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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. 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. 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. Therefore, a hybrid approach that automatically chooses between the Born approximation and the classical mechanics approximation depending on the parameters of the collision has been developed. When experimental data and theoretical calculations are not available, approximate formulas are frequently used. Based on experimental data and theoretical predictions, a new fit formula for ionization cross-sections by fully stripped ions is proposed. The resulting plots of the scaled ionization cross-sections of hydrogen by fully stripped ions are presented. The new fit formula has also been applied to the ionization cross-sections of helium. Again, the experimental and theoretical results merge close together on the scaled plot.

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1. Introduction

Ion beams lose electrons when passing through a background gas in accelerators, beam transport lines, and target chambers. As a result, the ion

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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 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]. 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 [2,3]. In most cases, both approximations give similar results. 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 [4]. Therefore, a hybrid approach that automatically chooses between the Born approximation and the classical mechanics approximation depending on the parameters of the collision [5] has been developed.

While specific values of the cross-sections for various pairs of projectile ions and target atoms have been measured at several energies [2,3,6,7], the study of the scaling of cross-sections with energy and target or projectile nucleus is only now underway [8,9]. 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 [10]. 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 Gryzinski'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 [11]. 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 the present paper, we describe a new fit formula [6] for the ionization cross-section which has no fitting parameters and is correct at small energies. The formula has been 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 are the standard notations for the principal quantum number and the orbital angular momentum quantum number, respectively, and $v_0 = 2.2 \times 10^8\,\text{cm/s}$ is the atomic velocity scale [12]. The collision dynamics is very different, depending on whether v is smaller or larger than v_{nl}.

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

$$\sigma^{\text{Bohr}}(v, I_{nl}, Z_\text{p}) = 2\pi Z_\text{p}^2 a_0^2 \frac{v_0^2 E_0}{v^2 I_{nl}} \tag{1}$$

where $a_0 = 0.529 \times 10^{-8}\,\text{cm}$ 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

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

Here, the scaling function $G^{\text{GGV}}(x)$ is defined in Ref. [6]. At high projectile velocity $v \gg v_{nl}$, Eq. (2) tends to Eq. (1) but with an additional multiplying coefficient of $\frac{5}{3}$. This is a consequence of the fact that for an electron with nonzero velocity, less velocity transfer is required for ionization, which gives rise to a larger cross-section.

Bethe made use of the Born approximation of quantum mechanics to calculate cross-sections [12]. The Born approximation is valid for $v/v_0 > 2Z_p$ and $v \gg v_{nl}$ [12]. This yields the relation

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

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

Gryzinski 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, Gryzinski assumed an artificial electron velocity distribution function (EVDF) instead of the correct EVDF. After a number of additional simplifications and assumptions, Gryzinski suggested an approximation for the cross-section in the form given by Eq. (2) with another function $G^{\text{Gryz}}(x)$, which is specified in Refs. [6,10]. The Gryzinski 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 $v < v_{nl}$.

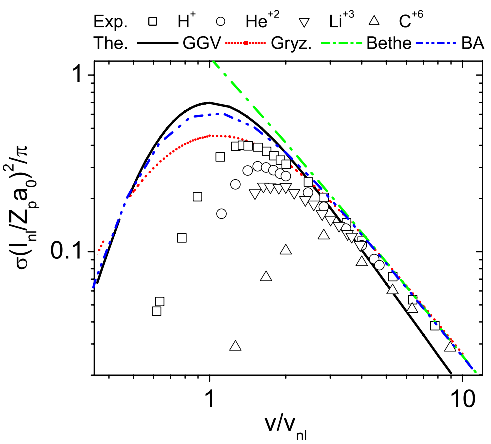

Fig. 1. Ionization cross-sections of atomic hydrogen by fully stripped ions showing both experimental data and theoretical fits. GGV stands for the classical calculation by Gerjuoy using the fit of Garcia and Vriens. Gryz denotes the Gryzinski approximation. Bethe stands for Bethe's quantum-mechanical 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 $I_{nl} = \frac{1}{2}$, $v_{nl} = v_0 = 2.19 \times 10^8$ cm/s, and the cross-section is normalized to $a_0^2 = 0.529^2 \times 10^{-16}$ cm^2 [6].

