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Electron impact broadening of multicharged neon spectral lines

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Abstract. In this work, we present an amelioration of the Dimirijević 84 formula of electron collisional Stark line widths based on modification of the semi empirical approach using collision strength values between initial, final and their perturbing levels. We have applied this method for calculation of Stark widths of some lines of neon. The obtained results were compared with experimental and other theoretical results.

Key words. Stark broadening- plasma spectroscopy- collision strengths

1. Introduction

Stellar and laboratory plasma diagnostic, atomic abundances, opacity calculations, all have led to a need for knowledge about Stark broadening of multicharged ion spectral lines. For the calculations of the Stark broadening parameters, sophisticated quantum-mechanical and semiclassical methods (Griem 1974) exist, but they often require a considerable labor even for the evaluation of a single line width. Moreover, when quick estimate is needed, the approximate approaches may be very useful.

One such approximate method is the modified (Dimitrijević & Konjević 1980; 1981) semi-empirical (Griem 1968) formula suitable for singly as well as for multiply charged ion lines. In this work, we use electron impact excitation collision strengths instead of the semiempirical Gaunt factor used by Dimitrijević & Konjević (1980), (1981), these collision strengths are obtained in the distorted wave approximation in *LS* coupling schema. They are of higher accuracy than semiempirical Gaunt factor.

2. Theory

In the modified semiempirical method, the full Stark width W of an ionic line can be calculated from the following expression (Dimitrijević & Konjević 1980; 1981):

$$\begin{aligned} W \;=\; & N\frac{8\pi}{3}\frac{\hbar^2}{m^2}\left(\frac{2m}{\pi KT}\right)^{\frac{1}{2}}\frac{\pi}{\sqrt{3}}\left[R^2_{l_i,l_{i+1}}\widetilde{g}\left(\frac{E}{\Delta E_{l_i,l_{i+1}}}\right)\right. \\ & +R^2_{l_i,l_{i-1}}\widetilde{g}\left(\frac{E}{\Delta E_{l_i,l_{i-1}}}\right)+R^2_{l_f,l_{f+1}}\widetilde{g}\left(\frac{E}{\Delta E_{l_f,l_{f+1}}}\right) \\ & +R^2_{l_f,l_{f-1}}\widetilde{g}\left(\frac{E}{\Delta E_{l_f,l_{f-1}}}\right) \\ & +\sum_{i'}\left(R^2_{ii'}\right)_{\Delta n\neq 0} g\left(\frac{3kTn_i^3}{4z^2E_H}\right) \end{aligned}$$

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$$+ \sum_{f'} \left(R^2_{ff'}\right)_{\Delta n \neq 0} g\left(\frac{3kTn_f^3}{4z^2 E_H}\right)\Bigg] \quad (1)$$

In this expression, $E \approx 3kT/2$ is the energy of the perturbing electrons, $\Delta E_{jj'} = |E_{j'} - E_j|$ is the energy difference between the initial ($j = i$) or final ($j = f$) levels, and their perturbing levels ($j' = i', f'$), n is the effective principal quantum number, z is the charge "seen" by the optical electron ($z = 2$ for singly-, 3 for doubly-charged ions etc...) and E_H is the ionization energy of hydrogen. The semiempirical procedure for the calculation of electron impact widths accounts explicitly for interactions from "weak" collisions only (Griem 1974). It is assumed (Griem 1968) that the contribution of elastic collisions can be neglected for higher energies.

In Eq. (1), all perturbing levels with $\Delta n \neq 0$ are lumped together and the corresponding nearest perturbing level is estimated from $\Delta E_{n,n+1} \approx 2z^2 E_H/n^3$. The effective Gaunt factors $\widetilde{g}(x)$ for the transitions with $\Delta n = 0$ (Dimitrijević & Konjević 1980) is taken as

$$\widetilde{g}(x) = 0.7 - \frac{1.1}{z} + g(x) \quad (2)$$

At high temperatures, say ($x \geq 50$), all Gaunt factors are calculated in accordance with the GBKO high temperature limit (Griem et al. 1962)

$$\widetilde{g}_{jj'} = g_{jj'} = \frac{\sqrt{3}}{\pi}\left[\frac{1}{2} + \ln\left(\frac{2zkT}{n^2 \Delta E_{jj'}}\right)\right] \quad (3)$$

