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Relative cross-sections of charge transfer and ionization processes between multiply-charged ions and He at low and intermediate energies

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ABSTRACT

The relative cross-sections of double (DI) to single ionization (SI) σ_{DI}/σ_{SI}, transfer ionization (TI) to single capture (SC) σ_{TI}/σ_{SC} and double capture (DC) to single capture σ_{DC}/σ_{SC} of helium by multiply-charged ions A^{q+} (q = 2–5) at low and intermediate energies are calculated by considering the distribution of target electron and the interaction time between the projectile and the target electron. The calculated results are compared with published experimental data by our group and others.

1. Introduction

The investigation of charge transfer and ionization in collisions of multiply-charged ions with atoms is of considerable interest, because of both the pure physics interest in clarifying the relevant mechanisms and the importance in different applications including plasma and astrophysics as well as atomic physics. In collisions of multiply-charged ions and atoms, there are several channels which can be identified and measured by means of coincidence techniques. It is now believed that one-electron processes are rather well understood. At the same time, the multiple-electron processes, which involve the electron-electron correlation, are much more complicated. At very low ($v_p \ll 1$ a.u.) and very high ($v_p \gg 1$ a.u.) velocities, capture and ionization are the dominant mechanisms, respectively. However, at low to intermediate velocities, ionization and capture are comparable and also strongly couple each other. Up to now, theoretical calculations have not been well explored for double- or multiple-electron systems yet. It is well known that helium is the simplest target atom on studying the double-electron processes. In the past, a number of relevant experiments [1–16] were performed, which included the measurements by our group [1,8,9,11] for C^{q+}, O^{q+} and F^{q+} + He collisions at low to intermediate velocities. In general, the processes in collisions of projectiles A^{q+} with He can be described by the following reactions:

$$\text{single ionization (SI)}: \quad A^{q+} + He \rightarrow A^{q+} + He^{+} + e^{-} \tag{i}$$

$$\text{double ionization (DI)}: \quad A^{q+} + He \rightarrow A^{q+} + He^{2+} + 2e^{-} \tag{ii}$$

$$\text{single capture (SC)}: \quad A^{q+} + He \rightarrow A^{(q-1)+} + He^{+} \tag{iii}$$

$$\text{transfer ionization (TI)}: \quad A^{q+} + He \rightarrow A^{(q-1)+} + He^{2+} + e^{-} \tag{iv}$$

$$\text{double capture (DC)}: \quad A^{q+} + He \rightarrow A^{(q-2)+} + He^{2+} \tag{v}$$

In the Bohr–Lindhard (B–L) model [17], two critical distances, i.e., the release radius R_r and capture radius R_c, are proposed. At R_r, the Coulomb force from the projectile with the charge q attracting the target electron equals its the binding force in the target: $q/R_r^2 = v_e^2/a$, i.e., $R_r = (qa)^{1/2}/v_e$, where v_e and a are the electron velocity and its orbital radius, respectively. When the potential energy of this released electron in the projectile frame is larger than its kinetic energy, the capture then occurs possibly. The capture distance R_c is determined by $R_c = 2q/v_p^2$ in which v_p is the projectile velocity. If $R_c > R_r$, one released electron will be absolutely captured by the projectile and the capture cross-section σ_c is given by $\sigma_c = \pi R_r^2$. This means the capture cross-section is independent of the impact velocity. However, because $R_c < R_r$ for higher energies, both ionization and capture are possible for a released electron. Supposed that

