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SOME EFFECTS OF PRESSURE BROADENING IN SOLAR AND STELLAR CURVES OF GROWTH

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Summary

It is shown that the elementary theory of line broadening by collision damping provides adequate explanation of the various bifurcations of the empirical solar curve of growth. The apparent dependence of damping constant of a line on the parity of its lower level also follows. Applications are made to other stars and some early laboratory results by Babcock of pressure shifts in FeI are qualitatively explained.

1. *Introduction.* Various studies of solar and stellar curves of growth for FeI have shown anomalous behaviour among the strong lines. Adams & Russell (1928) and Koelbloed (1953) drew attention to the fact that in cool giant stars lines arising from low- and high-voltage levels have different curves of growth. Similar effects in early-type stars have been reported by Abt (1960) and Groth (1961). A particularly intensive study was carried out by Helfer & Wallerstein (1964).

Carter (1949), using laboratory *f*-values, showed that for the sun the deviation of lines from a mean curve of growth apparently depends on the parity of the lower level of the transition, and Wright (also using experimental *f*-values) found a similar effect in K-stars. Studies by Weidemann (1955) and Warner (1964a) have suggested that for the sun there is an increase of damping constant with low excitation potential, and this has been interpreted as a consequence of the lines of higher E.P. being formed deeper in the photosphere where the pressure is higher.

However, the contribution functions of strong lines are almost identical, so that they are all formed at approximately the same mean depth. In addition, Gokdogan & Pecker (1964) have re-emphasised the dependence of damping constant on parity by showing that lines from the lower terms b^3P and z^7F^0, which have almost identical E.P., have grossly different empirical solar curves of growth. The latter authors have claimed that classical van der Waals broadening cannot account for this phenomenon and have suggested other (unknown) damping effects or departures from L.T.E. as a cause.

Finally, Pagel (1965, 1966) has stressed the importance of allowing for furcation of the solar curve of growth when making differential studies of other stars. Non-allowance can result in transfering the solar anomalies to other stars, and may therefore obscure interesting properties of some stellar curves of growth.

2. *Broadening theory.* The form of the strong and medium-strong portions of the curve of growth are determined by the value of the damping constant Γ. Γ is given by summing the effects of collisions by neutral particles (van der Waals), by ionized particles (Stark) and of intrinsic line width (radiation damping) i.e.

$$\Gamma = \Gamma_W + \Gamma_{St} + \Gamma_{Rad}. \qquad (1)$$

In dwarf star atmospheres Γ_W is usually the dominant term in (1), though for some lines Γ_{St} may also be important. In giant atmospheres all three terms may contribute, and in supergiants only Γ_{Rad} is usually of importance.

The impact approximation (see Unsold 1955, Aller 1963) gives, for a given level,

$$\Gamma_W = 17{\cdot}0 C_6^{2/5} \bar{v}_H^{3/5} N_H \qquad (2)$$

for collisions with neutral hydrogen; $\bar{v}_H$ is the mean velocity of the perturbing atoms and N_H is the number density. The van der Waals constant C_6 is given (for hydrogen) by

$$C_6 = 6{\cdot}46 \times 10^{-34}\, \overline{r^2} \qquad (3)$$

where $\overline{r^2}$ is the mean square radius (in atomic units) of the level. For a particular *line* C_6 is found by differencing the respective values for the upper and lower levels of the transition, so we may write

$$C_6 = 6{\cdot}46 \times 10^{-34} \Delta\overline{r^2} \qquad \text{(for line)}. \qquad (4)$$

The value of $\overline{r^2}$ is calculated from

$$\overline{r^2} = \int_0^\infty P^2(r) r^2\, dr \qquad (5)$$

where $P(r)$ is the wavefunction for the level. For non-penetrating orbits (a suitable criterion is $n^* > l+1$) we can adopt the coulomb approximation (Bates & Damgaard 1949) to obtain

$$\overline{r^2} = \frac{n^{*2}}{2\, Z^2}\{5n^{*2} + 1 - 3l(l+1)\} \qquad (6)$$

where n^* and l are the effective and angular quantum numbers.

