On the Stark Broadening of Singly Ionized Argon Lines

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Using a semi-classical formalism which includes Debye shielding, Stark broadening parameters of various components within the $4s\,^2P-4p'\,^2P^0$ multiplet and the $4p-4d$ ($^2P^0-^2P$, $^2D^0-^2P$, $^2D^0-^2D$) supermutiplet of Ar II are computed. We show that when various components of a multiplet (supermultiplet or transition array) are broadened inequally by an embedded close-lying perturbing level, use of a perturber parameter cut-off at the Debye length can restrain the calculated differences between Stark widths within the multiplet.

1. Introduction

It was recently reported [1] that the Stark widths (in angular frequency units) can differ in the limit of ± 30% within a supermultiplet, while inside of a transition array this limit is extended to ± 40%. For the Stark shifts, however, we often observed much larger differences [2–3].

Within a multiplet, the Stark widths are nearly the same [4] if the structure of the atomic energy levels is regular [5], otherwise differences may exist in special cases [5]. A typical example is reported [6] for the $4s\,^2P-4p'\,^2P^0$ Ar II multiplet whose observed differences, up to 39%, are explained by the irregular positions of the $3d'\,^2D$ levels [7]. However the latter semi-empirical treatment neglected Debye shielding, which is only negligible in usual cases. In the actual case, the $3d'\,^2D_{3/2}$ perturbing level is so close that one can expect a strong sensitivity to the screening effect: if we drop out the influence of electron perturbers beyond the Debye sphere centered on the emitter, it may happen that the electron broadening contributed by the close perturbing level is considerably reduced. Hence the relationship between the Stark components can be affected strongly with and without the Debye effect.

The knowledge of the behaviour of the Stark broadening parameters within a multiplet or supermultiplet may be useful for a critical evaluation of existing data and for a quick estimation of new data by interpolations [8, 9]. Numerical results for the $4p-4d$ ($^2P^0-^2P$, $^2D^0-^2P$, and $^2D^0-^2D$) supermultiplet of Ar II are useful for astrophysical and plasma diagnostic requirements. In this work, we performed these calculations by one of the most involved semi-classical theories [4, 10]. The case of the $4s\,^2P-4p'\,^2P^0$ Ar II multiplet is of particular interest for a new physical insight. The results help us to judge the importance of Debye shielding as well as its inclusion procedure in the calculations. Since an analytical solution to this complex problem is difficult, here we utilized the widely-adopted procedure [11] which uses an upper cut-off at the Debye length for the electron-impact parameter in the Stark broadening integrations.

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2. Theory

Within the frame of the semi-classical broadening theory [12], the full half-width (W) and shift (d) of an electron-impact broadened line can be expressed in terms of cross-sections for elastic (σ_{el}) and inelastic ($\sigma_{jj'}$) processes [4, 10]:

$$W = N_e \int_0^\infty v f(v)\,dv \left| \sum_{i' \neq i} \sigma_{ii'}(v) + \sum_{f' \neq f} \sigma_{ff'}(v) + \sigma_{el} \right|, \quad (1)$$

$$d = N_e \int_0^\infty v f(v)\,dv \int_{R_3}^{R_d} 2\pi\varrho\,d\varrho \sin 2\Phi_p \quad (2)$$

with

$$\sum_{j' \neq j} \sigma_{jj'}(v) = \tfrac{1}{2}\pi R_1^2 + \int_{R_1}^{R_d} 2\pi\varrho\,d\varrho \sum_{j' \neq j} P_{jj'}(\varrho, v), \quad (3)$$

$$\sigma_{el} = 2\pi R_2^2 + \int_{R_2}^{R_d} 8\pi\varrho\,d\varrho \sin^2(\Phi_p^2 + \Phi_q^2)^{1/2}. \quad (4)$$

