Scaling law for total electron-impact ionization cross sections of Li-like ions

L. U. Ancarani[1] and P.-A. Hervieux[2]
[1]*Laboratoire de Physique Moléculaire et des Collisions, Institut de Physique, Technopôle 2000, 57078 Metz, France*
[2]*Institut de Physique et Chimie des Matériaux de Strasbourg, GONLO, 23 rue du Loess, 67034 Strasbourg, France*
(Received 5 April 2005; published 15 September 2005)

Experimental total cross sections for direct electron-impact ionization of the valence electron of several Li-like ions are seen to follow a new *ab initio* scaling law which is inspired by a Coulomb-Born model and the frozen-core Hartree-Fock approximation. The predictive character of this scaling law should be very useful to experimentalists and can be used to complete data tables needed for plasma or astrophysical studies. A single-parameter fit of the best available experimental data, once scaled, provides us with a single formula, for moderately charged Li-like ions, which is more accurate than Lotz semiempirical formula.

DOI: 10.1103/PhysRevA.72.034701 PACS number(s): 34.80.Kw

The electron-impact ionization of positive ions plays a very important role in many areas of plasma physics. In particular, total cross sections (TCS's) are needed for the diagnostics of high-temperature plasma occurring in fusion-plasma devices like ITER. Measurements of TCS's are difficult and costly, particularly for highly charged ions because of the low target densities of ion beams when compared to gas targets. Theoretical calculations are therefore useful not only to understand ionization but also to complement experimental data and to design future experiments. However, it is not always easy to state which theoretical model should be chosen as they are based on different approaches and approximations. Thus, one of the most important challenges in the field of electron-impact ionization of ions is to develop a general theoretical framework within which accurate cross sections for many ions can be computed.

One way to complement experimental data is based on the use of predictive semiempirical formulas, such as that proposed by Lotz [1] or its variants (see the review in [2]), which incorporate the correct behavior at high incident energy and possibly close to threshold. More recently, with the aim of searching for universal TCS shapes, new semiempirical formulas have been proposed [3,4]. They are built upon the analysis of experimental data and the use of a fitting procedure (empirically obtained parameters).

An alternative method to predict cross sections relies on the use of scaling laws for ions belonging to isoelectronic sequences. Let $V_{\rm ion}$ denote the ionization potential, X the incident energy E_i in $|V_{\rm ion}|$ units, and $\mathcal{Z}$ the ionicity of the ion. For the ionization of H-like ions Thomson's theoretical classical approach [5] predicts that TCS's scale according to $V_{\rm ion}^2$ and that they depend only on X. Quantal Coulomb calculations [6] have shown that, although the classical formula may be very inaccurate, it has the merit of indicating that the TCS's, when multiplied by $V_{\rm ion}^2$, are a function of X and vary slowly with $\mathcal{Z}$ along the H-like sequence. This has been confirmed experimentally [3]. The $V_{\rm ion}^2$ scaling has been extensively applied to other isoelectronic sequences [2], and generally TCS's follow the trend, although approximately. Hence, it is often embedded in semiempirical formulas.

In this paper we question whether the $V_{\rm ion}^2$ scaling is sufficiently appropriate for Li-like ions. Generally, for alkali-metal-like ions, a scaling law is not obvious because of the *nonhydrogenic character* of the targets. In a previous paper [7], we have made a systematic analysis for the direct ionization (DI) of the valence electron of ions belonging to H-, Li-, Na-, and K-like isoelectronic sequences. Within a nonrelativistic theoretical model, based on the use of frozen-core Hartree-Fock (HF) bound wave functions and the Coulomb-Born approximation (CBA), we have identified an approximate scaling law for the triple-differential cross sections (TDCS's). Unfortunately, no experimental data exist today to confirm this predictive scaling. In recent years, however, several experimental groups have measured absolute total-ionization cross sections for H- and Li-like ions (and to a lesser extent of Na- and K-like ions). With further approximations, it is possible to extend our prediction and obtain—for the ionization of the valence electrons of alkali-metal-like ions—a new *ab initio* scaling law for TCS's which differs from that in $V_{\rm ion}^2$. In this paper, rather than trying to justify our CBA model [7], we would like to show that the best available experimental data for the DI of Li-like ions satisfy quite well this new scaling law. As a consequence, a single parameter Lotz-type fit of these data yields a single formula, for moderately charged Li-like ions, which is more accurate than Lotz semiempirical formula [1]. The latter has been, and is, widely used by atomic and plasma physicists because of its simplicity and, in many cases, remarkable predictions.

