Scaling law for helium double ionization by impact of ions from H^+ to U^{92+} in the strong-coupling regime

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Based on our previous classical over-barrier-ionization model, a universal scaling law of double-to-single-ionization cross-section ratios R_{21} for impact by nearly stripped ions in the strong-coupling regime ($0.5 < q/\upsilon < 5$) is found. The scaling law is consistent with extensive experimental data from proton to U^{92+}. A fitting curve to the predictions of the theory is also proposed for application convenience.

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The most widely used scaling law of a single-ionization cross section in the velocity range $\upsilon \gg \upsilon_{\text{Bohr}}$, where υ_{Bohr} is the Bohr velocity, was proposed by Gryzinski. Assuming an artificial electron velocity distribution function (EVDF) instead of the correct EVDF, Gryzinski obtained a scaling law that matches the asymptotic behavior of the Bethe formula [1]. However, as the collision velocity υ declines to υ_{Bohr}, the scaling formula is no longer suitable because the circulation period of the target electron should be taken into account. In the velocity range of $\upsilon \approx \upsilon_{\text{Bohr}}$, because the electron is attracted by both projectile and target nuclei, the "easiest" way to release from the nuclei corresponds to electron ejection into a region where the attracting force exerted by the projectile balances the binding force exerted by the target near the saddle point [2,3]. In addition, the maximum single-ionization cross section is scaled by the term $\sqrt{Z_p/Z_T}$ accordingly. After analyzing extensive experimental data, Kaganovich *et al.* found that the maximum-ionization cross section occurred at $\sqrt{Z_p/Z_T+1}$ and proposed a valid scaling formula over a wide velocity range by use of the term $\frac{\upsilon}{\upsilon_e\sqrt{Z_p/Z_T+1}}$, which is the normalized velocity. More details about the scaling laws of the single-ionization cross section can be found in Refs. [3,4].

Multiple ionization is a subject of considerable interest, which is conducive to understanding the two-electron transition process and electron-electron correlation. The helium atom is an ideal example because it has only two electrons. McGuire pointed out that there are two mechanisms: shake-off (SO) and two-step (TS2) processes [5]. In SO, the first electron is directly ionized by the projectile, while the second electron gets ionized when it is released from the influenced orbit. In TS2, two electrons are ionized by separate binary encounters with the projectile. Later on, the two-step with one interaction (TS1) mechanism was proposed as follows: The first electron is ejected by the interaction of the projectile and the second electron, which is left in a bound state of He^+, will be ionized due to the interaction with the outgoing electron [6]. Knudsen *et al.* argued that the cross sections for TS1 and SO would have dependences similar to that of the single-ionization cross sections in their range of q and υ, whereas the TS2 would lead to the $(q/\upsilon)^4$ dependence of double-ionization cross sections [7]. Hence, the ratio R could be determined by

$$R = A + B\frac{q^2}{\upsilon^2 \ln(2.08\upsilon)}. \tag{1}$$

The Bethe formula is used to establish Eq. (1) for the dipole transition. By adding the quadrupole transition term to the single-ionization cross section, Bapat and Krishnakumar [8] obtained the improved scaling law of helium double ionization in the range $q/\upsilon < 0.5$. The scaling law of helium double ionization in the strong perturbative range $q/\upsilon > 1$ is still in dispute. Our previous work had suggested that the scaling formula of R_{21} for the extremely-high-q limit within the strong-couple regime could be written as $0.28\sqrt{q}/\upsilon$ [9].

In this Brief Report a universal scaling formula of R_{21} for impact by nearly stripped ions ranging from proton to U^{92+} in the regime $0.5 < q/\upsilon < 5$ is obtained based on our classical over-barrier-ionization (COBI) model. The theoretical results are in good accord with extensive experimental data. Moreover, an empirical formula is proposed through the fitting curve for application convenience and it is equivalent to the derived formula in the same regime.

The COBI model is based on Bohr's classical over-barrier model (COBM) [10]. In the COBM, two important ion-atom–interaction distances are introduced. The first is the release distance R_r,

$$R_r = \frac{Z + 2\sqrt{qZ}}{I}, \tag{2}$$

which shows that the target electron can be released to the side of the projectile when the internuclear distance is smaller than R_r. The second is the capture distance R_c,

$$R_c = \frac{2q}{\upsilon^2}, \tag{3}$$

which shows that the released electron can be captured by the projectile if the potential energy in the ionic field of the electron is greater than its kinetic energy in the projectile's frame. In COBI [9,11], we considered that the released but uncaptured electron would be accelerated continuously by the approaching ion. When the ion enters the ionization distance R_I, where the Stark energy converted into the kinetic energy of the released electron is greater than its ionization energy in the quasimolecular state, the electron will get enough kinetic

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energy to escape. Thus, the ionization distance R_I satisfies

$$\frac{q}{R_I} \geqslant I + \frac{q}{R_r}. \tag{4}$$

In other words, electrons that are released within the capture distance will be captured; those released electrons outside the capture distance will not be ionized until the ion approaches the distance R_I.

