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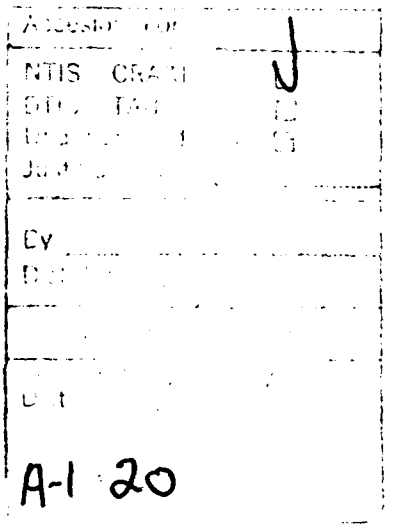

BROADENING AND SHIFT OF Fe I LINES PERTURBED BY ATOMIC HYDROGEN

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Abstract. The broadening and shift parameters for a number of Fe I lines perturbed by atomic hydrogen are computed using the interatomic potential due to Hindmarsh *et al.* (1967, 1970). It is also shown that the rms radius and the effective radius of the radiating atom, which determine the force constants in the interatomic potential, can be simply related each other, depending on the orbital quantum number of the atomic level.

1. Introduction

The collisions with neutral hydrogen in the solar photosphere broaden and shift the absorption lines. While the pressure shift is commonly neglected in the line synthesis (Beckers and De Vegvar, 1978), the pressure broadening compete with the velocity broadening (granulation, waves, and turbulence) in determining the wings of medium and strong lines. The classical formula used to compute the pressure broadening by neutral particles is based on the Van der Waals attraction between the colliding atoms (e.g., Unsöld, 1955). The broadening values obtained in this way appeared to be generally too low, about a factor 2, in comparison with the experiment and with the values inferred from the analysis of the solar lines (Holweger, 1971a, b).

Hindmarsh *et al.* (1967, 1970) extended the classical Van der Waals broadening considering both attractive and repulsive terms in the interaction potential between radiating and perturbing atoms. O'Neill and Smith (1980a, b) have shown that this

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semi-empirical theory predicts the broadening of a number of Ca I and Fe I lines by noble gases generally with an underestimate of only 20%.

We used the theory of Hindmarsh *et al.* to compute the values of the damping and shift for a number of Fe I lines produced by neutral hydrogen perturbers at temperatures typical of the solar photosphere. Some of the broadening parameters computed in this note have been already used for the line synthesis in the presence of velocity fields (e.g., Gomez *et al.*, 1987).

2. Method

The damping constant, or half width at half intensity maximum, γ, and the shift, β, in angular frequency unit, appear in the Lorentzian line profile

$$I(\omega) = \frac{\gamma/\pi}{(\omega - \omega_0 - \beta)^2 + \gamma^2}\,, \tag{1}$$

where ω is the angular frequency of the radiation and ω_0 refers to the line center.

According to Hindmarsh *et al.* (1970), the damping γ_1 and the shift β_1 per unit number of perturbers are

$$\gamma_1 = \frac{\gamma}{N} = 4\pi\left(\frac{3\pi}{8}\right)^{0.4} \bar{v}^{0.6}\,|C_6|^{0.4}\,B(\alpha,\xi)\,, \tag{2}$$

$$\beta_1 = \frac{\beta}{N} = 2\pi\left(\frac{3\pi}{8}\right)^{0.4} \bar{v}^{0.6}\,|C_6|^{0.4}\,S(\alpha,\xi)\,. \tag{3}$$

Here $\bar{v}$ is the relative velocity of the colliding atoms and $\hbar C_6$ is the differential force constant of the term r^{-6} in the potential of interaction of two atoms separated by distance r. The factors B and S have the values 0.3 and -0.44, respectively, in the case of a pure van der Waals potential (r^{-6}); in general they are the integrals

$$B(\alpha,\xi) = \int_0^\infty x \sin^2[\tfrac{1}{2}(\alpha x^{-11} - \xi x^{-7} - x^{-5})]\,dx\,, \tag{4}$$

$$S(\alpha,\xi) = \int_0^\infty x \sin(\alpha x^{-11} - \xi x^{-7} - x^{-5})\,dx\,, \tag{5}$$

and the parameters α and ξ are

$$\alpha = 0.539\bar{v}^{1.2}\,|C_{12}|/|C_6|^{2.2}\,, \tag{6}$$

$$\xi = 0.780\bar{v}^{0.4}\,|C_8|/|C_6|^{1.4}\,, \tag{7}$$

where $\hbar C_8$ and $\hbar C_{12}$ are the force constants of the terms r^{-8} and r^{-12}, respectively, in the interatomic potential. The contribution of the term r^{-8} is negligible in the case

of light perturbers. In the solar photosphere the main perturber is hydrogen, then we assume $\xi = 0$.

