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LETTER

Letter to the Editor

Self broadening of hydrogen lines: initial results

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Abstract. For the first time broadening by both resonance and dispersive-inductive interactions with H-atoms are included in the formation of Balmer lines in cool stars, without the use of a multipole expansion. Comparison of synthetic profiles with observed profiles for the Sun and two late F dwarfs shows that this improvement in broadening theory accounts for some of the problems found in previous work. It is anticipated that planned future developments in the theory of self broadening will lead to further improve ments in the modelling of cool star atmospheres.

Key words: atomic processes – line: profiles

1. Introduction

Profiles of hydrogen lines in stellar spectra are determined solely by properties of the hydrogen atom and the atmospheric structure as hydrogen is both the source of the continuous and line opacity. Hydrogen line profiles are therefore a very important diagnostic tool in stellar modelling. In cool stars like the Sun, hydrogen is largely neutral with a number density about ten thousand times larger than the electron and ion densities produced by ionization of metals. Although, broadening by electrons and io ns is still very important, it is essential to include the effects of collisions with hydrogen atoms due to their high number density. Past efforts to do so have been inadequate for two reasons:

1. Resonance broadening of p–states has been included using the theory of Ali & Griem (1966) which assumes the interaction can be represented by a multipole expansion, which can be shown to be valid only for the $2p$ state.
2. Broadening by dispersive and inductive interactions between the atoms, so called van der Waals broadening, is entirely neglected.

The importance of this latter contribution to the line broadening has been stressed by Lortet & Roueff (1969) who warn that, "the broadening of H-lines in the presence of H or He is nowhere completely treated, as the van der Waals interaction has always been omitted". They conclude that such broadening is likely to be important in Balmer lines and dominant in Paschen lines relative to resonance broadening.

In this work the multipole expansion is removed from the theory of all broadening mechanisms. The enhanced broadening which results is a first step in the development of a complete theory which should make a significant contribution to our understanding of the structure of cool star atmospheres.

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2. Theory

The broadening of H-lines is extremely complex. The quasi-static ion field splits the lines up into overlapping Stark components which are broadened by collisions with electrons and H-atoms, the resulting profile has then to be averaged over the ion field distribution. All sources of broadening are included when we later consider the synthesis of stellar spectra. Here we treat the effects of H-atom collisions in isolation, to focus attention on their effect alone.

2.1. Overlapping lines in the impact approximation

Balmer lines are comprised of three overlapping components s–p (18.79), p–s (1.761), and p–d (90.17). The strength of the components in atomic units is shown in parentheses, the p–d component being by far the strongest. In the notation of Peach (1981) the line shape is given by

$$L(\omega) = \frac{1}{\pi}\mathrm{Re}\sum_{l_i l_j l_i' l_j'} \langle\langle n_i l_i (n_j l_j)^* || \boldsymbol{\delta} || n_i l_i' (n_j l_j')^* \rangle\rangle \times \langle\langle n_i l_i' (n_j l_j')^* || \left[\boldsymbol{h} - i(\omega - \mathbf{h_0}/\hbar)\right]^{-1} || n_i l_i (n_j l_j)^* \rangle\rangle \quad (1)$$

in the reduced line/doubled-atom space (see Peach 1981), with $\boldsymbol{\delta}$ the electric dipole operator, and $\mathbf{h_0}$ the Hamiltonian for the unperturbed atoms. In terms of the $\mathbf{S}$-matrix for each subspace $\mathbf{S}_i$ and $\mathbf{S}_j$, $\boldsymbol{h}$ is the operator corresponding to $N\{1 - \mathbf{S}_i \mathbf{S}_j^*\}_{\mathrm{av}}$ in line space, where N is the perturber density and $\{\}_{\mathrm{av}}$ indicates averaging over all possible orientations of the collision. The dipole operator determines the strength of each component's contribution to the complete line, including possible interference between components.