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Here N_e is the electron density; $f(v)$ is the Maxwellian velocity distribution function for electrons; ϱ the impact parameter of the incoming electron; i and f denote the initial and final atomic energy levels; and i′ and f′ are their corresponding perturbing levels. The polarisation (Φ_p) and quadrupole (Φ_q) phase shifts are given by [10]

$$\Phi_p = \sum_{i' \neq i} \Phi_{ii'} - \sum_{f' \neq f} \Phi_{ff'}, \qquad (5)$$

$$\Phi_q = [(B_i \overline{r_i^2})^2 + (B_f \overline{r_f^2})^2 - B_{if} \overline{r_i^2}\,\overline{r_f^2}]\, F(\varepsilon, v), \qquad (6)$$

where B are the quadrupole coupling constants [10, 13]; $\overline{r^2}$ are the average of r^2 (the square of the coordinate vector matrix-element of the optical electron) in a j state; and $F(\varepsilon, v)$ is a function depending on the perturber hyperbolic orbit of semi major axis a and eccentricity ε. With the energies in Rydbergs and a in a_0 (Bohr orbit) units, the transition probability $P_{jj'}$ in (3) and the phases $\Phi_{jj'}$ in (5) are defined by the real and imaginary part, respectively, of

$$\tfrac{1}{2} P_{jj'} + i\,2\Phi_{jj'} = \frac{2}{E\,\Delta E_{jj'}} f_{jj'} \frac{1}{a^2 \varepsilon^2} [A(\xi, \varepsilon) + i B(\xi, \varepsilon)] \qquad (7)$$

with

$$a = \frac{1}{E}; \quad E = \tfrac{1}{2} m v^2; \quad \varepsilon = \left(1 + \frac{\varrho^2}{a^2}\right)^{1/2};$$

$$\xi = \tfrac{1}{2} \Delta E_{jj'} E^{-3/2}. \qquad (8)$$

for singly ionized emitters.

Here $F_{jj'}$ is the oscillator-strength; and $A(\xi, \varepsilon)$ and $B(\xi, \varepsilon)$ are the Stark broadening functions [14, 15]. The energy conservation suggests to replace in E the velocity v by its mean value before (v) and after (v') collision:

$$E = \tfrac{1}{2} m v v'; \quad \tfrac{1}{2} m v^2 - \Delta E_{jj'} = \tfrac{1}{2} m v'^2. \qquad (9)$$

The upper cut-off R_d is at the Debye length and the lower cut-offs R_1, R_2, and R_3 are defined by examining the transition probability properties [4]

$$\sum_{j' \neq j} P_{jj'}(R_1, v) = \tfrac{1}{2}, \qquad (10)$$

$$[\Phi_p^2(R_2) + \Phi_q^2(R_2)]^{1/2} \equiv \delta(R_2) = 1, \qquad (11)$$

$$2\Phi_p(R_3) = 1. \qquad (12)$$

The contribution of resonances of elastic cross-sections is taken into account in the linewidth calculations according to [16].

3. Results and Discussions

The data for Ar II atomic energy levels were taken from Bashkin and Stoner [17]. We computed the required oscillator-strengths by using a scaled Thomas-Fermi model [18] and the results for many transitions induced by collisions are similar to those obtained from Coulomb approximation.

In Table 1, our semi-classical results for the $4s\,^2P - 4p'\,^2P^0$ multiplet are compared with previous works: Hey's semi-empirical values (without Debye shielding) [7] and Behringer and Thoma measurements [6]. Our complete results for this multiplet and for the $4p-4d$ ($^2P^0-^2P$, $^2D^0-^2P$, $^2D^0-^2D$) supermultiplet are listed in Table 2.

For the multiplet $4s\,^2P - 4p'\,^2P^0$, Hey's calculated results seem to confirm the observed differences because the level $3d'\,^2D_{3/2}$ is particularly closer to the perturbed level $4p'\,^2P^0_{1/2}$ than the level $3d'\,^2D_{5/2}$ to the perturbed level $4p'\,^2P^0_{3/2}$ (see Figure 1a). However, our calculations with Debye shielding show (Table 1) only a slight difference.

We note that both the upper cut-off R_D and the functions in (3) and (4) are fixed by the plasma temperature T and the electron density N_e. In these equations, replacing R_D by an arbitrary higher value would mathematically give a higher result for the width or shift. However, this procedure is only physically consistent if the modification introduced by the arbitrary cut-off is negligible. This is generally true in the usual cases where no important close perturbing level is present [11].