The expression of C_6 (Unsöld, 1955) is

$$C_6 = \frac{e^2}{\hbar}\,\sigma(\overline{r_u^2} - \overline{r_l^2})\,, \tag{8}$$

where σ is the dipole polarizability of the perturbing atom, which has the exact value of 0.67×10^{-24} cm^3, and $\overline{r_u^2}$ and $\overline{r_l^2}$ are the quantum mechanical average values of r^2 for the upper and lower states of the transition, respectively. Accurate values of the mean square radii for all assigned terms in the Fe I energy diagram were calculated by Warner (1969) and we used these values in our calculations. Hindmarsh *et al.* (1967) suggest for C_{12} the expression

$$\hbar C_{12} = 0.9 \times 10^{-16}(R_r + R_p)^{12}\,, \tag{9}$$

TABLE I

Lines and atomic parameters

λ (Å)	n_l^*	n_u^*	l_l	l_u	$\overline{r_l^2}$ (a_0^2)	$\overline{r_u^2}$ (a_0^2)	R_{eff} (a_0)
5074.75	1.923	3.319	1	2	23.77	124.90	22.59
5137.39	1.912	3.226	1	2	23.77	145.20	23.70
5198.72	1.548	2.033	0	1	11.36	19.76	10.38
5217.40	1.704	2.426	1	0	17.25	94.38	16.41
5250.22	1.323	1.585	0	1	9.83	13.48	9.24
5250.65	1.704	2.426	0	1	11.36	19.76	10.38
5263.31	1.714	2.444	1	0	17.25	94.38	16.41
5302.31	1.717	2.444	1	0	17.25	94.38	16.41
5379.58	1.799	2.777	0	1	9.73	23.89	11.02
5395.22	1.985	3.432	1	2	25.23	140.90	23.48
5434.53	1.405	1.719	0	1	11.78	17.25	9.95
5506.79	1.403	1.709	0	1	11.78	17.25	9.95
5576.10	1.745	2.462	1	0	18.09	94.38	16.41
5635.83	1.934	3.077	1	1	17.30	196.40	23.43
6240.65	1.548	1.920	0	1	11.36	17.30	9.96
6246.33	1.780	2.426	1	0	20.04	94.38	16.41
6252.56	1.574	1.968	0	1	9.77	26.11	11.34
6297.80	1.548	1.916	0	1	11.36	23.01	10.89
6301.51	1.790	2.444	1	0	20.04	94.38	16.41
6302.50	1.797	2.462	1	0	20.04	94.38	16.41

where the numerical constant (in erg) was fixed empirically and R_r and R_p are the distances, from the nucleus of the radiating and perturbing atoms, respectively, at which the unperturbed radial charge density has the value 0.012 atomic units. We used the Coulomb approximation (e.g., Seaton, 1958) to compute the effective radius, since its definition involves the knowledgement of the atomic wavefunction at long distances from the nucleus.

3. Results

In Table I we list the 20 Fe I lines whose broadening and shift parameters were computed for this note. For each line we report the effective principal quantum number, n^*, and the orbital quantum number, l, of both energy levels, which are needed to specify the corresponding Coulomb wavefunction. The 6th and 7th columns of the table contain the mean square radius of the lower and upper level respectively, derived from Warner (1969). The last column contains the values of the effective radius of the radiating atom, R_{eff}. The effective radius for atomic hydrogen is 4.38 atomic units.

In Table II we list for each line the multiplet number, the level notation, the damping

TABLE II

Broadening and shift parameters

λ (Å)	Multiplet No.	level *lower*	level *upper*	γ/N (10^{-8} rad cm^3 s^{-1})	γ_{VdW}/N (10^{-8} rad cm^3 s^{-1})	β/N (m/s)
5074.75	1094	y^5F_4	e^3G_5	6.06	2.30	64.0
5137.39	1090	y^5F_5	h^5D_4	6.59	2.48	70.9
5198.72	66	a^5P_1	y^5P_2	1.59	0.85	14.8
5217.40	553	z^5D_4	e^5D_3	3.31	2.07	26.8
5250.22	1	a^5D_0	z^7D_1	1.36	0.61	13.7
5250.65	66	a^5P_2	y^5P_3	1.59	0.85	15.0
5263.31	553	z^5D_2	e^5D_2	3.31	2.07	27.0
5302.31	553	z^5D_1	e^5D_2	3.31	2.07	27.2
5379.58	928	b^1G_4	z^1H_5	1.73	1.05	14.5
5395.22	1143	z^5G_2	g^5F_1	6.49	2.43	74.3
5434.53	15	a^5F_1	z^5D_0	1.50	0.72	15.7
5506.79	15	a^5F_2	z^5D_3	1.50	0.72	15.9
5576.10	686	z^5F_1	e^5D_0	3.32	2.06	28.4
5635.83	1088	z^3P_1	w^5P_1	2.58	2.95	24.3
6240.65	64	a^5P_1	z^3P_2	1.50	0.74	17.6
6246.33	816	z^5P_3	e^5D_3	3.32	2.04	33.1
6252.56	169	a^3H_6	z^3G_5	1.80	1.11	17.4
6297.80	62	a^5P_1	y^5D_2	1.71	0.97	17.8
6301.51	816	z^5P_2	e^5D_2	3.32	2.04	33.4
6302.50	816	z^5P_1	e^5D_0	3.32	2.04	33.4

