Ionization Cross Sections for Ion-Atom Collisions in High Energy Ion Beams

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Abstract

Knowledge of ion-atom ionization cross sections is of great importance for many accelerator 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. The Born approximation and classical trajectory calculations are frequently used to estimate the cross sections. Neither approximation is expected to be valid over the entire range of projectile ions and target atoms. Aspects of both models must be included in order to address the shortcomings in the underlying assumptions. A large difference in cross section, up to a factor of six, calculated in quantum mechanics and classical mechanics, has been obtained for 3.2GeV I^- and Cs^+ ions. Because at such high velocities the Born approximation is well validated, the classical trajectory approach fails to correctly predict the stripping cross section at high energies for electron orbitals with low ionization potential.

INTRODUCTION

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 [1]. While specific values of the cross sections for various pairs of projectile ions and target atoms have been measured at several energies [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 [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 [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 [8] 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.

The typical scale for the electron orbital velocity with ionization potential I_{nl} is $v_{nl} = v_0\sqrt{2I_{nl}/E_0}$. Here, n, l is the standard notation for the main quantum number and the orbital angular momentum quantum number, and $v_0 = 2.2 \cdot 10^8 cm/s$ is the atomic velocity scale [9]. The collision dynamics is very different, depending on whether v is smaller or larger than v_{nl}.

We first summarize the scaling of ionization cross section by the fully stripped ions. More than a century ago, Thompson calculated the ionization cross section in the limit $v >> v_{nl}$ [1]. This treatment neglected the orbital motion of the target electrons and assumed a straight-line trajectory of the projectile, which gives [1]

$$\sigma^{Bohr}(v, I_{nl}, Z_p) = 2\pi Z_p^2 a_0^2 \, \frac{v_0^2 E_0}{v^2 I_{nl}}, \qquad (1)$$

where $a_0 = 0.529 \cdot 10^{-8} cm$ is the Bohr radius. Subsequent treatments accounted for the effect of finite electron orbital velocity. The most complete and accurate calculations were done by Gerjuoy, by averaging the Rutherford cross section over the phase space of the atomic electrons leading to ionization. The result of the calculations can be expressed as

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

Here, the scaling function $G^{GGV}(x)$ is defined in [8].

Bethe made use of the Born approximation of quantum mechanics to calculate cross sections [9]. The Born approximation is valid for $v/v_0 > 2Z_p$ and $v >> v_{nl}$ [9]. This yields the relation

$$\sigma^{Bethe} = \sigma^{Bohr} \times \left[0.566 \ln\left(\frac{v}{v_{nl}}\right) + 1.26\right]. \qquad (3)$$

Note that for $v >> v_{nl}$, the logarithm term on the right-hand side of Eq.(3) contributes substantially to the cross

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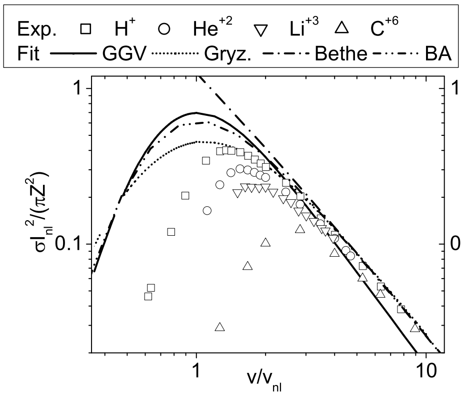

Figure 1: Ionization cross sections of atomic hydrogen by fully stripped ions showing both experimental data and theoretical fits. GGV stands for the classical calculation by Gerjuoy using the fit of Garcia and Vriens. Gryz denotes the Gryzinski approximation. Bethe stands for Bethe's quantum-mechanical calculation in the Born approximation, limited to $v > v_{nl}$ in Eq.(3). Finally, BA denotes the Born approximation in the general case. All values are in atomic units. For hydrogen, the ionization potential is $I_{nl} = 1/2$, $v_{nl} = v_0 = 2.19 \cdot 10^8 cm/s$, and the cross section is normalized to $a_0^2 = 0.529^2 \cdot 10^{-16} cm^2$.

section, and as a result the quantum mechanical calculation in Eq.(3) gives a larger cross section than the classical trajectory treatment in Eq.(1) (see Fig.1).

Gryzinsky attempted to obtain the ionization cross section using only classical mechanics, similar to Gerjuoy. But, in order to match the asymptotic behavior of the Bethe formula in Eq.(3) 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.(2) with another function $G^{Gryz}(x)$, which is specified in [6, 8]. The Gryzinsky formula can be viewed as a fit to the Bethe formula at large velocities $v >> v_{nl}$ 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,

$$X^{q+} + H(1s) \rightarrow X^{q+} + H^{+} + e, \tag{4}$$

where X^{q+} denotes fully stripped ions of H, He, Li, C atoms, and $(1s)$ symbolizes the ground state of the hydrogen atom. The experimental data are taken from the data of Shah *et al.* (see details in [8]).

From Fig.1 it is evident that the Bethe formula describes well the cross sections for projectile velocities larger than the orbital velocity $v >> v_{nl}$. 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 $v < v_{\max}$, Gillespie proposed to decrease the results of the Born approximation at low velocities by an exponential factor [7]. Although Gillespie's fit proved to be very useful, the fitting parameters are not available for most target atoms. Based on the results of the classical trajectory approximation, Olson developed a scaling for the total electron loss cross section [10], which includes both the charge exchange cross section and the ionization cross section. Unfortunately, application of the scaling to the ionization cross sections does not yield good agreement [8].

