A&A 566, L8 (2014)
DOI: 10.1051/0004-6361/201424242

Astronomy & Astrophysics

Letter to the Editor

Infrared absorption of dense helium and its importance in the atmospheres of cool white dwarfs★

Piotr M. Kowalski

IEK-6 Institute of Energy and Climate Research, Forschungszentrum Jülich, Wilhelm-Johnen-Strasse, 52425 Jülich, Germany
e-mail: p.kowalski@fz-juelich.de

Received 20 May 2014 / Accepted 9 June 2014

ABSTRACT

Aims. Hydrogen-deficient white dwarfs are characterized by very dense, fluid-like atmospheres of complex physics and chemistry that are still poorly understood. The incomplete description of these atmospheres by the models results in serious problems with the description of spectra of these stars and subsequent difficulties in derivation of their surface parameters. Here, we address the problem of infrared (IR) opacities in the atmospheres of cool white dwarfs by direct ab initio simulations of IR absorption of dense helium.

Methods. We applied state-of-the-art density functional theory-based quantum molecular dynamics simulations to obtain the time evolution of the induced dipole moment. The IR absorption coefficients were obtained by the Fourier transform of the dipole moment time autocorrelation function.

Results. We found that a dipole moment is induced due to three- and more-body simultaneous collisions between helium atoms in highly compressed helium. This results in a significant IR absorption that is directly proportional to $\rho_{\rm He}^3$, where $\rho_{\rm He}$ is the density of helium. To our knowledge, this absorption mechanism has never been measured or computed before and is therefore not accounted for in the current atmosphere models. It should dominate the other collisionally induced absorptions (CIA), arising from H−He and H_2−He pair collisions, and therefore shape the IR spectra of helium-dominated and pure helium atmosphere cool white dwarfs for He/H > 10^4.

Conclusions. Our work shows that there exists an unaccounted IR absorption mechanism arising from the multi-collisions between He atoms in the helium-rich atmospheres of cool white dwarfs, including pure helium atmospheres. This absorption may be responsible for a yet unexplained frequency dependence of near- and mid-IR spectra of helium-rich stars.

Key words. atomic processes – dense matter – stars: atmospheres – white dwarfs

1. Introduction

Being billions of years old, cool white dwarfs with $T_{\rm eff}$ < 8000 K have received significant attention because they can be used as cosmochronometers (Lebofsky & Liebert 1984; Fontaine et al. 2000). Their spectra carry important information that, when correctly decoded, can tell us about physical parameters, such as $T_{\rm eff}$, gravity, and chemical composition of their atmospheres, which reveals in return information about past stellar and planetary formation processes prevailing in our Galaxy (Farihi 2009; Fontaine et al. 2000; Richer et al. 2006). This information could be correctly deciphered only when a reliable set of the atmosphere models is used in the analysis (Kowalski et al. 2013; Kowalski 2007). Unfortunately, having fluid-like densities of up to a few g/cm^3 (see Fig. 1), the atmospheres of helium-rich white dwarfs are very difficult to model. Over the last decade, several dense-fluid effects were introduced into the modeling that substantially improved the description and understanding of the atmospheres of these stars. These include the pressure-induced absorption mechanisms (Iglesias et al. 2002; Kowalski & Saumon 2006; Kowalski 2006b, 2010; Gustafsson & Frommhold 2001), the refractive radiative transfer equation (Kowalski & Saumon 2004), the non-ideal equation of state and chemistry of spectroscopically important species (Kowalski et al. 2007; Kowalski 2006a) and also the recently improved H_2–He collision induced absorption (Abel et al. 2012). However, because of their complex physics and chemistry, the atmospheres of helium-rich, cool white dwarfs are still poorly understood, which is indicated by poor fits to the spectral energy distributions of these stars by models (Bergeron & Leggett 2002; Kilic et al. 2009; Kowalski et al. 2013). Most of these problematic stars, such as LHS3250 (Harris et al. 1999; Bergeron & Leggett 2002), or the several so-called ultra-cool white dwarfs that were discovered thanks to the Sloan Digital Sky Survey (Gates et al. 2004; Bergeron & Leggett 2002) show significant near- and mid-IR flux depletion that is thought to be caused by the strong H_2−He and H−He collisionally induced absorptions (CIA) in extremely dense, helium-dominated atmospheres (He/H $\gg 10^3$). However, none of such spectra, especially their near- and mid-IR parts, could be successfully fitted by the current models.

