 2Z_p/v_p^2$ is defined as the capture radius, which means that the electron will be captured once it enters this capture distance. In this low energy region, the capture radius is larger than the release radius, $R_c > R_r$, and the probability of electron release is larger than that of electron capture. When the incident energy is getting higher, the capture distance R_c will be smaller than the release distance R_r, $R_c < R_r$. At that time, the probability of electron capture will be less than the probability of electron release. Thus, some of the released electrons will not be captured, but be ionized.

Therefore, we define the ionization distance, R_i, where the electron releases from the target but is not be captured by the projectile.[21] The ionization distance should satisfy, $Z_p/R_i \geq E_n + Z_p/R_r$.

The ionization probability could be written as

$$P_i(b) = \exp\left(-\int_{-\infty}^{t_i} \frac{N_\Omega}{T}\,\mathrm{d}t\right)\left[1 - \exp\left(-\int_{-t_r}^{+t_r} \frac{N_\Omega}{T}\,\mathrm{d}t\right)\right]. \quad (4)$$

The capture probability could be written as

$$P_c(b) = \exp\left(-\int_{-\infty}^{t_c} \frac{N_\Omega}{T}\,\mathrm{d}t\right)\left[1 - \exp\left(-\int_{-t_r}^{+t_r} \frac{N_\Omega}{T}\,\mathrm{d}t\right)\right]. \quad (5)$$

Here, a hypothesis was made: an electron crossing the potential barrier would be either ionized or captured. In Eqs. (4) and (5), the integration time, $t_k = \sqrt{R_k^2 - b^2}/v_p$ ($k = r, c, i$), are the release radius, the capture radius, and the ionization radius, respectively. The cross section of electron capture or electron ionization could be numerically calculated by the integration of the impact parameter.

Similar to what was done in the molecular over-barrier model (MOBM), we developed a "string", (P_1, T_1, T_2), to explain the channels of projectile one-electron loss.[26] Here, P_1, T_1, and T_2 donate the projectile electron, the first ionized target electron, and the second ionized target electron, respectively. Once one of the three electrons appears in the strings, that electron has ionized already, and the charge state of the ionized projectile or target will be increased by one "1". If the character "0" appears in the strings, it means that the electron was not ionized, and the charge state of the projectile or the target does not change. For instance, the string $(P_1, 0, 0)$ demonstrates a channel where only the projectile electron is ionized (SL0I) and the charge state of the target atom does not change.

The SLSI channel includes ionizations of both the projectile electron and the target electron. One could not recognize the two electrons, because the two electrons are identical. Hence the total probability of SLSI should be the sum of the two probabilities of $(P_1, T_1, 0)$ and $(T_1, P_1, 0)$. The order of the electrons in a particular string does not mean that the time stamp of the ionization happened, but only the charge state of projectile or target. For example, the string $(P_1, T_1, 0)$ means that the projectile electron P_1 was ionized by the effective charge state $Z_T^{\mathrm{eff}}(b)$ of the target; and the target electron T_1 was ionized by the charge state of projectile $(q+1)+$, instead of $q+$. The character "0" means that the second target electron

was still bounded in the potential barrier. On the other hand, the string of $(T_1, P_1, 0)$ demonstrates that the target electron T_1 was ionized at the projectile charge state $q+$, the projectile electron P_1 was ionized under the charge state of target $1+$.

The SLDI channel could be explained by the strings of (P_1, T_1, T_2), (T_1, P_1, T_2), and (T_1, T_2, P_1) In these three strings, all three electrons will be ionized, and all three electrons are identical. The probability of SLDI would be the sum of the three probabilities. In the calculation, the ionization of projectile electron P_1 was induced by the target atom under effective charge states, charge state $1+$, and charge state $2+$, respectively. The second target electron T_2 was ionized at the projectile charge states of $(q+1)+$ and $q+$ when the target charge state was increased to $1+$.