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

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

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 Ref. [6]).

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 Gryzinski's formula gives results close to the Bethe formula and the experimental data.

The Bethe, GGV and Gryzinski formulas fail at small velocities because they assume free electrons, neglecting the influence of the target atom potential on the electron motion during the collision. Apparently the assumption of free electron motion fails if the circulation period of the electron around the atom's nucleus is comparable with the interaction time of an ion with the electron. Let us now estimate the projectile velocities at which the electron circulation needs to be taken into account. The typical impact parameter leading to ionization is

$$\rho_{\text{ioniz}} \simeq \sqrt{\frac{\sigma^{\text{Bohr}}}{\pi}} = \frac{2a_0 v_0^2 Z_p}{v v_{nl}} \quad (5)$$

and the interaction time is of order ρ_{ioniz}/v. The electron circulation time $\tau_{nl} \simeq a_{nl}/v_{nl}$, where v_{nl} is the electron orbital velocity, which scales as $v_{nl} = Z_T v_0$, and the ion radius $a_{nl} = a_0/Z_T$ [12]. Therefore the condition $\tau_{nl} > \rho_{\text{ioniz}}/v$ holds for $v > v_{\max}$, where

$$v_{\max} = v_{nl}\sqrt{2Z_p/Z_T}. \quad (6)$$

Here, Z_p is the charge of the fully stripped projectile and Z_T is the nuclear charge of the target atom or ion. For velocities larger than v_{max}, the ionization cross-section decreases as the velocity increases (see Eq. (3)) due to the decreasing interaction time with an increase in velocity. On the other hand, for velocities less than v_{max}, the collision becomes more adiabatic. The influence of the projectile is averaged out due to the slower motion of the projectile compared with the electron orbital velocity, and the ionization cross-section decreases with decreasing projectile velocity. Thus, the cross-section has a maximum at $v \simeq v_{max}$ (Eq. (6)).

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 [11]. Although Gillespie's fit proved to be very useful, the fitting parameters are not available for most target atoms.

A universal curve is expected if both the cross-sections and the square of the impact velocity are divided by Z_p [13]. 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 the classical trajectory approximation, Olson developed a scaling for the total electron loss cross-section [14], which includes both the charge exchange cross-section and the ionization cross-section. Unfortunately, application of the scaling to only the ionization cross-sections does not yield good agreement, as is shown in Ref. [6].

2. New fit formula for the ionization cross-section

The following scaling has been proposed [6]

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

where

$$G^{new}(x) = \frac{\exp(-1/x^2)}{x^2}[1.26 + 0.283\ \ln(2x^2+25)]. \tag{8}$$

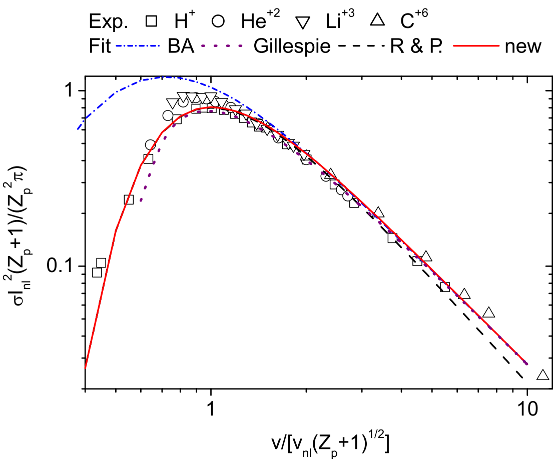

Fig. 2. Ionization cross-sections of hydrogen by fully stripped ions showing the scaled experimental data and the theoretical fits [6]. BA denotes the Born approximation. Gillespie denotes Gillespie's fit. R.&P. denotes the fit proposed by Rost and Pattard [15]. "New" denotes the new fit given by Eq. (8).