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the release is a gradual process, it takes place with a probability per unit time of the order of v_e/a. Within R_c, the release probability is in the order of $(R_c/v_p)(v_e/a)$. In this case, the capture cross-section is obtained as $\sigma_c = 8\pi q^3 \cdot (v_e/a) \cdot v_p^{-7}$. Thus, the B–L model predicts the capture cross-section at higher velocities decreases as v_p^{-7}. Ionization occurs when the energy transferred exceeds the ionization potential. Therefore, the ionization cross-section σ_i is obtained by the integration of the Rutherford cross-section from the ionization potential I to the maximum transferable energy $2v_p^2$, $\sigma_i = 4\pi q^2 \cdot v_p^{-2} \cdot [(2I)^{-1} - (2v_p)^{-2}]$. Following Bohr and Lindhard, Brandt [18] and Ben-Itzhak et al. [19] calculated the capture cross-sections in fast collisions using the impact-parameter dependences by taking into account the different times spent by projectiles with different impact parameters, respectively. Within the classical frame and the independent electron approximation (IEA), we have evaluated the cross-section ratios for double to single ionization and transfer ionization to single capture using the Lenz–Jensen (L–J) model of the atom [1,8]. In one of our recent papers [20], we also calculated the absolute cross-sections of ionization and transfer in collisions of various ions with atomic hydrogen by replacing the L–J model of the atom with a simple exponential function, which gave a more realistic electron distribution. The satisfactory results were obtained. In this work, this method is extended to calculate the cross-section ratios of double to single ionization σ_{DI}/σ_{SI}, transfer ionization to single capture σ_{TI}/σ_{SC} and double to single capture σ_{DC}/σ_{SC} in collisions of ions with He. The electron–electron correlation is taken into account in some way. In the next section, the calculation method will be described in detail. Throughout this paper, atomic units are used unless otherwise stated.

2. Calculation method

A target atom is assumed to be static in the origin of the coordinates and a projectile moves along a linear trajectory. The coordinate of the projectile nucleus is given by $\mathbf{S} = \mathbf{v}_p t + \mathbf{b}$ where $\mathbf{b}$ is the impact parameter with respect to the target nucleus. The release and capture conditions that are derived from the B–L model turn into, respectively,

$$\frac{q}{|\mathbf{S}-\mathbf{r}|^2} = \frac{v_e^2}{|\mathbf{r}|} \tag{1}$$

and

$$\frac{q}{|\mathbf{S}-\mathbf{r}|} = \frac{1}{2}v_p^2 \tag{2}$$

where $\mathbf{r}$ is the coordinate of the target electron. Only when the impact parameter of the projectile with respect to the target electron, ρ, is less than the release distance, $|\boldsymbol{R}_r| = |\mathbf{S}-\mathbf{r}|$, the release of a target electron is possible. Then one-electron-release probability $f_r(\rho, q, v_p, r)$ is given by

$$f_r(\rho, q, v_p, r) = \frac{1}{\tau} \cdot 2\frac{\sqrt{R_r^2 - \rho^2}}{v_p} \tag{3}$$

with $1/\tau$ being the release rate. Here a simple form of the release rate, $1/\tau \sim v_e$, is employed. The released electron may be captured if it is in the capture sphere. Thus the capture probability is given by

$$f_c(\rho, q, v_p, r) = \frac{1}{\tau}2\frac{\sqrt{R^2 - \rho^2}}{v_p} \tag{4}$$

where R satisfies $R = R_r$ if $R_c > R_r$ and $R = R_c$ otherwise. We suppose that when the projectile approaches the target nuclei, the released electron will move together with the projectile, and only when it moves away from the nuclei, the ionization is classically allowed. Thus the ionization probability $f_i(\rho, q, v_p, r)$ is given by

$$f_i(\rho, q, v_p, r) = \frac{[f_r(\rho, q, v_p, r) - f_c(\rho, q, v_p, r)]}{2} \tag{5}$$

The electron density, $|\psi(\mathbf{r})|^2$, of the target atom is supposed as a simple exponential function of the distance:

$$|\psi_{1s}(\mathbf{r})|^2 = \left(\frac{Z^{*3}}{\pi}\right) \exp(-2Z^* r) \tag{6}$$

where Z^* is the effective nuclear charge. The probability that the electron is in $d^3\mathbf{r}$ at $\mathbf{r}$ is $|\psi(\mathbf{r})|^2\, d^3\mathbf{r}$. Thus release, ionization and capture probabilities are expressed as

$$P_{r,i,c}(b, q, v_p) = \int f_{r,i,c}(\rho, q, v_p, r)|\psi(\mathbf{r})|^2\, d^3\mathbf{r} \tag{7}$$