The electron-impact ionization of Li-like ions can occur through both direct and indirect channels. While DI describes only part of the process, its accurate knowledge is very important for atomic physicists, both experimentalists and theoreticians. An accurate DI single formula can therefore be useful (i) as an improvement of Lotz formula when excitation-autoionization (EA) is absent or at very high energies when elaborate calculations cannot be performed because of computational difficulties, (ii) as a possible tool for collision experimentalists to normalize their relative TCS's, and (iii) as an accurate estimate of the DI background when EA (or other indirect contributions) comes into play. Indeed, the analysis and understanding of EA is very difficult both from an experimental and theoretical points of view. Even when EA is important, the estimate of the DI background is useful since it allows, by subtraction from experimental TCS's, to isolate the contributions from indirect channel

mechanisms. This has been done in many theory-experiment papers on Li-like ions (e.g., [8–10]), where the subtracted DI cross sections were estimated by the Lotz formula, by simple theoretical calculations, or by experimental extrapolation. The knowledge of DI cross sections is therefore useful to study EA and, consequently, the total-ionization cross sections.

For H-like ions, the $V_{\rm ion}$'s of the $1s$ state ($n=1$) are given by the exact quantal formula $V_{\rm ion}=-(\mathcal{Z}+1)^2/2n^2$ (atomic units are used throughout unless otherwise specified). For alkali-metal-like ions, the $V_{\rm ion}$'s of the valence electrons ($ns, n\geqslant 2$) do not obey the same exact formula because of screening effects. However, for such ions, it is known that the frozen-core HF approximation is well suited and can be safely used to get the $V_{\rm ion}$'s. The latter can be reasonably represented by a two-parameter fit [7]

$$V_{\rm ion}=-\frac{\tilde{z}^2}{2\tilde{n}^2}, \tag{1}$$

where $\tilde{z}$ can be regarded as an effective charge and $\tilde{n}$ as an effective quantum number. For Li-like ions we have found [7] $\tilde{z}=\mathcal{Z}+1+0.330\,49$ and $\tilde{n}=1.989\,92$, the $V_{\rm ion}$ for $\mathcal{Z}=1$ being the worst reproduced by the fit. The frozen-core HF approximation (the closed shell is considered as a spectator) can also be used for the wave function of the bound valence electron $\varphi_a(\boldsymbol{r})=R_{n_a s}(r)Y_{00}(\hat{r})$.

Consider now two ions, labeled N and M, belonging to the same isoelectronic sequence and define the ratio

$$\gamma^{NM}=\tilde{z}^{(N)}/\tilde{z}^{(M)}. \tag{2}$$

For H-like ions ($\tilde{n}=1$, $\tilde{z}=\mathcal{Z}+1$), we have

$$R^{(N)}_{n_a s}([\gamma^{NM}]^{-1}r)=(\gamma^{NM})^{\beta}R^{(M)}_{n_a s}(r), \tag{3}$$

with $\beta=3/2$, $n_a=1$, and $\gamma^{NM}=(\mathcal{Z}^{(N)}+1)/(\mathcal{Z}^{(M)}+1)$ is simply the ratio of the nuclear charges of ions N and M. In [7] we have shown that relation (3) also holds for alkali-metal-like ions—though approximately—if one takes a different value of β (this is another manifestation of screening effects in the target ions). For Li-like ions we have found $\beta=1.678\,21$. The fact that the ionization potentials and the bound wave functions approximately satisfy the general relations (1) and (3) has led us to investigate a possible scaling law for TDCS's corresponding to the ionization of sequences of ions.