Equation (2) can be written (Aller 1963)

$$\log \Gamma_W = 19{\cdot}61 + 0{\cdot}40 \log C_6 + \log P_g - 0{\cdot}70 \log T$$

and substitution from (4) gives

$$\log \Gamma_W = 6{\cdot}33 + 0{\cdot}40 \log \Delta\overline{r^2} + \log P_g - 0{\cdot}70 \log T. \qquad (7)$$

3. *Calculation of mean square radius.* We have calculated values of $\overline{r^2}$ from (5) using wavefunctions derived from Scaled Thomas–Fermi (STF) method (Stewart & Rottenberg 1965), which is superior to the coulomb approximation for $n^* < l+1$ but which gives identical results for $n^* > l+1$. As with the Bates–Damgaard method, the eigenvalue of the one-electron Schrodinger equation is taken to be the (observed) energy needed to remove an electron from the given atomic level, so that

$$n^{*2} = \frac{RZ^2}{I-E} = \frac{RZ^2}{\Delta E}$$

where R is Rydberg's constant, E is the energy of the level and I is the appropriate series limit.

We give in Fig. 1 the ratio of $\overline{r^2}$ calculated from the STF and the coulomb approximation methods. Only $4p$ and $4d$ electrons need be illustrated as the criterion $n^* > l+1$ is satisfied for all s electrons in the iron group, and no f electrons are involved in strong transitions. Fig. 1 was constructed for FeI, but as the

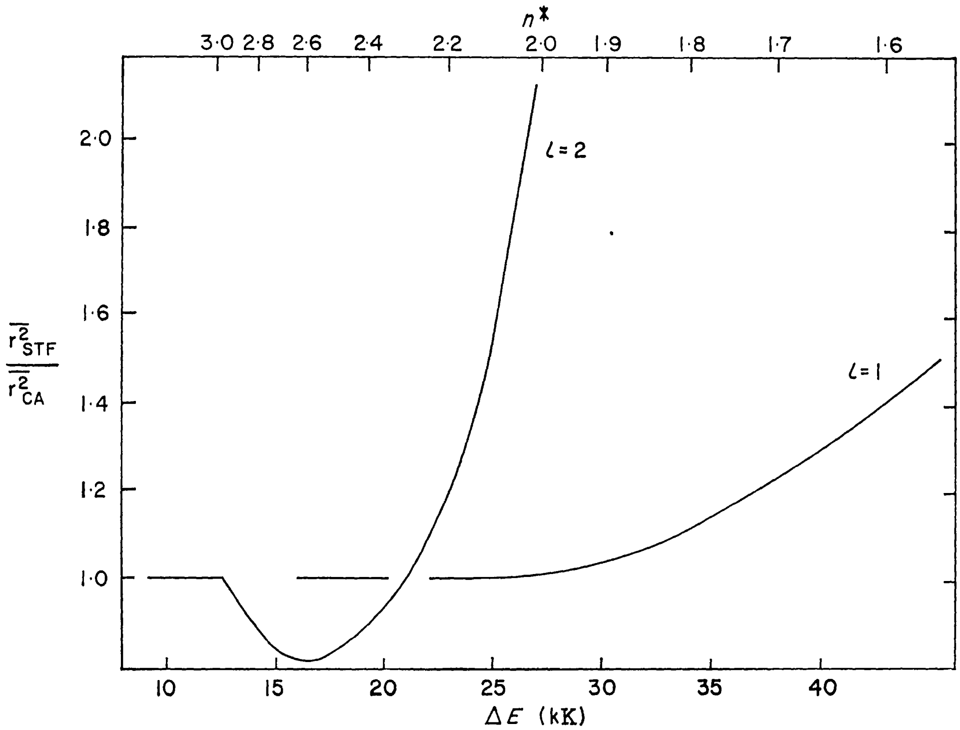

FIG. 1. *Ratio of mean square radius, calculated by the Scaled Thomas–Fermi and coulomb approximation methods.*

dependence of $P(r)$ on nuclear charge is weak in the STF method, it may be used for the entire neutral iron group.

