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THEORETICAL ANALYSIS OF THE HE_2 LINE AT 585 Å

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Abstract. Pressure broadening by molecular hydrogen and helium is one of the major broadening mechanism in the atmosphere of brown dwarfs. He(1 ^{1}S)-He(2 ^{1}P) collisional line profiles are determined in a unified theory of spectral line broadening using very recent *ab initio* potential energies. Results are reported for the conditions prevailing in brown dwarf atmospheres.

Keywords: line: profiles, stars: low mass, brown dwarfs, stars: atmospheres

1 Introduction

A unified theory of spectral line broadening has been developed to calculate neutral atom spectra given the interaction and radiative transition moments for relevant states of the radiating atom with other atoms in its environment. Complete details and the derivation of the theory are given in Allard et al. (1994, 1999). The interatomic interactions are the main physical quantities needed for a good understanding of collisional processes, they are now computed with high accuracy.

2 Molecular potentials

The *ab initio* computation of the adiabatic potential energy curves of He_2 have been carried out using the MOLPRO 2009 package *. A huge Multi Reference Configuration Interaction (MRCI) has been performed starting from a very large Multi Configuration Self Consistent Field (MCSCF). The MCSCF calculation involved 26 active orbitals and a very large basis set (called basis E) composed of 118 orbitals for each He atom $(21s, 12p, 8d, 3f)$. For the lowest quintet state this approach was shown (Deguilhem 2009) to be very effective compared to full CI results, leading to differences much less than a tenth of a wavenumber.
We have also checked that using orbitals optimised from state averaged or the ones of the quintet state, lead to almost identical results, a strong indication that we are very close to the full CI results.
Therefore the main limitation in the accuracy of these adiabatic potential curves resides in limitation due to the finite basis set used, however considering the quality of the basis set this error appears to be small.

There are 2 transitions which contribute to the $1s\ ^1S \rightarrow 2p^1P$ line profile:

$$1s\ X^1\Sigma_g^+ \rightarrow 2p\ F^1\Pi_u \quad \text{noted } (X-F)$$
$$1s\ X^1\Sigma_g^+ \rightarrow 2p\ D^1\Sigma_u^+ \quad \text{noted } (X-D).$$

The involved molecular potentials are shown in Fig. 1.

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*http://www.molpro.net.

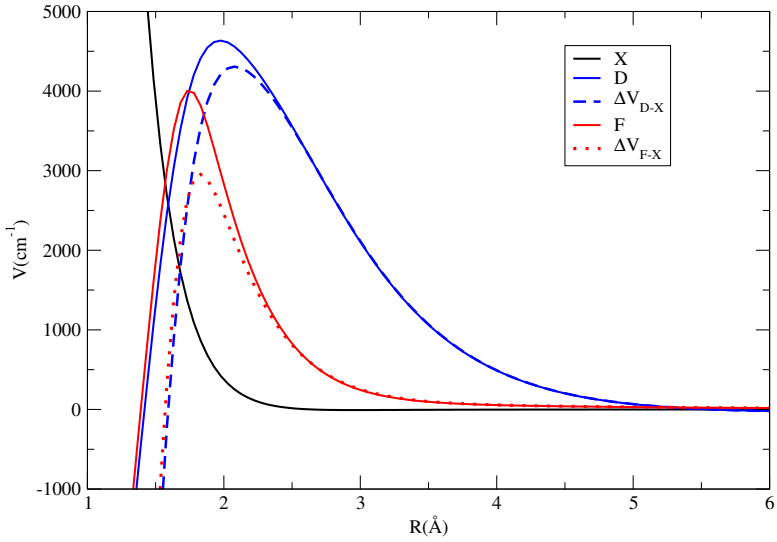

Fig. 1. *Ab initio* potential energy curves and the corresponding energy differences of the $1s\ ^1S \rightarrow 2p\ ^1P$ line.

3 Theoretical spectra

In radiative collision transitions it is the difference potential between the final and initial states that determines the frequency and the energy emitted or absorbed by a single photon. The shape of the line wing is sensitive to $\Delta V(R)$, the difference between the ground and excited state interaction potential. For the transitions $X \rightarrow D$ and $X \rightarrow F$ the difference potential maxima are respectively 4300 and 3000 cm^{-1} (Fig. 1) which lead to far blue satellite respectively at 4000 cm^{-1} (571.4 Å) and 2600 cm^{-1} (576 Å)(Fig. 2).

