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# Broadening of Spectral Lines by Collisions with H-atoms

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**Abstract.** Pressure broadening of metallic lines in cool stars is dominated by collisions with hydrogen atoms. A universal theory for broadening of neutral metallic lines by this mechanism developed by Anstee, Barklem, and O'Mara is briefly reviewed. Several examples of successful application of the data are presented and future applications discussed. Line broadening data from this theory for a large sample of lines can be obtained by accessing the Vienna Atomic Line Database (www.astro.univie.ac.at/∼vald) or for individual lines by using software available at www.astro.se/∼barklem.

## 1. Importance

In cool stars like the Sun neutral hydrogen atoms outnumber electrons by four orders of magnitude. Consequently, the broadening of strong spectral lines is dominated by collisions with neutral hydrogen atoms. Development of a satisfactory line broadening theory is important as it allows strong lines, which often have the advantage of well determined $f$–values and wings independent of non-thermal photospheric motions, to be used to determine abundances. Such lines can also be used to determine surface gravities, and have been shown to be important in determining semi-empirical temperature distributions in cool stars.

## 2. Theory Outline

In stellar atmospheres, neutral hydrogen atoms move sufficiently rapidly for the impact approximation to be valid. This leads to a Lorentz profile

$$L(\omega) = \frac{w}{\pi} \frac{1}{(\omega - \omega_0)^2 + w^2}$$

with a half half-width which is given by

$$w = N_H \int_0^\infty v f(v) \sigma_{br}(v) dv$$

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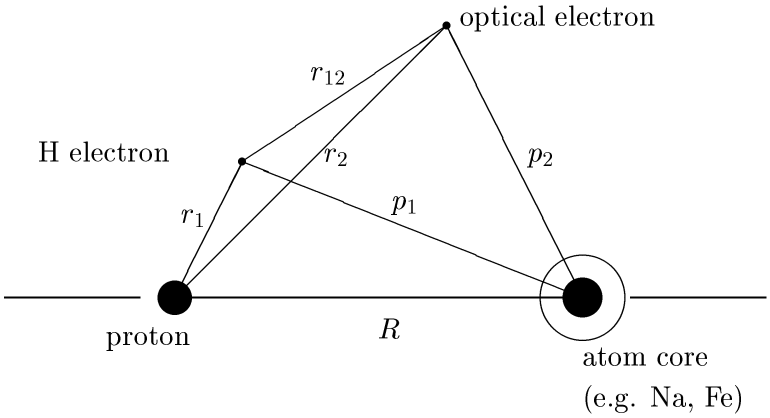


Figure 1. Model of the electrostatic interaction for the two atom system.

where $N_H$ is the hydrogen atom number density, $v$ the relative collision speed, $f(v)$ the speed distribution and $\sigma_{br}$ is the line broadening cross-section given by

$$\sigma_{br}(v) = 2\pi \int_0^\infty \langle \Pi(b,v) \rangle_{av} b db$$

where $b$ is the impact parameter. The line broadening efficiency factor $\Pi(b,v)$ is averaged over all orientations of the atoms, and is expressed in terms of the $S$–matrix for the collision, which is in turn functionally dependent on the interaction energy between the hydrogen atom and the perturbed atom in its upper and lower states. *The only essential difference between various treatments is the method used to determine this interaction energy.* The perturbed atom is modelled as a positive atom core with an optical electron, which with reference to figure 1 is

$$V = \frac{1}{R} + \frac{1}{r_{12}} - \frac{1}{r_2} - \frac{1}{p_1}$$

for the case of a neutral perturbed atom, in atomic units.

## 3. Classical van der Waals theory

In classical theory the interaction is determined through the multipole expansion of $V$, retaining only the dipole-dipole term, and the potential is averaged over all orientations. This leads to

$$\langle \Delta E \rangle_{av} \sim \frac{-\alpha_H \langle p_2^2 \rangle}{R^6}$$

where $\alpha_H$ is the polarisability of hydrogen. This is the *van der Waals interaction.* In line broadening, the multipole expansion is only valid if the atoms have non-overlapping electronic clouds at the separations important in the broadening. A simple calculation based on the Lindholm–Foley line broadening theory

(Lindholm 1942, Foley 1946) shows for typical velocities of interest in cool stellar atmospheres the multipole expansion is only valid if

$$\langle p_2^2 \rangle^{1/2} \ll 10.5$$

This is *never* satisfied for lines of astrophysical interest. The van der Waals theory predicts its own failure. Therefore, *"van der Waals broadening" is a misnomer!*

## 4. ABO theory

The main features of the potentials in the Anstee, Barklem & O'Mara (ABO) theory are:

- The multipole expansion is *not* used.
- Spin, exchange effects and avoided ionic crossings neglected.
- Perturbation theory is employed,

$$\Delta E_i = \langle i|V|i\rangle + \sum_{j\neq i} \frac{\langle i|V|j\rangle\langle j|V|i\rangle}{E_i - E_j}$$

  with the Unsöld approximation,

$$\Delta E_i \approx \langle i|V|i\rangle + \frac{1}{E_p}\left[\langle i|V^2|i\rangle - \langle i|V|i\rangle^2\right]$$

  solved *analytically* until a final numerical integration,

$$\Delta E_i \approx \frac{1}{E_p}\int_0^\infty P_{nl}^2(p_2) I_{l|m|}(R, p_2)\, dp_2$$

- Coulomb wavefunctions are used, enabling calculations independent of atomic element.

It is an important feature of the method that the interaction energy is determined analytically to within a single numerical integration over the radial wavefunction of the perturbed atom.