However, in using I from spectroscopic energy levels we are neglecting an important effect (Layzer 1961). If the wavefunction of the optical electron overlaps that of the core to any great extent, then the core will change energy by a significant amount when the atom is ionized, and it is readily seen that the ΔE deduced from spectroscopic data will be too small. In simple atoms this will be important only when the optical electron is a member of a shell or subshell. Provided the principal quantum number of the active electron exceeds that of all the core electrons ΔE may be obtained by spectroscopic methods. In the iron group, however, the competition between the $3d$ and $4s$ states indicates that overlap occurs and hence ΔE will be underestimated. The important iron group transition types are given in Table I.

TABLE I

Transition types in the iron group

	Array	Type	Parity of low state
(i)	$d^{n+1}-d^np$	$d\to p$	even
(ii)	$d^ns-d^{n-1}sp$	$d\to p$	even
(iii)	d^ns-d^np	$s\to p$	even
(iv)	$d^{n-1}s-d^{n-1}sp$	$s\to p$	even
(v)	$d^{n-1}sp-d^{n-1}ss$	$p\to s$	odd

We note that $\overline{r^2}(3d)$ cannot be calculated reliably from the STF method; Hartree–Fock calculations (e.g. Garstang 1962) give $\overline{r^2}(3d)\sim 2$ in the iron group. Those configurations involving a $4s$ (and also, but less marked, a $4p$) electron will have ΔE underestimated, i.e. n^* overestimated. From (6) we see that since $\overline{r^2}$ is very sensitive to n^*, the resulting mean square radii may be seriously overestimated. Finally, only for the $d^{n-1}ss$ configuration (involving a $5s$ active electron) will the value of $\overline{r^2}$ be nearly correct.

4. *Applications to the Sun.* We take $\tau = 0{\cdot}20$ as a representative optical depth for the formation of the wings of strong lines, at which depth in the sun $P_g \sim 8{\cdot}7 \times 10^4$ dynes cm^{-2} and $T \sim 5490\,^\circ$K. Then, from (7)

$$\log \Gamma_W^\odot = 8{\cdot}65 + 0{\cdot}40 \log \Delta\overline{r^2}. \tag{8}$$

Equation (8) is a reasonably accurate formula applicable to most strong solar lines. Curves of growth are usually characterized by the value of a $(=\Gamma/4\pi\Delta\nu_0$, where $\Delta\nu_0 = v/\lambda$ in the usual notation.) Then

$$\log a_W^\odot = 0{\cdot}40 \log \Delta\overline{r^2} + \log\left(\frac{\lambda}{5\,000}\right) - 2{\cdot}00. \tag{9}$$

Table 2 illustrates values of $\Delta\overline{r^2}$, for various strong multiplets, calculated by the use of STF wavefunctions. The inequality signs are assigned according to the precepts of the previous Section.

Table II

Mean square radii for terms in FeI

Multiplet number	Transition type (see Table 1)	$\overline{r^2}_{\mathrm{low}}$	$\overline{r^2}_{\mathrm{up}}$	$\Delta\overline{r^2}$
1001	(i)	2	$<24{\cdot}9$	<23
1002	(i)	2	$<21{\cdot}9$	<20
339	(ii)	2	$<16{\cdot}8$	<15
350	(ii)	2	$<15{\cdot}3$	<13
342	(iii)	$<17{\cdot}3$	$<30{\cdot}1$	<13
268	(iii)	$<16{\cdot}6$	$<27{\cdot}0$	<10
111	(iv)	$<11{\cdot}8$	$<16{\cdot}8$	<5
152	(v)	$<13{\cdot}5$	$78{\cdot}3$	$>64{\cdot}8$
318	(v)	$<15{\cdot}1$	$78{\cdot}3$	$>63{\cdot}2$
1052	(v)	$<22{\cdot}2$	$98{\cdot}5$	$>76{\cdot}4$
1078	(v)	$<22{\cdot}9$	$98{\cdot}5$	$>75{\cdot}6$

We may summarize Table 2 by concluding that for multiplets with *even* low terms $\Delta\overline{r^2} \sim 10$, and for those with *odd* low terms $\Delta\overline{r^2} \sim 70$–$90$. This difference, a factor of ten, shows from equation (9) that $\log a_W^\odot$ will be $\sim -1{\cdot}8$ to $-1{\cdot}6$ for "even" multiplets, and $\sim -1{\cdot}2$ for "odd" multiplets. These values are closely those found from coarse analyses by Warner (1964a) and Pagel (1966) for transitions of the types given in Table II.