The second matrix in Eq. 1 determines the broadening and shift characteristics of each component. We compute this matrix in the semiclassical approximation assuming straight line trajectories for the perturbers. Thus the problem is essentially reduced to computing the S–matrix for the collision given appropriate interatomic potentials. We compute the S–matrix *under the assumption of adiabatic collisions* in the same way as the Anstee & O'Mara (1991) theory for isola ted metallic lines (see Barklem & O'Mara (1997) for d–state details). The final matrix is a complex square matrix of order $n_i n_j$, and once computed can be inverted easily by standard numerical techniques.

2.2. Interaction potentials

We assume that the ℓ-degeneracy has been lifted by the static ion field and use methods developed by Anstee & O'Mara (1991) and Barklem & O'Mara (1997) to determine the dispersive-inductive contribution to the interaction. For p–states, the resonance interaction is calculated without the use of a multipole expansion which is valid only for the $2p$ state.

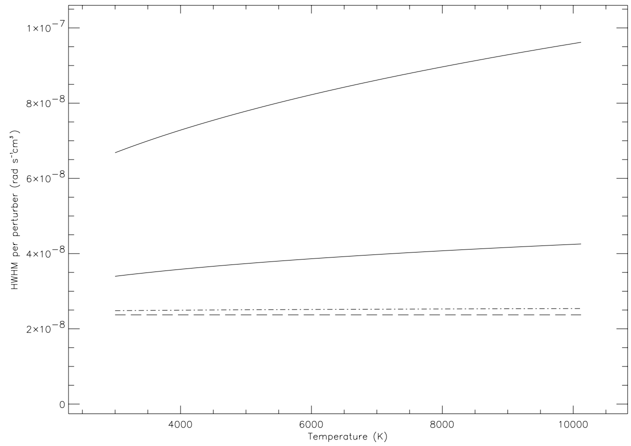

Fig. 1. Comparison of the line width (HWHM) per perturber due to H collisions with temperature computed in this work for the dominating $2p$–$3d$ component of Hα (lower full) and $2p$–$4d$ component of Hβ (upper full) with that of the resonance broadening theory of Ali & Griem (dashed) for the $2p$–state, and our calculation of the resonance broadening (dot-dash) for this state.

3. Results

Fig. 1 compares the results with the theory of Ali & Griem which considers only resonance broadening and treats the interaction using the first two terms of the multipole expansion. We find that our results are in quite good agreement with the Ali & Griem file theory when we only consider the resonance interactions as they did. However, we found that the effect of the dispersive–inductive interaction of other states involved in the transition is quite substantial, particularly that resulting from the d–state of the upper level in Balmer lines. Note that resonance broadening alone is temperature independent. The dispersive contribution relative to the resonance contribution for Hβ is greater than for Hα and this is reflected in the stronger temperature dependence of the line width.

4. Synthetic stellar spectra and comparison with observations

We have used the above work to compute synthetic stellar line profiles. We use the Stark broadening calculations of Stehle (1994) which include thermal broadening and convolve them with the self broadening profiles and radiative damping profiles. We use the SYNTH code of Piskunov (1992) for the radiative transfer which assumes astrophysical LTE.

4.1. Solar models

Castelli et al. (1997) found that the ATLAS9 solar model (Kurucz 1993) with convective overshooting fits the observed solar energy distribution and limb-darkening quite well but leads to Balmer line profiles which are too weak. In contrast models without overshooting fit the Balmer lines but little else. Any process which increases the line strength, such as the increased H-atom broadening discussed here, will result in a better fit when the model with overshooting is used.

Fig. 2 compares two synthetic solar profiles for Hα and Hβ obtained using the Kurucz ATLAS9 model with overshooting, the stronger profiles are a result of using our model of H-atom broadening while the weaker profiles correspond to the use of the Ali & Griem theory.