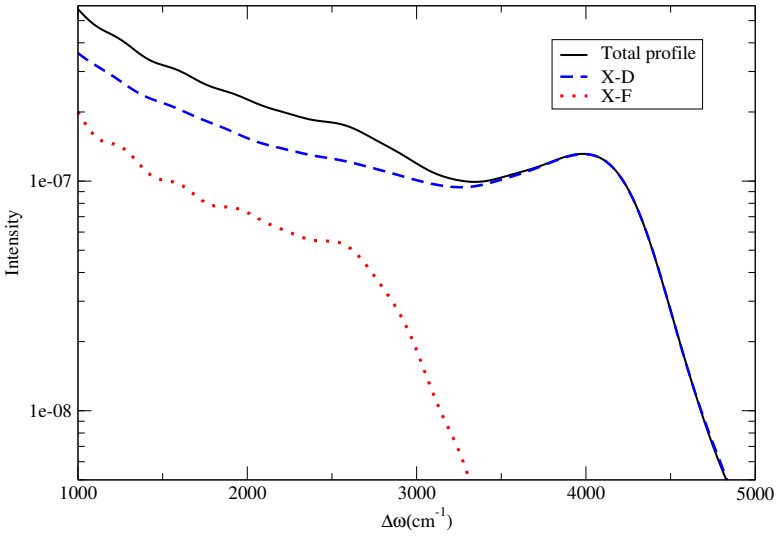

Fig. 2. Individual components of the blue far wing compared to the total one (T=1000 K and n_{He}= 10^{19} atoms cm^{-3}).

The unified profile, including the core of the line (Fig. 3), is asymmetrical and contributes only in the UV part. It is not correct to use Lorentzian profiles in the far wings, as is the standard practice in most stellar atmosphere work.

The cores are formed in the uppermost, lowest density atmospheric layers still dominated by He and H_2 collisions. Since in a model atmosphere calculation, the resulting line profile is the integration of the flux in all layers from the deepest to the uppermost, it is important that the centers be adequately represented, i.e., they can be non-Lorentzian at the high densities of the innermost layers, while Lorentzian in the upper atmosphere but with different widths than predicted by the hydrogenic van der Waals approximation usually used for the

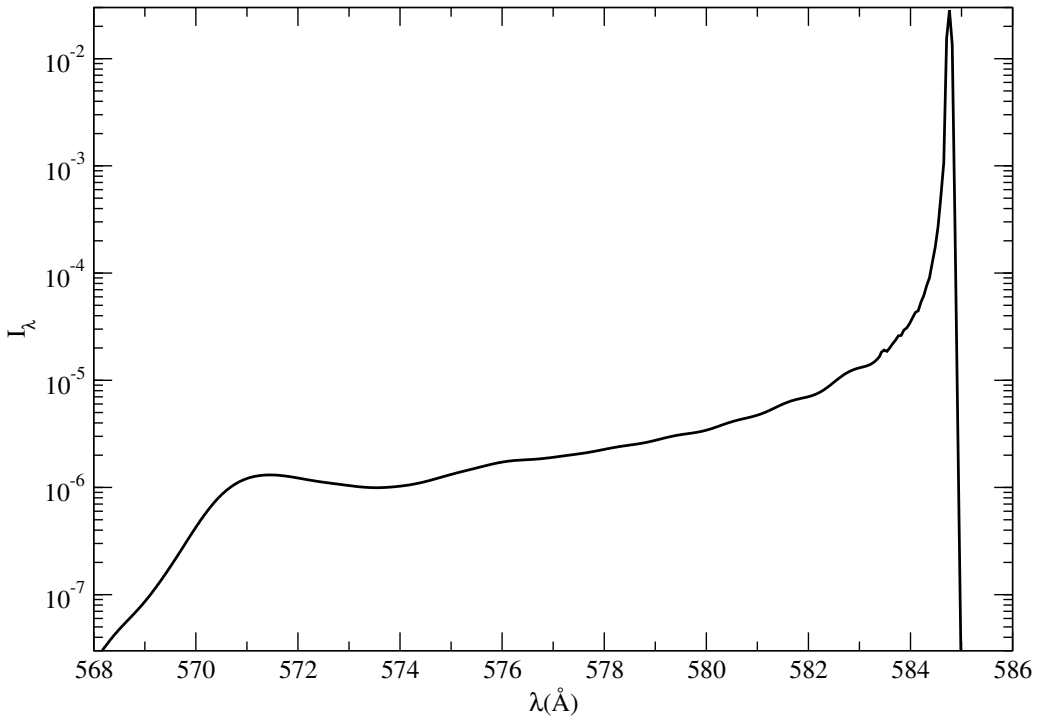

Fig. 3. Unified profile for T=1000 K and $n_{He}= 10^{20}$ atoms cm^{-3}.

Table 1: Variation with temperature of the full width at half maximum and shift (10^{-20} cm^{-1}/cm^{-3})

Line parameters	1000 K	2000 K	3000 K	4000 K	5000 K	6000 K
w_{imp}	2.44	2.6	2.77	2.86	2.97	3.12
d_{imp}	0.47	0.75	0.89	1.11	1.16	1.32

cores. At low densities, pressure broadening and shift of spectral lines are described by the well-known impact theory of Lindholm (1945). The variation of the impact width (full width at half maximum) and shift versus the temperature is given in Table 1.

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References

Allard, N. F., Koester, D., Feautrier, N., & Spielfiedel, A. 1994, A&A Suppl., 200, 58
Allard, N. F., Royer, A., Kielkopf, J. F., & Feautrier, N. 1999, Phys. Rev. A, 60, 1021
Deguilhem, B. 2009, in Ph. D. thesis (Toulouse, France: Université Paul Sabatier)
Lindholm, E. 1945, Ark. Fys. A, 32, 1