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THEORETICAL ANALYSIS OF THE MG(3 ^{3}P)-MG(4^{3}S) LINE SHAPE IN COOL DZ WHITE DWARFS

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Abstract. We present a determination of the Mg(3 ^{3}P)-Mg(4 ^{3}S) collisional line profiles using very recent *ab initio* potential energies. Results are reported for the conditions prevailing in cool DZ white dwarf atmospheres.

Keywords: white dwarfs - Stars: atmospheres - Lines: profiles

1 Introduction

Traces of heavy metal in cool DZ white dwarfs are now attributed to the accretion of circumstellar dust. This dust is thought to originate from the tidal disruption of some rocky material. They provide a unique opportunity to study the composition of extra-solar planetary systems. The determinations of precise atmospheric parameters and abundances require accurate description of the line profiles of the identified features. This work is a continuation of our studies of sodium and ionized calcium resonance lines perturbed by helium (Allard 2013; Allard & Alekseev 2014; Allard et al. 2014). The triplet $3p$-$4s$ line profiles of Mg perturbed by helium are calculated for the physical conditions encountered in the atmospheres of cool white dwarfs that exhibit a strong asymmetry in their spectra. We show that a line satellite band located in the near blue wing of the Mg line is responsible of an asymmetry not correctly considered by modelers of cool DZ white dwarfs. The asymmetrical shapes of spectral lines have been extensively investigated for many years because of their importance in experimental and theoretical work (Allard & Kielkopf 1982). Line profile calculations in our work have been done in unified line-shape semiclassical theory (Anderson 1952) using new *ab initio* potential energies that take into account the long range part. The analysis was based on line broadening theory reported in Allard et al. (1999). Several theoretical computed profiles are used to illustrate the evolution of the line satellite with pressure.

2 Potentials

The *ab initio* computation of the adiabatic potential energy curves of MgHe have been carried out using a large core pseudopotential for Mg complemented by operatorial Core Polarisation Potential (CPP) (Fuentealba et al. 1983) with the MOLPRO package. The large basis set we built was inspired from the standard (pseudopotential) basis set (Fuentealba et al. 1982) and the one used in rather high Rydberg calculations (Khemiri et al. 2013) leading to a 10s9p6d3f3g basis set. For He, the huge 30s17p10d6f3g basis set of Deguilhem and coworkers (Deguilhem et al. 2009) has been used. State specific orbitals were obtained from CASSCF calculations (Werner & Knowles 1985) , where the active space consisted of 4 electrons distributed in all orbitals up to the 4s orbital of Mg. These orbitals were then used in subsequent MRCI (Werner & Knowles 1988) calculations to obtain the potential energy curves as well as static and transition dipole moments for all allowed transitions. For this 4 electrons system, this leads to almost full CI quality calculations.

Potential energy curves $V(R)$ for the MgHe molecule in the $3p\,^3$P and $4s\,^3$S states are shown in Fig. 1, where R denotes the internuclear distance between the radiator and the perturber.