Fig. 3 compares profiles for Hα and Hβ from the solar flux atlas of Kurucz et al. (1984) with synthetic profiles obtained using our H-atom broadening, the Holweger–Müller (1974) model and Kurucz ATLAS9 models with and without convective overshooting. Note that Castelli et al. claim that the continuum for Hβ is drawn 1% too high in this atlas, hence we have adjusted the observations appropriately. The Holweger–Müller and the ATLAS9 model wi th overshooting produce profiles that are in good agreement with each other, are stronger than the profiles based on the Ali & Griem theory alone, but still weaker than the observed profiles. The ATLAS9 model without overshooting produces synthetic profiles that are now too strong, particularly for Hα. It is anticipated that planned extensions to the current work will increase the H-atom broadening further and perhaps result in better agreement between observed and synthetic profiles obtained with t he ATLAS9 model with overshooting thus resolving the gross discrepancy found by Castelli et al. However it is likely some of the remaining discrepancy lies in the models and the treatment of convection.

4.2. Other cool stars

Synthetic spectra were compared with observations for two other cool stars, β Com and χ Her. Stellar data for these stars from the literature are shown in Table 1.

The spectra were acquired at high resolution (R = 30000) using the MUSICOS spectrograph at the Isaac Newton Telescope

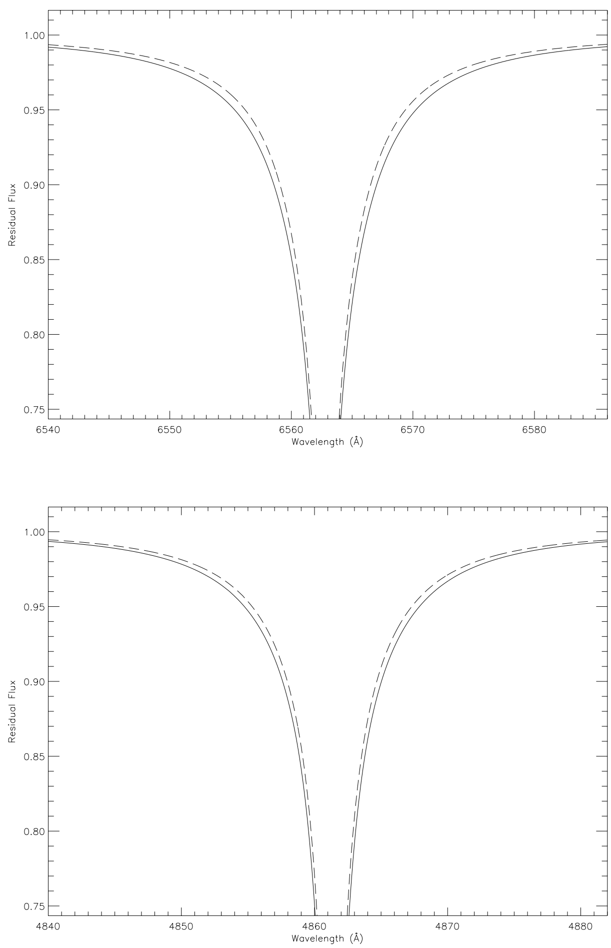

Fig. 2. Synthetic flux profiles for Hα (top) and Hβ (bottom) for the Kurucz ATLAS9 solar model with overshooting. The full lines show profiles which employ our self-broadening calculations and the dashed lines employ the Ali & Griem theory. The lines show a 11.3% and 9.2% increase in equivalent width respectively.

