CROSS–SECTIONS FOR IONIZATION OF ATOMS AND IONS BY ELECTRON IMPACT AT LOW ENERGIES

José Franco*

University of Wisconsin-Madison

Department of Physics

Madison, Wisconsin 53706

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ABSTRACT

It is shown that a semi-empirical expression for electron impact ionization cross-section, when averaged over the energy at which the maximum takes place, has a form similar to the classical Binary Encounter approximation. A compilation of the best experimental data is given. The new data supports the empirical relation given by Franco and Daltabuit, between the peak value for the cross-section and the energy at which the cross-section is maximum.

RESUMEN

Se muestra que una formulación semi-empírica para las secciones rectas de ionización por colisiones con electrones, puede ser comparada con la aproximación clásica de encuentros binarios. También, se presenta una recopilación de los mejores datos experimentales existentes. Los datos experimentales más recientes se ajustan a la relación empírica (entre el máximo de la sección recta y la energía en la cual ocurre dicho máximo), propuesta por Franco y Daltabuit.

* Becario del Consejo Nacional de Ciencia y Tecnología, México.

I. INTRODUCTION

Collisional ionization of atoms and ions by electrons is a fundamental process with very important applications to astrophysics and plasma physics. In recent years, the experimental work in this branch has increased and valuable information about cross-sections for several multicharged ions is now available. In plasma physics, the cross-section at low energies is most important because an ion generally achieves maximum concentration when $kT \sim 0.1\ I$ (the ground state ionization potential). At high electron incident energies, the agreement between experiments and the quantum mechanical approximations is remarkably good, but at low energies the semi-empirical and classical formulations give satisfactory results with the additional advantage that the computations are easier (Peart et al.[1], Tripathi and Rai[2], Burgess et al.[3], Barfield[4], Franco and Daltabuit[5]).

The semi-empirical formulations are made ad hoc to fit the experimental data; therefore, good results are expected when the empirical parameters can be chosen properly. However, it is not clear the reason why a given parameter will determine the agreement or disagreement with experiment. Then it is important to find links between the empirical and theoretical approaches in order to understand the physics behind phenomenological relations.

In the present communication, we discuss the connection between the semi-empirical formula proposed by Cantó and Daltabuit[6] and the classical binary encounter approximation (BEA) model (for a recent review on the general theory and approximate methods in collisional ionization, see Peterkop[7]).

II. EXPERIMENTAL INFORMATION

Cantó and Daltabuit[6] proposed the two parameter formula for the cross-section:

$$\sigma = \sigma_m \frac{4(x-1)(x_m-1)}{(x+x_m-2)^2} , \tag{1}$$

where σ_m is the maximum of the cross-section, x is the energy of the incident electron (in units of the ground state ionization potential) and x_m is the energy at which the maximum takes place. This formula gives a good fit at low energies when the empirical parameters σ_m and x_m are known. The available experimental information is given in Table I. Reported uncertainties are typically 10%, but in some cases can be as high as 40% (Li, Na, Ar^{3+}). The amount of reported measurements are sufficient for every experiment to determine σ_m and x_m with good confidence level $\sim$ 10% (except in the case of Ne^{+3}). The data for Al, Ca^+, Sr^+, Ba^+, Tl (which show dramatic enhancement due to autoionization) and for Cu, Au, Hg, Tl^+ (which have complex ground state structures) have been included for the sake of completeness, but are not considered in the discussion. E_m is the energy at maximum in eV.

Franco and Daltabuit[5], pointed out that σ_m and x_m obey the simple empirical relation:

$$x_m \sigma_m = c\, N_e/I^2 \quad , \tag{2}$$

where I is the ground state ionization potential, N_e is the available number of electrons in the shell and c is a constant. The above relationship is shown in Fig. 1 and with the inclusion of the new data we obtain $c = 3.8 \times 10^{-14}$ cm^2 eV^2, which is 10% smaller than the one given by Franco and Daltabuit[5]. The expected accuracy of Eq. (2) is 20%. Several atoms with complex ground state structures, such as Cu, Hg and Tl^+, follow this relation when N_e = 10 is used, but its validity for these types of species can be accidental. A simple interpretation of Eq. (2), follows from Thomson's classical formula at the maximum of the cross-section. Writing c in terms of a_o and I_H, Eq. (2) becomes:

$$\sigma_m = \left(\frac{2.69}{x_m}\right) \pi a_0^2 \, (I_H/I)^2 \, N_e \quad , \tag{3}$$

and it is remarkable that most of the experimentally tested species adjust to such a simple relation at maximum.