It is worthwhile to mention that a comparison between our calculations and Hey's is not easy. Basically Griem's semi-empirical approach [19], as utilized by Hey, used the same classical path assumption in the semi-classical theory. However its inelastic cross-sections come from the Born-Bethe

Table 1. Comparison between various full half-width results for lines within the $4s\,^2P - 4p'\,^2P^0$ Ar II multiplet. W_{sc}: semi-classical, present calculations; W_{se}: semi-empirical, Hey calculations [7]; W_m: Behringer and Thoma experiment [6]. Plasma conditions: $N_e = 10^{17}\,cm^{-3}$, and $T = 20\,000$ K.

λ (Å)	J_f	J_i	W_m (Å)	W_{se} (Å)	W_{sc} (Å)
2892	3/2	1/2	0.326	0.236	0.243
2943	3/2	3/2	0.202	0.194	0.240
2979	1/2	1/2	0.302	0.252	0.258
3034	1/2	3/2	0.222	0.206	0.255

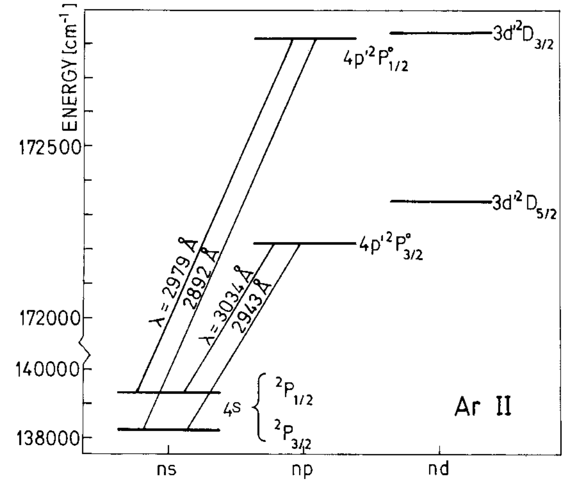

Fig. 1a. Energy level diagram for the 4s ^{2}P$-$4p′ ^{2}P^0 Ar II multiplet.

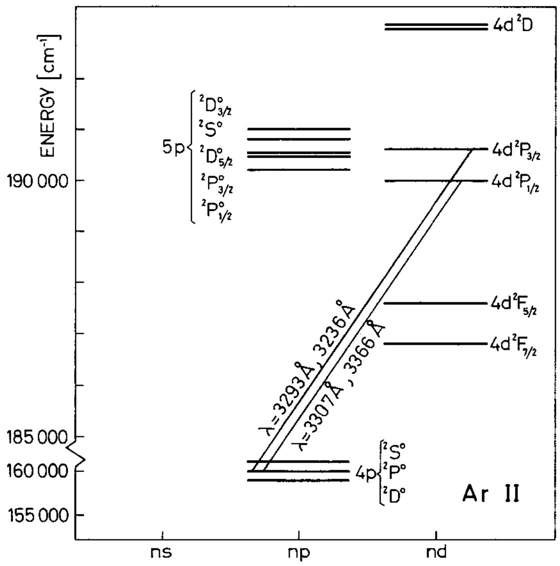

Fig. 1b. Energy level diagram for the 4p ^{2}P^0$-$4d ^{2}P and 4p ^{2}D^0$-$4d ^{2}D multiplets.

approximation which is only valid for high energy; and their expression is based upon the effective Gaunt factor $\bar{g}$ approximation [20, 21]. Also, the elastic part is omitted but compensated by putting $\bar{g} = 0.2$ for $E < \Delta E_{jj'}$ in the inelastic part. As for the calculational procedure, we computed oscillator-strengths from the Thoma-Fermi potential which is valid for heavy atoms whereas Hey used hydrogenic functions. Hey used the energy levels tabulated by Moore 1971 [22] and supplemented by simple