NEW FIT FORMULA FOR THE IONIZATION CROSS SECTION

We propose the following scaling [8]

$$\sigma^{ion}(v, I_{nl}, Z_p) = \frac{\pi a_0^2 N_{nl} Z_p^2}{(Z_p+1)} \frac{E_0^2}{I_{nl}^2} G^{new}\left(\frac{v}{v_{nl}\sqrt{Z_p+1}}\right), \tag{5}$$

where

$$G^{new}(x) = \frac{\exp(-1/x^2)}{x^2}\left[1.26 + 0.283 \ln\left(2x^2+25\right)\right]. \tag{6}$$

The resulting plots of the scaled cross sections are shown in Fig.2. Comparing Fig.1 and Fig.2, it is evident that all of the experimental data merge close together in the scaled plot based on Eqs.(5) and (6).

We have also applied the new fit formula in Eqs. (5) and (6) to the ionization cross sections of helium [8]. Again, all of the experimental and theoretical results merge close together on the scaled plot. The new proposed fit in Eq.(5) with the function in Eq.(6) gives very good results for both hydrogen and helium [8].

STRIPPING CROSS SECTIONS AT LARGE PROJECTILE VELOCITIES

We have investigated theoretically and experimentally the stripping of 3.4 Mev/amu Kr^{+7} and Xe^{+11} in N_2; and 10.2 MeV/amu Ar^{+6}, 19MeV/amu Ar^{+8}, 30 MeV He^{+}, and 38 MeV/amu N^{+6}, all in He, N_2, Ar and Xe [5]. Both the Born approximation and the classical trajectory calculation give very good estimates, except for the case of Xe. This is not expected to be the case for fully stripped target ions and/or low ionization potentials of the projectile ions. Tables 1 and 2 show the stripping cross sections for only one electron from the outer electron shell for different projectile ions with the same velocity $v = 32v_0$ ($25 MeV/amu$) colliding with a nitrogen atom (N) or bare nitrogen nucleus (N^{+7}).

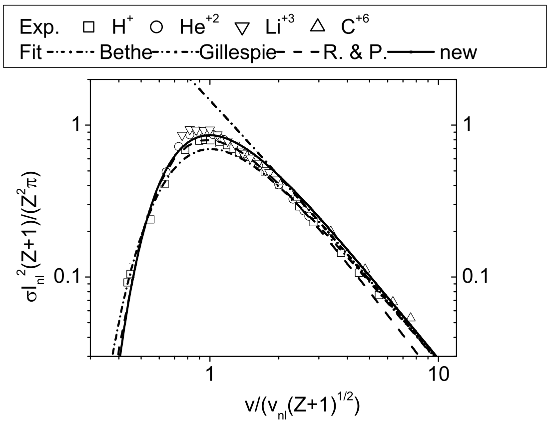

Figure 2: Ionization cross sections of hydrogen by fully stripped ions showing the scaled experimental data and the theoretical fits. BA denotes the Born approximation. Gillespie denotes Gillespie's fit. R.&P. symbolizes the fit proposed by Rost and Pattard [11]. ”New” denotes the new fit given by Eq.(6).

$\sigma, 10^{-16} cm^2$	Cs^+	I^-	H^- ions
N	0.045	0.08	0.10
N^{+7}	0.32	2.5	12.5

Table 1. Stripping cross sections of $3.35 GeV\ Cs^+$, $3.2 GeV\ I^-$ and $25 MeV\ H^-$ by N or N^{+7} calculated making use of the Born approximation in quantum mechanics (stripping of only one electron from the outer electron shell is considered here with ionization potentials: $22.4 eV$ for Cs^+; $3.06 eV$ for I^-; and $0.75 eV$ for H^-).

$\sigma, 10^{-16} cm^2$	Cs^+	I^-	H^- ions
N	0.10	0.47	1.34
N^{+7}	0.17	1.29	5.05

Table 2. The same stripping cross sections as in Table 1 but calculated making use of the classical trajectory approximation.

The result of cross sections calculations using Eq.(1) with a factor $5/3$, and the result in Eq.(3), coincide with the results in Tables 1 and 2 for the stripping cross sections by a fully stripped nitrogen ion calculated in the classical trajectory approximation and the Born approximation of quantum mechanics, respectively. The stripping cross sections calculated in the classical trajectory approximation for Cs^+ and I^- ions by fully stripped nitrogen ions is only factor 2-3 larger than the stripping cross sections by neutral nitrogen atoms, which is in qualitative agreement with the observations in [3]. However, there is a large difference, up to a factor 100 (for H^-), in the same stripping cross sections calculated in the Born approximation of quantum mechanics. It is evident that the stripping of Cs^+ ions by N^{+7} decreases by a factor of $22.4 eV/3 eV = 7.5$ compared with I^- ions, which is in agreement with the Bohr [Eq.(1)] and Bethe [Eq.(3)] formulas. However. the stripping cross sections for Cs^+ and I^- ions by a neutral nitrogen atom differ by only a factor of 2 in the Born approximation.

CONCLUSIONS

The new scaling formulas in Eqs. (5) and (6) for the ionization and stripping cross sections of atoms and ions by fully stripped projectiles has been proposed. We have recently investigated theoretically and experimentally the stripping of more than 18 different pairs of projectile and target particles in the range of 3-38 MeV/amu to study the range of validity of both the Born approximation and the classical trajectory calculation. In most cases both approximations give similar results [2, 5]. However, for fast projectile velocities and low ionization potentials, the classical approach is not valid and can overestimate the stripping cross sections by neutral atoms by an order-of-magnitude [13].

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