From Table I, it can be noted that x_m is typically about 3 This fact has already been pointed out by several authors (i.e., Lotz [8], Peart and Dolder[9], Franco and Daltabuit[5]), and it is a well known feature displayed by collisional excitation cross-section curves (Lin[10]).

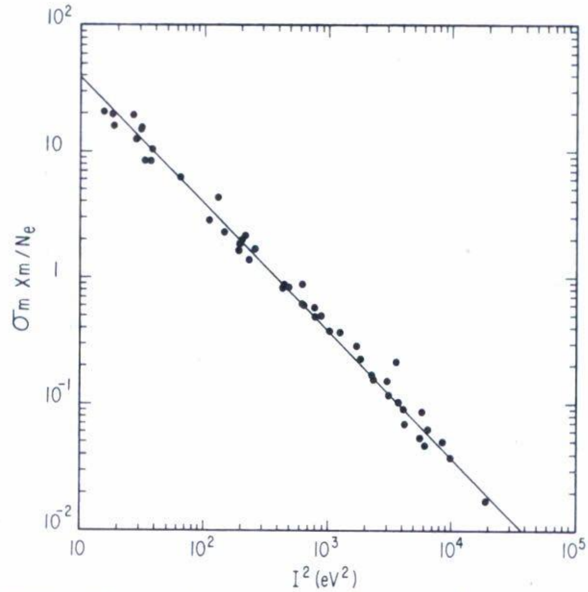

Fig. 1. Empirical relation between $\sigma_m x_m/N_e$ and I^2 (the ground state ionization potential). The experimental data are taken from Table I (see remarks).

For alkali-type species the average value of x_m is 2.7 with little scatter (except for H and Ba^+). For other configurations the scatter is larger and the averaged x_m is higher than 3, however, x_m decreases rather smoothly along isoelectronic sequences (as pointed out by Franco and Daltabuit[5]). The average value over all the configurations considered in Fig. 1 is $\langle x_m \rangle = 3.5$. Most of the measurements have been limited to neutral atoms, or once and twice ionized (with large x_m), and the higher ionization stages (with small x_m) are under-represented in our sample. Hence, it is foreseen that $\langle x_m \rangle$ will decrease when new high ionization data (more than doubly ionized) can be available. In order to consider this effect, we are going to use $x_m = 3$ as a typical value (to differenciate it from the sample's average).

With the aid of Eq. (3), we can rewrite Eq. (1) in the standard form:

$$\sigma(x) = N_e \pi a_o^2 \quad (I_H/I)^2 \quad \bar{\sigma}_E(x) \quad , \tag{4}$$

where the empirical reduced cross-section is:

$$\bar{\sigma}_E(x) = \frac{4}{x_m} \frac{(x-1)}{(x+x_m-2)^2} \quad [2.69(x_m - 1)] \tag{5}$$

Taking $x_m = 3$, the typical reduced cross-section is:

$$\langle \bar{\sigma}_E (x) \rangle_{x_m} \simeq 7.1 \frac{(x-1)}{(x+1)^2} \quad , \tag{6}$$

and represents the mean behavior over all configurations. From Eq. (2), the scaling law between isoelectronic sequences at maximum is:

$$\frac{\sigma_1}{\sigma_2} \sim \left[\frac{I_2}{I_1}\right]^2 \frac{x_{m,2}}{x_{m,1}} \quad , \tag{7}$$

for higher ionized species and alkali-type species x_m is about the same, then Thomson's classical scaling law is recovered.