and

$$R^2_{l,l'} \simeq \left(\frac{3n}{2z}\right)^2 \frac{\max(l,l')}{2l+1}\left[n^2 - \max{}^2(l,l')\right]\phi^2 \quad (4)$$

where, the symbol ϕ represents the Bates and Damgaard (1949) factor, tabulated by Oertel and Shomo (1968), and

$$\sum_{j'} \left(R^2_{jj'}\right)_{\Delta n \neq 0} \simeq \left(\frac{3n_j}{2z}\right)^2 \frac{n_j^2 + 3l_j^2 + 3l_j + 11}{9} \quad (5)$$

Using the relation between the Gaunt factor, the collision strength Ω and the line strength S:

$$g = \frac{3\sqrt{3}}{8\pi}\frac{\Omega_{jj'}}{S_{jj'}} \quad (6)$$

and the relation:

$$S_{jj'} = g_j R^2_{jj'} \quad (7)$$

where g_j is the statistical weight of the initial level j (j can be equal to i or to f). With Eqs. (6 and 7) we find that:

$$R^2_{jj'} g = \frac{3\sqrt{3}}{8\pi}\frac{\Omega_{jj'}}{g_j}. \quad (8)$$

Finally, the formula calculating full Stark width of ionic spectral lines in terms of the collision strengths for transitions with the same principal quantum number and in terms of Gaunt factors for transitions with $\Delta n \neq 0$ is:

$$W = N\left(\frac{\hbar}{m}\right)^2\left(\frac{2m\pi}{KT}\right)^{\frac{1}{2}}\left[\frac{1}{g_i}\sum_{i'}\Omega_{ii'} + \frac{1}{g_f}\sum_{f'}\Omega_{ff'}\right.$$
$$+ \frac{8\pi}{3\sqrt{3}}\sum_{i'}\left(R^2_{ii'}\right)_{\Delta n \neq 0} g\left(\frac{3kTn_i^3}{4z^2 E_H}\right)$$
$$\left. + \frac{8\pi}{3\sqrt{3}}\sum_{f'}\left(R^2_{ff'}\right)_{\Delta n \neq 0} g\left(\frac{3kTn_f^3}{4z^2 E_H}\right)\right] \quad (9)$$

In a previous paper (Dimitrijević 1984), the author used a particular case of expression (9) to calculate electron impact widths of the resonance lines $2s^2\,{}^1S - 2s2p\,{}^1P^0$ of Be-like ions ($g_i = 1$ and $g_f = 3$):

$$\frac{1}{g_i}\sum_{i'}\Omega_{ii'} + \frac{1}{g_f}\sum_{f'}\Omega_{ff'} = \frac{4}{3}\Omega. \quad (10)$$

The simplified formula employed in the work of Dimitrijević to evaluate the collision strength Ω, according to Younger (1980) for this transition is:

$$\Omega = \alpha_1 + \frac{\alpha_2}{2} + \alpha_3 \ln(x) \quad (11)$$

$$\alpha_1 = \frac{0.0348}{Z} + \frac{65.9}{Z^2} - \frac{174}{Z^3}$$
$$\alpha_2 = \frac{3.37}{Z} + \frac{45.7}{Z^2} - \frac{115}{Z^3}$$
$$\alpha_3 = \frac{0.897}{Z} + \frac{38.1}{Z^2} - \frac{58.6}{Z^3}$$

where $x = \dfrac{E}{\Delta E_{jj'}}$ and Z is the effective charge of the ion ($z = Z + 1$).

In order to take elastic collisions and resonance effects into account, the collision strength is extrapolated below the threshold for corresponding inelastic process: $\Omega = \alpha_1 + \alpha_2$ for $0 \leq x \leq 1$.

Here, the collision strength is different from that of Dimitrijević (1984). We begin by the calculation of the atomic data, the wavefunctions, the energy levels, the wavelengths....using the SUPERSTRUCTURE code (Eissner et al. 1974). First, this program determines a set of non relativistic wavefunctions by diagonalisation of the non-relativistic Hamiltonian using orbitals calculated in a scaled potential $V_{\lambda_l}(r)$; the scaling parameters λ_l being obtained by a self consistent energy minimization procedure. In the second step, the program diagonalises the relativistic Breit-Pauli Hamiltonian, and the multiconfigurational wave functions obtained, contain both the correction and relativistic effects (spin-orbit, mass, Darwin and one-body).

