THE FREE-FREE OPACITY IN WARM, DENSE, AND WEAKLY IONIZED HELIUM

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Abstract. We investigate the ionization and the opacity of warm, dense helium under conditions found in the atmospheres of cool white dwarf stars. Our particular interest is in densities up to 3 g/cm³ and temperatures from 1000K to 10000K. For these physical conditions various approaches for modeling the ionization equilibrium predict ionization fractions that differ by orders of magnitudes. Furthermore, estimates of the density at which helium pressure-ionizes vary from 0.3 to 14 g/cm³. In this context, the value of the electron-atom inverse bremsstrahlung absorption is highly uncertain. We present new results obtained from a non-ideal chemical model for the ionization equilibrium, from Quantum Molecular Dynamics (QMD) simulations, and from the analysis of experimental data to better understand the ionization fraction in fluid helium in the weak ionization limit.

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INTRODUCTION

We are interested in the opacity of He and He/H mixtures for densities up to 3 g/cm³ and temperatures of $T = 1000K$ to 10000K to model the atmospheres of very cool white dwarf stars. Our work is motivated by the fact that there exists a wide range of predictions for the density at which helium pressure-ionizes (Table 1). This translates into large uncertainties in the number of free electrons and the value of the free-free opacity in the regime of our interest. We approach this problem by constructing more reliable models for ionization equilibrium of He on the basis of a chemical model, QMD simulations, and available experimental data [1].

The current state of modeling

There is a large span in predictions for the density at which the pressure ionization phenomenon occurs in helium (Table 1).

For the chemical models [1]-[5], this arises from oversimplified treatments of the physics and the presence of free parameters. The interactions between atoms and ions are usually described by a polarization potential with a hard sphere cut off at short dis-
tance (e.g., [5]), which varies between models. Often they are simply neglected (see [4]). In particular, it is not correct to treat the e − He interaction with a polarization potential [7], as we discuss below.

The more sophisticated quantum calculations of the $T = 0$ K solid predict a high density for pressure ionization [6], which we confirm with QMD simulations. On the other hand the only published experimental data [1] suggest that this phenomenon occurs at density $\sim 1.5 - 2.0$ g/cm$^3$.

THE ELECTRON-HELIUM INTERACTION

The energy of a free electron in cryogenic helium has been shown experimentally to be as large as $V_e \sim +1.5$ eV (positive) at densities of $\sim 0.2$ g/cm$^3$ [8]. This is in the quantitative agreement with the prediction of the Lenz potential energy [9]

$$V_e = 2\pi \hbar^2 n(\text{He}) a / m_e,$$

where $a \sim 1.3$ a.u. is the scattering length [9], and $n(\text{He})$ is the number density of helium. This is because the e − He interaction is strongly repulsive for $r > 1$ a.u. [10], and significantly different from the polarization interaction [7] (Fig. 1a, solid & dotted curves). The quantum mechanical calculations for the energy of an electron in dense helium, using the potential of [10], are in good agreement with experimental data [11]. This shows that free electrons interact strongly with the atoms in dense He, but not through an attractive polarization potential. This is an important element in chemical models.

To introduce the interaction of quantum mechanical electrons with the atoms in a chemical model of the thermodynamics, we performed Density Functional Theory (DFT) calculation of the free energy of free electron in dense He. The results are well approximated by the Lenz formula (Fig. 1b), which we adopt in the chemical model.

