Semiempirical Formulas for Dipole Excitation Cross Sections and the Gaunt Factor for Ions

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Semiempirical formulas for dipole excitation cross sections necessary in solving plasma kinetics problems are mainly based on the Bethe approximation or its modifications, for example the effective Gaunt factor approximation. The published values for the effective Gaunt factor, $g(x)$, are the same for all ions irrespective of the ionic charge or the orbital moments involved in the transitions in contradiction with experimental results. For explaining this difference we use a simple analytical representation of cross sections for ions based on a modification of Born approximation. An expression for the Gaunt factor is obtained that for high energies coincides with previous results, but for low energies shows a noticeable difference depending of the type of transitions (ns-np or np-nd, for example) and also a certain dependence of $g(x)$ on the atomic number, Z, and the core charge Z_c. The formula for cross sections contains two parameters C and φ; C can be calculated from the Bates-Damgaard approximation whereas φ is calculated using the general expression for the Born approximation.

I. Introduction

The optically allowed dipole transitions ($\Delta\ell = \pm 1$, $\Delta S = 0$) induced by electron impact on ions are very important processes in different branches of gas discharge and plasma physics. Due to the scarcity of experimental values, the data on cross sections and excitation rates are generally taken from theoretical calculations.

There are several semiempirical formulas for estimating dipole excitation cross sections in neutral atoms and ions[1]. For high energies of the incident electron, the excitation cross section for optically allowed transition is expressed in terms of the oscillator strength by means of the Bethe approximation. The widely used semiempirical formula of Van Regemorter is based on the Bethe formula[1,2] and reads, in atomic units,

$$\sigma = (8\pi/\sqrt{3}) f (Ry/\Delta E)^2 g(x)/x, \qquad (1)$$

with $x = \epsilon/\Delta E$, where ϵ is the incident electron energy, f is the absorption oscillator strength, Ry is the Rydberg energy and $g(x)$ is the Gaunt factor. When $x \to \infty$ we obtain

$$g(x) \to (\sqrt{3}/2\pi) \ln x, \qquad (2)$$

and eq. (1) becomes the Bethe formula.

Closely related with cross section calculations is the semiempirical approach of Griem for linewidths calculations based in the impact approximation,[3,4] where the thermally averaged Gaunt factor is given by

$$< g >= \int g(\epsilon) \exp(-\epsilon/kT) d(\epsilon/kT), \qquad (3)$$

where the notation of Ref. [5] is used.

The tabulated values of $g(x)$[1,4] are the same for all types of ions and transitions. However, in published papers experimental dependences of $g(x)$ on the core charge Z_C [5] and the orbital quantum numbers of the transition[6] were showed.

The above mentioned dependences are hidden in numerical calculations, but it is possible to find them

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when cross sections are expressed in analytical formulae. In this paper we start from a semiempirical dependente of a (~in a modified Born approximation, valid also for ions and an expression for $g(x)$ is obtained that for x $\rightarrow \infty$ coincides with eq. (2) and for low x values is dependent of the type of transition explaining the experimental diference between g_{s-p} and g_{p-d}.

We systematize and generalize the results presented for Sobelman et al.[1] using the Born approximation (not valid for ions near the threshold) and a few values quoted using the Coulomb approximation.

II. Theory

Cross sections (or collision strengths) calculated by means of diverse approaches can be expressed in various analytical simple forms[7-10] but for the purposes of this paper a form similar to the expression given hy Sobelman et al.[1] is choosen. The cross sections can be expressed for the multipole order $\mathcal{H} = |\ell_0 - \ell_1|$ (for simplicity, the case $\mathcal{H} = 1$ is evaluated) in the Born approximation as

$$\sigma^{\mathbf{B}} = C(Ry/\Delta E)^2(D^2_{LS}/g_0) [(x-1)/x)]^{1/2} \ln(15+x)/(x-1+\varphi), \quad (4)$$

where φ and C are related to the constants tabulated in Ref. [1] (after adjustments by the method of least squares), D^2_{LS} is the angular part of the line strength S, and g_0 is the degeneracy of the initial level. As it is well known, this approximation is not suitable for ionic lines but the empirical modification

$$\sigma(x) = \sigma^{\mathbf{B}}[x + 3/(1+x)] , \quad (5)$$

gives a good description of the cross sections including the finite values at threshold[11].