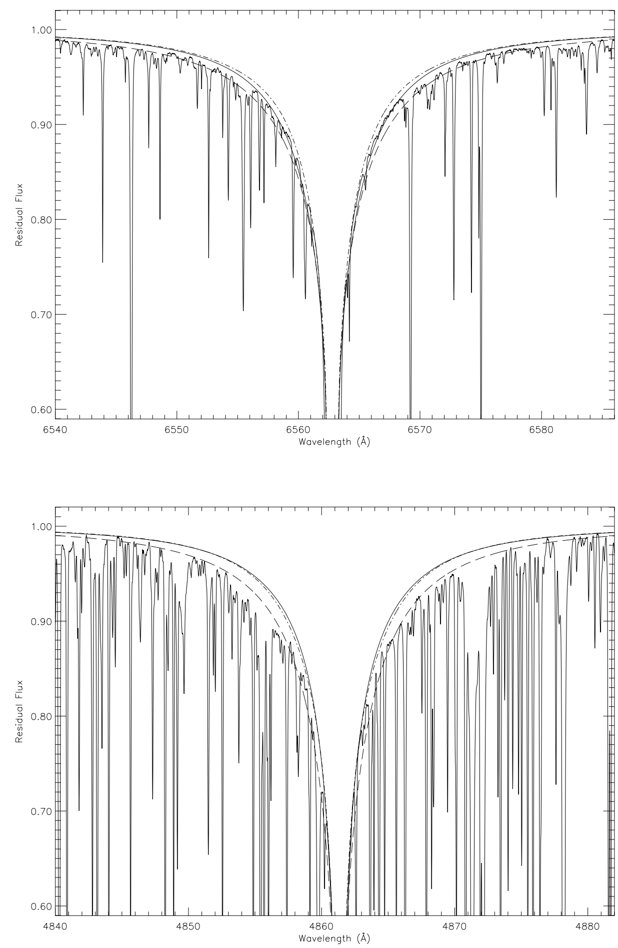

Fig. 3. Comparisons of synthetic flux profiles with observations for the Sun for Hα (top) and Hβ (bottom). Full and dashed lines use the Kurucz ATLAS9 model with and without overshooting respectively, and the dot–dashed lines use the Holweger–Müller model.

Table 1. Stellar parameters for comparison stars from the literature. $T_{\rm eff}$ is from Blackwell & Lynas-Gray (1998) using the infrared flux method. Gravities and metallicities are all taken from Edvardsson et al. (1993).

Star	Spectral Type	$T_{\rm eff}$ (K)	$\log g$	[Fe/H]
β Com (HR 4983)	F9.5V	5959$\pm$30	4.38	0.01
χ Her (HR 5914)	F9V	5745$\pm$35	4.34	-0.47

in May 1999. The data were carefully reduced and compared with synthetic spectra using the ATLAS9 models with parameters in Table 1. The results were consistent with those found for the Sun, namely models without overshooting produce profiles that are too strong. For both stars, models with overshooting produce Hα profiles that are in reasonable agreement with o bservations while the synthetic Hβ profile is too weak in χ Her and marginally so in β Com. To fit the Hα profiles using the models without overshooting we needed to reduce $T_{\rm eff}$ by approximately 110 K and 140 K in β Com and χ Her respectively, values which are much greater than the estimated errors in the $T_{\rm eff}$ values from the infrared flux method (around 30 K). However the fitting is somewhat subjective due to differences in line shapes and he nce the fitting error perhaps is of the order of 50 K. Roughly the same order of temperature correction was required in Hβ profiles, however the models never reproduce the line shape well (as we see in Fig. 3 for the Sun), making the determination much less reliable.

4.3. $T_{\rm eff}$ Determinations using Balmer lines in cool stars

We computed a grid of MARCS models (Asplund et al. 1997) over a range of temperatures, with solar gravity, for metallicities of [Fe/H]=0.0 and -2.0. We used the grid to estimate the difference in determined $T_{\rm eff}$ from our theory and the Ali & Griem theory. For each model we computed synthetic profiles for Hα and Hβ as described above using both theories. For each profile resulting from our theory we then found the best matching profile (in the line wings) using the Ali & Griem theory, and

