Ab initio Stellar Astrophysics: Reliable Modeling of Cool White Dwarf Atmospheres

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Abstract. Over the last decade ab initio modeling of material properties has become widespread in diverse fields of research. It has proved to be a powerful tool for predicting various properties of matter under extreme conditions. We apply modern computational chemistry and materials science methods, including density functional theory (DFT), to solve lingering problems in the modeling of the dense atmospheres of cool white dwarfs ($T_{\text{eff}} < 7000$ K). Our work on the revision and improvements of the absorption mechanisms in the hydrogen and helium dominated atmospheres resulted in a new set of atmosphere models. By inclusion of the Ly-α red wing opacity we successfully fitted the entire spectral energy distributions of known cool DA stars. In the subsequent work we fitted the majority of the coolest stars with hydrogen-rich models. This finding challenges our understanding of the spectral evolution of cool white dwarfs. We discuss a few examples, including the cool companion to the pulsar PSR J0437-4715. The two problems important for the understanding of cool white dwarfs are the behavior of negative hydrogen ion and molecular carbon in a fluid-like, helium dominated medium. Using ab initio methods we investigate the stability and opacity of these two species in dense helium. Our investigation of C$_2$ indicates that the absorption features observed in the “peculiar” DQp white dwarfs resemble the absorption of perturbed C$_2$ in dense helium.

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INTRODUCTION

Cool White dwarfs are among the oldest stars in the Galaxy. Being Gyrs old these stellar remnants are of importance for dating old stellar populations and understanding their star formation history. We are interested in understanding the physical properties of the atmospheres and the spectra of cool white dwarfs. Over the last years we have introduced several improvements in the physics of dense media in our atmosphere models, including the radiative transfer in the refractive atmosphere, the non-ideal chemical equilibrium abundances of spectroscopically important species and the opacity of dense helium. Identification of the missing absorption mechanism at short wavelengths in the models of hydrogen-rich atmospheres as the Ly-α red wing opacity as well as better description of helium-rich atmospheres have a significant impact on our understanding of cool white dwarfs. These improvements dramatically change the predicted flux at short wavelengths (especially in the Johnson U and B, and SDSS u and g filters). The hydrogen atmosphere models follow the observed sequence of cool white dwarfs on various color-color diagrams (Fig. 1). The best fits to the spectral energy distributions of the individual stars with $T_{\text{eff}} < 6000$ K have been obtained with hydrogen-rich models. This suggest that most of the cool stars possess hydrogen-rich atmospheres, which challenges...
the current picture of the spectral evolution of cool white dwarfs.

In order to investigate the chemical evolution of white dwarf atmospheres the more extreme, fluid-like atmospheres of helium-rich stars have to be better understood. The atmospheres of these stars have extreme pressures and densities of a few g/cm$^3$ and can not be described by ideal gas laws but must rather be treated as a helium-rich fluid in which the strong inter-particle interactions determine its physics and chemistry. The conditions prevailing at the surfaces of the helium-rich atmosphere stars could be diagnosed with trace species such as H$^-$ and C$_2$, through the impact of dense fluid on their absorption and the resulting white dwarf spectra. Using modern methods we compute the properties of these species in dense helium. The resulted high-pressure-induced spectral distortions are then matched with absorption signatures observed in the spectra of helium-rich stars (like distorted Swan bands in DQp stars) to derive the atmospheric parameters of the stars.

VALIDATION OF THE MODELS

With a grid of improved atmosphere models we have analyzed large samples of cool white dwarfs. The colors of the new models are compared to a large SDSS sample in Figure 1. The new pure-H models not only reproduce the observed sequence of white dwarfs better than previous models but also show the need to include extreme line broadening of Ly-$\alpha$ to characterize white dwarfs with $T_{\text{eff}} < 6000$K when the short wavelength filters are used ($\lambda < 8000$ Å). We also fitted the individual SEDs of a large
sample of cool white dwarfs. We found that most of the stars we fitted have pure-H atmospheres, with several having mixed H/He atmospheres dominated by H. Most of the stars previously identified as having pure-He atmospheres [1, 2] turn out to be hydrogen-rich stars in our analysis [3, 4, 5, 6]. Two examples of such fits are given in figure 2. We also observe that the amount of helium in mixed stars seems to decrease with the decrease in the effective temperature and the coolest stars ($T_{\text{eff}} < 4500$ K) possess pure-H atmospheres. The interpretation of these results requires further investigation and new, targeted observations to further validate the models.

The dependence of the derived atmospheric parameters on the atmosphere models used in the investigation is also evident for the low-mass, He-core white dwarfs. These under-massive white dwarfs evolve through mass transfer in binary systems. One of the best known such system is a cool white dwarf orbiting the millisecond pulsar PSR J0437-4715. Using the atmosphere models of Bergeron et al. [7] the white dwarf was assigned a helium-rich atmosphere [8], which is at odds with the evolutionary models of such stars. We fitted the entire spectral energy distribution of the star, including HST UV, optical, near- and mid-infrared spectra with our models. The result is shown in figure 3. An excellent fit is obtained with a pure-H atmosphere model with $T_{\text{eff}} \sim 4000$ K. The presence of hydrogen is indicated by the flux suppression in the UV because the Ly-$\alpha$ opacity and near-IR because of CIA opacity from molecular hydrogen [9], comparing with the fit by the pure-He atmosphere model.