THE CHEMICAL MODEL FOR THE IONIZATION EQUILIBRIUM

We constructed a chemical model considering the following species: He, He$^+$, He$^+_2$, e$^-$. The interactions between atoms and ions are described by the potentials shown in Fig. 1a. In the chemical picture, the non-ideal effects can be treated as a shift in the ionization/dissociation energies [3]. Considering the reactions He $\leftrightarrow$ He$^+$ + e$^-$ and He$^+_2 \leftrightarrow$ He$+$ + e$^-$ the shifts are $\Delta I_1 = \mu^{\text{id}}(\text{He}) - \mu^{\text{mid}}(\text{He}^+) - \mu^{\text{mid}}(e)$ and $\Delta I_2 = \mu^{\text{mid}}(\text{He}^+_2) - \mu^{\text{mid}}(\text{He}) - \mu^{\text{mid}}(\text{He}^+)$. The non-ideal contributions to the chemical potentials for the He atom and the ions where obtained through the numerical solution of the Ornstein-Zernike equation in the Percus-Yevick approximation [15]. This approach is valid in the low ionization limit. The results are shown in Fig. 2a, where they are compared with the shift in the ionization energy extracted from conductivity data [1] through the relation $\sigma_{\text{exp}} / \sigma_{\text{id}} = e^{\Delta I_1 / k_B T}$, where $\sigma_{\text{id}}$ is the ideal gas conductivity. The agreement with the experiment is good. In this model He pressure-ionizes at $\sim 2$ g/cm$^3$ because of strong attractive He − He$^+$ interaction (Fig. 1a), which favors ionization. This model is questionable, however, because this He − He$^+$ potential inevitably leads to a bound state (He$^+_n$), which would greatly reduce the interaction with the other neighboring He atoms.

QUANTUM MOLECULAR DYNAMICS RESULTS

We also conducted QMD-DFT calculations of dense helium, using the Viena Ab-initio simulation package. The results in terms of band gap (ionization energy) is presented on Figure 2b. We find that in this model, helium pressure-ionizes above a density of $10$ g/cm$^3$. The resulting conductivities at the experimental conditions are 2 orders of magnitude smaller and show a very strong temperature dependence rather than the strong density dependence reported in [1]. It is well known that band gaps are underestimated using GGA functional. More accurate functionals would only increase the gap and worsen the disagreement with the experimental data.

THE FREE-FREE OPACITY FROM HELIUM

The free-free (inverse bremsstrahlung) opacity of dense helium is determined by the ionization fraction and e − He collisions. In a dense medium, the collisions can be described with the classical Drude model [17]. On Figure 3 we compare the QMD ab-
FIGURE 1. (a) The interaction potentials for the chemical model. The lines represent the following potential curves: $e-\text{He}$ of [10] (solid) and [7] (dotted), $\text{He}-\text{He}$ of [12] (dashed), $\text{He}-\text{He}^+$ of [13] (long dashed), and $\text{He}-\text{He}^+$ of [14] (dash-dotted). (b) The DFT free energy of a free electron in helium. The line represents the Lenz potential energy (Eq. 1).

FIGURE 2. (a) The change in the ionization/dissociation potential predicted by the chemical model. The lines represent the results for $\Delta I_1$ (solid, dotted) and $\Delta I_2$ (dashed, dash-dotted) for $T = 1.0$ eV and $T = 2.0$ eV respectively. The filled circles represent the value of $\Delta I_1^{exp}$ extracted from the experimental data of [1]. (b) The QMD bandgap for $T = 0.5$ eV (solid line) and $T = 1.5$ eV (dotted line). The filled circles represent the effective value of ionization energy $24.6$ eV $- \Delta I_1^{exp}$. 
FIGURE 3. The absorption coefficient of He obtained from QMD simulations (solid lines) for temperature $T = 0.5$ eV and densities $\rho = 0.5, 2.0$ and $4.0$ g/cm$^3$ (from the bottom to top). The dotted line represents the standard free-free absorption coefficient for $\rho = 0.5$ g/cm$^3$ [19], adopting the density of free electrons of the QMD simulation.

CONCLUSIONS

Our goal is to calculate the free-free absorption from dense, non-ideal, weakly ionized helium. This source of opacity depends on the ionization fraction and the frequency of $e - He$ collisions. We use two different approaches to solve for the number density of free electrons in dense helium: a chemical model and QMD-DFT simulations. In the first method we have introduced a new description of the $e - He$ interaction and use ab initio potentials for the He-ions interactions. This gives us a good agreement with the experiment, but the result is driven by a questionable He$^+ - He^+$ potential. On the other hand, the more sophisticated QMD simulations suggest that pressure ionization of He does not occur below 10 g/cm$^3$, which is inconsistent with the conductivity data. This large discrepancy between models and the conductivity measurements is astrophysically significant. New experiments that probe the pressure ionization of dense He are essential in finding a resolution of this problem.

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