The resulting plots of the scaled cross-sections are shown in Fig. 2. Comparing Figs. 1 and 2, it is evident that all of the experimental data merge close together in the scaled plot based on Eqs. (7) and (8).

We have also applied the new fit formula in Eqs. (7) and (8) to the ionization cross-sections of helium [6]. Again, all of the experimental data and theoretical results merge close together on the scaled plot. The new proposed fit in Eq. (7) with the function in Eq. (8) gives very good agreement for both hydrogen and helium [6].

3. 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}, 19 MeV/amu Ar^{+8}, 30 MeV He^{+}, and 38 MeV/amu N^{+6}, all in He, N_2, Ar and Xe [3]. Data for He^{+}, and N^{+6} are shown in Tables 1 and 2, respectively, together with theoretical calculations. Here, the label BA refers to the theoretical calculations made using the Born approximation (described in detail in Appendix A of Ref. [6]), and CT refers to the

Table 1
Stripping cross-sections of 30 MeV/amu He^+ in collisions with He, Ar and Xe

$\sigma, 10^{-16}\,cm^2$	Exp.	BA	CT	Hybrid
He	0.4 ± 0.1	0.30	0.69	0.30
Ar	7.3 ± 0.4	9.0	11.5	9.1
Xe	$23. \pm 1$	47	36	33

Exp. denotes the experimental data from Ref. [3]; BA denotes the cross-sections calculated making use of the Born approximation of quantum mechanics; CT refers to calculations making use of the classical mechanics only; and Hybrid is a combination of both as described in the text.

Table 2
Similar to Table 1 but stripping cross-sections of 38 MeV/amu N^{+6} in collisions with He, Ar and Xe

$\sigma, 10^{-16}\,cm^2$	Exp.	BA	CT	Hybrid
He	0.06 ± 0.01	0.044	0.046	0.044
Ar	1.64 ± 0.03	1.58	1.58	1.68
Xe	6.29 ± 0.04	10.30	6.50	6.9

theoretical calculations made using classical mechanics only (described in detail in Appendix B of [6]); and the label Hybrid is a combination of both as described below. Note that the cross-sections calculated in the Born approximation agree better with experimental data for light target atoms, whereas the classical mechanics results agree better with the experimental data for xenon. The disagreement between the calculations and the experimental data is due to the application of approximations outside their validity range. To overcome this shortcoming, we have developed the "hybrid method". The cross-section can be represented as an integral over the impact parameter (ρ). The simplest method to calculate the cross-section is to use both the classical and Born approximations, but only for the regions in which they are valid, and sum the results to obtain the total cross-section. But at what point is one method favored over the other? The range of validity of both approximations can be estimated by evaluating the action $S(\rho) = \int_{-\infty}^{\infty} V[r(\rho,t)]\,dt$ along the trajectory $r(\rho,t) = [\rho^2 + (vt)^2]^{1/2}$. At small impact parameters ($\rho < \rho^*$), where ρ^* is determined by the condition

$$\int_{-\infty}^{\infty} V[r(\rho^*, t)]\,dt = \hbar, \tag{9}$$

the target atom potential $[V(r)]$ is large and the corresponding change in action is large; thus, we can apply classical mechanics for $\rho < \rho^*$. Similarly, the Born approximation fails if $S(\rho) > \hbar$. Thus, as a natural cutoff, we shall use the Born approximation for the regions where $S(\rho) < \hbar$, and we shall use the classical approach for the regions where $S(\rho) > \hbar$. The total cross-section can then be written as a sum of the classical cross-section for the region $\rho < \rho^*$ and the cross-section calculated in the Born approximation for the region $\rho > \rho^*$.

Using the procedure outlined above, the cross-sections presented in Table 1 have been recalculated. Results of the hybrid calculations are shown in the last columns of Tables 1 and 2. Note that the cross-sections involving He as the target atom are identical for calculations making use of the Born approximation and for the calculations using the hybrid method. This is because $S(\rho)/\hbar$ is small for this parameter range, and the Born approximation remains valid throughout the entire region of integration. This suggests that the Born approximation should be more accurate than the classical approximation in this case. In the opposite case of xenon, the hybrid method gives results close to the calculations performed using classical mechanics, because $S(\rho)/\hbar$ remains larger than unity for most impact parameters, leading to ionization. In summary, the hybrid method helps to identify which method is more trustworthy. Moreover, it produces more reliable results than either of the approximations separately (see, for example, Ar case in Table 2).

