BRIEF COMMUNICATIONS

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Scaling cross sections for ion-atom impact ionization

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Knowledge of ion-atom ionization cross sections is of great importance for many applications. When experimental data and theoretical calculations are not available, approximate formulas are frequently used. Based on experimental data and theoretical predictions, a new fit for ionization cross sections by fully stripped ions is proposed.
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Ion beams lose electrons when passing through a background gas in accelerators, beam transport lines, and target chambers. As a result, the ion confinement time and beam focusability are decreased. An unwanted electron population, produced in ion-atom collisions, may also lead to the development of collective two-stream instabilities. Therefore it is important to assess the values of ion-atom ionization cross sections. In contrast to the electron and proton ionization cross sections, where experimental data or theoretical calculations exist for practically any ion and atom, the knowledge of ionization cross sections by fast complex ions and atoms is far from complete (see, for example, Ref. 1). While specific values of the cross sections for various pairs of projectile ions and target atoms have been measured at several energies in Refs. 2–5, the scaling of cross sections with energy and target or projectile nucleus charge has not been experimentally mapped. When experimental data and theoretical calculations are not available, approximate formulas are frequently used. The most popular formula for ionization cross section was proposed by Gryzinski in Ref. 6. The ''web of science'' search engine shows 457 citations of this paper, and most of the citing papers use Gryzinski's formula to evaluate the cross sections. In this approach, the cross section is specified by multiplication of a scaling factor and a unique function of the projectile velocity normalized to the orbital electron velocity. The popularity of Gryzinsky's formula is based on the simplicity of the calculation, notwithstanding the fact that the formula is not accurate at small energies. Another fit, proposed by Gillespie, gives results close to Gryzinski's formula at large energies and makes corrections to Gryzinski's formula at small energies as given in Ref. 7. Although more accurate, Gillespie's fit is not frequently used in applications because it requires a knowledge of fitting parameters not always known *a priori*. In this paper, we present a new fit formula for the ionization cross section which has no fitting parameters and is correct at small energies. The formula is checked against available experimental data and theoretical predictions.

We first provide a brief overview of the theoretical models and experimental data for ionization cross sections. The typical scale for the electron orbital velocity with ionization potential I_{nl} is

$$v_{nl}=v_0\sqrt{2I_{nl}/E_0}. \tag{1}$$

Here, n,l is the standard notation for the main quantum number and the orbital angular momentum quantum number, $v_0=2.2\times10^8$ cm/s and $E_0=27.2$ eV are the atomic velocity and energy scales, respectively (see, for example, Ref. 8). The collision dynamics is very different, depending on whether projectile particle velocity v is smaller or larger than v_{nl}.

Here, we summarize the scaling of ionization cross section by the fully stripped ions. The stripping cross sections by neutral atoms were discussed in Ref. 4. A reader who is interested in additional details is referred to our longer report.[9] More than a century ago, Thompson calculated the ionization cross section in the limit $v \gg v_{nl}$ (see, for example, Ref. 1). This treatment neglected the orbital motion of the target electrons and assumed a straight-line trajectory of the projectile, which gives[1]

$$\sigma^{\mathrm{Bohr}}(v,I_{nl},Z_p)=2\pi Z_p^2 a_0^2\frac{v_0^2E_0}{v^2I_{nl}}, \tag{2}$$

where $a_0=0.529\times10^{-8}$ cm is the Bohr radius. Subsequent treatments accounted for the effect of finite electron orbital velocity. In Ref. 10, Gerjuoy calculated the stripping cross section by averaging the Rutherford electron-ion scattering cross section over the phase space of the atomic electrons leading to ionization. The result of the calculations can be expressed as

$$\sigma^{\mathrm{GGV}}(v,I_{nl},Z_p)=\pi a_0^2 Z_p^2\frac{E_0^2}{I_{nl}^2}G^{\mathrm{GGV}}\left(\frac{v}{v_{nl}}\right). \tag{3}$$