The collision strengths Ω in Eq. (9) are calculated using the distorted wave program DISWAV (Eissner 1998). It is a non relativistic code which calculates the transition matrix T elements in LS coupling and so the collision strengths in this coupling.

Collision strengths used here were calculated in this work, however our objective is to demonstrate how collision strengths existing in literature, which are of higher accuracy than semiempirical Gaunt factors, might be used to increase the accuracy of the modified semiempirical approach. We note also that we take into account the elastic collision contribution to the width implicitly, by calculating the collision strengths at the threshold energy and extrapolating them below the threshold as in Dimitrijević & Konjević (1980) and Griem (1968). It has been shown that the elastic contribution to the line width becomes less important with the increase in temperature (Ralchenko et al. 1999).

3. Result and discussion

We present in the Table (1) our theoretical width, experimental (Wrubel et al. 1996; 1998) and other theoretical (Griem (1974), Dimitrijević & Konjević (1980), Seaton (1988), Ralchenko et al. (1999)) Stark widths of the investigated $2s3s - 2s3p$ transitions of berylliumlike neon (Ne VII). The average of W_{exp}/W between our theoretical calculations and the experimental ones for the two transitions is 1.58, while, this average is about 1.74 for Dimitrijević & Konjević (1980).

In the same Table (1) are presented our theoretical, experimental (Glenzer et al. 1992) and other theoretical (Griem (1974), Dimitrijević & Konjević (1980), Seaton (1988), Dimitrijević & Sahal-Bréchot (1993b), (1994b), Ralchenko et al. (2003)) results for $3s - 3p$ transition of lithiumlike neon (Ne VIII). The average of W_{exp}/W between our theoretical calculations and the experimental ones for the three temperatures is about 2.08. For Dimitrijević & Konjević (1980) this average is about 2.31. We can see that our results are closer to the experimental ones than those of Dimitrijević & Konjević (1980), so on the basis of presented analysis, we can suggest that the presented method can be used for Stark line width calculations. It is demonstrated here, how one can include in the modified semiempirical method (Dimitrijević & Konjević 1980) the data on collision strengths available in the literature, which are of higher accuracy than semiempirical Gaunt factors. In such a way one may obtain results with better accuracy.

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Table 1. Stark line width in Å for Ne VII and Ne VIII, the present calculations (W) and calculated widths evaluated by (Dimitrijević & Konjević 1980) (index DK), after (Griem 1974) (index G), (Seaton 1988) (index S), semi-classical calculations of (Dimitrijević & Sahal-Bréchot 1993b; 1994b) (index DSB), (Ralchenko et al. 1999, 2003) (index R) are compared with experimental widths (W_m) of (Wrubel et al. 1996; 1998; Glenzer et al. 1992; Hegazy et al. 2003).

Transition	$T(K)$	$N_e(cm^{-3})$	W	$\frac{W_m}{W}$	$\frac{W_m}{W_{DK}}$	$\frac{W_m}{W_G}$	$\frac{W_m}{W_S}$	$\frac{W_m}{W_{DSB}}$	$\frac{W_m}{W_R}$
Ne VII	1.205E05	3.5E18	1.578						
$2s3s\,^1S - 2s3p\,^1P^\circ$	2.205E05	3.5E18	1.167	1.51	1.57	1.28	-	-	1.70
$\lambda = 3643.6Å$	3.205E05	3.5E18	0.967						
Ne VII	1.380E+5	3.0E18	0.361						
$2s3s\,^3S - 2s3p\,^3P^\circ$	2.380E05	3.0E18	0.275	1.64	1.91	1.53	-	-	1.96
$\lambda = 1981.97Å$	3.380E05	3.0E18	0.231						
Ne VIII	3.447E05	2.8E18	0.544	2.20	2.55	2.22	3.29	1.91	-
$3s\,^2S - 3p\,^2P^\circ$	4.642E05	1.0E18	0.168	1.73	1.92	1.65	2.58	1.36	2.30
$\lambda = 2820.7Å$	4.932E05	3.2E18	0.520	2.31	2.45	2.07	3.47	1.67	-

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