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Line shapes for the spectra of Brown Dwarfs

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Abstract. Highly accurate calculations of the central cores of pressure broadened alkali resonance doublets due to H_2 and He perturbers are needed in order to estimate the effects of dust in brown dwarf atmospheres. We report results for Lorentzian alkali-line profiles broadened by helium perturbers. They are based on a fully quantum-mechanical close-coupling description of the colliding atoms, the Baranger theory of lineshapes and new *ab initio* potentials for the alkali-rare gas interaction.

Key words. Brown Dwarfs: alkali resonance doublets – Brown Dwarfs: synthetic spectra – Spectral line broadening: calculations

1. Introduction

Accurate pressure broadened profiles of alkali resonance doublets perturbed by H_2 and He are of crucial importance for the modelling of atmospheres of late M, L and T type brown dwarfs and for generating their synthetic spectra in the region 600 - 900 nm. The dominant lines are the Na I 589.0/589.6 nm and K I 766.5/769.9 nm doublets (Pavlenko et al. 2000) but there can also be significant contributions from less abundant alkalis such as Li, Rb and Cs, and from subordinate doublets such as Na I 818.3/819.5 nm. The non-Lorentzian profiles of the strongly broadened Na I and K I doublets have been recently studied by Burrows, & Volobuyev (2003) and Allard et al. (2003), with the emphasis on approximate or unified semiclassical models that can describe the far wings of the profiles. Also Zhu et al. (2005) have carried out quantum mechanical calculations of emission and absorption spectra for the wings of the lithium resonance line. However highly accurate calculations of the central Lorentzian cores are needed (Pavlenko 2004) in order to estimate the effects of dust in brown dwarf atmospheres.

We report results for the Lorentzian alkali-line profiles broadened by helium perturbers. The calculations extend our previous study (Leo et al. 2000) of pressure broadening of the Na I doublets by He at laboratory temperatures up to 500 K and are based on a fully quantum-mechanical close-coupling description of the colliding atoms and the Baranger (1958) theory of lineshapes. As input for our calculations we have computed new *ab initio* potentials for the alkali-rare gas interaction.

2. Spectral line profiles

The width and shift of the spectral lines have been calculated using the quantum-mechanical

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impact theory of Baranger (1958) for non-overlapping spectral lines in which the profile of each isolated line is a Lorentzian. The half width w and shift d of the Lorentzian spectral profile for a line involving initial and final emitter states $|j_i\rangle$ and $|j_f\rangle$ respectively of total electronic angular momentum $\mathbf{j} = \mathbf{L} + \mathbf{S}$ (we suppress the quantum numbers (n, L, S) for convenience) is given by (Leo et al. 2000)

$$w + id = N \int_0^\infty f(E)\, S(E)\, dE \tag{1}$$

where $f(E)$ is the normalized Maxwellian perturber energy distribution:

$$f(E) = 2\pi(\pi k_B T)^{-3/2} \sqrt{E}\, \exp(-\frac{E}{k_B T}), \tag{2}$$

N is the perturber number density and

$$\begin{aligned} S(E) \;=\; & \frac{\hbar^2 \pi}{M^2} \sqrt{\frac{M}{2E}} \sum_{l,l'} \sum_{J_i,J_f} (2J_i + 1)(2J_f + 1) \\ & \times(-1)^{l+l'} \begin{Bmatrix} J_f & J_i & 1 \\ j_i & j_f & l \end{Bmatrix} \begin{Bmatrix} J_f & J_i & 1 \\ j_i & j_f & l' \end{Bmatrix} \\ & \times\{\delta_{l,l'} - \langle j_i\ l'\ J_i|S|j_i\ l\ J_i\rangle \\ & \times\langle j_f\ l'\ J_f|S|j_f\ l\ J_f\rangle^*\}. \end{aligned} \tag{3}$$

Here l and l' are the values of the relative emitter-perturber angular momentum $\mathbf{L}_R$ before and after the collision, $\mathbf{J} = \mathbf{L}_R + \mathbf{j}$ is the total angular momentum of the emitter-perturber system, $\langle j'\ l'\ J|S|j\ l\ J\rangle$ is the interaction picture scattering matrix in the coupled $\{|j\ l\ J\rangle\}$ representation, $\left\{\begin{smallmatrix} a & b & c \\ f & g & h \end{smallmatrix}\right\}$ is the $6 - j$ symbol and M is the reduced mass of the emitter-perturber system.