Wu *et al.* [12] obtained the scaling law of single ionization of helium for impact by ions of various charge states with the approximate form

$$R_r \approx \frac{2\sqrt{qZ}}{I}. \tag{5}$$

Here we use the same expression of R_r as that used by Wu *et al.* in deriving the single-ionization scaling law of helium in the similar q and υ regimes. From Eqs. (4) and (5) we get the expression of the ionization distance R_I,

$$R_I \approx \frac{q}{I\left(1+\frac{1}{2}\sqrt{\frac{q}{Z}}\right)}. \tag{6}$$

Note that the release and capture processes do not take place instantly but occur gradually; the release and capture probabilities P_r and P_c should be taken into account. For the single-electron system, the probabilities are given as, respectively,

$$P_r(b) = \frac{2\sqrt{R_r^2 - b^2}}{\upsilon}\frac{1}{T} \quad \text{for } b \leqslant R_r, \tag{7}$$

$$P_c(b) = \frac{2\sqrt{R_c^2 - b^2}}{\upsilon}\frac{1}{T} \quad \text{for } b \leqslant R_c. \tag{8}$$

Equations (7) and (8) show the ratio of the collision duration to the orbital period T of the target electron. Thus, the ionization probability P_I is

$$P_I(b) = P_r(b) - P_c(b) \quad \text{for } b \leqslant R_I. \tag{9}$$

Many theories have manifested that the independent event model [13] is more suitable for calculating the cross section of multiple ionization than the independent-particle model.

The double-to-single-ionization cross-section ratio R_{21} is given as

$$R_{21} = \frac{\sigma^{2+}}{\sigma^{+}} = \frac{\int P_{I1}P_{I2}2\pi b db}{\int P_{I1}(1-P_{I2}-P_{C2})2\pi b db + \int P_{I2}(1-P_{I1}-P_{C1})2\pi b db}. \tag{10}$$

Here σ^{2+} and σ^{+} are the double- and single-ionization cross sections, respectively, P_{r1}, P_{c1}, and P_{I1} are the release, capture, and ionization probabilities for the first released electron, and P_{r2}, P_{c2}, and P_{I2} are those for the second released electron.

For the concerned regime of q and υ in this work, several approximations can be made.

(i) Experimental data have indicated that when the collision velocity is larger than 2 or 3 a.u., the capture cross sections are much smaller than the ionization cross sections [14]. Therefore, the capture terms P_{C1} and P_{C2} are neglected in the denominator of Eq. (10).

(ii) Those experimental data also showed that the double-ionization cross section σ^{2+} is at least one order of magnitude smaller than the single-ionization cross section σ^{+}. Thus, the term P_{I2} in the denominator of Eq. (10) is neglected [14–19]. Then we get an approximate form R_{21} in Eq. (11) and this approximated expression has been proved to be valid [9]:

$$R_{21} = \frac{\sigma^{2+}}{\sigma^{+}} \approx \frac{\int_0^{R_{r2}} P_{I1}P_{I2}2\pi b db}{\int_0^{R_{r1}} P_{I1}2\pi b db}. \tag{11}$$

(iii) According to Eqs. (7)–(9), the probabilities of release, capture, and ionization decrease slowly and smoothly when the collision parameter b increases, so the integrated reaction probabilities will be close to the mean value of the reaction probability multiplied by the geometric ionization cross section. Thus, the double- and single-ionization cross sections σ^{2+} and σ^{+} can be estimated well by the following expressions [9]:

$$\sigma^{2+} \approx \pi R_{I2}^2 \times \tfrac{1}{2}P_{r1}(0)P_{r2}(0), \tag{12}$$

$$\sigma^{+} \approx \pi R_{I1}^2 \times \tfrac{1}{2}P_{r1}(0). \tag{13}$$

Finally, we get the approximate expression of R_{21}:

$$R_{21} \approx \frac{R_{I2}^2}{R_{I1}^2}[P_{r2}(0)] = 2\frac{Z_2}{Z_1}\frac{q_2^2}{q_1^2}\frac{I_1^2}{I_2^2}\left(\frac{2\sqrt{Z_1}+\sqrt{q_1}}{2\sqrt{Z_2}+\sqrt{q_2}}\right)^2 \times \frac{2\sqrt{q_2 Z_2}}{I_2 \upsilon T} = fm, \tag{14}$$