III. DISCUSSION

The classical binary encounter approximation (BEA) originally formulated by Gryzinsky[11], has been modified to take into account the atomic electron's kinetic energy and the acceleration of the incident electron due to the atomic field near the point where the impact occurs (Ochkur and Petrun'kin[12], Stabler[13], Thomas and Garcia[14], Vainshtein et al.[15]). The reduced cross-section in the BEA model, with all these modifications included, is (see Peterkop[7]):

$$\bar{\sigma}_{BEA}(x) = \frac{4}{3x} \frac{(x-1)}{(x+2)} \left[5 + \frac{2}{x}\right] \quad , \tag{8}$$

whose maximum is centered at $x \sim 2.67$.

The Exchange Classical Impact Parameter (ECIP) method, formulated by Burgess[16] (see also Burgess and Percival[17]) is also based in the BEA model, but including quantum-type corrections. The corresponding reduced cross-sections can be written in a similar form to Eq. (8) with the addition of a term for the interference between direct and exchange scattering, and a term expressed as an integral over the photo-ionization cross-section, χ_{ph}, which corresponds to the treatment of collisional ionization as a radiactive process (Seaton[18]):

$$\bar{\sigma}_{ECIP}(x) = \frac{4}{3x}\,\frac{(x-1)}{(x+2)}\left[5 + \frac{2}{x} - \frac{3x\,\ell n x}{(x^2-1)}\right] + \chi_{ph} \quad ,$$

at high energies the contribution to the total cross-section from χ_{ph} is of the order of 20%, but near the threshold it is negligible (Burgess et al.[3], Barfield[4]). The function $\frac{2}{x} - \frac{3x\ell nx}{(x^2-1)}$ takes values near -0.6 for the range of energies of interest (x close to x_m). Then, we can approximate the ECIP case as:

$$\bar{\sigma}_{ECIP}(x) = 6\,\frac{(x-1)}{x(x+2)} \quad , \tag{9}$$

with the maximum centered at $x_m \sim 2.73$.

We can conclude that the empirical reduced cross-section here discussed, averaged over the parameter x_m, provides a link between the mean behavior of the experimentally tested species and the classical binary encounter approximation (ECIP included). This can explain the results obtained by Burgess et al.[3], whose comparison of the collisional ionization cross-sections at low energies (near the maximum) favoured (on the average) the ECIP method.

A comparison of this kind with the quantum mechanical approximation is not possible at the present time. The radial wave functions used are independent of the ion configuration, total angular momentum and spin. Hence, such calculations are not expected to be more accurate than simpler classical methods. Recent computations using the Coulomb-Born approximation for C^{2+}, C^{3+}, N^{3+} and N^{4+} (Moores[19]), are in better agreement with experiments. This is encouraging, but it is not the general case as was shown by Burgess et al.[3], and improvements are needed in the quantum mechanical treatment.

From a practical point of view, accurate cross-sections (and their corresponding ionization rates) can be easily obtained with Eqs. (4) and (5) using the experimentally determined values of x_m, in the absence of experimental data, $x_m = 3$ will provide a reasonable estimate for most ions. Finally, further analysis based on empirical relations with emphasis on particular electronic configurations (as those obtained by Hasted and Awad[20]) will shed more light on the phenomena of electron-atom collisions.

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Table I. Experimental Data

Ion	Ground State	σ_m (10^{-16} cm^2)	E_m (eV)	x_m	Remarks	Reference
H	$1s^1$	0.67	56	4.1		21
He^+	$1s^1$	0.048	178	3.3		21
Li	$2s^1$	5.3	15	2.8	f	8
C^{3+}	$2s^1$	0.025	180,300	2.8	a,c	37,42
N^{4+}	$2s^1$	0.015	270,500	2.6,5.1	a,c	37,42
O^{5+}	$2s^1$	0.008	300,700	2.2,5.1	a	42
Na	$3s^1$	7.3	14	2.6	f	21
Mg^+	$3s^1$	0.51	40	2.7		25
K	$4s^1$	7.8	9.5,32	2.2,7.4	a	38
Ca^+	$4s^1$	1.75	100	9	b	9
Rb	$5s^1$	8.2,10.5	10,30	2.4,7	a	38
Sr^+	$5s^1$	2.5	100	9	b	9
Cs	$6s^1$	7.5,9.7,10	11,15,30	2.8,3.9,7.7	a	38
Ba^+	$6s^1$	4.25	18,20,40	1.8,2,4	b	26,27,29
Cu	$3d^{10}4s^1$	7.6	95	12.3	e	41
Au	$5d^{10}6s^1$	15.3	100	10.8	e	41
He	$1s^2$	0.37	120	4.9	c	21,30
Li^+	$1s^2$	0.04	325	4.3		26,27
C^{2+}	$2s^2$	0.11	140	2.9	c	34,35
Mg	$3s^2$	7.8,(4.2)	12,(26)	1.6,(3.4)	a,d	15,32
Ca	$4s^2$	6.5,7	20,26	3.3,4.2	a	15
Sr	$5s^2$	8.7,10	20,26	3.5,4.6	a	15