## 5. ABO theory results

The results of ABO theory are presented as cross-sections $\sigma$ for a given relative velocity $v_0 = 10^4$ m/s. The velocity dependence is well described by

$$\sigma(v) \propto v^{-\alpha}$$

and thus each result for $\sigma(v_0)$ has a corresponding velocity parameter $\alpha$. The line-width can then be obtained from a simple analytic formula, namely

$$w/N = \left(\frac{4}{\pi}\right)^{\alpha/2} \Gamma\left(\frac{4-\alpha}{2}\right) v_0 \sigma(v_0) \left(\frac{\bar{v}}{v_0}\right)^{1-\alpha}$$

where $\bar{v} = \left(\frac{8kT}{\pi\mu}\right)^{1/2}$ is the average velocity for temperature $T$ and reduced mass of the two atoms $\mu$. The computed line broadening data available are:

- General results for neutrals, tabulated with effective principal quantum number $n^*$ for s-p, p-d and d-f transitions (code to interpolate these data and compute line-widths is available at www.astro.uu.se/~barklem)
- Specific results for important lines of Ba II, Be II, Ca II, Mg II, Sr II.
- Data for approximately 5000 lines in VALD (Vienna Atomic Line Database, Kupka *et al* 1999, www.astro.univie.ac.at/~vald)

See Barklem et al (2000) and references therein for details, of ABO theory and results.

## 6. Some Results of Application to Solar Spectra

A number of applications to solar spectra have been made, which we briefly summarise. In all the following cases LTE and the Holweger & Müller (1974) model were assumed. The main results have been:

- Neutral lines show general agreement with meteoritic abundances (Na I example shown in figure 2).
- Strong Fe I lines reveal:
  - A "low" meteoritic abundance of $\log(N_{\rm Fe}/N_{\rm H}) + 12 \sim 7.51$.
  - A quantitative explanation of the Carter (1949) effect, i.e. Fe I lines of similar excitation but differing parity of the upper state are differently broadened in the solar spectrum.
- Ba II, Ca II and Sr II lines find:
  - Abundances consistent with meteoritic values.
  - No significant variation of Ca and Sr abundances with line strength, or between ionisation stages.

The ABO theory has also been employed by Allende Prieto *et al* (2001) in a semi-empirical determination of the solar photospheric $T$-$\tau$ relationship by inversion of solar spectral lines. Some key results related to the broadening theory were found. Firstly, the $T$-$\tau$ structure derived from 7 strong lines was the same as the structure from 55 weak lines. Secondly, the abundances derived from only strong lines is in good agreement with those from the weak lines. Finally, and perhaps the strongest test, the known value of the surface gravity ($\log g = 4.44$) provides the best fit to observations, as seen from figure 3.

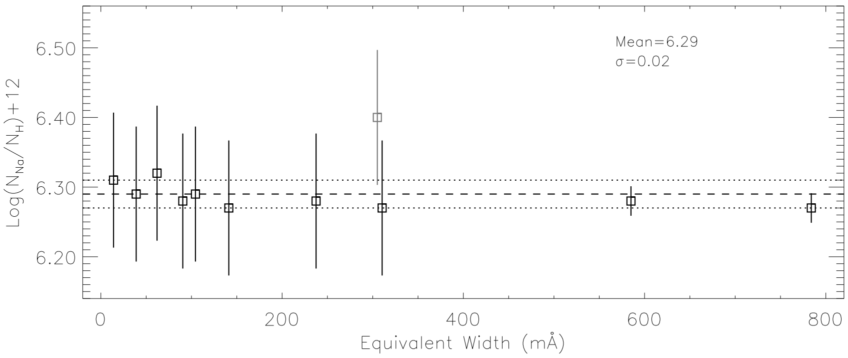


Figure 2. The solar abundances derived from the Na I solar spectrum plotted with line strength. Error bars shown only account for the error in $f$–values. The meteoritic abundance from Grevesse *et al* (1996) is 6.32±0.02.

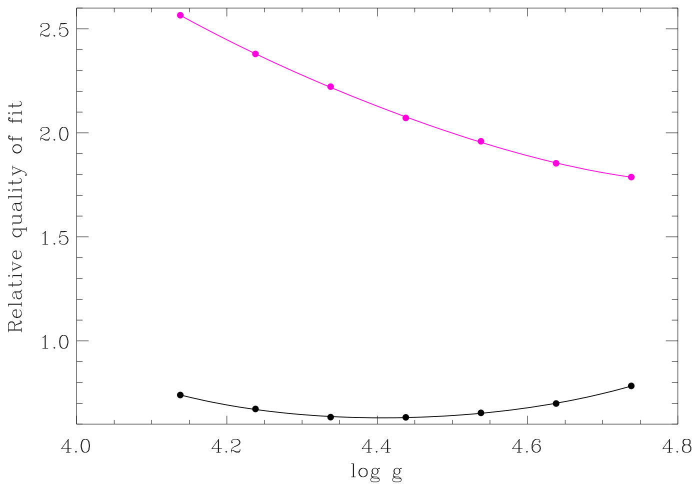


Figure 3. The quality of fits from inversion of the solar spectral lines using classical van der Waals theory (upper pink line) and ABO theory (lower black line) for various assumed surface gravities. Figure courtesy Carlos Allende Prieto.

## 7. Summary

ABO theory provides a universal theory for collisional broadening of by H-atoms of neutrals, which easy to apply. Individual results for important lines of singly ionised species are also available. The estimated accuracy of the calculations is better than 10%. There is now no need or excuse for using *van der Waals theory* and arbitrary fudge factors!

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