In this contribution, we address the problem of IR absorption by performing state-of-the-art ab initio molecular dynamics simulations of the IR opacities of dense helium. Because IR opacities from pure helium have never been reported before, we were looking for any IR absorption signatures caused by fluctuations of the dipole moments induced in highly compressed helium. We were especially interested in its strength and importance in the atmospheres of helium-rich, cool white dwarfs. Our ab initio simulations have revealed the then unknown infrared absorption mechanism that shapes the

★ The opacity table is only available at the CDS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5) or via http://cdsarc.u-strasbg.fr/viz-bin/qcat?J/A+A/566/L8

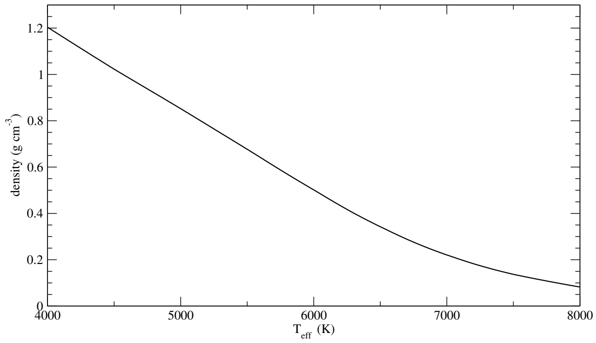

Fig. 1. Photospheric density ($\tau_r = 2/3$) in the pure He white dwarf atmospheres of given $T_{\rm eff}$, as predicted by our atmosphere models (see the text for models details).

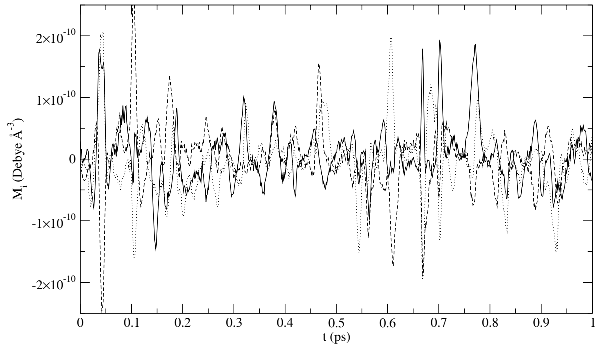

Fig. 2. Time evolution of the components of the dipole moment vector $\boldsymbol{M}$ in dense helium of $T = 5000$ K and $\rho_{\rm He} = 514$ amagat, where amagat $= 2.68678 \times 10^{19}$ cm^{-3}. The lines mark M_x (solid), M_y (dotted), and M_z (dashed) components.

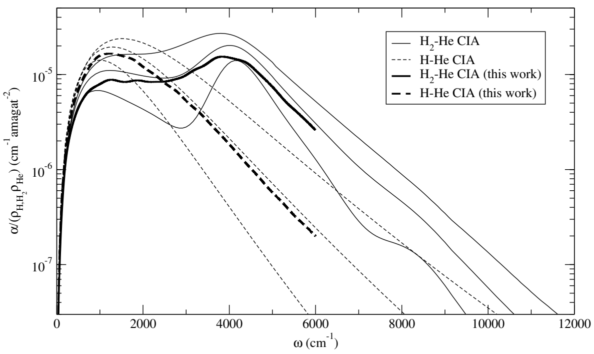

Fig. 3. H_2−He (thin solid lines, Abel et al. (2012)) and H−He (thin dashed lines, Gustafsson & Frommhold (2001)) CIA opacities. The results for $T = 7000$ K, 5000 K and 3000 K are presented (*from top to bottom*). The thick lines represent the result of our simulation performed for $T = 5000$ K, $\rho_{\rm H_2,H} = 16$ amagat, and $\rho_{\rm He} = 498$ amagat, where amagat $= 2.68678 \times 10^{19}$ cm^{-3}.