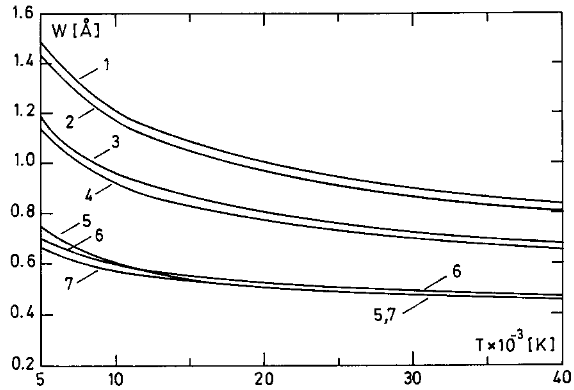

Fig. 2. Electron-impact full half-widths W of Ar II lines within the 4p$-$4d (doublets) supermultiplet at $N_e = 10^{17}$ cm^{-3} as a function of temperature. We denote

Line 4p ^{2}P^0$-$4d ^{2}P			
1	2	3	4
$J = 3/2-3/2$	$1/2-3/2$	$3/2-1/2$	$1/2-1/2$
Line 4p ^{2}D^0$-$4d ^{2}D			
5	6	7	
$J = 3/2-3/2$	$3/2-5/2$	$5/2-5/2$	

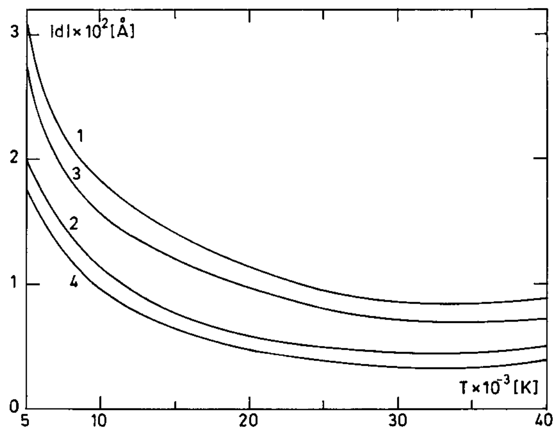

Fig. 3. Stark shifts d within the 4s ^{2}P$-$4p′ ^{2}P^0 Ar II multiplet as a function of temperature and at $N_e = 10^{17}$ cm^{-3}. We denote

Line 4s ^{2}P$-$4p′ ^{2}P^0			
1	2	3	4
$J = 1/2-3/2$	$1/2-3/2$	$3/2-3/2$	$3/2-1/2$

quantum defect estimates. Since for Ar II the compilation in [22] was indeed achieved in 1949 (Re-edition), we utilized the recent tabulation of Bashkin and Stoner 1975 [17]. The 5p ^{2}P$^0_{3/2}$ energy level is 190507.36 cm^{-1} in [17] but 190106.84 cm^{-1} in [22]. Hence this interacting energy level can

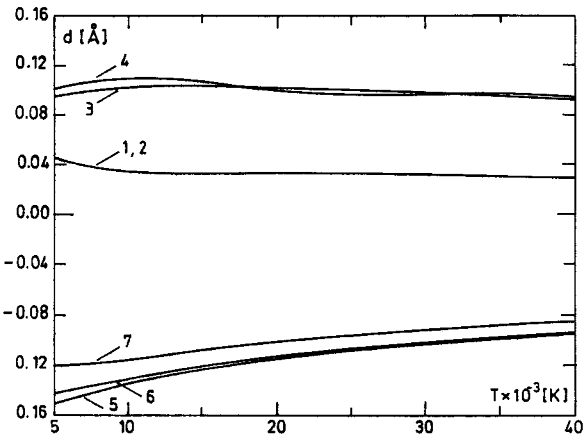

Fig. 4. Stark shifts d within the 4p−4d (doublets) supermultiplet as a function of temperature and at $N_e = 10^{17}$ cm^{-3}. We use the same nomenclature as in Figure 2.

Table 2. Electron-impact full half-width W (FWHM) and shift d for Ar II at electron density $N = 10^{17}$ cm^{-3} and temperature $T = 5000-40\,000$ K. E.g., for the line $\lambda = 2892$ Å, $J_f = 3/2$, $J_i = 1/2$, the full half-width is read $W = 0.300$ Å and the shift is $d = -0.0095$ Å for the plasma temperature $T = 10\,000$ K.