There is clear evidence (see discussion and references in [7]) that a CBA should be suitable for describing the ionization of valence electrons of H-like and alkali-metal-like ions, at least when the ionicity is sufficiently important and for intermediate to high incident energies. As collision model we have therefore considered [7] a nonrelativistic, first-order perturbation theory and the CBA without exchange. The ejected and scattered electrons are then treated on equal footing. The long-range Coulomb attraction in the initial (final) channel due to the charge of the target (residual) ion is taken into account by the description of the continuum electrons by Coulomb wave functions corresponding to two constant effective charges obtained within the frozen-core HF approximation: one for the initial channel and one for the final channel ($\tilde{z}$). The details of the short-range effects and the final-state correlation between the two outgoing electrons are ignored in the model. They may play a role for singly ionized ions, but the effect should be progressively smaller relatively to that of the strong Coulomb field as the ionicity of the ions increases.

Provided the incident and ejected energies are properly scaled, an approximate scaling law has been predicted for ionization TDCS's of the valence electron of isoelectronic H-like and alkali-metal-like ions [see Eq. 25 of [7]]. In the case of H-like ions, the scaling factor $(\gamma^{NM})^{2\beta-9}$ becomes $(\gamma^{NM})^{-6}$. While the results for H-like ions may have been expected [because $V_{\rm ion}\sim(\mathcal{Z}+1)^2$], we have observed [7] that the scaling law is well verified also for calculated TDCS's for alkali-metal-like sequences (Li-, Na-, and K-like ions), the larger the ionicity the better since the long-range Coulomb interactions are then dominant. In all cases the TDCS for the singly charged ion is separated from those for higher multiplicity which are closely bunched together.

The scaling law is not modified by integrating the TDCS over the solid angles of the ejected or scattered electrons: it therefore applies in exactly the same manner for the double- and single-differential cross sections. For the TCS, one has to further integrate over all possible ejected energies. Assuming our model, with the two escaping electrons treated equally, to be acceptable over the whole physical integration range, one finds [7]

$$\sigma^{(N)}[(\gamma^{NM})^2E_i^{(M)}]\simeq(\gamma^{NM})^{2\beta-7}\sigma^{(M)}[E_i^{(M)}]. \tag{4}$$

For H-like ions, $\beta=3/2$, the scaling factor $(\gamma^{NM})^{-4}$ is in agreement with Thomson's classical scaling prediction in $V_{\rm ion}^2$ [5]. For alkali-metal-like ions, our result goes further by providing a law with modified ratios γ^{NM} and noninteger powers. The approximate nature of the scaling (4) is related to the fact that the bound wave functions do not obey Eq. (3) exactly and to the choice of effective charges within the CBA.

Let us now consider experimental data. The magnitude of measured TCS's for the ionization of H-like ions [3] decreases very rapidly for increasing ionicity, but the shapes remain similar. Once scaled according to Thomson's law [i.e., multiplied by the factor $(\gamma^{NM})^4$] and plotted versus X, the data are bunched together [3]. The data for the neutral (H) and for the singly charged ion (He^+) deviate from the bunch because the screening of the incident electron is relatively more important.

After a thorough bibliographic research, we found that quite a few experimental papers have now been published on the DI of Li-like ions. We have chosen to select the most recent set for each ion—i.e., Be^+ [11], B^{2+} [12], C^{3+} [8], N^{4+} [9], O^{5+} [9], and Ne^{7+} [10] (previous measurements have been reported; see the above references). The selected unscaled cross sections are plotted (symbols) in Fig. 1 as a function of X: similarly to the case of the H-like sequence the TCS's decrease very rapidly in magnitude with increasing ionicity, but maintain the same shape. Since here we are interested only in the DI of the valence electron (the dominant ionization mechanism), we have not included experimental points for which other channels like the ionization of