IR spectra of helium-rich atmosphere, cool white dwarfs. We show that this absorption, which is a few orders of magnitude weaker in absorption cross-section than already accounted for in the models H−He and H_2−He CIA opacities, dominates the IR absorption when He/H > 10^4, including the pure He case.

2. Computational approach

Our simulations were performed by application of density functional theory (DFT) method, which is widely used in the quantum mechanical computations of dense, complex, many particle systems (Koch & Holthausen 2000). The DFT methods are appropriate for calculations of the ground state energies of multi-electron systems, and have proven to be very useful in calculations of various chemical and physical properties of atoms, molecules, solids, and matter under high compression (Jahn & Kowalski 2014), including those constituting the atmospheres of cool white dwarfs (e.g., Kowalski et al. 2007; Kowalski 2010). In our work, we used one of the most common implementations of DFT, the generalized gradient approximation (GGA) with PBE exchange-correlation functional (Perdew 1996). We used plane-wave DFT CPMD code (Marx & Hutter 2000) with ultrasoft pseudopotentials (Vanderbilt 1990), and the energy cut-off of 340 eV. The Born-Oppenheimer molecular dynamics simulations were performed on 32 atoms containing supercells, and in each simulation, a 160 ps long trajectory was generated. The total dipole moment of the supercell was computed in every step with the timestep of 1.2 fs. We notice that we neglect the higher frequency simulation results in the analysis because this timestep gives good sampling of frequencies up to about 6000 cm^{-1}.

The IR spectrum is represented by the frequency-dependent absorptivity coefficient, $\alpha(\omega)$, that was computed through the Fourier transform of the dipole moment time autocorrelation function (Guillot 1991; Silvestrelli et al. 1997; Jahn & Kowalski 2014) as

$$\alpha(\omega) = \frac{2\pi\omega^2}{3ck_{\rm B}TV} \int_{-\infty}^{\infty} {\rm d}t \exp(-{\rm i}\omega t) \langle \boldsymbol{M}(t) \cdot \boldsymbol{M}(0) \rangle, \quad (1)$$

where c, $K_{\rm B}$ and V are the speed of light, the Boltzmann constant, and the supercell volume respectively. The vector $\boldsymbol{M}(t)$ is the total dipole moment of the simulation cell at a time t. The method of computing IR opacities by the means of molecular dynamics simulations has been used in the past, for instance for calculation of IR spectrum of water (Silvestrelli et al. 1997; Iftimie & Tuckerman 2005; Guillot 1991). We note that the real absorption coefficient that is used in the modeling is given by $\alpha(\omega)/n(\omega)$, where $n(\omega)$ is the index of refraction, because an atmosphere of a cool, helium-rich white dwarf is a refractive medium (Kowalski & Saumon 2004). In Fig. 2, we show an example of the time evolution of the $\boldsymbol{M}(t)$ vector components that gives rise to the non-negligible IR absorption by dense helium.

To compute the atmosphere models we used our own stellar atmosphere code that accounts for various dense medium effects, like the refraction (Kowalski & Saumon 2004), the non-ideal equation of state and chemical equilibrium (Kowalski 2006a; Kowalski et al. 2007) and the high density corrections to the important absorption mechanisms (Iglesias et al. 2002; Kowalski & Saumon 2006; Kowalski 2006b). It also includes the recently improved H_2−He CIA opacities of Abel et al. (2012).