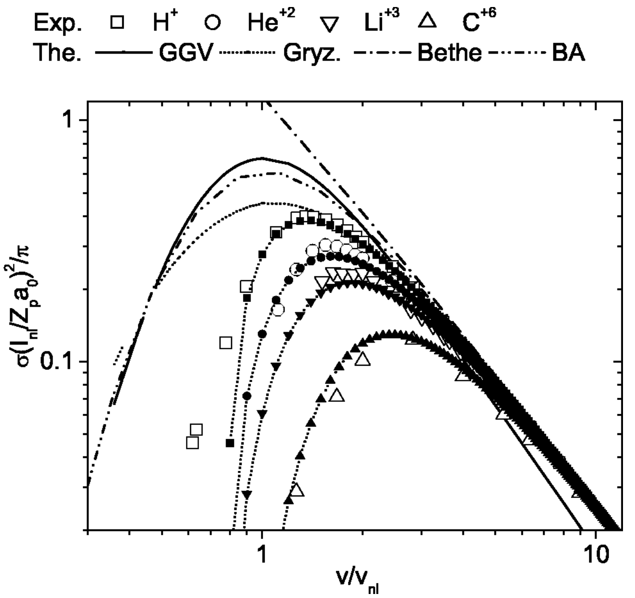

FIG. 1. Ionization cross sections of atomic hydrogen by fully stripped ions showing both experimental data and theoretical predictions. GGV stands for the classical calculation by Gerjuoy using the fit of Garcia and Vriens. Gryz denotes the Gryzinski approximation. Bethe stands for Bethe's quantum-mechanical calculation in the Born approximation, limited to $v > v_{nl}$ in Eq. (4). Finally, BA denotes the Born approximation in the general case. Open symbols show experimental data. Closed symbols and dotted lines are Gillespie's fit.

Here, the scaling function $G^{\mathrm{GGV}}(x)$ is defined in Ref. 9.

Bethe made use of the Born approximation of quantum mechanics to calculate cross sections (see, for example, Ref. 8). The Born approximation is valid for $v/v_0 > 2Z_p$ and $v \gg v_{nl}$.[8] This yields the relation

$$\sigma^{\mathrm{Bethe}} = \sigma^{\mathrm{Bohr}} \times \left[0.566 \ln\left(\frac{v}{v_{nl}}\right) + 1.26 \right]. \tag{4}$$

Note that for $v \gg v_{nl}$, the logarithmic term on the right-hand side of Eq. (4) contributes substantially to the cross section, and as a result the quantum mechanical calculation in Eq. (4) gives a larger cross section than the classical trajectory treatment in Eq. (2) (see Fig. 1).

In Ref. 6 Gryzinsky attempted to obtain the ionization cross section using only classical mechanics, similar to Gerjuoy. However, in order to match the asymptotic behavior of the Bethe formula in Eq. (4) at large projectile velocities, Gryzinsky assumed an artificial electron velocity distribution function (EVDF) instead of the correct EVDF. After a number of additional simplifications and assumptions, Gryzinsky suggested an approximation for the cross section in the form given by Eq. (3) with another function $G^{\mathrm{Gryz}}(x)$, which is specified in Refs. 6 and 9. The Gryzinsky formula can be viewed as a fit to the Bethe formula at large velocities $v \gg v_{nl}$ with some rather arbitrary continuation to small velocities $v < v_{nl}$.

Figure 1 shows the experimental data for the cross sections for ionizing collisions of fully stripped ions colliding with a hydrogen atom,

$$X^{q+} + H(1s) \rightarrow X^{q+} + H^{+} + e, \tag{5}$$

where X^{q+} denotes fully stripped ions of H, He, Li, and C atoms, and $(1s)$ symbolizes the ground state of the hydrogen atom. For hydrogen, the ionization potential is $I_{nl} = (1/2)E_0$ and $v_{nl} = v_0 = 2.19 \times 10^8$ cm/s. The cross section is normalized to $\pi Z_p^2 a_0^2 / I_{nl}^2 = 3.51 Z_p^2 \times 10^{-16}$ cm^2. The experimental data for H^{+} are from Ref. 11; He^{+2} and C^{+6} from Ref. 12, and Li^{+3} from Ref. 13.