We see immediately where the apparent dependence on parity arises. The only low lying odd terms are those in $d^{n-1}sp$, so odd multiplets are essentially $p \to s$ transitions; from (6) and Table I we see that these are the only transitions for which the $3l(l+1)$ factor is zero in the upper state, thus leading to large values of $\Delta\overline{r^2}$.

In Fig. 2 we illustrate some curves of growth for FeI calculated from the Mutschlecner model (Muller & Mutschlecner 1964), with full allowance for variation in damping constant as a function of optical depth. Comparison with the empirical curves given by Pagel (1966, Fig. 1) shows that the model, together with adequate allowance for broadening, has accounted for the variety of curves of growth found in FeI. The study by Gokdogan & Pecker (1964) failed to reach a similar conclusion because they used the wrong form of equation (6), confused principal and effective quantum numbers, and did not allow for broadening of the upper levels.

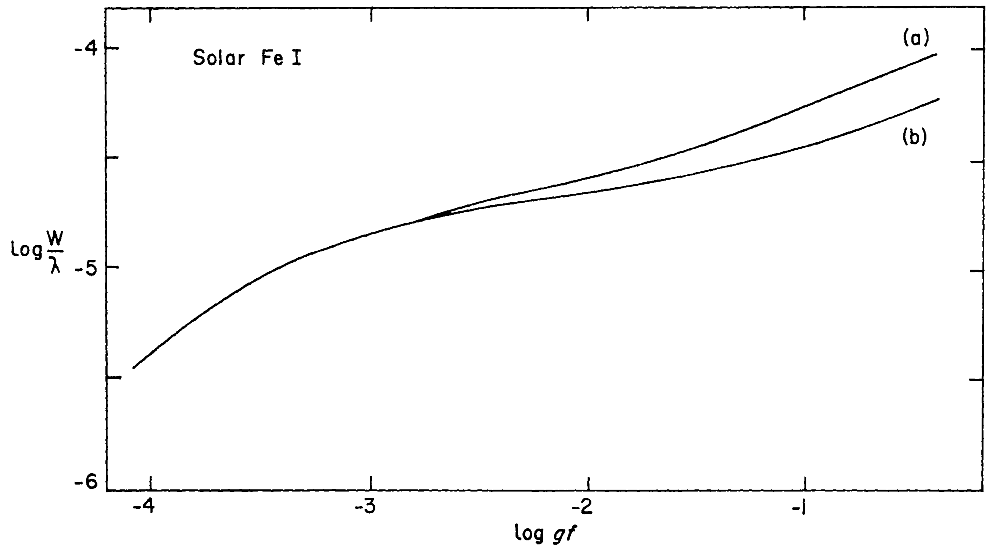

FIG. 2. *Solar FeI curves of growth at* 6 000 Å. *Curve* (*a*) *has E.P.* = 3 V, $\Delta\overline{r^2} = 70$; *curve* (*b*) *has E.P.* = 1 V, $\Delta\overline{r^2} = 10$.