3. Results and discussion

3.1. H–He and H_2–He CIA opacities

To test the applied IR absorption simulation method, we first computed the IR absorption of a supercell containing one H atom or H_2 molecule and 31 He atoms. Such a simulation should result in the reproduction of already known H−He and H_2−He CIA opacities. The comparison of the result of our simulations that were performed for $T = 5000$ K, with the H−He and H_2−He CIA profiles of Gustafsson & Frommhold (2001) and Abel et al. (2012) is given in Fig. 3. The simulated IR absorptions reproduce the shapes of both CIA absorption profiles well. The simulations underestimate the absorption profiles by a factor of up to ∼1.25, but they correctly predict the magnitude of the

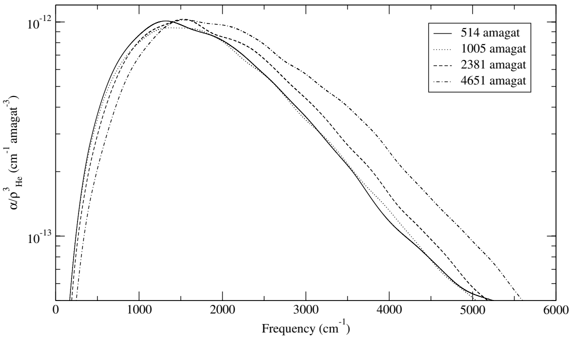

Fig. 4. Simulated IR absorption profiles of dense helium obtained for T = 5000 K and various helium densities indicated in the figure legend. The densities are expressed in amagat = 2.68678×10^{19} cm^{-3}.

absorption strength and the higher frequency profiles are also relatively well reproduced. Overall, this exercise shows that the DFT-based simulations of IR spectra are able to predict correctly the strength and shape of the IR absorption of dense H/He.

3.2. CIA opacity of dense helium

First, we computed the absorption coefficients for temperature of 5000 K and several densities. The result is given in Fig. 4. We found that the absorption coefficient is proportional to the cube of density, which is different from the case of H−He and H_2−He CIA opacities, where the relative absorption coefficients are proportional to the square of density (Gustafsson & Frommhold 2001; Abel et al. 2012). This is expected because the power of density indicates the multiplicity of collisions that contribute to the induction of the dipole moment. During a collision of a pair of identical atoms, such as two He atoms, the net dipole moment is zero and such a collision-pair is IR inactive. Therefore, the result given in Fig. 4 shows that the IR absorption arises mainly from ternary collisions in dense helium. It is therefore much weaker by about four orders of magnitude than the H−He and H_2−He CIA absorptions (comparing results given in Figs. 3 and 4 and assuming the density of perturbers of about 1000 amagat). For the most extreme densities represented in Fig. 4 we notice that the absorption profile becomes slightly blueshifted, which is most probably due to contributions from multiple collisions beyond the ternary ones. Because this effect becomes significant at the most extreme densities (>0.8 g/cm^3), at which it should cause just a 400 Å blueshift of the absorption spectrum, this is a second order effect, and we neglect it in further analysis. The accurate analysis of the contribution to the IR opacity from more than ternary collisions would require more extensive studies with larger simulations cells that contain more He atoms, which may be a topic of the subsequent studies. On the other hand, neglecting this pressure-induced blueshift does not affect the conclusions of the paper.

Having found the density dependence of the helium IR absorptivity coefficient we simulated the absorption coefficients for several temperatures of 1000 K, 2000 K, 2500 K, 3000 K, 4000 K, 5000 K, 6000 K, 7500 K, 8000 K, 9000 K and 10 000 K and fixed helium density of ρ = 514 amagat = 1.38 × 10^{22} cm^{-3} = 0.092 g/cm^3. The resulted absorption profiles were then fitted to the analytical formula:

$$\alpha(\omega)/\rho^3_{\rm He} = \beta\omega^{2.5}{\rm e}^{\gamma(T)\omega} \text{ for } \omega < \omega_0\,, \quad (2)$$

$$\alpha(\omega)/\rho^3_{\rm He} = \beta\omega_0^{2.5}{\rm e}^{\gamma(T)\omega_0}{\rm e}^{(\gamma(T)+6.25\times10^{-4})(\omega-\omega_0)} \text{ for } \omega > \omega_0\,, \quad (3)$$