By using our proposed "string", the three categories of projectile one-electron loss that we defined in the beginning of this section could be written as follows:

$$\begin{aligned} &(P_1,0,0), && && \text{SL0I},\\ &(P_1,T_1,0), && (T_1P_1,0), && \text{SLSI},\\ &(P_1,T_1,T_2), && (T_1,P_1,T_2), && (T_1T_2P_1), && \text{SLDI}. \end{aligned}$$

In the current calculation, we used the effective charge state $Z_{\mathrm{T}}^{\mathrm{eff}}(b)$ from Ref. [6] for the target atom. We define three radii of the projectile electron, release radius, capture radius, and ionization radius as

$$R_{\mathrm{r}} = \frac{Z_{\mathrm{P}} + \sqrt{Z_{\mathrm{T}} Z_{\mathrm{P}}}}{E_{\mathrm{ie}}}, \quad R_{\mathrm{c}} = \frac{2Z_{\mathrm{T}}^2}{v_{\mathrm{rel}}^2}, \quad \frac{Z_{\mathrm{T}}}{R_{\mathrm{i}}} \geq E_{\mathrm{ie}} + \frac{Z_{\mathrm{T}}}{R_{\mathrm{r}}}. \tag{6}$$

Here, v_{rel} is the relative velocity of target, E_{ie} is the ionization energy of the projectile electron. We define the cross sections of the channels SL0I, SLSI, and SLDI as σ_{SL0I}, σ_{SLSI}, and σ_{SLDI}.

$$\sigma_{\mathrm{SL0I}} = 2\pi \int_0^{\infty} P_{\mathrm{Pi}}(b)(1 - P_{\mathrm{T1r}}(b))(1 - P_{\mathrm{T2r}}(b)) b \mathrm{d}b, \tag{7}$$

$$\sigma_{\mathrm{SLSI}} = 2\pi \sum \int_0^{\infty} P_{\mathrm{Pi}}(b) P_{\mathrm{T1i}}(b)(1 - P_{\mathrm{T2r}}(b)) b \mathrm{d}b, \tag{8}$$

$$\sigma_{\mathrm{SLDI}} = 2\pi \sum \int_0^{\infty} P_{\mathrm{Pi}}(b) P_{\mathrm{T1i}}(b) P_{\mathrm{T2i}}(b) b \mathrm{d}b, \tag{9}$$

where $P_{\mathrm{Pi}}(b)$ and $P_{\mathrm{Ti}}(b)$ are the ionization probabilities of the projectile electron and target electron, which are calculated using Eq. (4) under the framework of "string", $P_{\mathrm{Tr}}(b)$ is the release probability of the target electron, calculated by the formula (3). The total cross section of projectile one-electron loss in $A^{q+} + \mathrm{He}$ system could be described as

$$\sigma_{\mathrm{Single\text{-}loss}} = \sigma_{\mathrm{SL0I}} + \sigma_{\mathrm{SLSI}} + \sigma_{\mathrm{SLDI}}. \tag{10}$$

It should be noted that the effectiveness of the "string" description in this paper is based on the two-step theory[27] and the independent electron approximation[10] We use "string" to explain the projectile one-electron loss of $A^{q+} + \mathrm{He}$ because only three electrons were involved. It would be wrong to use such a "string" to explain manyelectron systems.

3. Results and discussion

As shown in the Figs. 2–5, the cross section of projectile ionization is charge state dependent and related with the incident velocity, $\sigma_{\mathrm{LOSS}} = f(v^2, q)$. In the low energy region, figures show that the cross section of projectile electron loss is increasing with the increase of the incident energy. On the other hand, in the high energy region, the cross section of projectile electron loss will decrease with the increase of incident energy. Experiments have proved that the maximum cross section will be achieved when the incident energy of ions is 200–300 keV/amu.[11,21,25] This phenomenon was well predicted by our theoretical calculation.

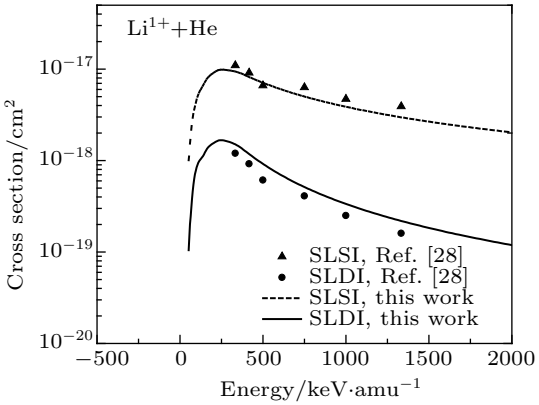


Fig. 2. Cross sections of SLSI and SLDI of helium in $\mathrm{Li}^{1+} + \mathrm{He}$ collision. Dots (▲) and (●) are the cross sections of SLSI and SLDI from Ref. [28], respectively. Lines are the theoretical calculations of this work.