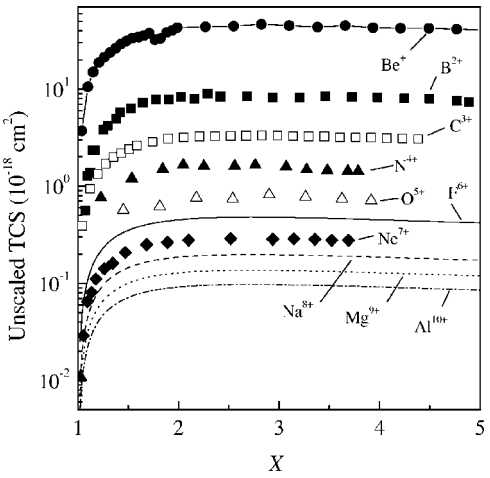

FIG. 1. Experimental TCSs for Li-like ions (Be^+ [11], B^{2+} [12], C^{3+} [8], N^{4+} [9], O^{5+} [9], and Ne^{7+} [10]) as a function of X. The TCS's for F^{6+}, Na^{8+}, Mg^{9+}, and Al^{10+}, shown with lines, are estimated through the single formula (6).

K-shell electrons or indirect ionization contribute.

To represent the experimental TCS's on a linear graph (Fig. 2), we have scaled them according to the law (4). The first ion Be^+ ($M=1$, $\mathcal{Z}^{(1)}=1$)—taken as the reference—is plotted on an absolute scale. The raw experimental data (symbols) for $\mathcal{Z}^{(N)}>1 (N>1)$ are multiplied by the factor $(\gamma^{N1})^{-2\beta+7}>1$ where γ^{N1} is given by Eq. (2). The two panels—shown with the same scale—correspond to two choices of $\tilde{z}$ and β: (i) in the left panel (Thomson), the data are scaled with $\tilde{z}=\mathcal{Z}+1$ and $\beta=3/2$ so that $(\gamma^{N1})^{-2\beta+7}=[(\mathcal{Z}^{(N)}+1)/2]^4$ which is Thomson's scaling law; (ii) in the right panel (present), the same data are scaled with $\tilde{z}=\mathcal{Z}+1+0.330\,49$ and $\beta=1.678\,21$ so that $(\gamma^{N1})^{-2\beta+7}=[(\mathcal{Z}^{(N)}+1+0.330\,49)/2.330\,49]^{3.64358}$.

In the left panel we observe that, once scaled, the cross sections have the same order of magnitude. In spite of the error bars, however, the spread is quite important when compared with the equivalent scaling of experimental TCS's for H-like ions (see Fig. 5 of [3]). Thomson scaling is therefore seen to break down for Li-like ions.

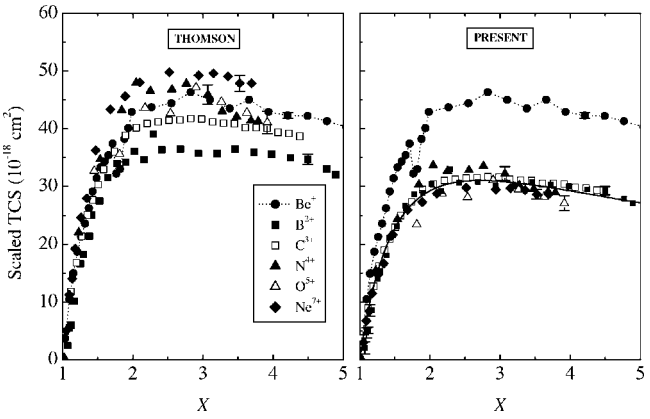

FIG. 2. Scaled experimental TCS's for Li-like ions. For reasons of clarity, only one typical error bar is shown for each ion, except for C^{3+} for which it is smaller than the size of the symbol. The data for Be^+ ($\mathcal{Z}=1$) are shown on an absolute scale (solid circles plus dotted line). The data for other ions $\mathcal{Z}>1$ (symbols) are scaled (see text) according to Eg. (4): in the left panel (Thomson) and in the right panel (present). The solid line in the right panel is the single parameter Lotz-type fit (5) with $A=84.3$.