5. *Applications to other stars.* Allowing for differences in temperature and pressure between star and sun we have, from (7) and (9)

$$\log a_W^* = 0{\cdot}40 \log \Delta\overline{r^2} + \log \frac{P_g^*}{P_g^{\odot}} + 0{\cdot}70 \log \theta^*/\theta^{\odot} - \log \frac{v^*}{v_{\odot}} + \log\left(\frac{\lambda}{5\,000}\right) - 2{\cdot}00 \tag{10}$$

where $\theta = 5040/T$. Warner (1964b) has shown that for the outer parts of a stellar atmosphere, where strong lines are formed, we may use the relationship

$$\log \frac{P_g^*}{P_g^{\odot}} \simeq -\tfrac{5}{4} \log \frac{\theta^*}{\theta^{\odot}} - 0{\cdot}37\left(\frac{\theta^*}{\theta^{\odot}} - 1\right) + \tfrac{1}{2} \log \frac{g^*}{g^{\odot}}.$$

Inserted into (10) this gives

$$\log \frac{a_W^*}{a_W^{\odot}} = 0{\cdot}50 \log \frac{g^*}{g^{\odot}} - 0{\cdot}92(\theta^*/\theta^{\odot} - 1) - \log \frac{v^*}{v^{\odot}}. \tag{11}$$

For typical K giant stars $g^* \sim 0{\cdot}01\, g^{\odot}$ and $\theta^* \sim 1{\cdot}2\, \theta^{\odot}$, which results in $\log a_W^*/a_W^{\odot} \sim -1{\cdot}4$. Comparison with the solar values given above shows that $\log a_W^*$ will lie in the range $-2{\cdot}6$ to $-3{\cdot}2$. Typical values for the other broadening agents are $\log a_{\mathrm{Rad}}^* \sim -2{\cdot}5$ (for $\Gamma_{\mathrm{Rad}} = 10^8\,\mathrm{s}^{-1}$) and $\log a_{\mathrm{St}}^* \sim -5$ in K giants. Hence we may expect that in some cases the differential effects due to van der Waals broadening may be obscured by radiation damping. In Fig. 3 we illustrate a curve of growth for γ Tau, using the equivalent widths published by Helfer & Wallerstein (1964) and the FeI *f*-values given by Corliss & Warner (1964). No discernible bifurcation appears, showing that some of the difficulties experienced by Helfer & Wallerstein in their analyses of the Hyades K giants lies in the adoption of a *mean* solar curve of growth.

Applying (10) to an M5 dwarf, for which $\log P_g^*/P_g^\odot \sim 0{\cdot}5$ and $\log \theta^*/\theta^\odot \sim 0{\cdot}33$ (Allen 1963) we have $\log a_W^*/a_W^\odot \sim 0{\cdot}9$. It would therefore appear that the differential effects already noted in the solar curve of growth may increase manyfold in cooler dwarf stars. The detailed intercomparison of spectra of cool stars by Beatty (1951) contains information on just such effects. Thus in the comparison between giant and dwarf K stars, she says of the FeI lines:

"All lines arising from levels with E.P. less than 3·1 V are strengthened in the giant, while those arising from higher levels are strengthened in the dwarf. Several multiplets of high E.P. are considerably winged in the dwarf".

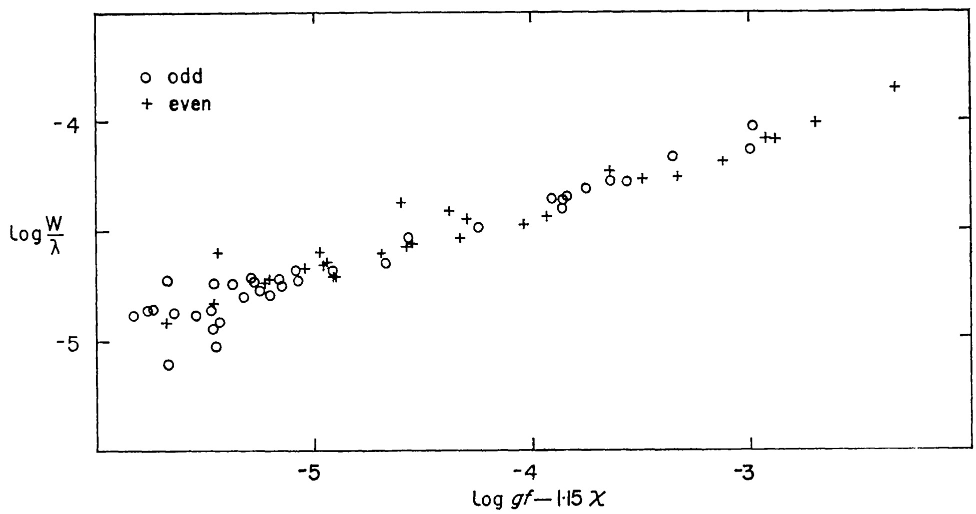

FIG. 3. *Curve of growth for the Hyades K-giant γ Tau. The value* $\theta = 1{\cdot}15$ *is that found from weak lines by Helfer & Wallerstein.*

