A NEW HYDROGEN EQUATION OF STATE FOR LOW MASS STARS

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1) INTRODUCTION

Studies of the structure and evolution of low mass stars, brown dwarfs and giant planets require an equation of state (EOS) that includes a detailed, accurate model of the strongly non-ideal behavior of matter in these cool, compact objects [Fig. (1)]. Physical processes in the outer layers of white dwarfs, especially the analysis of the pulsation properties of ZZ Ceti stars, depend sometimes critically on the thermal properties of partially ionized hydrogen. In view of the substantial developments in the statistical physics of dense fluids and plasmas over the past decade, the computation of a new, independent EOS for astrophysical applications is justified. The statistical mechanical models which we present for hydrogen can be adapted to treat both pure helium and hydrogen-helium mixtures.

2) DESCRIPTION OF THE MODEL FREE ENERGY

We have developed two different models to compute the EOS of pure hydrogen. At low density ($\log \rho < 0$), low temperature ($\log T < 4$), we consider a mixture of hydrogen atoms and molecules. At high densities ($\log \rho > 0$) and at high temperatures ($\log T > 5$), we use a model of protons interacting with a responsive, neutralizing electron background. In the intermediate region of partial ionization, the two models are combined as described below.

a) The Neutral Model

Assuming factorization of the partition function of the system, the free energy of the H/H_2 mixture becomes:

$$F_I = F_{trans} + F_{conf} + F_{int} + F_{qm}. \quad (1)$$

The translational free energy, F_{trans} is the ideal gas contribution of all particles. The configuration term, F_{conf}, represents the interactions between the different particles in their ground states. It is evaluated in the framework of the WCA fluid perturbation theory (Weeks, Chandler and Andersen 1971) In this theory, the interaction potential $\phi(r)$ is split into a repulsive reference potential $\phi^{ref}(r)$, and a weak, attractive, perturbation potential $\phi^{pert}(r)$. We approximate the free energy of the reference system by that of a hard sphere fluid, which is known analytically (Mansoori *et al.* 1971), whereas the contribution of the perturbation potential is given by the first term of the

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free energy expansion:

$$F_{conf}(N,V,T,x_1,x_2) = F_{hs}(\sigma_{\rm H},\sigma_{\rm H_2}) + \frac{1}{2}\frac{N^2}{V}\sum_{i,j=1}^{2} x_i x_j \int \phi_{ij}^{pert}(r) g_{ij}^0(r)\, d^3r. \qquad (2)$$

In Eq. (2), N is the total number of particles, V is the volume of the system and $g_{ij}^0(r)$ represents the pair correlation functions of the reference system. The concentrations x_H and x_{H_2} in the H/H_2 fluid are determined by the condition of chemical equilibrium, with the temperature- and density-dependent hard sphere diameters $\sigma_{\rm H}$ and $\sigma_{\rm H_2}$ *calculated through a thermodynamic criterion* (Weeks, Chandler and Andersen 1971). The internal energy and pressure obtained by numerically differentiating Eq. (2) are in excellent agreement with the results of Monte Carlo simulations of the H/H_2 mixture (Saumon, Chabrier and Weis 1988). The potential functions $\phi_{ij}(r)$ are fitted to realistic potentials obtained from *ab initio* calculations (Kolos and Wolniewicz 1965, Porter and Karplus 1964) and from experiments (Ross, Ree and Young 1983).

The internal free energy, F_{int}, includes all known levels for H_2 (Huber and Herzberg 1979). The effects of interparticle interactions upon the internal levels are treated with the formalism of Hummer and Mihalas (1988). In their approach, the energy of the bound states is unperturbed, but each level is assigned an occupation probability which ensures self-consistency between the interaction terms [Eq. (2)] and their effect on the internal partition function. The occupation probability provides a smooth cutoff of the otherwise diverging H partition function.

Quantum diffraction effects are included in F_{qm}, the first term of the Wigner-Kirkwood $\hbar^2$ expansion.

Figure 2 shows the concentration of atoms in the H/H_2 mixture as given by the condition of chemical equilibrium, using Eq. (1) for the free energy. We find that pressure-dissociation of molecules is significant in regimes characteristic of giant planets and brown dwarfs.

b) The Fully Ionized Model

In this regime, the ions are classical particles, while the electrons – which constitute a polarizable, inhomogeneous medium – range from a fully degenerate to a nearly classical state. The hamiltonian of this system is:

$$H = H_i + H_e + V_{ie}, \qquad (3)$$

where H_i is the hamiltonian of the ions in a uniform neutralizing background, H_e is the jellium hamiltonian for the electrons (Pines and Nozières 1966) and V_{ie} describes the ion-electron interaction. Assuming this last term to be small and thereby retaining only the linear contribution, Eq. (3) can be rewritten (Ashcroft and Shroud 1978):

$$H = H^{eff} + H_e, \qquad (4)$$

where

$$H^{eff} = \sum_i \frac{p_i^2}{2m_i} + \frac{Z^2}{2V}\sum_{k\neq 0}\frac{4\pi e^2}{k^2}\left[\frac{\rho_{\vec{k}}\rho_{\vec{k}}^*}{\epsilon(k,\omega=0)} - N_i\right] \qquad (5)$$

is the hamiltonian of the screened ionic fluid. In Eq. (5), N_i is the number of ions, $\rho_{\vec{k}}$ is the Fourier component of the ion density and $\epsilon(k,0)$ is the temperature- and density-dependent Lindhard