where

$$f(q_1,q_2) = 2\frac{Z_2}{Z_1}\frac{q_2^2}{q_1^2}\frac{I_1^2}{I_2^2}\left(\frac{2\sqrt{Z_1}+\sqrt{q_1}}{2\sqrt{Z_2}+\sqrt{q_2}}\right)^2 \frac{2\sqrt{Z_2}}{I_2 T}, \tag{15a}$$

$$m(q_2) = \frac{\sqrt{q_2}}{\upsilon}, \tag{15b}$$

where $Z_1 = 1.3$, $Z_2 = 2$, $I_1 = 25$ eV, $I_2 = 54$ eV, $T = \pi/E_{1s}$, and q_1 and q_2 are the effective charges of the projectile that are experienced by the first and the second released electron.

Note that the picture of the COBI model is the sequential release process of target electrons in which two electrons escape from the target nucleus one by one. When the projectile enters the ionization distance R_{I1}, the first target electron whose ionization energy is lower is ionized. So the first effective charge q_1 is the charge of projectile nucleus. As the projectile enters R_{I2}, the first ejected electron will move to the side of projectile and screen its nucleus. The second effective charge of the projectile will decline to q_2. The method to estimate the values of q_2 is $q_2 = q_1 - 1$. In the work of Barany *et al.* [15], this estimation method is adopted to deal with multiple capture processes. It is emphasized that the value of q_2 for the H^+ ion is estimated to be 0.3 from the 1s binding

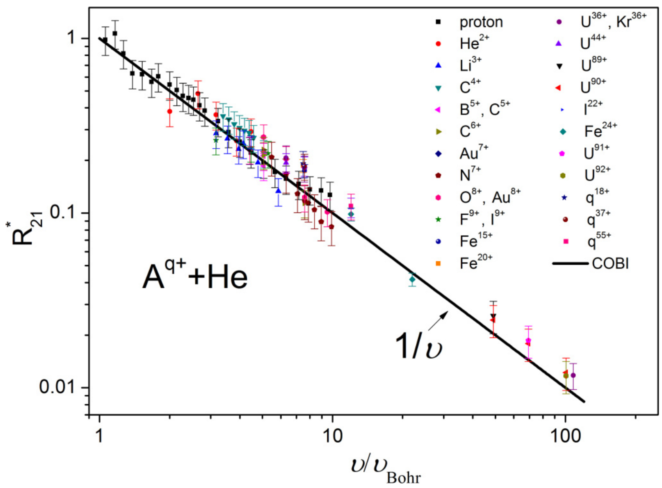

FIG. 1. (Color online) Scaled double to single ionization ratio $R_{21}^{*} = R_{21}/[f(q_1,q_2)\cdot\sqrt{q_2}]$ of helium impacted by nearly stripped ions from the proton to U^{92+} ($0.5 < q/\upsilon < 5$). Dots with error bars are experimental data taken from Refs. [9,11,14–19] and the line is derived from Eq. (14).

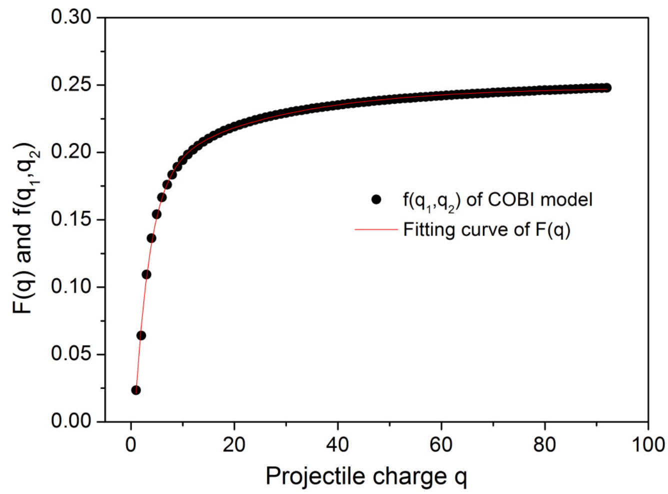

FIG. 2. (Color online) Fitting curve $F(q)$ as a function of projectile charge q and the results obtained using $f(q_1,q_2)$ given by Eq. (15a).

energy of the negative hydrogen ion [11]. As a result, the relationship between q_1 and q_2 is

$$q_2 = \begin{cases} 0.3 & \text{for} \quad q_1 = 1 \\ q_1 - 1 & \text{for} \quad 2 \leqslant q_1 \leqslant 92. \end{cases} \tag{16}$$

It should be mentioned that we had done the direct integration to Eq. (11) and found that for all ions considered here, the integrated results are just slightly different, no more than $\pm 3\%$, from the values calculated from Eqs. (12)–(14). At the same time, the integrated results are too complicated to apply in practical works. So we chose to present the results of Eq. (14) for convenient applications with good accuracy.