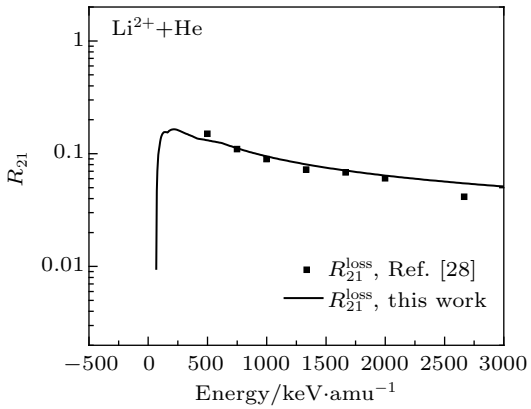


Fig. 3. Ratios of double-to-single helium ionization associated with projectile one-electron loss in $\mathrm{Li}^{2+} + \mathrm{He}$ collision. Dots (■) are the experimental results from Ref. [28]. The line is the theoretical calculations of this work.

Figures 2 and 3 show the cross section of projectile loss of $\mathrm{Li}^{1+,2+}$ in collisions with helium. For Li^{1+}, cross sections of helium double and single ionizations associated with projectile single loss (SLSI and SLDI) are calculated based on theoretical calculation. It is clear that the cross section of SLDI is one to two orders of magnitude bigger than the cross section of SLSI. For Li^{2+}, figure 3 shows the cross section ratio of double-to-single helium ionization associated with projectile one-electron loss, $R_{21}^{\mathrm{loss}} = \sigma_{\mathrm{SLDI}}/\sigma_{\mathrm{SLSI}}$. Both the calculated

cross section and cross section ratio are in good agreement with the experimental data from Ref. [28].

Figure 4 shows our experimental results and the theoretical calculation of this work. The details of the experimental setup can be found in a previous paper.[21–23] A collision system of $C^{2+,3+}$ and $O^{2+,3+}$ with helium was investigated. Figures show the cross section ratios of double-to-single ionization of helium associated with direct ionization ($R_{21}^{\rm direct}$) and one-electron loss ($R_{21}^{\rm loss}$) of projectile. For the process of direct ionization of helium, the charge state of the projectile is unchanged, and only two electrons from the target were involved in the calculation. The experimental data were from Refs. [21] and [22]. Theoretical calculations are in very good agreement with the experimental results. Some observations are confirmed from these figures: 1) $R_{21}^{\rm direct} < R_{21}^{\rm loss}$, the ratio of target double to single ionization associated with one projectile electron loss is larger than the ratio with direct ionization; 2) Both $R_{21}^{\rm direct}$ and $R_{21}^{\rm loss}$ show maximum values when incident energy are 200–300 keV/amu. Due to the limitations of our experimental setup, we could only record the charged ions. The data from the SL0I channel was not measured, and is not included in the figure.