It is more convenience to perform the integral in Eq. (7) in cylinder coordinate. For this purpose, the formula (7) can be rewritten as

$$P_{r,i,c}(b, q, v_p) = \int_0^{R_{r,r,c}} \rho\, d\rho \int_0^{2\pi} d\varphi \int_{-\infty}^{+\infty} f_{r,i,c}[\rho, q, v_p, r(b, \rho, \varphi, z)] \cdot C\, e^{-2Z \cdot r(b,\rho,\varphi,z)}\, dz \tag{8}$$

Since the probabilities P_c and P_i may be larger than unity, we use the unitarized formula described by Sidorovich et al. [21]

$$P_{ui,uc}(b, q, v_p) = \left[\frac{P_{i,c}}{P_i + P_c}\right] \cdot [1 - \exp(-(P_i + P_c))] \tag{9}$$

in which the subscript 'u' denotes the corresponding unitarized probability. The electrons are supposed to get away from the target one by one. Two target electrons have the same ionization potential at the beginning, and then once one of the target electrons is removed, the other will be exposed to a stronger field due to the Coulomb force from the target nucleus. In other words, the ionization potential of the second electron will have an increase. It needs to be noted that the ionization potential I is associated with the effective charge state Z^* that the electron feels as well as the spatial distribution of the target electron. On the other hand, if the first electron is captured by the projectile, the projectile charge state will be reduced by one, otherwise it has no change. In addition, just as mentioned in the last section, we suppose the ionization only occur in the way-out stage. That is, the capture occurs prior to the ionization.

3. Results and discussion

Within the IEA, the probability functions for SC, DC, TI, SI and DI processes are given as

$$P_{SC}(b, q, v_p) = 2P_{uc1}(b, q, v_p)[1 - P_{uc2}(b, q, v_p) - P_{ui2}(b, q, v_p)] \tag{10}$$

$$P_{DC}(b, q, v_p) = P_{uc1}(b, q, v_p)P_{uc2}(b, q, v_p) \tag{11}$$

$$P_{TI}(b, q, v_p) = 2P_{uc1}(b, q, v_p)P_{ui2}(b, q, v_p) \tag{12}$$

$$P_{SI}(b, q, v_p) = 2P_{ui1}(b, q, v_p)[1 - P_{uc1}(b, q, v_p) - P_{ui2}(b, q, v_p)] \tag{13}$$

$$P_{DI}(b, q, v_p) = P_{ui1}(b, q, v_p)P_{ui2}(b, q, v_p) \tag{14}$$

where subscripts 1 and 2 represent the first and second electrons removed from the target, respectively. For simplicity, we use $Z_1^* = 1.345$ and $Z_2^* = 2$ for P_{SC}, P_{DC}, P_{SI} and P_{DI}, and $Z_1^* = 1.345$ and

$Z_2^* = 1.6875$ for P_{TI}. The total cross-sections σ can be calculated by integrating the corresponding probabilities over the impact parameter:

$$\sigma(q, v_p) = 2\pi \int_0^\infty P(b, q, v_p) b\, db \tag{15}$$

Fig. 1 shows the impact parameter dependence of various reaction channels in collisions of A^{3+} with He at (a) $v_p = 3$ and (b) $v_p = 4$, respectively. It can been seen that for the case of pure capture processes (SC and DC) and TI the impact-parameter ranges decrease with the increasing energy, which is due to the fact that the capture distance R_c is in inverse proportion to v_p^2. However, for the case of pure ionization channels (SI and DI) the impact-parameter ranges are constant by reason of the velocity independence of release distances. It can be also seen that the calculated probability values depend strongly on the impact velocity, which should been contributed into the changes in both the projectile-target interaction time and the capture distance induced by the projectile-velocity change.