Then, it is possible to write eq. (4) in form

$$\sigma = (Ry/\Delta E)^2(D^2_{LS}/g_0)CF(x) , \quad (6)$$

where

$$F(x) = \{[(x^2+2)/(x^2+x+3)]^{1/2}(x+1) \ln[(x^2+16x+18)/(1+x)]\}/(x^2+2+\varphi+\varphi x). \quad (7)$$

From the behavior of $\sigma(x \rightarrow \infty)$ and the relation $f = S(\Delta E/Ry)/3g_0$ it follows that

$$C = (4/3)(\Delta E/Ry) l_> I_1^2, \quad (8)$$

where $l_>$ is the greater of the angular moments involved in the transition and

$$I_1 = \int P_0(r)P_1(r)rdr , \quad (9)$$

and in the Bates-Damgaard approximation they can be calculated in function of effective quantum numbers, the core charge and the tabulated function Φ[12]. It must be noted that the quoted values of C[1] after multiplication by $(T_0/T_1)^{3/2}$ are similar to those calculated . using eq. (9), although the discrepancy can be of the order of 10%, where T_0 and T_1 are the term values of the initial and final levels.

On the other hand, from eqs. (1), (2) and (7) results

$$g(x) = (\sqrt{3}/2\pi)xF(x), \quad (10)$$

and, at the threshold ($x = 1$)

$$g(1) = 1.22/(3 + 2\varphi). \quad (11)$$

The evaluation of φ is more involved and we generalize the quoted values from Ref. [1] after least squares fitting. Cross sections calculated with eqs. (6) and (7) at x = 1 correspond to the calculation using the general expression of Born

$$\sigma^{\mathbf{B}} = (8Ry/\epsilon)(D^2_{LS}/g_0)(2\mathcal{H}+1)(2\ell_0+1)(2\ell_1+1) \begin{pmatrix} \ell_0 & \ell_1 & \mathcal{H} \\ 0 & 0 & 0 \end{pmatrix}^2 \int [R(q)]^2 q^{-3} dq, \quad (12)$$

with

$$R(q) \equiv \int_0^\infty P_{n\ell}(r) j_1(qr) P_{n'\ell'}(r) dr, \qquad (13)$$

for $E = 2.5\Delta E$ (x = 2.5), as can be viewed from eq. (5).

In Eq. (12) $P_{n\ell}$ and $P_{n'\ell'}$ are expressed in terms of Whittaker functions as in the method of Bates-Damgaard; j (qr) is tlie spherical function of order 1: $j_1(x) = [(\sin x)/x - \cos x]/x$. The integral (13) is solved usinq Gauss-Laguerre method and further integration of eq. (12) between $k_{\max} = \epsilon^{1/2} + (c - \Delta E)^{1/2}$ and $k_{\min} = \epsilon^{1/2} - (\epsilon - \Delta E)^{1/2}$ is carried out using the Simpson's rule. It was verified that for $x \to \infty$ the proper limit for tlie collision strength given by the Bethe formula

$$x\sigma = 4f(Ry/\Delta E)^2 \ln x \qquad (14)$$

is consistent with the f values obtained from the Bates-Damgaard method[12], as it must be.

Introducing the quantity

$$\begin{aligned} B(\ell_0, \ell_1; 2.5) &= (2\mathcal{H} + 1) \ldots \int [R(q)]^2 q^{-3} dq \\ &= 2.5(\Delta E/Ry) g_0 \sigma^{\mathbf{B}}(2.5)/8 D_{LS}^2 , \end{aligned} \qquad (15)$$

the final result for φ is

$$\varphi = 0.5 \left[\frac{5.91 \ell_> I_1^2 Ry D_{LS}^2}{\Delta E g_0 \sigma^{\mathbf{B}}(2.5)} - 3 \right] . \qquad (16)$$

After integrations, the values of φ can be adjusted in terms of ν_0 (the effective principal quanturn number of the initial level) and $Av = \nu_1 - \nu_0$ with tlie following polynomials

$$g(s - p) = \sum_{i=0}^{4} P_i(\nu_s)(\Delta\nu_{s-p})^i, \qquad (17)$$

and

$$g(p - d) = \sum_{i=0}^{4} Q_i(\nu_p)(\Delta\nu_{p-d})^i, \qquad (18)$$

valid at least for $\nu_0 = 1 - 5$ and $Av = 0.1 - 1.0$. In Eqs. (17) and (18) P and Q are polynomials in ν_0 (v, and ν_p respectively), whose values are in Table 1.