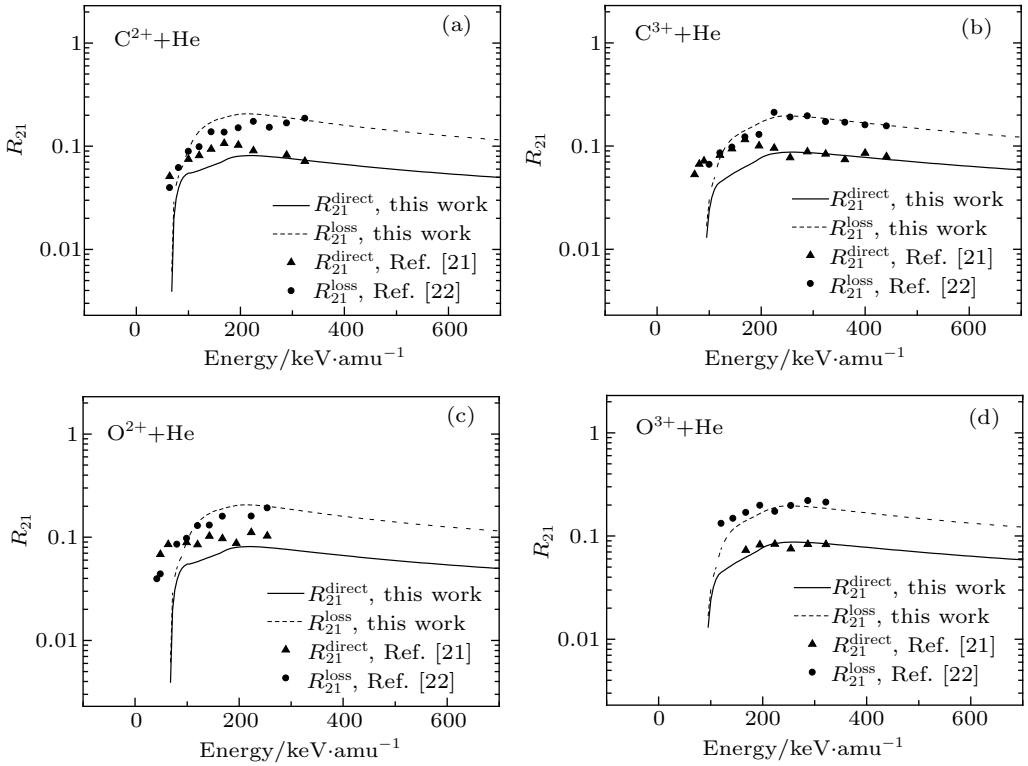


Fig. 4. Ratios of double-to-single ionization of helium associated with direct ionization and one-electron loss of projectile in (a) C^{2+} + He collision, (b) C^{3+} + He collision, (c) O^{2+} + He collision, and (d) O^{3+} + He collision. Dots (▲) and (●) are the experimental results for $R_{21}^{\rm direct}$ and $R_{21}^{\rm loss}$ respectively. Lines are the theoretical calculations.

In this work, we treated the projectile as a hydrogen-like ion when it suffers one-electron loss. Therefore, in the theoretical calculation, we used the ionization energy of a hydrogen-like ion, instead of the ionization energy of a projectile atom. This hypothesis would be one of the contributions to the difference between theoretical calculations and the experimental results. Figure 5 shows an application example, for the collision systems of C^{5+} with helium in present energy regime. We compare our calculation with the well-known plane-wave Born approximation (PWBA), which included the effects of screening and anti-screening. The experimental data and the PWBA calculation were quoted from the papers of Montenegro *et al.*[11,29] Very good agreement is found among the experimental data, PWBA calculation, and our calculation.

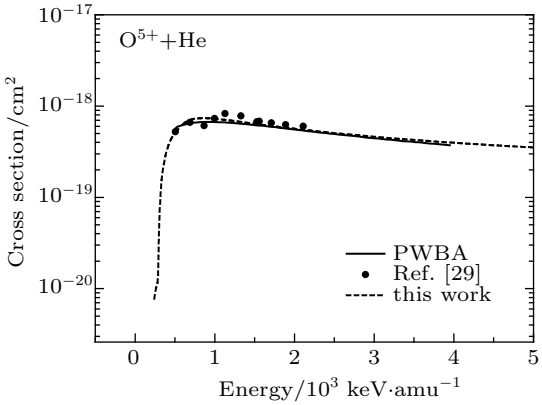


Fig. 5. Cross section of the projectile single-electron loss in the O^{5+} + He collision system. Dots (●) are the experimental results from Ref. [29]. Dash line and solid line are the theoretical calculations of this work and PWBA, respectively.

4. Conclusions

We have proposed a classical method to calculate the cross section of the projectile electron loss in the collision of light charged ions with helium. This method is based on the classical over-barrier model and the molecular over-barrier model. The collision systems of $Li^{1+,2+}$, $C^{2+,3+,5+}$, and $O^{2+,3+}$ with helium were investigated. Theoretical calculations are in good agreement with the experimental results. We also compared our method with the PWBA calculation.

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