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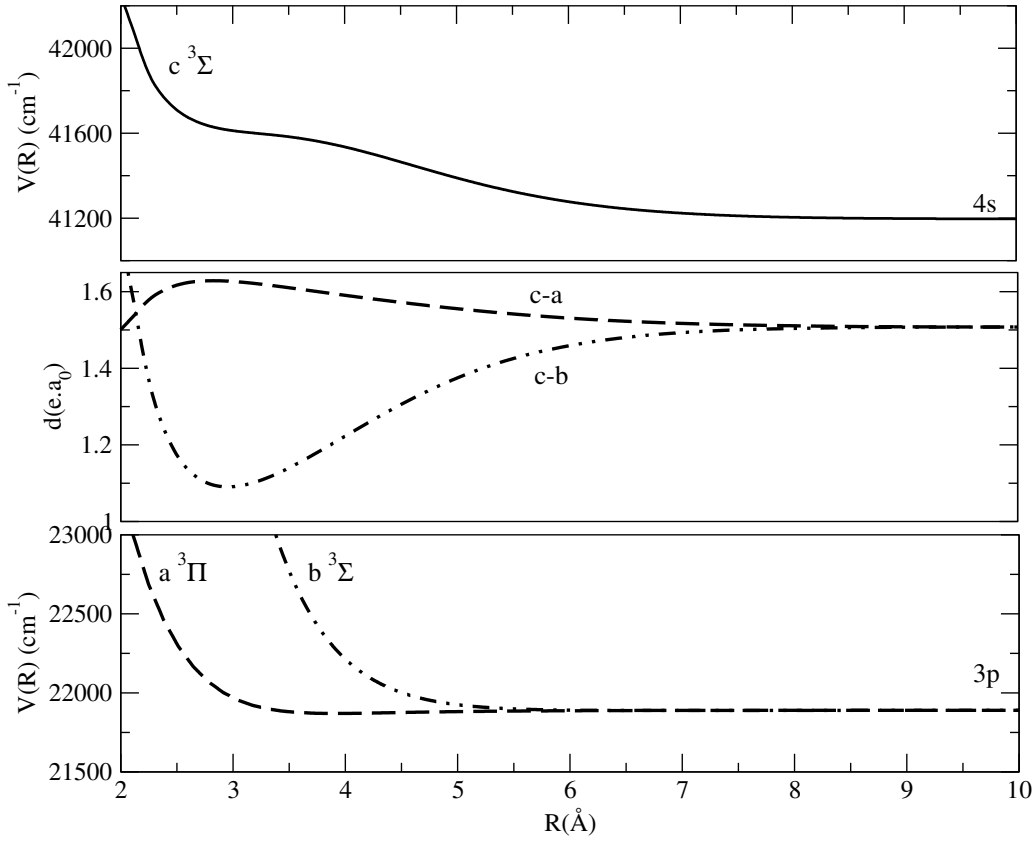

Fig. 1. Potential energies for the triplet $4s$ and $3p$ states of the Mg–He molecule and transition dipole moments.

3 Density dependence of the line profile

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 unified theory of Anderson (1952) predicts that there will be satellites centered periodically at frequencies corresponding to the extrema of the difference potential between the upper and lower states. Hence the interpretation of the asymmetrical shape of the $3p \rightarrow 4s$ line requires us to study ΔV, as shown in Fig. 2-left. The difference potential maxima are respectively 400 and 165 cm^{-1} for $3p\,^3\Pi \rightarrow 4S\,^3\Sigma$ and $3p\,^3\Sigma \rightarrow 4s\,^3\Sigma$. Figure 2-right shows the individual components for comparison, weighted as if they were the only contribution to the profile. The distinct wide shoulder at about 240 cm^{-1} due to the $3p\,^3\Pi \rightarrow 4S\,^3\Sigma$ transition, yields unresolved line satellite in the blue wing about 5120 Å (Fig. 3-right). The other maximum at ΔV= 165 cm$^-$1 does not give the slightest hint of a blue shoulder, the corresponding individual profile simply appears to have a blue asymmetry.

In Fig. 3 we show the variation of the line profiles at 6000 K with increasing helium density. When the density is about $1.75\times\ 10^{21}$ cm^{-3} the development of the blue wing leads to the overwhelming of the line by the satellite. The line satellite becomes higher than the main line for $n_{He} = 2.5\times\ 10^{21}$ cm^{-3} which has totally disappeared for $n_{He} = 4\times\ 10^{21}$ cm^{-3}.

4 Conclusion

The purpose of this study was to establish the link of the strong asymmetry observed in spectral features observed in cool DZ white dwarfs with the existence of an unresoved blue satellite. This effect is of increasing importance with He density, and as a result, the profile shifts towards the position of the satellite band. The asymmetry in the Mg profile is uncorrectly identified as due to quasistatic broadening since Wehrse & Liebert (1980) but the line shape does not depend on the assumption that the interaction is given by a van der Waals approximation.