The scaled double-to-single-ionization ratios R_{21}^{*} of helium impacted by ions ranging from proton to U^{92+} are calculated by Eq. (14) and compared with extensive experimental data, as shown in Fig. 1. It is found that the overall agreement is good and the experimental data and theory show the $1/\upsilon$ dependence. Equation (14) shows that the double-to-single-ionization ratios R_{21} in the strong-coupling regime are determined by $f(q_1,q_2)$, the geometrical cross-section ratios of double and single ionization, and the ionization probability $m(q_2)$ of the second released electron. The picture of sequential over-barrier-ionization processes indicates that the ionization probability $m(q_2)$ should be proportional to $1/\upsilon$ and that the coefficient $f(q_1,q_2)$ is determined by the ionization distances R_I of the two released electrons and the strong correlation between them ($q_2 = q_1 - 1$).

In order to apply the ratio R_{21} conveniently, a fitting polynomial $F(q)$ is introduced to replace $f(q_1,q_2)$. In Fig. 2, the closed circles are the values of the $f(q_1,q_2)$ function given by Eq. (15a) and the solid line is the fitting curve $F(q)$:

$$F(q) = 0.25 - 0.068e^{-0.041q} - 0.23e^{-0.34q}. \tag{17}$$

In an application way, the scaling law of double ionization of helium in the strong-coupling regime can be rewritten as

$$R_{21} \approx F(q)\frac{\sqrt{q-\alpha}}{\upsilon}, \quad \alpha = \begin{cases} 0.7 & \text{for proton} \\ 1 & \text{for other ions.} \end{cases} \tag{18}$$

In summary, we draw a universal scaling law of helium double ionization for nearly stripped ions ranging from proton to U^{92+} in the strong-coupling regime ($0.5 < q/\upsilon < 5$). The theoretical law is in good accord with extensive experimental data. An empirical formula is also proposed for convenient application.

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APPENDIX: THE INTEGRAL FORMULA OF DIRECT IONIZATION CROSS SECTIONS

The approximate expression of double- and single-ionization cross sections are presented in the main text. Here the integral formulas of double- and single-ionization cross sections in Eq. (11) by use of *Mathematica* 9.0.1 are given as, respectively,

$$\begin{aligned}\sigma^{2+} &= \int_0^{R_{I2}} \frac{2\sqrt{R_{r1}^2 - b^2} \times 2\sqrt{R_{r2}^2 - b^2}}{(\upsilon T)^2} 2\pi b\, db \\ &= \frac{8\pi}{(\upsilon T)^2}\left[\left(-\frac{1}{8}\right) \times \left(R_{r1}^2 + R_{r2}^2 - 2R_{I2}^2\right) \times \left(R_{r1}^2 - R_{I2}^2\right)^{0.5} \times \left(R_{r2}^2 - R_{I2}^2\right)^{0.5}\right.\end{aligned}$$

$$- \frac{1}{16}\left(R_{r1}^2 - R_{r2}^2\right)^2 \times \ln\left[-R_{r1}^2 - R_{r2}^2 + 2R_{I2}^2 + 2\left(R_{r1}^2 - R_{I2}^2\right)^{0.5} \times \left(R_{r2}^2 - R_{I2}^2\right)^{0.5}\right] + \frac{1}{8}\left(R_{r1}^2 + R_{r2}^2\right) \times R_{r1} \times R_{r2} + \frac{1}{16},$$
$$\times \left(R_{r1}^2 - R_{r2}^2\right)^2 \ln\left(-R_{r1}^2 - R_{r2}^2 + 2R_{r1}R_{r2}\right)\Bigg], \tag{A1}$$

$$\sigma^+ = \int_0^{R_{I1}} \frac{2\sqrt{R_{r1}^2 - b^2}}{\upsilon T} 2\pi b\, db = \frac{4\pi}{\upsilon T}\left[\left(-\frac{1}{3}\right) \times \left(R_{r1}^2 - R_{I1}^2\right)^{1.5} + \frac{1}{3} \times \left(R_{r1}^2\right)^{1.5}\right]. \tag{A2}$$

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