**AB INITIO INVESTIGATIONS**

*Ab initio* methods represent a novel approach to the modeling of the properties of fluid-like stellar atmospheres. In combination with the methods of the classical theory of
**FIGURE 3.** The measured spectrum of the pulsar and cool white dwarf binary system PSR J0437-4715 [21]. Lines represent the fits by pure-H and pure-He models. The short wavelength flux is a contribution from the pulsar. The unit of the flux is erg cm$^{-2}$ s$^{-1}$ Å$^{-1}$.

Fluids they are a powerful tool for predicting the thermodynamical, optical and chemical properties of cool white dwarf atmospheres. In our work we use the density functional theory, the most common *ab initio* method (PBE functional and plane wave codes, see Koch & Holthausen [10]). Below we briefly discuss two examples of our recent *ab initio* work (see also Kowalski, these proceedings).

### $H^-$ in dense helium

By the time it reaches $T_{\text{eff}} \sim 6000$K a white dwarf with an initial pure-He atmosphere should have accreted enough hydrogen from the interstellar medium for the latter to be detectable through the prominent bound-free opacity from the negative hydrogen ion. Bergeron et al. [1] suggested that the negative hydrogen ion undergoes pressure ionization in the dense helium atmospheres, which could explain the absence of hydrogen in the spectra of helium-rich, cool white dwarfs. In order to address this problem, we performed quantum mechanical calculations of $H^-$ in dense helium. Surprisingly, at least up to the density of helium of 4 g/cm$^3$ (which is the highest density reached in the cool white dwarfs atmospheres) the negative hydrogen ion remains bound, which is indicated by the presence of two electrons around the proton.

### $C_2$ in dense helium

Some helium-rich atmosphere white dwarfs (DQ/DQp) show the $C_2$ bands in the optical (Swan bands). This gives the opportunity not only to investigate the properties
of molecular heads in their atmospheres, but to use $C_2$ as a probe of the physical conditions in cool helium-rich atmospheres, which are still poorly understood. There are two noteworthy observational facts about the DQ/DQp white dwarfs. Cutoff in their cooling sequence at $T_{\text{eff}} \sim 6000\, \text{K}$ [11, 12] and the appearance of so called DQp stars, which show distorted Swan-bands-like spectral features in the optical, at lower effective temperatures [13, 1]. The examples of spectra of both types of stars are given in figure 4. Two different explanations for the origin of the spectral features have been discussed in the literature. Lebofsky & Liebert [14], Hall & Maxwell [15] speculated that the DQp stars show pressure shifted bands of $C_2$, while other researchers point to a different molecular species [13, 1, 16]. The second idea was critically reviewed by Hall & Maxwell [15]. To elucidate the nature of the spectral features observed in DQp stars we performed an extensive investigation of spectroscopic properties of $C_2$ in dense helium, the electronic transition energy for the Swan bands and the vibrational frequencies, in dense fluid helium [17]. Our calculations show that the electronic transition energy for the Swan absorption increases significantly with the density ($\Delta T_e \sim 1.6\rho_{\text{He}} \,(\text{eV})$), causing a blueward shift of the Swan bands in the spectra of DQp stars. The observed shifts of about 0.08 eV for most of the DQpes indicate that the bands form at density of $\sim 0.05\, \text{g/cm}^3$, which is an order of magnitude lower than the one predicted by pure-He/C atmosphere models. This suggest pollution by hydrogen, which even in small amounts increases the opacity and can lower the atmospheric density to the required values.

Our result shows that the optical bands observed in DQp stars are pressure shifted $C_2$ bands as was originally proposed by Lebofsky & Liebert [14]. The same approach to the $^3\Pi_u \rightarrow ^3\Sigma_g^-$ Ballik-Ramsay absorption (10000-18000 $\AA$ bands, Ballik & Ramsay [18]) gives the blueward shifts of at least 1000 $\AA$ ($\Delta T_e = 2.2\rho_{\text{He}} \,(\text{eV})$) for these bands in DQpes. The distortion of the Ballik-Ramsay bands may produce the spectral depression observed at $\sim 1\, \mu\text{m}$ for the DQp star LHS2293 [19].
CONCLUSIONS

The atmospheres of cool white dwarfs could be understood only by having a reliable set of both hydrogen- and helium-rich atmosphere models, and modern ab initio methods of computational quantum mechanics are powerful tools to generate the necessary constitutive physics. With our improved models we have fitted the entire SEDs of various types of white dwarfs. Most of the white dwarfs with $T_{\text{eff}} < 5000\,\text{K}$ show H-rich atmospheric composition and the coolest stars could be fitted only with the pure-H models. This indicates that the accretion of hydrogen from the ISM plays an important role in the evolution of white dwarf atmospheres. Our investigation of the properties of molecular carbon in the helium-rich atmosphere DQ/DQp stars shows that the molecular bands observed in the optical spectra of DQp stars are the pressure shifted Swan bands.

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