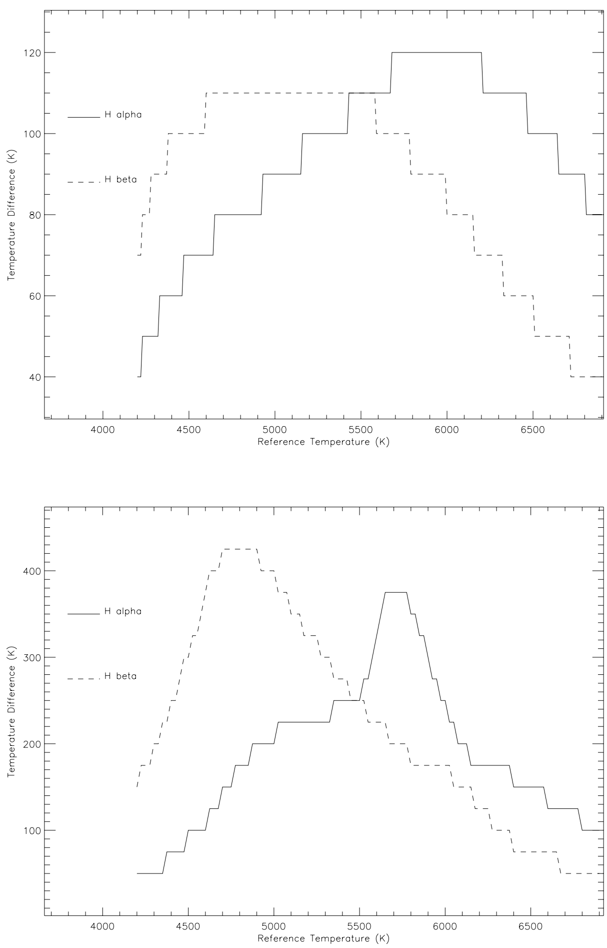

Fig. 4. The predicted difference in effective temperature determinations from our new calculations, and calculations using the resonance broadening theory of Ali & Griem for Hα and Hβ. Plots are shown for solar metallicity (top) and 1/100 solar metallicity (bottom), in both cases for solar surface gravity. The "reference temperature" is that which would be found using our broadening theory. The plot then predicts how much higher the effective temperature derived using the Ali & Griem eory is expected to be.

recorded the temperature difference between the models used to generate the two profiles. The results, plotted in Fig. 4, indicate that the new line broadening calculations lead to a significant lowering of the derived effective temperature.

Of particular interest is the presence of a peak temperature "error" and the difference in location of the peak for Hα and Hβ. As is clear in Fig. 2, due to enhanced H-atom broadening, synthetic profiles obtained using our theory are always stronger than those obtained using Ali & Griem theory. In Ali & Griem theory the H-atom broadening is resonance broadening only and is therefore temperature independent while in our theory the dispersive-inductive contribution l eads to an increase with temperature. At low $T_{\rm eff}$, H-atom broadening makes its greatest contribution and as $T_{\rm eff}$ is raised the temperature "error" increases because of the growth in the H-atom broadening in our theory. Eventually Stark broadening begins to dominate accounting for the peak followed by a decline as Stark broadening becomes more and more dominant as $T_{\rm eff}$ increases. As Stark broadening in Hβ is greater than in Hα the peak occurs at a lowe r $T_{\rm eff}$ for Hβ. The higher peak temperature "error" for metal deficient stars reflects the higher temperature required to increase the ion/electron density sufficiently. This can be tested observationally. In agreement with this result Gardiner et al. (1999, Fig. 9) found using the Ali & Griem theory that $T_{\rm eff}$ obtained using Hα is larger than for Hβ at $T_{\rm eff}$ = 6000–7000K while the situation is reversed for stars with a lower $T_{\rm eff}$. It is perhaps significant to note that Castelli et al. find, using Ali & Griem theory and the solar ATLAS9 model with overshooting, that $T_{\rm eff}$ has to be raised by 100–150K (close to the peak of 120K in Fig. 4) in order to fit the observed solar profiles.

5. Conclusions and future directions

Without resort to the use of a questionable multipole expansion, both resonance broadening and dispersive-inductive broadening by H-atoms have, for the first time, been included in the broadening of Balmer lines. For Balmer line formation in cool stars dispersive-inductive interactions with H-atoms are important. Their inclusion goes part of the way to resolving current problems with Balmer line formation in cool stars. It is hoped that future work, which will include the contribution of diabatic ℓ-cha nging collisions, will remove the remaining discrepancies and establish H-line profiles as a reliable diagnostic tool in cool stars.

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