J_f J_i	λ (Å)	5000 K	10 000 K	20 000 K	30 000 K	40 000 K
4s ^{2}P−4p′ ^{2}P^0						
3/2−1/2	2892	0.375	0.300	0.243	0.219	0.207
		−0.0174	−0.0095	−0.0047	−0.0034	−0.0038
3/2−3/2	2943	0.388	0.302	0.240	0.215	0.203
		−0.0273	−0.0157	−0.0097	−0.0070	−0.0072
1/2−1/2	2979	0.397	0.317	0.258	0.233	0.221
		−0.0198	−0.0114	−0.0058	−0.0046	−0.0050
1/2−3/2	3034	0.411	0.320	0.255	0.229	0.216
		−0.0308	−0.0181	−0.0113	−0.0086	−0.0088
4p ^{2}P^0−4d ^{2}P						
3/2−1/2	3366	1.180	0.956	0.799	0.725	0.679
		0.0953	0.1030	0.1010	0.0972	0.0933
1/2−1/2	3307	1.140	0.923	0.771	0.700	0.656
		0.1010	0.1090	0.0983	0.0949	0.0912
3/2−3/2	3293	1.480	1.210	0.999	0.899	0.834
		0.0449	0.0348	0.0338	0.0319	0.0289
1/2−3/2	3236	1.430	1.170	0.966	0.869	0.807
		0.0446	0.0353	0.0335	0.0317	0.0290
4p ^{2}D^0−4d ^{2}P						
3/2−1/2	3273	1.070	0.892	0.756	0.689	0.646
		0.1090	0.0998	0.0931	0.0849	0.0805
5/2−3/2	3138	1.310	1.090	0.909	0.819	0.762
		0.0221	0.0152	0.0177	0.0176	0.0153
4p ^{2}D^0−4d ^{2}D						
3/2−3/2	3000	0.749	0.601	0.513	0.477	0.455
		−0.150	−0.134	−0.115	−0.103	−0.0957
5/2−5/2	2955	0.660	0.572	0.505	0.473	0.454
		−0.121	−0.116	−0.101	−0.091	−0.085
3/2−5/2	3014	0.695	0.595	0.522	0.488	0.467
		−0.142	−0.131	−0.113	−0.102	−0.095

largely influence the relationship within the multiplets involved. E.g., the distance of this level to the 4d $^2P_{3/2}$ state is 84.81 cm^{-1} instead of 485.33 cm^{-1} from [22], and we can expect to see the $\lambda = 3236$ Å line broader than the $\lambda = 3307$ Å line (Table 2).

For the supermultiplet of the transition array 4p−4d, Fig. 2 shows nearly the same line-widths within the $^2D^0-^2D$ multiplet. However, the same figure indicates significant differences of line-widths within the $^2P^0-^2P$ multiplet. Unlike the previous case (4s ^{2}P−4p′ ^{2}P^0 multiplet) which has only one close perturbing level, here the situation becomes more complex because of the various close perturbing levels 5p (Figure 1 b).

The shifts within the 4s ^{2}P−4p′ ^{2}P^0 multiplet vary up to a factor of 2 (see Figure 3). Within the supermultiplet considered, the shifts are inverted in sign (Fig. 4) for the $^2D^0-^2D$ multiplet as compared to the $^2P^0-^2P$ and $^2D^0-^2P$ multiplets. This inversion occurs because the upper states 4d ^{2}D and 4d ^{2}P are not perturbed in the same direction: Figure 1 b shows that the main perturbing levels 5p ^{2}P^0 are lower than 4d ^{2}D for the first multiplet, whereas the principal perturbing level 5p ^{2}S^0 is higher than 4d ^{2}P for the last multiplets.

In conclusion, within the semi-classical approach irregularities in energy-level positions can induce different Starks widths (or shifts) for the components of one and the same multiplet, supermultiplet, or transition array. The shifts are generally more sensitive to the irregularities than the widths, and their signs may be even inverted. However, when an important perturbing level is embedded close to some energy levels of a multiplet (supermultiplet or transition array) causing differences between Stark parameters of various components, a Debye shielding cut-off may limit considerably such differences.

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