In the right panel, the data appear quite differently. We observe that the cross section for the singly charged ion (Be^+) is separated from the others ($\mathcal{Z}=2,3,4,5,7$) which are nicely bunched together. This indicates that the scaling law (4)—with our values of $\tilde{z}$ and β—is adequate. The fact that the data for $\mathcal{Z}=1$ are isolated should not surprise as the same has been observed for H-like ions [3]. Moreover, one should not forget that the scaling is based on the CBA which is more valid for highly charged ions (the same applies for H-like ions [3]).

The experimental confirmation of our *ab initio* scaling could be done only because of sufficient data being available and to the latest measurement on C^{3+} [8]. Indeed, in the measurements preceding it, the experiments did not allow for the separation of ions $^{12}C^{3+}$ and $^{16}O^{4+}$ in the beam since these two species have the same charge-to-mass ratio. This weakness resulted in measured cross sections about 30% lower than those of Ref. [8] which have been obtained with a isotopically clean $^{13}C^{3+}$.

From the observations made in the right panel of Fig. 2, one is naturally led to predict that TCS for other Li-like ions, once scaled (present), would be placed in the same bunch. To make this prediction practical, we have made a single-parameter Lotz-type fit [1]

$$\sigma_{scaled}[10^{-18}\ \mathrm{cm}^2]=A\frac{\ln(X)}{X} \tag{5}$$

of all scaled experimental data with $\mathcal{Z}>1$: we found $A=84.3$. This fit is illustrated in the right panel of Fig. 2 by a solid curve and yields therefore a single formula for electron-impact ionization TCS's of moderately charged Li-like ions with $\mathcal{Z}>1$.

With a reverse scaling, it is easy to predict the TCS for other Li-like ions,

$$\sigma_{unscaled}[10^{-18}\ \mathrm{cm}^2]=A^{(N)}\frac{\ln(X)}{X}, \tag{6}$$

where $A^{(N)}=A[(\mathcal{Z}^{(N)}+1+0.330\,49)/(2+0.330\,49)]^{-3.64358}$ provides the coefficient $A^{(N)}$ for each ion labeled N. The unscaled TCS's for F^{6+}, Na^{8+}, Mg^{9+}, and Al^{10+} predicted in this way are shown in Fig. 1 with lines (there no experimental data on a broad range of X). TCS's fall rapidly for higher ionicities and would be difficult to measure, but can be easily estimated with the proposed formula. Note that, for $\mathcal{Z}>25$, relativistic effects come into play, and our scaling may break down as it is based on a nonrelativistic model.

Let us now compare formula (6) with that of Lotz [1]. In the case of Li-like ions, the latter is given by Eq. (6) with $A^{(N)}_{Lotz}=4.5\times10^4/V^2_{\mathrm{ion}}$ where V_{ion} of ion N is expressed in eV [1,2]. In Fig. 3 we show the ratio $A^{(N)}_{Lotz}/A^{(N)}$ as a function of the ionicity $\mathcal{Z}$. Although the orders of magnitude of $A^{(N)}$ and $A^{(N)}_{Lotz}$ are the same, we see that the prediction of TCS amplitudes can vary up to 40%. Hence, the Lotz semiempirical

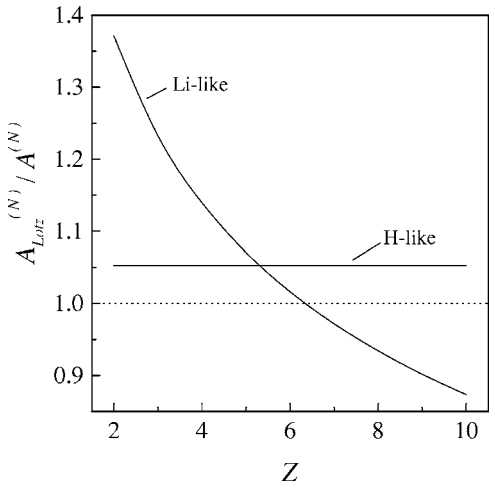

FIG. 3. Ratio $A_{Lotz}^{(N)}/A^{(N)}$ of the factors appearing in (6) as a function of the ionicity $\mathcal{Z}$.

formula will be sufficiently accurate for $\mathcal{Z}$ values around 6, but will overestimate or underestimate the TCS amplitude for smaller or larger values of $\mathcal{Z}$. Experimental evidence indicates that formula (6) for Li-like ions is seen to be more accurate than the Lotz semiempirical formula.