Fig. 2(a)–(d) show our calculated ratios σ_{DI}/σ_{SI} together with the experimental data of helium by $A^{q+}(q = 2–5)$, respectively, as a function of $E/q^{1/2}$ (E is the projectile energy in keV/u). In general, the present calculations can qualitatively reproduce the energy dependence of the ratios σ_{DI}/σ_{SI}. It is found that theories is in better agreement with the experimental data induced by fully stripped ions ($Z = q$) than those by partially stripped ions ($Z > q$). This is reasonable because the projectile in the present calculations is

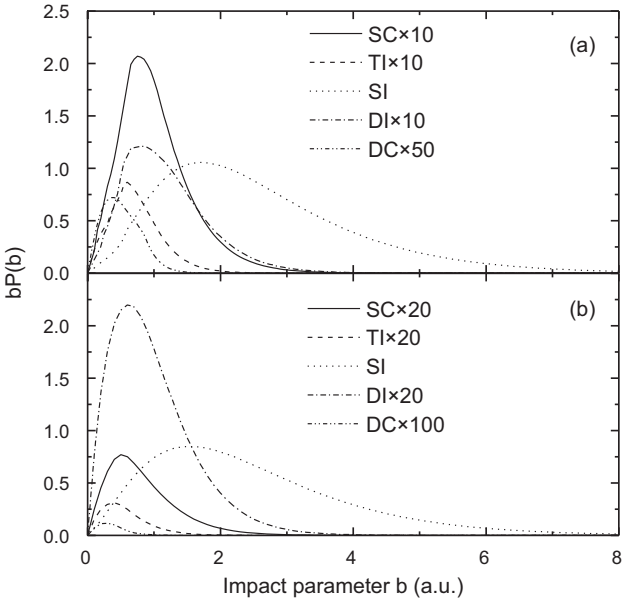

Fig. 1. The impact-parameter dependence of various reaction channels for A^{3+} + He collisions at (a) $v_p = 3$ and (b) $v_p = 4$.