constant (full width at half intensity maximum) and the shift in velocity unit. The damping constant is calculated at the temperature T = 5000 K and per unit number of neutral hydrogen atoms. To change the temperature it is sufficient to multiply by $(T/5000)^{0.4}$ (O'Neill and Smith, 1980a). As a matter of comparison, we report also the broadening computed with the pure Van der Waals theory. It appears that the Van der Waals values are generally smaller than the values calculated by including the term r^{-12} in the interatomic potential, which confirms the results of O'Neill and Smith (1980b). A comparison with the empirical damping constants determined by Simmons and Blackwell (1982) for lines 5434.53, 6252.56 and multiplet 62 indicates that our data are slightly larger ($\sim 25\%$) than the data based on the fit of solar lines. The shift parameter has been computed at the temperature of 5000 K and for a perturber number density of 10^{17} neutral H per cm^3. This density corresponds to a depth between 0 and 50 km in the VALC atmospheric solar model. Since the hydrogen number density decreases exponentially with depth in the photosphere, the values we found for the pressure shift of Fe I lines confirm the findings of Beckers and De Vegvar (1978) that for the Fe I lines the pressure shift is negligible with respect to the convective blueshift produced by the solar granulation.

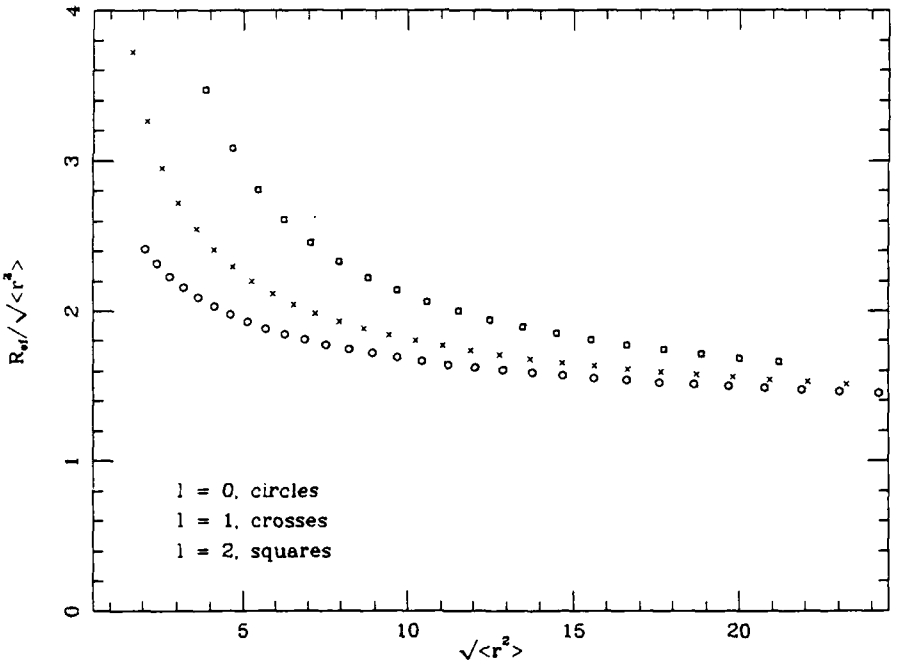

Fig. 1. Ratio of the effective radius, R_{eff}, to the r.m.s. radius, $\sqrt{r^2}$, of an atomic level versus the r.m.s. radius. Circles refer to l = 0, crosses to l = 1, and squares to l = 2, with l being the orbital quantum number of the level. Both radii were computed on the base of the Coulomb approximation to the atomic wavefunction.

Finally, Figure 1 shows the relation existing between the effective radius and the mean square radius of a level when both are computed on the base of the Coulomb approximation. Usually the ratio of the effective radius to the r.m.s. radius is approximated by 2 (e.g., Hart, 1974). However, Figure 1 shows that this ratio is a monotonic decreasing function of the r.m.s. radius which depends on the orbital quantum number of the level. This relation provides a quick way to estime the effective radius, e.g., by using the Unsöld (1955) formula to evaluate the mean square radius.

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