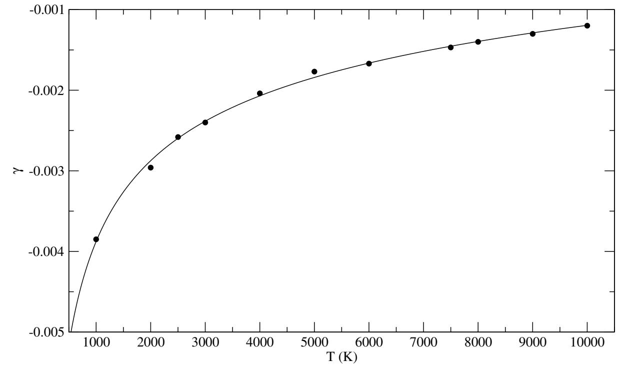

Fig. 5. Temperature-dependent parameter γ as a function of temperature. The points represent the computed values and the line is the best fit given by Eq. (4).

where ω_0 = 4000 cm^{-1} and $\alpha(\omega)/\rho^3_{\rm He}$ is given in cm^{-1}*amagat*$^{-3}$. The high frequency approximation is constructed, so the value and the derivative over ω of the two expressions match at $\omega = \omega_0$ and the $\log(\alpha(\omega)/\rho^3_{\rm He})$ is a linear function of ω for large ω. We selected this simple model to represent the results of the simulations, so it resembles the shape of the simulated absorption and the already known absorption profiles of H−He CIA (Gustafsson & Frommhold 2001). The initial fits suggested that the numerical prefactor β is temperature independent. Therefore, we decided to fix it to the average value of 1.56×10^{-19}, which was obtained by fitting all the simulated results. Then we performed one-dimensional fit of $\gamma(T)$ function to the data. The obtained $\gamma(T)$ as a function of temperature is

$$\gamma = \left(-0.0601248 + 1.55103 \times 10^{-6}T\right) \cdot T^{-0.393053} \quad (4)$$

and is visualized in Fig. 5 with the simulation results. Although complex models of the CIA profiles exist, such as the enhanced Birnbaum-Cohen line shape model used by Gustafsson & Frommhold (2001), we found the outlined simple model adequate for our purpose. The modeled $\alpha(\omega)$ of dense helium is given in Fig. 6, where we also included the simulated absorption profiles for selected temperatures. One can see that the overall match of the model to the simulated profiles is pretty good.

3.3. New synthetic spectra of He-rich white dwarfs

Having the new IR absorption, in the next step we tested its importance in the atmospheres of cool white dwarfs. In Fig. 7, we plotted the synthetic spectra of cool, helium-rich stars computed with and without the new opacity. On the left panel, we plotted the sequence of $T_{\rm eff}$ = 5300 K and $\log g = 8\,(cgs)$ models. Because of its weaker strength comparing to H−He and H_2−He CIA opacities, the new absorption reveals itself in models with He/H > 10^4. It also significantly reduces the IR fluxes of pure He atmospheres, as shown in the right panel. Because the atmosphere becomes more extreme with lowering $T_{\rm eff}$ (see Fig. 1), the effect increases with a decrease in $T_{\rm eff}$, and it reduces the IR flux by ~50% for $T_{\rm eff}$ = 4000 K. On the other hand, it starts to become important only for $T_{\rm eff}$ < 8000 K. This is because the atmosphere is significantly less dense at higher $T_{\rm eff}$ and other absorption mechanisms, such as He^- free-free absorption (Iglesias et al. 2002), whose strength rises exponentially with temperature, become dominant.