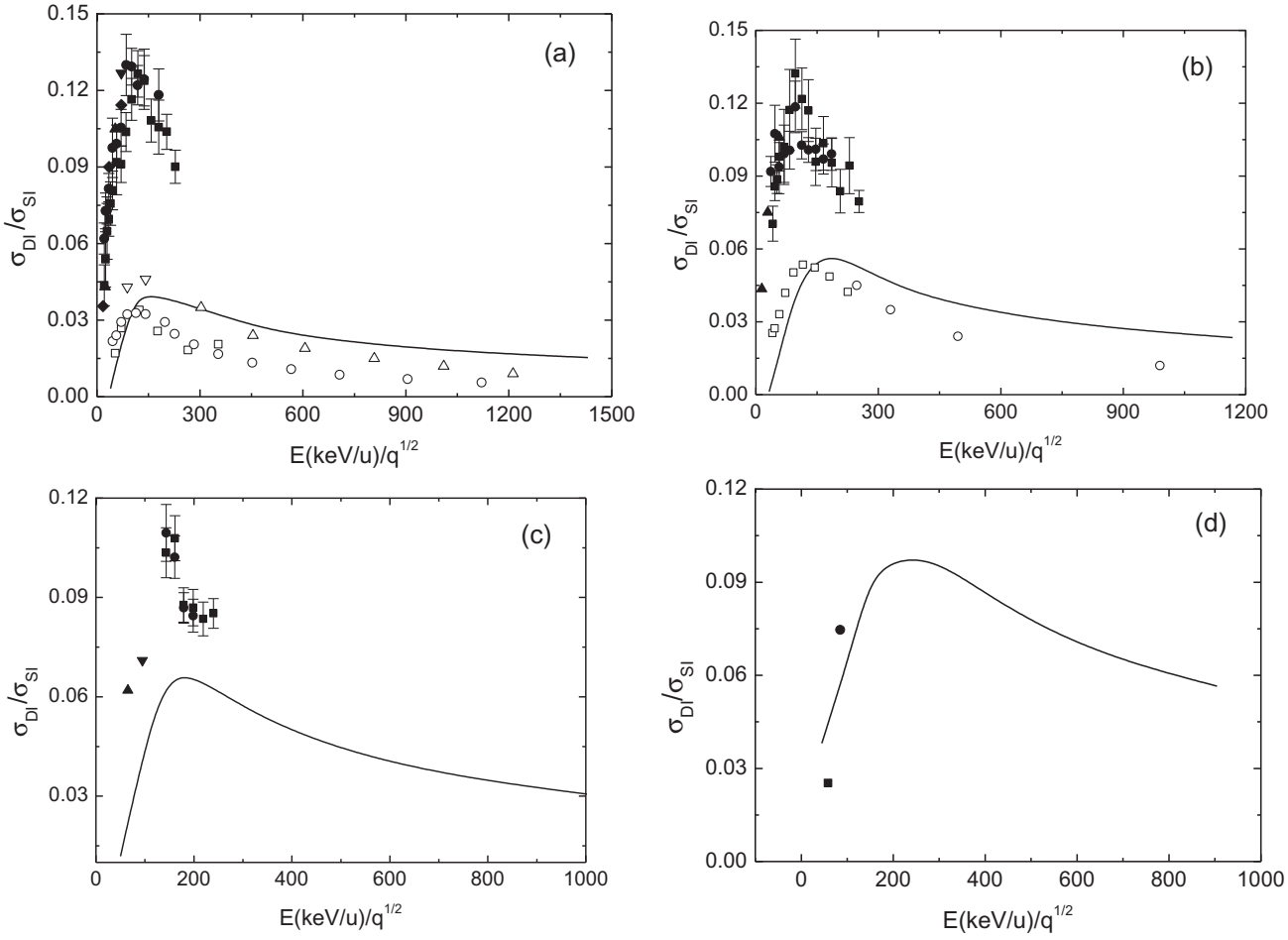

Fig. 2. Cross-section ratios σ_{DI}/σ_{SI} of He by ions A^{q+} (a) $q = 2$, (b) $q = 3$, (c) $q = 4$ and (d) $q = 5$ as functions of projectile energy. *Calculations*: solid lines; *Experiments*: (a) C^{2+} (■ [1], ▲ [2]), O^{2+} (● [1], ▼ [2]), N^{2+} (♦ [2]), He^{2+} (□ [3], ○ [4]), Li^{2+} (△ [5], ▽ [6]); [b] C^{3+} (■ [1]), O^{3+} (● [1]), N^{3+} (▲ [2]), Li^{3+} (□ [4], ○ [5]); (c) C^{4+} (■ [1], ▲ [1]), O^{4+} (● [7]), B^{4+} (▼ [7]); (d) C^{4+} (■ [7]), B^{4+} (● [7]).