The difference between the classical mechanics calculations and the Born approximation becomes more significant for fast projectiles. As envisioned in heavy ion fusion, a driver will accelerate heavy ions up to energies 25 MeV/amu. For beam–plasma interaction issues, it is important to evaluate stripping cross-sections by neutral atoms and plasma ions. As a limiting case, we shall evaluate cross-sections for projectiles with low ionization potentials colliding with neutral target atoms or

Table 3
Stripping cross-sections of 3.35 GeV Cs^+, 3.2 GeV I^- and 25 MeV H^- by N or N^{+7} calculated making use (left) of the Born approximation in quantum mechanics, and (right) the classical trajectory approximation (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^-
BA:	N	0.045	0.08	0.10
	N^{+7}	0.32	2.5	12.5
CT:	N	0.10	0.47	1.34
	N^{+7}	0.17	1.29	5.05

fully stripped target ions. Table 3 shows results of calculations of 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}). At these energies $S(\rho)/\hbar$ remains much less than unity and the Born approximation is valid, whereas the classical mechanics calculations is not. For the experimental data in Tables 1 and 2, the difference between the two approximations is a factor 2 at most. We now study the difference for projectiles with much lower ionization potentials than in Tables 1 and 2. For example, Cs^+ has ionization potential 22.4 eV, I^- has ionization potential 3 eV and H^- has ionization potential 0.75 eV, whereas He^+ and N^{+6} have ionization potentials 54.4 eV and 666 eV, respectively.

At these high energies, the results of cross-section calculations agree well with the Bohr formula (Eq. (1)) with a multiplicative factor $\frac{5}{3}$ for the classical trajectory approximation, and with the Bethe formula (Eq. (3)) for the Born approximation of quantum mechanics, respectively.

First, note in Table 3 that the classical trajectory approximation gives cross-sections a factor of 2 less than the Born approximation for the stripping cross-sections by a fully stripped nitrogen ion. This is due to the presence of the logarithmic term in the Bethe formula (Eq. (3)) compared to the Bohr formula (Eq. (1)). This term describes classically forbidden transitions at large impact parameters.

However, there is a large difference, up to a factor 10 (for H^-), in the value of the stripping cross-sections by neutral atoms calculated in the classical trajectory approximation and the Born approximation of quantum mechanics. The reason for this is the quantum mechanical uncertainty of the electron location. At high energies, classical mechanics overestimates the probability of ionization, presuming that the electron can be located at a prescribed impact parameter (see details in Ref. [4]).

Similar to large projectile velocities, ionization occurs only at small impact parameters close to the nucleus in classical mechanics. As a result, the stripping cross-sections calculated in the classical trajectory approximation for Cs^+ and I^- ions by fully stripped nitrogen ions are only a factor of 2–3 larger than the stripping cross-sections by neutral nitrogen atoms. This is in qualitative agreement with the calculations of Ref. [7]. However, the correct quantum mechanical calculations show a large difference between the stripping cross-sections by neutral atoms and fully stripped ions as targets, because classical mechanics overestimates the probability of ionization, presuming that the electron can be located at prescribed impact parameter [4].

We now examine the dependence of the stripping cross-section on ionization potential. Both the Bohr (Eq. (1)) and Bethe (Eq. (3)) formulas predict that the cross-section is inversely proportional to the ionization potential. Table 3 shows that the stripping of Cs^+ ions by N^{+7} decreases by a factor of $22.4/3\,eV = 7.5$ compared with I^- ions. However, the dependence of the stripping cross-section on ionization potential by neutral atoms is much weaker. For example, 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.

4. Conclusions

The new scaling formulas in Eqs. (7) and (8) 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 [2,3]. 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 [4].

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