Table 1. Fitting polynomials for φ_{s-p} and φ_{p-d}

a. φ_{s-p}

Power of ν_s

i	4	3	2	1	0
4	-0.78	-8.80	82.87	-174.74	126.27
3	1.36	18.62	-162.55	347.56	-251.30
2	-0.81	-12.50	104.44	-224.50	162.20
1	0.18	3.10	-25.50	57.40	-39.25
0	-0.04	0.12	0.27	-1.07	0.92

i.e.: $P_4(\nu_s) = -0.78\,\nu_s^4 - 8.80\,\nu_s^3 + 82.87\,\nu_s^2 - 174.74\,\nu_s + 126.27$

a. φ_{p-d}

Power of ν_p

1	4	3	2	1	0
4	15.3	-238.3	1350.3	-3212.5	2672.6
3	-24.0	383.5	-2208.7	5316.1	-4443.9
2	9.2	-157.8	962.5	-2403.3	2042.1
1	-0.07	8.3	-81.5	255.1	-237.4
0	-0.24	2.8	-10.7	16.8	-9.5

III. Results and conclusions

Tables 2a and 2b show tlie calculated values for $\varphi(s - p)$ and $\varphi(p - d)$ in terms of ν_0 and Av. In Table 3, φ values and $g(x = 1)$ are shown for several strong ns-np and np-nd transitions of one, two and three times ionized nohle gases using the very well studied spectra of these elements[6]. Despite the fact that radial integrals I_1 and $B(\ell_0, \ell_1; 2.5)$ are calculated using Whittaker functions (and not Hartree-Fock values for example) is noticeable that for a same element, $g(1)$ follows a trend of the form[5] $g(1) \simeq a - b/Z_c$, and for a same ion $g_{sp} \simeq 1.5$ g_{pd} Ref. [6]. Furthermore, linewidths for single ionized noble gases calculated using the present

Table 2a. Transition s-p, parameter ϕ

$\Delta\nu$	The effective principal quantum number ν_s							
	1.50	2.00	2.50	3.00	3.50	4.00	4.50	5.00
.10	.32	0.47	0.60	0.73	0.87	1.00	1.13	1.25
.20	.74	1.02	1.27	1.52	1.77	2.01	2.26	2.51
.30	1.15	1.56	1.93	2.31	2.69	3.08	3.47	3.88
.40	1.57	2.13	2.63	3.18	3.73	4.31	4.91	5.53
.50	2.02	2.75	3.45	4.20	4.99	5.83	6.73	7.68
.60	2.53	3.48	4.44	5.50	6.64	7.88	9.24	10.75
.70	3.13	4.41	5.75	7.25	8.94	10.83	12.97	15.33
.80	3.89	5.67	7.59	9.84	12.46	15.50	19.06	23.10
.90	4.93	7.51	10.42	13.96	18.17	23.15	28.94	35.59
1.00	6.68	10.44	14.89	20.00	25.42	30.69	35.33	38.81

Table 2b. Transition s-p, parameter ϕ

$\Delta\nu$	The effective principal quantum number ν_p						
	2.00	2.50	3.00	3.50	4.00	4.50	5.00
.10	.47	0.56	0.61	0.77	0.91	1.50	1.18
.20	.86	1.07	1.29	1.57	1.82	2.09	2.34
.30	1.23	1.53	1.93	2.34	2.75	3.16	3.57
.40	1.59	2.00	2.60	3.16	3.76	4.37	5.00
.50	1.48	2.50	3.26	4.11	4.94	5.84	6.76
.60	1.86	3.53	4.11	5.34	6.44	7.77	9.15
.70	2.29	4.57	5.17	6.92	8.46	10.46	12.55
.80	2.80	5.70	6.58	9.10	11.42	14.56	17.97
.90	3.44	7.08	8.61	12.40	16.18	21.42	27.38
1.00	4.28	6.53		16.96	24.32	32.56	41.70

formalism[11] are in very good agreement with experiments where the ratio experimental widths/calculated widths is ≈ C.9.

In conclusion, the empirical modification (5) applied to the analyt.cal expression of Sobelman et al. for Born cross sections[1] permits to explain several experimental results and i: is useful for rapid computations in gas discharges and plasma modeling.

Table 3. Gaunt factor for selected strong lines of ionized noble gases

Element	s-p transitions φ	g(1)
Ne II (3s-3p)	1.85	0.18
(4s-4p)	2.75	0.14
Ne III (3s-3p)	1.44	0.21
(4s-4p)	2.07	0.17
(5s-5p)	2.71	0.15
Ar II (4s-4p)	2.06	0.17
Kr II (5s-5p)	2.43	0.16
(6s-6p)	3.54	0.12
Kr III (5s-5p)	1.98	0.18
Xe II (6s-6p)	2.53	0.15
(7s-7p)	3.73	0.12
Xe III (6s-6p)		0.15

Element	p-d transitions φ	g(1)
Ne II (3p-3d)	2.86	0.14
(4p-4d)	4.97	0.09
(5p-5d)	7.37	0.07
Ne III (3p-3d)	2.28	0.16
(4p-4d)	3.16	0.13
(5p-5d)	4.37	0.10
Ar II (4p-4d)	5.70	0.08
Kr II (5p-5d)	7.69	0.07
(6p-6d)	11.80	0.05
Xe II (6p-6d)	7.11	0.07
Xe III (6p-6d)	6.16	0.08

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