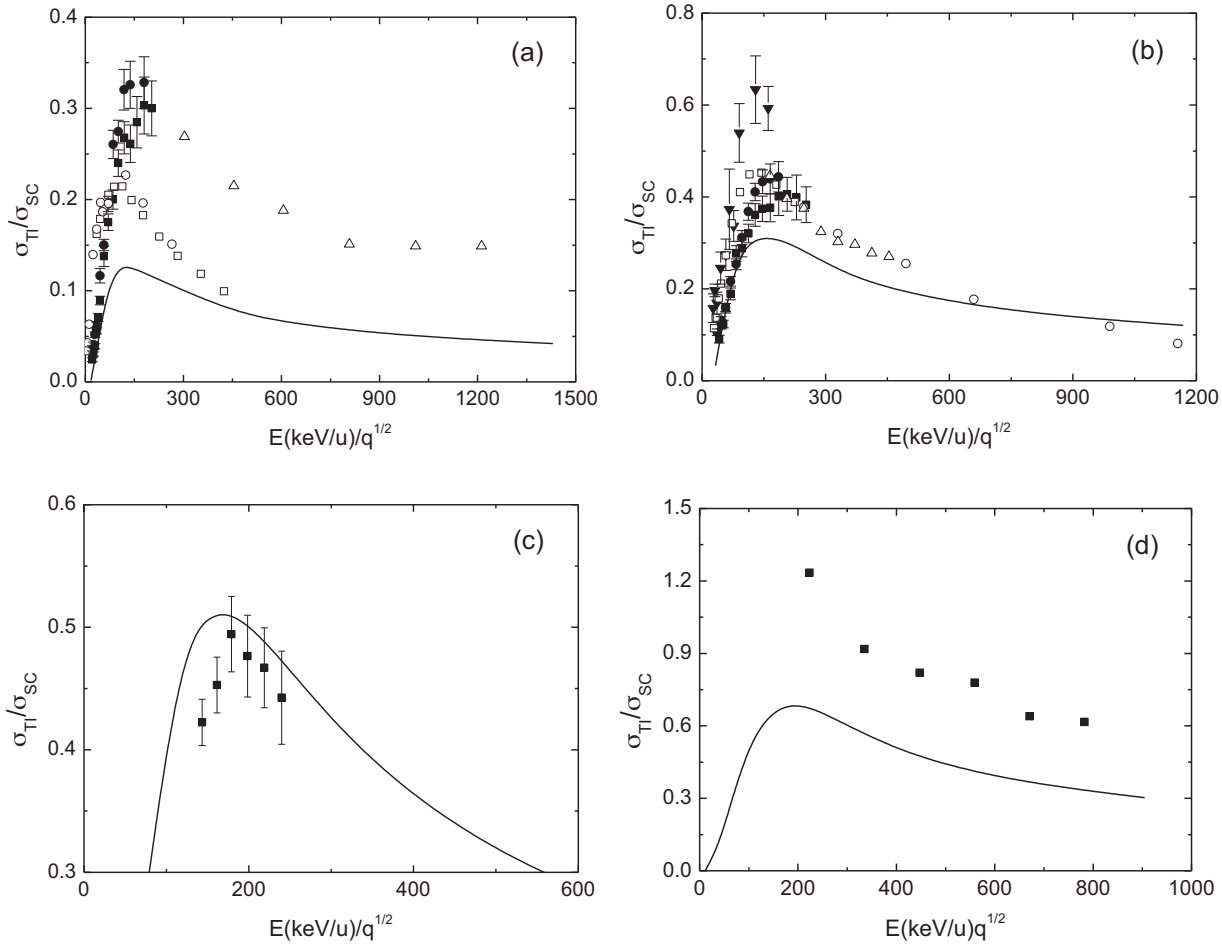

Fig. 3. Cross-section ratios σ_{TI}/σ_{SC} of He by ions A^{q+} (a) $q=2$, (b) $q=3$, (c) $q=4$ and (d) $q=5$ as functions of projectile energy. *Calculations*: solid lines; *Experiments*: (a) C^{2+} (■ [8]), O^{2+} (● [8]), He^{2+} (□ [4], ○ [3]), Li^{2+} (△ [5]); (b) C^{3+} (■ [8]), O^{3+} (● [8]), F^{3+} (▼ [9]), Li^{3+} (□ [4], ○[5], △ [10]); (c) C^{4+} (■ [11]); (d) F^{5+} (■ [12]).

simply treated as a structureless bare ion with the nuclear charge $Z=q$. For the partially stripped ion A^{q+}, because the nuclear is not fully shielded by the extranuclear electron(s), the average effective charge q_{eff} on the target electron usually larger than q, i.e., $q_{eff}>q$. On the other hand, the interaction between the projectile electron and the target electron (antiscreening mode) also contributes to the target ionization. The maximum value of σ_{DI}/σ_{SI} is located at $E_{max}\sim 150$–$200q^{1/2}$ keV/u, which indicates that E_{max} is about several hundreds keV/u and approximately in proportion to $q^{1/2}$. As an approximation to interpret this $q^{1/2}$-scaling roughly, according to Eqs. (1)–(5) f_i ($\rho=0$) will reach a maximum when