The scattering matrix elements in (3) are determined from the asymptotic behaviour of the radial functions $G^J_{jl}(R)$ for each scattering channel (j, l, J) which satisfy the coupled equations (Leo et al. 2000)

$$\begin{aligned} & [\frac{\partial^2}{\partial R^2} - \frac{l(l+1)}{R^2} + k_j^2]\, G^J_{jl,j''l''}(R) \\ & = \frac{2M}{\hbar^2} \sum_{j',l'} V^J_{jl,j'l'}(R)\, G^J_{j'l',j''l''}(R) \end{aligned} \tag{4}$$

where (j'', l'') labels the linearly independent solutions of (4) and the Born-Oppenheimer coupling terms have been neglected. The parameter

$$k_j^2 = 2M[E - (E^{(L,S)} + \varepsilon_j(\infty))]/\hbar^2 \tag{5}$$

is positive for open scattering channels and negative for closed channels. Here E is the total energy of the emitter-perturber system, $E^{(L,S)}$ is the energy of the state of the separated atoms to which the molecular state dissociates adiabatically and the fine structure parameter $\varepsilon_j(R)$ has been assumed to have its asymptotic value $\varepsilon_j(\infty)$.

The interaction potential matrix elements $V^J_{jl,j'l'}(R)$ (Leo et al. 2000) are, for the ${}^2S_j$ level,

$$V^J_{jl,j'l'}(R) = \delta_{j,j'}\delta_{l,l'}\ {}^2V_\Sigma(R), \tag{6}$$

for the ${}^2P_j$ levels,

$$\begin{aligned} V^J_{jl,j'l'}(R) \;=\; & \delta_{j,j'}\delta_{l,l'}\ {}^2V_\Pi(R) \\ & + C^{(1)}_{jl,j'l'}[{}^2V_\Sigma(R) - {}^2V_\Pi(R)] \end{aligned} \tag{7}$$

and, for the ${}^2D_j$ levels,

$$\begin{aligned} V^J_{jl,j'l'}(R) \;=\; & \delta_{j,j'}\delta_{l,l'}\ {}^2V_\Delta(R) \\ & + B_{jl,j'l'}(-1)^{j'-j}[1 + (-1)^{l'+l}] \\ & \times[{}^2V_\Pi(R) - {}^2V_\Delta(R)] \\ & + C^{(2)}_{jl,j'l'}[{}^2V_\Sigma(R) - {}^2V_\Delta(R)] \end{aligned} \tag{8}$$

where the coefficients

$$\begin{aligned} C^{(n)}_{jl,j'l'} \;=\; & \sum_\Omega (-1)^{j'-j} C(J\ j\ l; -\Omega\ \Omega\ 0) \\ & \times C(J\ j'\ l'; -\Omega\ \Omega\ 0) C(n\ \frac{1}{2}\ j; 0\ \Omega\ \Omega) \\ & \times C(n\ \frac{1}{2}\ j'; 0\ \Omega\ \Omega) \end{aligned} \tag{9}$$

and

$$\begin{aligned} B_{jl,j'l'} \;=\; & \sum_\Omega C(J\ j\ l; -\Omega\ \Omega\ 0) \\ & \times C(J\ j'\ l'; -\Omega\ \Omega\ 0) \\ & \times C(2\ \frac{1}{2}\ j; 1\ \Omega - 1\ \Omega) \\ & \times C(2\ \frac{1}{2}\ j'; 1\ \Omega - 1\ \Omega) \end{aligned} \tag{10}$$

Table 1. Coefficients w_i for temperature dependence of line widths (in units of 10^{-21} MHz m^3/atom)

Transition	w_0	w_1	w_2	w_3	w_4
3p $^2P_{1/2}$– 3s $^2S_{1/2}$	0.094	1.09	−1.27	0.576	−0.095
3d $^2D_{3/2}$– 3p $^2P_{1/2}$	0.500	2.09	−1.49	0.521	−0.084