Ion	Ground State	σ_m (10^{-16} cm^2)	Em (eV)	x_m	Remarks	Reference
Ba	$6s^2$	12.5	10,26	2,4.9	a	15
Hg	$5d^{10}6s^2$	5.5	55	5.27	e	21
Tl^+	$5d^{10}6s^2$	1.7	100	4.9	e	24
C^+	$2p^1$	0.57	78	3.2	c	23,35
N^{2+}	$2p^1$	0.18	140	2.9	c	23,20
O^{3+}	$2p^1$	.056	200	2.6		36
Al	$3p^1$	4,7	15,90	2.5,15	a,b	40
Ar^{5+}	$3p^1$	0.07	250	2.7	a	43
Ga	$4p^1$	6,7	25,100	4.2,16.7	a	40
In	$5p^1$	7.3,8	20,90	3,5,15.6	a	40
Tl	$6p^1$	16	80	13	b	40
C	$2p^2$	3.3	60	5.3	c	30,31
N^+	$2p^2$	0.52	112	3.8	c	21,20
O^{2+}	$2p^2$	0.18	145,(190)	2.6,(3.5)	d	22,35
Ar^{4+}	$3p^2$	0.09	190	2.5	a	43
N	$2p^3$	1.57	100	6.9	c	21,30
O^+	$2p^3$	.40,(.48)	148,(110)	4.2,(3.1)	c,d	22,35,43
Ne^{3+}	$2p^3$	0.13	300	3.1	g	35
Ar^{3+}	$3p^3$	0.17,(.38)	170	2.9	d	35,20,43
O	$2p^4$	1.5	90	6.6	c	21,30
Ne^{2+}	$2p^4$	0.16	220	3.5	c	35,20
Ar^{2+}	$3p^4$	0.45	90,(160)	2.4,(3.9)	c,d	35,20,43
Ne^+	$2p^5$	0.30	200	4.9	c	21,35,20,43

Ion	Ground State	σ_m (10^{-16} cm^2)	E_m (eV)	x_m	Remarks	Reference
Ar^+	$3p^5$	1.1,(1.5)	76,(110)	2.8,(4)	c,d	33,35,20,43
Xe^+	$5p^5$	1.84	70	3.3	c,d	43
Ne	$2p^6$	0.86	170	7.9		21
Na^+	$2p^6$	0.26	250	5.3		26,27
Mg^{2+}	$2p^6$	0.14	300	3.7		28
Ar	$3p^6$	3.1	70	4.4		21
K^+	$3p^6$	0.99	100	3.1		26.27
Kr	$4p^6$	4.2	55	3.9		21
Rb^+	$4p^6$	1.7,1.2	80,155	2.9,4.2	a,c	9,39
Xe	$5p^6$	5.7	40	3.3		21
Cs^+	$5p^6$	1.7,1.2	70,100	2.8,4	a	9

Remarks:

a) More than one peak due to inner-shell direct ionization. Only the first peak was used in Fig. 1.
b) Autoionization effects are very important. Not included in Fig. 1.
c) Values are average of the experimental data.
d) Numbers in parenthesis have larger uncertainties and are not considered in Fig. 1 due to large discrepancy with the more accurate information.
e) Not considered in Fig. 1.
f) Experimental errors $\sim$40%.
g) The number of points reported is not enough to find σ_m and E_m with confidence. Not considered in Fig. 1.