$$\frac{df_i}{dv_p}(\rho=0)=0 \tag{16}$$

We have a simple formula

$$E_{max}=\frac{1}{2}mv_p^2=3mv_e r^{-1/2}q^{1/2} \tag{17}$$

which may be helpful for us to understand the structure of curves to some extent. For a given charge state, the release distance is constant, while the capture distance is in inverse proportion to v_p^2. This implies that the ionization space will increase with the impact energy, which is responsible for the increase of the ionization cross-section with the impact energy in the lower energy range. On the other hand, because the mean release radius for double ionization is smaller than that of single ionization, the decrease of the capture radius has a more important influence on double ionization than single ionization. As seen from the energy-dependence curves of the ratio σ_{DI}/σ_{SI}, the cross-section for double ionization increases faster than that for single ionization with the increasing impact energy when the energy is lower than E_{max}. However, at higher energies ($E>E_{max}$), because the capture radius has been very small, the ionization space is expected to get a small or even negligible increase caused by the change of the projectile velocity. At the same time, as the impact velocity increases, the collision time between the projectile and the target electron gradually plays a major role on the collision process, in particular on the double electron process. Therefore, the trend of ratio σ_{DI}/σ_{SI} with the increasing energy at $E>E_{max}$ is mainly determined by the lack of the collision time.

Our calculated ratios σ_{TI}/σ_{SC} of He by A^{q+} ($q=2$–5) together with the related experimental data are shown in Fig. 3(a)–(d), respectively, as a function of $E/q^{1/2}$. The calculations can follow the trend of the experimental data qualitatively. The general shape of the whole curves is similar to that of the ratio σ_{DI}/σ_{SI}. The E_{max} value also approximately conforms to the $q^{1/2}$ scaling. The peak position of TI cross-sections may be evaluated roughly by $f_i=f_c$ ($\rho<R_c$). For simplicity, when $\rho=0$, according to Eqs. (1)–(5) we have $E_{max}\propto q^{1/2}$. According to our calculations if one of the target electrons is captured by the projectile, and then the second electron will be affected by a projectile with the charge $(q-1)$. This electron may be ionized or still stay in the target so that TI or SC occurs. Therefore, the trend of the ratio σ_{TI}/σ_{SC} with the increasing energy is determined by the behavior of the second electron. As the impact energy increases, the release probability for the second electron decreases, while its ionization probability firstly increases due to the rapid decrease of the capture distance and then goes down by the reason of the lack