We have carried out a similar analysis with the measured cross sections for H-like ions ($\mathcal{Z}=2$ [13], $\mathcal{Z}=4,5,6,7$ [3]) for which only DI is possible. As mentioned after Eq. (4), in this case, the scaling is just Thomson's V_{ion}^2 scaling. A single-parameter Lotz-type fit (5) of the scaled data yields $A=14.4$. Our predictive formula for unscaled H-like TCS's is therefore given by Eq. (6) with $A^{(N)}=A[(\mathcal{Z}^{(N)}+1)/2]^{-4}$. The Lotz semiempirical formula [1] predicts $A_{Lotz}^{(N)}$ given by exactly the same expression but with $A=15.2$—i.e., about 5% more of the value obtained from the fit of the experimental data. Hence, the Lotz formula is seen to be quite accurate for H-like ions (see also [3]). Contrary to the Li-like case, the ratio $A_{Lotz}^{(N)}/A^{(N)}$ is constant (see Fig. 3).

We have also investigated the case of Na-like ions, though the measured TCS's are scarce and with quite large error bars. Moreover, contributions of indirect ionization channels intervene already at small values of X. As for Li-like ions, Thomson's V_{ion}^2 scaling is seen to break down. According to the $\tilde{z}$ and β values for Na-like ions [7], the scaling factor is given by $(\gamma^{N1})^{-2\beta+7}=[(\mathcal{Z}^{(N)}+1+1.167\,14)/3.167\,14]^{3.46338}$. Because of the lack of exploitable data, it is presently difficult (and would be inaccurate) to extract a meaningful value of A for Eq. (5). However, compared to the Li-like sequence, we expect the ratio $A_{Lotz}^{(N)}/A^{(N)}$ to deviate even more from 1.

In conclusion, the best available experimental TCS's for direct electron-impact ionization of the valence electron of several Li-like ions are seen to follow an *ab initio* scaling law which is inspired by a CBA model and the use of the frozen-core HF approximation [7]. The law can be used as a predictive tool for unmeasured TCS's. A single-parameter Lotz-type fit of the scaled TCS's has provided us with a single formula, for moderately charged Li-like ions, which is more accurate than Lotz semiempirical formula.

The authors would like to thank P. Defrance for his interest in this work and S. Schippers for providing tabulated data for C^{3+}.

[1] W. Lotz, Astrophys. J., Suppl. **14**, 207 (1967); Z. Phys. **216**, 241 (1968).
[2] P. Defrance, M. Duponchelle, and D. L. Moores, *Atomic and Molecular Processes in Fusion Edge Plasmas*, edited by R. K. Janev (Plenum, New York, 1995), p. 153.
[3] K. Aichele *et al.*, J. Phys. B **31**, 2369 (1998).
[4] M. Szluinska, P. Van Reeth, and G. Laricchia, J. Phys. B **35**, 4059 (2002).
[5] J. J. Thomson, Philos. Mag. **23**, 449 (1912).
[6] A. Burgess and M. R. H. Rudge, Proc. R. Soc. London, Ser. A **273**, 372 (1963).
[7] L. U. Ancarani and P.-A. Hervieux, J. Phys. B **36**, 4447 (2003).
[8] H. Teng *et al.*, Phys. Rev. A **61**, 060704(R) (2000).
[9] P. Defrance *et al.*, J. Phys. B **23**, 2333 (1990).
[10] M. Duponchelle *et al.*, J. Phys. B **30**, 729 (1997).
[11] R. A. Falk and G. H. Dunn, Phys. Rev. A **27**, 754 (1983).
[12] O. Woitke *et al.*, Phys. Rev. A **58**, 4512 (1998).
[13] K. Tinschert *et al.*, J. Phys. B **22**, 531 (1989).