From Fig. 1 it is evident that the Bethe formula describes well the cross sections for projectile velocities larger than the orbital velocity $v \gg v_{nl}$. At large energies, the GGV formula underestimates the cross section, whereas Gryzinsky's formula gives results close to the Bethe formula and the experimental data. Both the GGV and Gryzinsky formulas disagree with the experimental data at small energies because they assume free electrons, neglecting the influence of the target atom potential on the electron motion during the collision. To account for the difference between the Born approximation results and the experimental data for $v < v_{nl}$, Gillespie proposed to decrease the results of the Born approximation at low velocities by an exponential factor, as given in Ref. 7. Although Gillespie's fit proved to be very useful, the fitting parameters are not available for most target atoms and the fit cannot be applied to small velocities where the fit gives negative cross section (see Ref. 9 for details).

For $v \sim v_{nl}$, a universal curve is expected if both the cross sections and the square of the impact velocity are divided by Z_p.[14] This scaling was established for the total electron loss cross section σ^{el}, which includes both the charge exchange cross section σ^{ce} and the ionization cross section, based on the results of classical trajectory Monte Carlo (CTMC) calculations by Olson in Ref. 15. In Ref. 16 Janev showed that the Olson scaling can be written in the universal from similar to Eq. (3),

$$\sigma^{el}(v, Z_p) = \pi a_0^2 Z_p^2 \frac{E_0^2}{I_{nl}^2} G^{\mathrm{Olson}}\left(\frac{v}{v_{nl}}\right), \tag{6}$$

where

$$G^{\mathrm{Olson}}(x) = \frac{5}{3x^2}[1 - \exp(-4x^2/5)].$$

Quantum mechanical calculations[17] give the same scaling as in Eq. (6), but with a different scaling function.

Analysis of the experimental data in Fig. 1 shows that the maxima of the experimentally measured cross sections occur at $v_{\max} = v_{nl}\sqrt{Z_p + 1}$, not at $v_{nl}\sqrt{Z_p}$ as would be the case according to Olson's scaling in Eq. (6). Figure 2 illustrates the inadequacy of Olson's fit in Eq. (6) for the ionization cross section instead of the total electron removal cross section and shows that data are considerably scattered near the maxima of the cross sections.

We now propose a new fit formula for the ionization cross section. Based on experimental data, it is natural to plot cross sections as a function of the normalized velocity $v/(v_{nl}\sqrt{Z_p + 1})$. Note that at large velocities, according to Eq. (2) $\sigma \sim Z_p^2/v^2$. Therefore making use of the normalized velocity $v/(v_{nl}\sqrt{Z_p + 1})$ requires normalization of the cross sections according to $\sigma/[Z_p^2/(Z_p + 1)]$. As a consequence, instead of Eq. (6), we propose the following scaling:

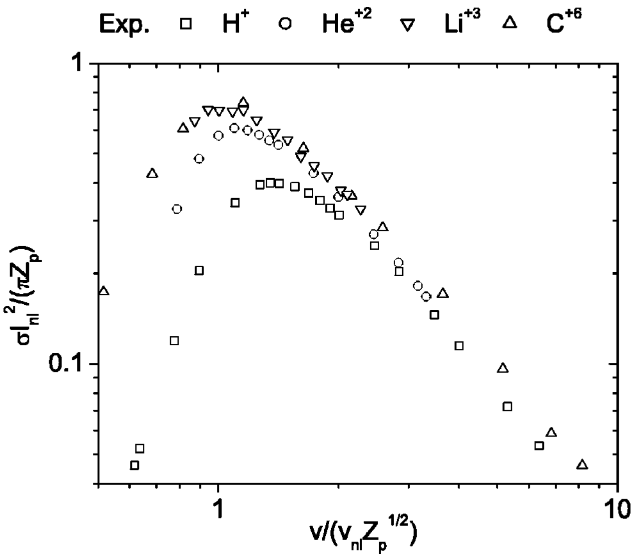

FIG. 2. Ionization cross sections of hydrogen by fully stripped ions. The scaled experimental data are from Fig. 1. Note that the data do not merge into a single curve.

$$\sigma^{\rm ion}(v,I_{nl},Z_p)=\pi a_0^2\frac{N_{nl}Z_p^2}{(Z_p+1)}\frac{E_0^2}{I_{nl}^2}G^{\rm new}\left(\frac{v}{v_{nl}\sqrt{Z_p+1}}\right), \quad (7)$$

where N_{nl} is the number of electrons in orbital nl. Resulting plots of the scaled cross sections are shown in Fig. 3. Comparing Figs. 2 and 3 one can clearly see that all of the experimental data merge together on the scaled plot based on Eq. (7).