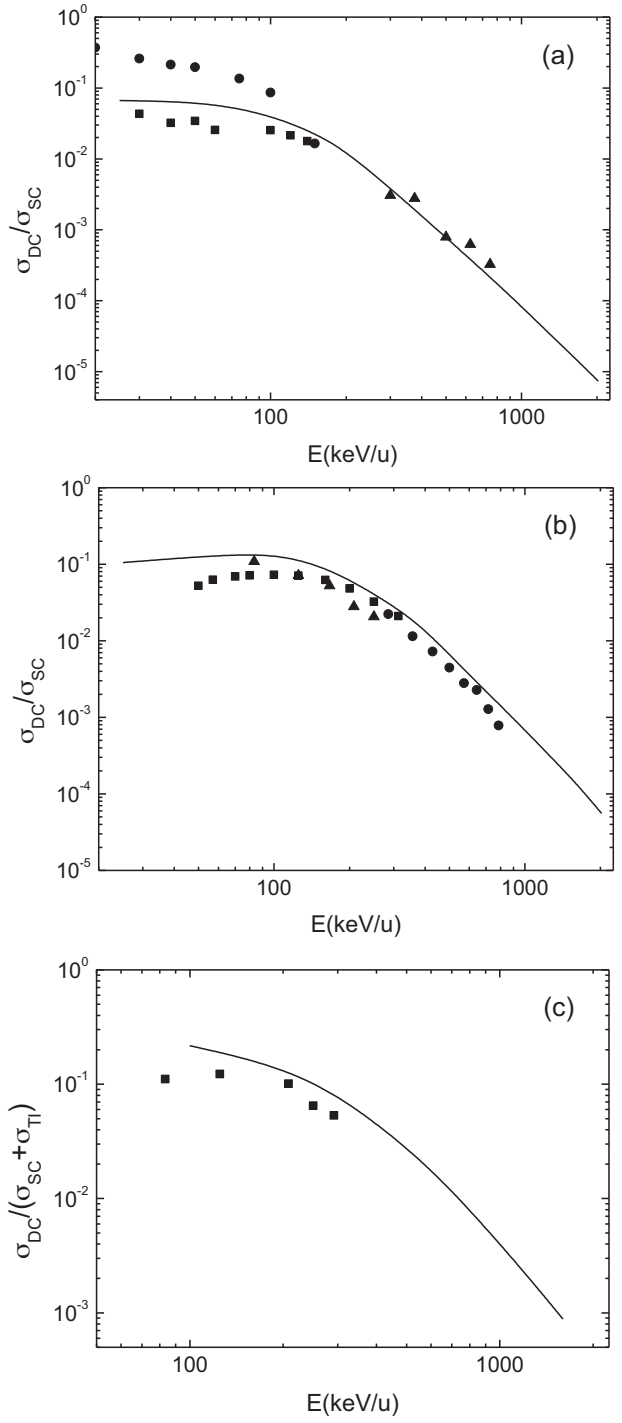

Fig. 4. Cross-section ratios σ_{DC}/σ_{SC} of He by ions A^{q+} (a) $q=2$, (b) $q=3$, and $\sigma_{DC}/(\sigma_{SC}+\sigma_{SC})$ by (c) A^{5+} as functions of projectile energy. *Calculations*: solid lines; *Experiments*: Ne^{2+} (■ [13]), He^{2+} (● [14], ▲ [15]); (b) Li^{3+} (■ [4]), Li^{3+} (● [10]), C^{3+}(▲ [16]); (c) O^{5+} (■ [16]).

of the impact time. It should be noted that autoionization (AI) of the projectile after capture of two electrons into a doubly excited state is thought of as an important TI mechanism at lower energies. However, in the present calculations, it is simply assumed that TI only comes from the combination of the independent-electron events, i.e., ionization plus capture.

The cross-section ratios σ_{DC}/σ_{SC} of He by A^{2+} and A^{3+} are shown in Fig. 4(a) and (b), respectively, and $\sigma_{DC}/(\sigma_{SC}+\sigma_{TI})$ for A^{5+} + He collisions in Fig. 4(c), as a function of projectile energy. Note that the experimental data of Ne^{2+} in Fig. 4(a) are the ratios for DC to total single capture. In terms of Eq. (4), at higher energies, the probability for total one-electron capture $f_c(\rho=0)=R_c/\upsilon_p^2\sim\upsilon_p^{-3}$. The probability f_{DC} ($\rho=0$) can then be approximated by the IEA probability f_{DC} ($\rho=0$). Therefore, the ratio of double capture to total one-electron capture σ_{DC}/σ_C behaves roughly as υ_p^{-3}. It is obvious that the cross-section for single capture decreases faster than that for total one electron capture. Thus when the impact energy is approximately larger than 200 keV/u, the ratio σ_{DC}/σ_{SC} will decay as $\upsilon_p^{-\alpha}$ ($\alpha<3$) which is slower than υ_p^{-3} for σ_{DC}/σ_C. On the other hand, because the capture radius R_c obtained through Eq. (2) is usually larger than the release radius R_r at lower energies, in this case the capture distance is treated in terms of Eq. (5), that is, the capture distance is constant. For this reason, as seen from Fig. 3, the curves for σ_{DC}/σ_{SC} and $\sigma_{DC}/(\sigma_{SC}+\sigma_{TI})$ are gentle relatively when the impact energy is lower.

4. Conclusions

In conclusion, we have considered a classical method, in which it is assumed that two electrons of target are removed one by one and the capture occurs prior to the ionization. This method have been applied to the evaluation of the cross-sections for single capture, double capture, single ionization, double ionization and transfer ionization in collisions of multiply-charged ions A^{q+} ($q=2$–5) with helium at low-to-intermediate velocities. The relative cross-sections are compared with the available experimental data. It is found that our results present a general good agreement with the experiments. It should also be emphasized that the present calculations are very simple and timesaving.

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