In Kowalski et al. (2013), we have demonstrated that our inability to fit the spectra of He-rich atmosphere stars, such as LHS1126 and LHS3250, shows that there may be a problem

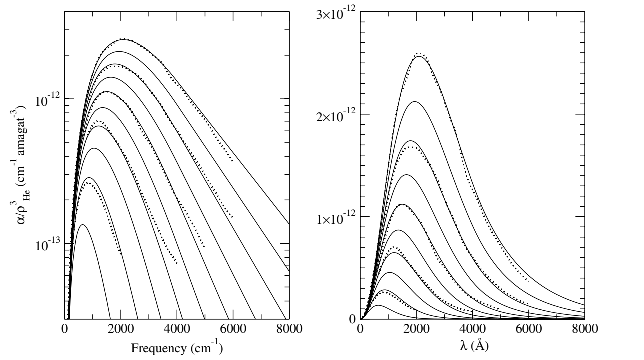

Fig. 6. IR opacity of dense helium for different temperatures given by our model (Eqs. (2)–(4)). The temperature T = 1000 K to 10 000 K by increments of 1000 K (from bottom to top). The dotted lines represent the results of the simulation for T = 2000 K, 4000 K, 6000 K, 8000 K, and 10 000 K. The vertical axis label of the *right panel* is identical to that of the *left panel*.

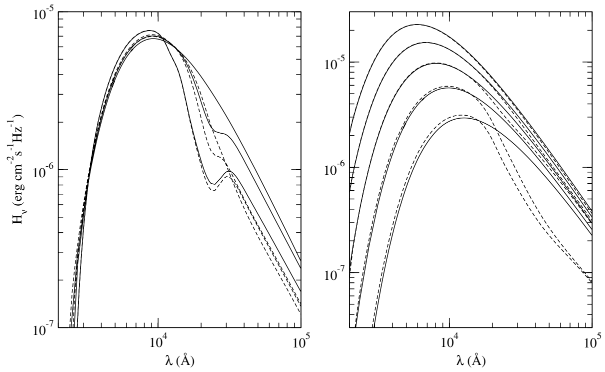

Fig. 7. *Left panel*: synthetic spectra of $T_{\rm eff}$ = 5300 K and log g = 8 (cgs) helium-rich white dwarfs computed without (solid lines) and with (dashed lines) the IR opacity of helium computed in these studies. The three sets of lines represent the models of He/H = 10^6 (resembling the pure He spectrum), 10^5 and 10^4, counting from top to bottom by taking the values at λ = 20 000 Å. *Right panel*: synthetic spectra of pure He atmosphere white dwarfs (log g = 8 (cgs)) computed without (solid lines) and with (dashed lines) the IR opacity of helium computed in these studies. The different sets of lines represent the results for $T_{\rm eff}$ = 8000 K, 7000 K, 6000 K, 5000 K and 4000 K (from top to bottom). The vertical axis label is identical to that of the left panel.

with the current IR opacities implemented in the atmosphere codes and that the additional IR absorption mechanisms may be present in the atmospheres of these stars. Indeed, with the reported CIA opacities of helium, the new synthetic spectra show substantially reduced fluxes in IR, and we suspect that the new absorption accounts for at least some of the discrepancy between models and the observed spectra. However, the detailed fitting of the spectra of cool white dwarfs requires reliable description of the ionization equilibrium in dense helium, which is still rather poorly constrained (Kowalski et al. 2007, 2013). This is because the ionization fraction determines the strength of the He^- free-free absorption (Kowalski et al. 2007), which interplay with the strength of the IR absorption shapes the spectra of these stars. We therefore avoid such an analysis in this study.

4. Conclusions

We report a previously unknown IR absorption mechanism resulting from the collisions between He atoms, which we simulated by the ab initio molecular dynamics method. The new CIA opacity is proportional to $\rho^3_{\rm He}$ and arises mainly from the ternary collisions between helium atoms. It should dominate the IR absorption in atmospheres of cool, He-rich white dwarfs with He/H > 10^4, including the pure He case, and it may be responsible for problems in fitting the spectra of such stars by current models. With the discovery of this new absorption mechanism, we are closer to understanding the absorption processes that prevail in dense helium at extreme conditions, which should result in a better description of the atmospheres of cool white dwarfs by models.

Acknowledgements. We thank Lothar Frommhold for discussing the issue of collisional induced absorption in dense helium and the manuscript, and the reviewer Pierre Bergeron as well as Didier Saumon for comments on the manuscript.

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