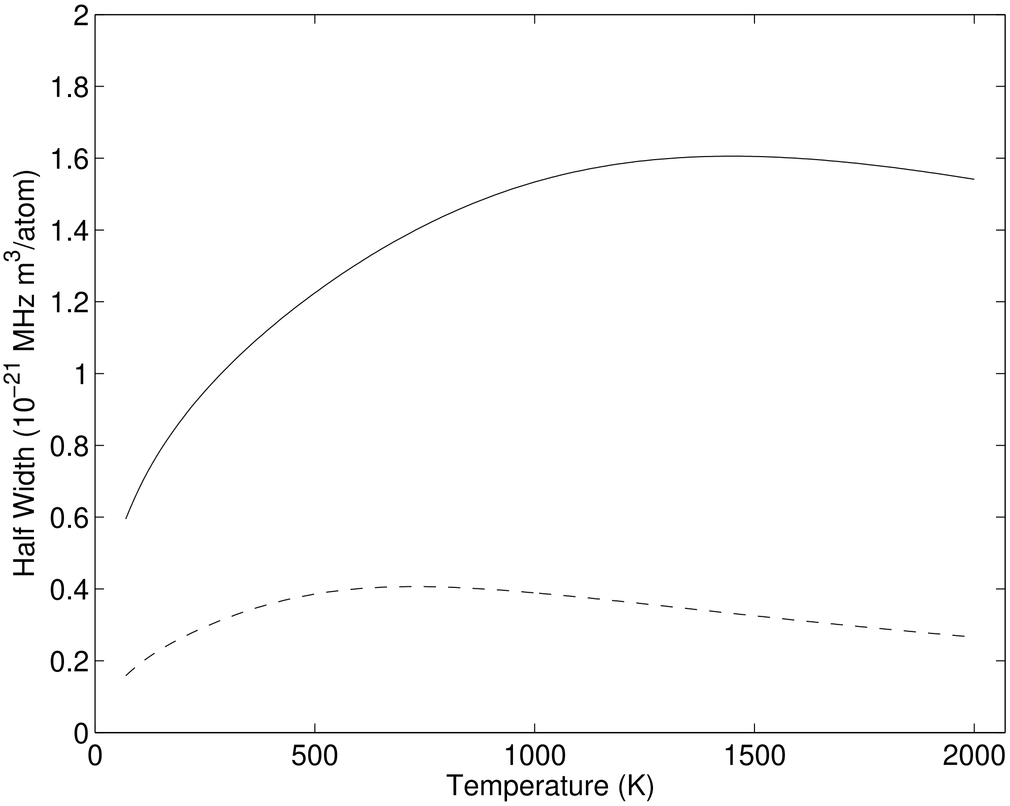

Fig. 1. Temperature dependence of Na I doublet lines half-widths (in units of 10^{-21} MHz m^3/atom) pressure broadened by He perturbers. The results shown are for 589.6 (dashed line), 818.3 (solid line) nm lines.

are symmetric with respect to the interchange $(j,l) \leftrightarrow (j',l')$. Here $C(j_1\ \ j_2\ \ j; m_1\ \ m_2\ \ m)$ is the Clebsch-Gordan coefficient, Ω denotes the projection of an angular momentum onto the internuclear axis $\mathbf{R}$ and $^{2S+1}V_\Lambda(R)$, where $\Lambda \equiv |\Omega_L|$, are the adiabatic molecular potentials.

The equations (4) decouple into two sets of opposite parity $(-1)^{J\pm1/2}$. Thus the $^2S_{1/2}$, $^2P_{1/2}$ and $^2D_{3/2}$ alkali states are represented by one, three and five coupled differential equations for each parity respectively.

The close-coupled equations (4) have been solved using a modified version of the FARM R-Matrix package, see Burke, & Noble (1995) and Venturi et al. (1999) and the solutions fitted to free-field boundary conditions to extract the scattering matrix elements. R-matrix techniques have high numerical stability and computational efficiency, especially where large numbers of scattering energies are needed. The FARM package incorporates a combination of R-matrix propagators (solution following at small distances where $V(R)$ is rapidly varying and potential following at larger distances where $V(R)$ is slowly varying) to integrate the coupled equations and an accelerated Gailitis expansion to minimize the distance at which the matching procedure is undertaken.

3. Interatomic potentials

The adiabatic molecular potentials $^{2S+1}V_{\Lambda}(R)$ for the X^*–He system (where X = Li, Na or K) have been obtained by using a three-body model in which the alkali X^* is treated as a X^+ ion plus an active electron and the perturbing He atom is represented by a polarisable atomic core. Model potentials are used to represent the electron-atom and electron-atomic ion interactions and the basic methods adopted for obtaining these model potentials are discussed by Peach (1982). The most important recent change from the earlier approach is that the core-core interaction is itself calculated directly using a three-body model composed of X^+ and He^+ cores plus one electron. A more detailed discussion of this development is given for the Li-He case by Behmenburg et al. (1996). Further numerical refinements have been incorporated into the computer program since then and new calculations carried out for the three alkali-helium systems considered in our study.

4. Results

Calculations have been completed for the sodium 3p $^2P_{\frac{1}{2}} \rightarrow$ 2s $^2S_{\frac{1}{2}}$ (589.6 nm) and 3d $^2D_{\frac{3}{2}} \rightarrow$ 3p $^2P_{\frac{1}{2}}$ (818.3 nm) lines. The main computational issues associated with extending our previous calculations up to the higher temperatures (2000 K) of astrophysical interest are convergence of the sum over partial waves in (3) and of the integration (1) over perturber energies. The present calculations required up to 1000 partial waves and energy nodes extending to 5000 K to obtain satisfactory convergence.

The temperature dependence of the computed half-widths is shown in Fig. 1 and the coefficients to the fit

$$w(T) = w_0 + w_1\hat{T} + w_2\hat{T}^2 + w_3\hat{T}^3 + w_4\hat{T}^4, \quad (11)$$

where $\hat{T} \equiv T/1000$, are given in Table 1.

5. Conclusions

The present calculations have demonstrated that the formalism, calculational techniques and potentials can be successfully applied to the computation of pressure broadening of alkali doublet lines by He perturbers at temperatures pertaining to the atmospheres of Brown Dwarfs. Extensions of the calculations to doublet lines in Li and K are currently underway.

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