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
complete. We have recently investigated the 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]:

\[
\sigma_{\text{Bohr}}(v, I_{nl}, Z_p) = 2\pi Z_p^2 a_0^2 \frac{v_0^2 E_0}{v^2 I_{nl}} \tag{1}
\]

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

\[
\sigma^{GGV}(v, I_{nl}, Z_p) = \pi a_0^2 Z_p^2 E_0^2 \frac{1}{I_{nl}^2} G^{GGV} \left( \frac{v}{v_{nl}} \right). \tag{2}
\]

Here, the scaling function \( G^{GGV}(x) \) 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 \( \frac{1}{x} \). 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

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

(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 \( v \ll v_{nl} \).

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

\[
X^q+ + H(1s) \rightarrow X^{q+} + H^+ + e,
\]

(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

\[
\rho_{\text{ioniz}} \approx \sqrt{\frac{\sigma_{\text{Bohr}}}{\pi}} = \frac{2a_0v_0^2Z_p}{vv_{nl}}
\]

(5)

and the interaction time is of order \( \rho_{\text{ioniz}}/v \). The electron circulation time \( \tau_{nl} \approx a_{nl}/v_{nl} \), where \( v_{nl} \) is the electron orbital velocity, which scales as \( v_{nl} = Z_Tv_0 \), and the ion radius \( a_{nl} = a_0/Z_T \) [12]. Therefore the condition \( \tau_{nl} > \rho_{\text{ioniz}}/v \) holds for \( v > v_{\text{max}} \), where

\[
v_{\text{max}} = v_{nl}\sqrt{2Z_p/Z_T}.
\]

(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 $v_{\text{max}}$, 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 $v_{\text{max}}$, 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 $v \approx v_{\text{max}}$ (Eq. (6)).

To account for the difference between the Born approximation results and the experimental data for $v < v_{\text{max}}$, 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 $\sigma^d$, which includes both the charge exchange cross-section $\sigma^{ce}$ 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]

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

where

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

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).

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
by evaluating the action validity of both approximations can be estimated total cross-section. But at what point is one they are valid, and sum the results to obtain the approximations, but only for the regions in which section is to use both the classical and Born

\[ S(r) = \int_{-\infty}^{\infty} V[r(t), t] \, dt = h, \]

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 \( S(\rho) > h \). Thus, as a natural cutoff, we shall use the Born approximation for the regions where \( S(\rho) < h \), and we shall use the classical approach for the regions where \( S(\rho) > h \). 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 \( S(\rho)/h \) 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 \( S(\rho)/h \) 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>
<thead>
<tr>
<th>( \sigma ), ( 10^{-16} ) cm²</th>
<th>Exp.</th>
<th>BA</th>
<th>CT</th>
<th>Hybrid</th>
</tr>
</thead>
<tbody>
<tr>
<td>He</td>
<td>0.4 ± 0.1</td>
<td>0.30</td>
<td>0.69</td>
<td>0.30</td>
</tr>
<tr>
<td>Ar</td>
<td>7.3 ± 0.4</td>
<td>9.0</td>
<td>11.5</td>
<td>9.1</td>
</tr>
<tr>
<td>Xe</td>
<td>23 ± 1</td>
<td>47</td>
<td>36</td>
<td>33</td>
</tr>
</tbody>
</table>

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>
<thead>
<tr>
<th>( \sigma ), ( 10^{-16} ) cm²</th>
<th>Exp.</th>
<th>BA</th>
<th>CT</th>
<th>Hybrid</th>
</tr>
</thead>
<tbody>
<tr>
<td>He</td>
<td>0.06 ± 0.01</td>
<td>0.044</td>
<td>0.046</td>
<td>0.044</td>
</tr>
<tr>
<td>Ar</td>
<td>1.64 ± 0.03</td>
<td>1.58</td>
<td>1.58</td>
<td>1.68</td>
</tr>
<tr>
<td>Xe</td>
<td>6.29 ± 0.04</td>
<td>10.30</td>
<td>6.50</td>
<td>6.9</td>
</tr>
</tbody>
</table>

Small impact parameters (\( \rho < \rho^* \)), where \( \rho^* \) is determined by the condition
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 \((N^+)\). At these energies \( S(\rho)/\hbar \) remains much less than unity and the Born approximation is valid, whereas the classical mechanics calculations is not. However, 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\(^-\)).

<table>
<thead>
<tr>
<th></th>
<th>( \sigma, 10^{-16} \text{ cm}^2 )</th>
<th>Cs(^+)</th>
<th>I(^-)</th>
<th>H(^-)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>BA:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>( N )</td>
<td>0.045</td>
<td>0.08</td>
<td>0.10</td>
</tr>
<tr>
<td></td>
<td>( N^+ )</td>
<td>0.32</td>
<td>2.5</td>
<td>12.5</td>
</tr>
<tr>
<td></td>
<td>CT:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>( N )</td>
<td>0.10</td>
<td>0.47</td>
<td>1.34</td>
</tr>
<tr>
<td></td>
<td>( N^+ )</td>
<td>0.17</td>
<td>1.29</td>
<td>5.05</td>
</tr>
</tbody>
</table>

Table 4. Cross-sections of 3.35 GeV Cs\(^+\), 3.2 GeV I\(^-\) and 25 MeV H\(^-\) by N or \((N^+)\) 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\(^-\)).

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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References