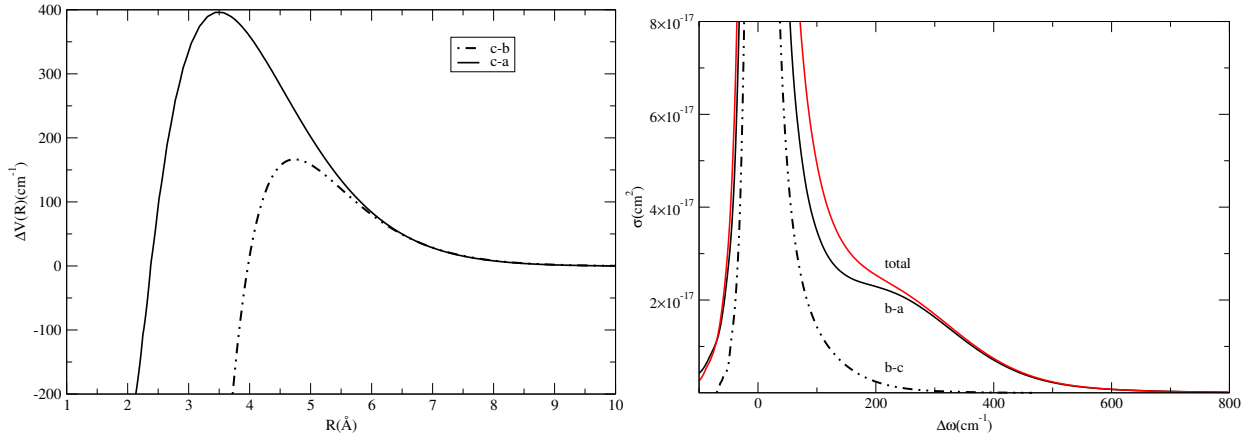

Fig. 2. Left: ΔV for the two transitions contributing to $3p \rightarrow 4s$ line. **Right:** Individual components of the line compared to the total profile. (T=6000 K and $n_{\rm He}$= 10^{20} cm^{-3}).

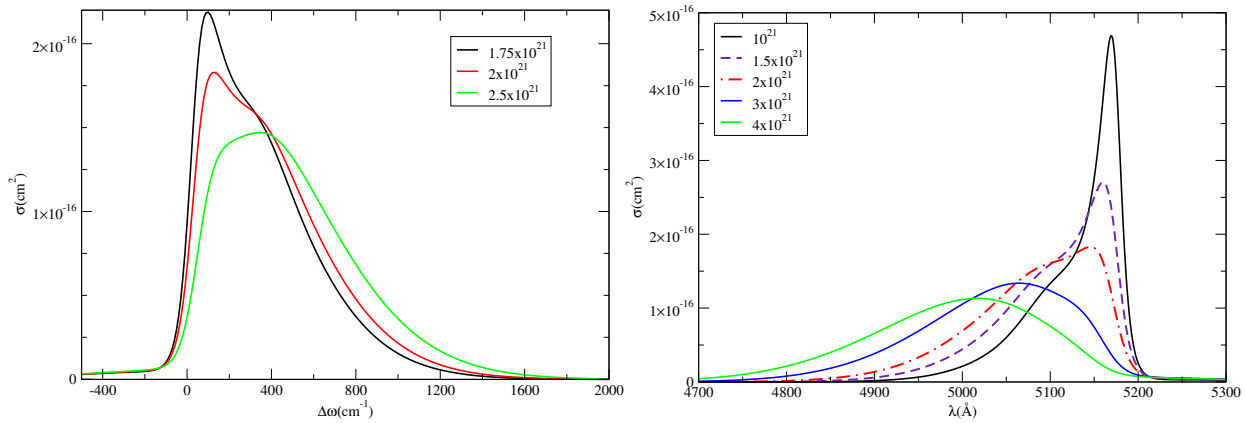

Fig. 3. Evolution of the unified profiles with increasing helium density. **Left:** $n_{\rm He}$= 1.75 to 2.5× 10^{21} cm^{-3}. **Right:** $n_{\rm He}$= 1 to 4× 10^{21} cm^{-3}.

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