6. *Other atoms and ions.* In ScI and TiI all strong multiplets arise from even multiplets and $\Delta\overline{r^2}$ will be small. In VI, CoI and NiI some multiplets will have large values of $\Delta\overline{r^2}$ and in CrI and MnI there are many multiplets for which $\Delta\overline{r^2} \sim 80$. It is clear that any use of these strong odd multiplets for abundance determinations must take into account the van der Waals broadening. An approximate criterion for importance of pressure broadening in the sun is $\Delta\overline{r^2} > 20$.

In the first ions of the iron group all multiplets have even low states, with the exception of a few in MnII. However, these latter are of type d^5p–d^5d, for which $\Delta\overline{r^2}$ will be small. For all of these ions the values of $\Delta\overline{r^2}$ are small partly because n^* tends to be smaller in the ions than in the neutrals, but principally because of the Z^{-2} factor in equation (6). In general $\Delta\overline{r^2}$ lies in the range 1–3.

7. *Experimental results.* Several recent papers have measured pressure shifts or broadening in FeI lines (Kusch 1958, Hey 1961, Chen & Chandrasekharan 1961). These experiments were carried out at high pressure (30–60 atmospheres) and it is unlikely that the simple impact approximation is valid under these conditions. Kusch found values of $\overline{r^2}$ considerably larger than calculated from equation (6), whereas Hey obtained better agreement.

The experiment most relevant to the discussion in this paper is that of pressure shifts in FeI measured at 0–1 atmosphere by Babcock (1928). He found a non-linear increase of shift $\Delta\nu$ with excitation potential and found that for a given E.P. $\Delta\nu$ is statistically greater for greater multiplicity of term. The first relationship is a natural consequence of the general increase of $\overline{r^2}$ with n^*, and the second arises because most triplet terms are in d^7s, d^6s^2 or d^7p, while quintet and septet terms arise predominantly from d^6sp and d^6ss—these latter have much larger values of $\overline{r^2}$. It is well known that the simple van der Waals formula for the pressure *shift* fails to give good agreement with experiment, and the writer's estimates of $\Delta\nu$ in Babcock's arc are an order of magnitude greater than those observed, but the qualitative explanation of Babcock's results seems sound enough.

Finally, it is of interest to note that the pressure classes *d* and *e*, assigned in the Revised Rowland (St John *et al.* 1928) and based on early work at Mount Wilson are defined as:

d high-temperature lines; asymmetrical toward red; pole effect large and positive; energy level high; pressure displacement large; limits of upper terms for Fe 41500–55000 cm^{-1},

e high-temperature lines; asymmetrical toward violet; pole effect large and negative; pressure displacement moderate; limits of upper terms for Fe 53500–55000 cm^{-1}.

The fact that all the lines falling on the higher branch of the bifurcated solar curve of growth are classified *d* or *e* (this was pointed out to the writer by Dr C. R. Cowley) was a strong indication at the beginning of the present study that the explanation of the phenomena must lie in the properties of the Fe atom (i.e. differential damping) and not in non-L.T.E. effects.

8. *Conclusion.* Far from indicating inadequacies in line broadening theory, or the existence of non L.T.E. effects in the solar photosphere, the long-known empirical bifurcation of the solar curve of growth provides a means of demonstrating the validity of the elementary theory of collision damping. These differential effects, of demonstrable importance in the sun and some giant stars, may assume considerable proportions in cooler dwarf stars, with possible effects on spectral classification or line blacketing. A study of the profiles of FeI lines in an *M* dwarf seems highly desirable.

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