The resulting universal function can be fitted with various functions, but the simplest fit was proposed by Rost and Pattard in Ref. 18. They showed that if both the cross section and the projectile velocity are normalized to the values of cross section and projectile velocity at the cross section maximum, then the scaled cross section $\sigma/\sigma_{\rm max}$ is well described by the fitting function

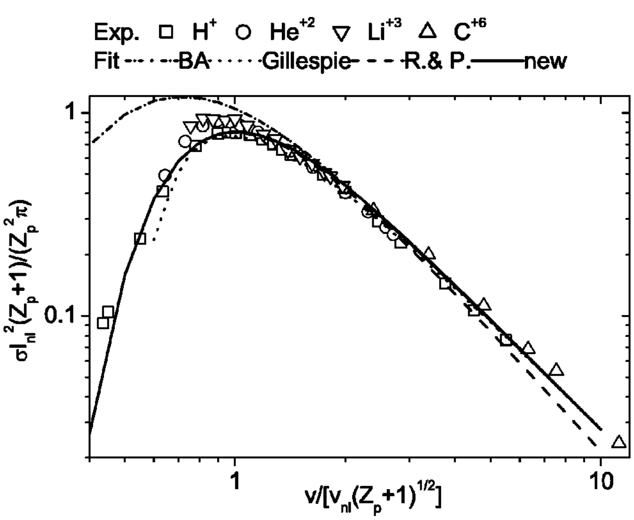

FIG. 3. Ionization cross sections of hydrogen by fully stripped ions showing the scaled experimental data and the theoretical fits. BA denotes the Born approximation. Gillespie denotes Gillespie's fit according to Ref. 7. R.&P. symbolizes the fit proposed by Rost and Pattard (Ref. 18) in Eq. (8). "New" denotes the new fit given by Eq. (11).

$$\sigma(v)=\sigma_{\rm max}\frac{\exp(-v_{\rm max}^2/v^2+1)}{v^2/v_{\rm max}^2}. \quad (8)$$

Here, $\sigma_{\rm max}$ is the maximum of the cross section, which occurs at velocity $v_{\rm max}$. For the present study (the case of the ionization cross section by the bare projectile), we obtain

$$\sigma_{\rm max}=\pi a_0^2\frac{Z_p^2}{(Z_p+1)}\frac{E_0^2}{I_{nl}^2}, \quad (9)$$

$$v_{\rm max}=v_{nl}\sqrt{Z_p+1}. \quad (10)$$

As can be seen from Fig. 3, the function in Eq. (8) with $\sigma_{\rm max}$ and $v_{\rm max}$ defined in Eqs. (9) and (10) describes well the cross sections at small and intermediate energies, but underestimates the cross section at high energies. The reason is that the function in Eq. (8) does not reproduce the logarithmic term in the Bethe formula in Eq. (4). To improve the agreement with the experimental data and the Bethe formula we propose a new scaling for the fitting function in Eq. (7) defined by

$$G^{\rm new}(x)=\frac{\exp(-1/x^2)}{x^2}[1.26+0.283\ln(2x^2+25)]. \quad (11)$$

At large $x\gg 1$, Eq. (11) approaches the Bethe formula in Eq. (4), and at small $x<1$, Eq. (11) approaches the result in Eq. (8). The resulting fit in Eq. (11) agrees well with experimental data for hydrogen as it is shown in Fig. 3.

We have also applied the new fit in Eqs. (7) and (11) to the ionization cross section of helium, which is shown in Fig. 4(a). The symbols denote the experimental data from Refs. 19 and 20, and the lines correspond to the continuum-distorted-wave-eikonal initial state (CDW-EIS) theory,[21] which is a generalization of the Born approximation. The CDW-EIS theory accounts for the distortion of the electron wave function by the projectile. From Fig. 4(a) one can see that the CDW-EIS theory overestimates the cross section near the maximum, and underestimates the cross section at small energies.

Direct application of the Olson scaling formula in Eq. (6) to the ionization of helium does not produce similarly good results as in the hydrogen case [see Fig. 4(b)]. But after applying the new scaling in Eq. (7), all of the experimental and theoretical results merge close together on the scaled plot, as is clearly evident in Fig. 4(c). Moreover, if we plot the cross sections as a function of velocity normalized to the orbital velocity v_{nl} estimated from the ionization potential of helium ($I_{\rm He}=24.6$ eV) making use of Eq. (1), the cross section is given by the same scaling as in Eq. (7) with the same function as in Eq. (11), as evident from Fig. 4(d). (The number of electrons in the helium atom is $N_{nl}=2$, and therefore the scaled cross section is twice that of hydrogen.) From Figs. 3 and 4(d) it is clear that the new proposed fit in Eq. (7) using the function in Eq. (11) gives very good results for both hydrogen and helium. Further verification of the new scaling is difficult at this time because reliable experimental data and numerical simulations for a broad range of projectile velocities are absent for other target atoms.

To summarize, the new scaling in Eq. (7) for the ionization and stripping cross sections of atoms and ions by fully

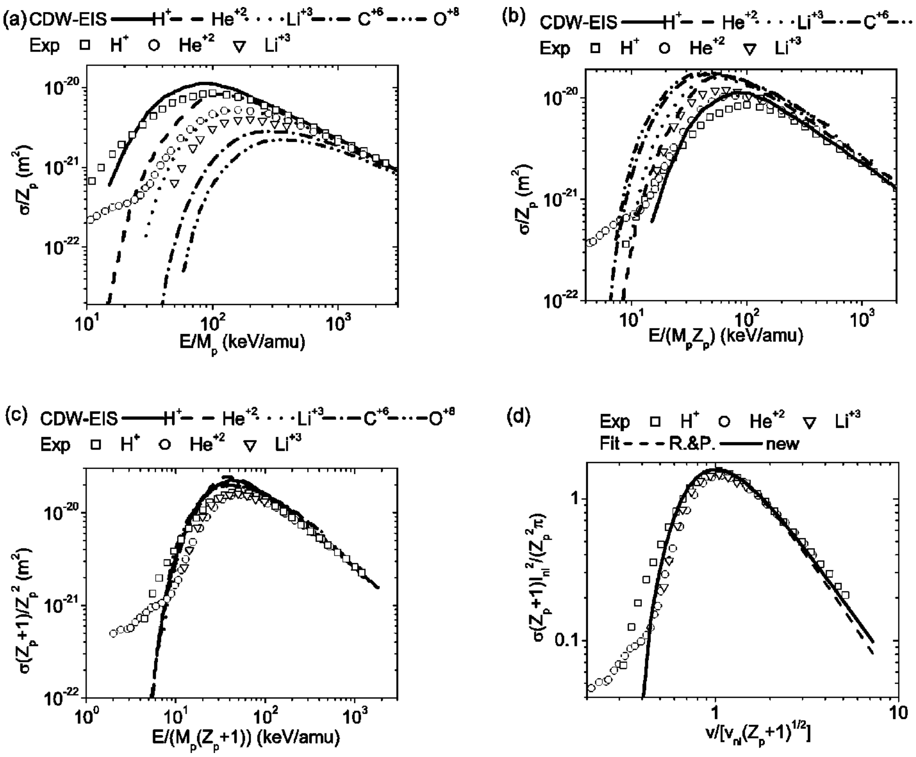

FIG. 4. Ionization cross sections of helium by fully stripped ions. The experimental data are from Refs. 19 and 20, and the theoretical calculations from Ref. 21. Shown in the figures are (a) the raw data; (b) the scaled data from (a), making use of Eq. (6); (c) the scaled data making use of Eq. (7); and (d) the experimental data only scaled using Eq. (7), and comparing with the fit functions. The notation R.&P. denotes Eq. (8), and ''new'' denotes Eq. (11).

stripped projectiles has been proposed. The new scaling does not have any fitting parameters and describes the shape of the cross section as a single function of the scaled projectile velocity [Eq. (11)]. The proposed scaling formula agrees well with theoretical predictions in the limit of large projectile velocities. The new scaling has been verified by comparison with available experimental data and theoretical simulations for the ionization cross sections of hydrogen and helium by H^{+}, He^{+2}, Li^{+3}, C^{+6}, and O^{+8}. The agreement between the new proposed scaling and experimental data is very good. The difference between the proposed fit and the experimental data is within 15% accuracy, which is similar to the estimated uncertainty in the measurements.

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