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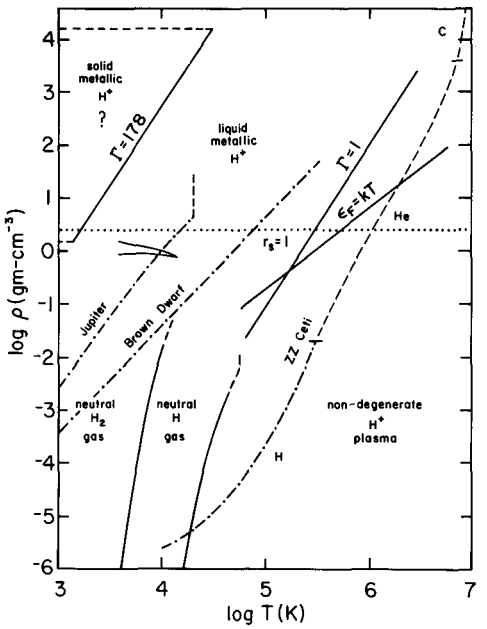

Figure 1. $(\rho - T)$ phase diagram of hydrogen. A few physical regimes are identified. Above the $\Gamma = 1$ line, the plasma is strongly coupled. Electrons are degenerate above the line $\epsilon_F = kT$. The narrow wedge near $\log T = 4$ and $\log \rho = 0$ indicates the location of the possible first-order phase transition. Adiabats of Jupiter and a brown dwarf are shown along with a ZZ Ceti model. Adapted from Fig. 2 of Van Horn (1986).

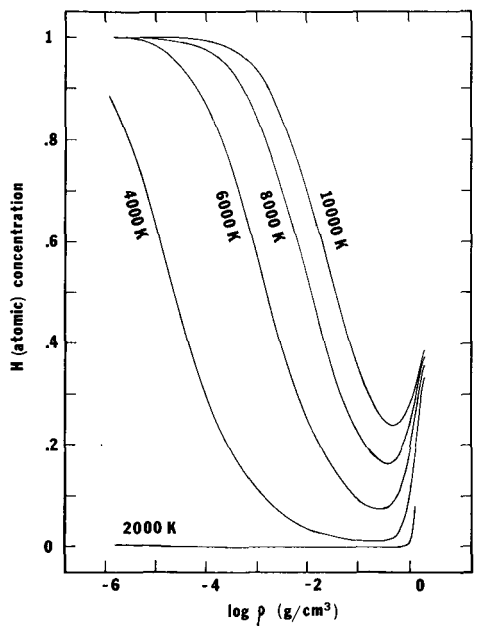

Figure 2. Atomic hydrogen concentration as a function of density and temperature, computed with the neutral model F_I . Note the effect of pressure dissociation near $\log \rho = 0$.

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screening function of the electron fluid in the adiabatic approximation (Lindhard 1954). As long as the dielectric function $\epsilon(k,0)$ includes a local field correction (LFC) to describe the exchange and short-range correlation effects in the quantum electron fluid, this model gives excellent results for the thermodynamics of a fully ionized hydrogen plasma, even in the low degeneracy, nearly classical regime for the electrons (Chabrier 1988). This LFC is an important contribution at intermediate densities ($\log \rho < 0.5$).

The free energy corresponding to the hamiltonian of Eqns (4) and (5) reads:

$$F_{II} = -kT \ln[Tr \exp^{-\beta H}] = F_i^0 + F_e^0 - kT \ln \int e^{-\beta U^{eff}} d^3 r_N + F_{xc} + F_{qm}, \qquad (6)$$

where the trace is taken over the states of the coupled ion-electron system, $\beta = 1/kT$, and U^{eff} represents the last term on the r.h.s. of Eq. (5). The superscript ^{0} denotes the perfect gas contribution (classical or degenerate). F_{xc} is the exchange and correlation free energy of the electron gas. We adopted the excellent analytical fit of Ichimaru, Iyetomi and Tanaka (1987) which is valid for any degree of degeneracy. Finally, F_{qm} represents the Wigner-Kirkwood quantum correction calculated for a screened ionic fluid.

At densities lower than $\log \rho = -0.5$, the linear approximation used in Eq. (5) is no longer valid. In this region, we use an interpolation between the free energy given by Eq. (6) and the low density ($\log \rho < 2$) limit given by the two-component Debye-Hückel free energy, corrected for the quantum nature of the electrons (DeWitt 1969, the reader should be aware of a misprint in the expression for βF_{ring}).

At high densities ($\log \rho > 0.5$), our model free energy recovers the results obtained by DeWitt and Hubbard (1976) with a zero temperature dielectric function in the RPA approximation. It also emcompasses the Thomas-Fermi model. In the region of intermediate density ($\log \rho \approx 0$) or intermediate degeneracy ($\epsilon_F \approx kT$), it represents a significant improvement over these models.

c) Partial ionization

The problem of temperature ionization, where the departures from the ideal gas behavior are small, is well understood. We recover the known limits by combining F_I and F_{II} with appropriate concentration factors and imposing the conditions of chemical equilibrium.

The pressure ionization problem, however, is more delicate. The simplest way to treat it is to interpolate smoothly between the two model free energies along isotherms. Another possibility, suggested by different authors (Robnik and Kundt 1983, Ebeling and Richert 1985, Marley and Hubbard 1988), is that pressure ionization is a first-order phase transition between a mostly neutral fluid and a fully ionized plasma.

Following standard procedure (Landau and Lifshitz 1959), we explored this possibility, using a superposition of F_I and F_{II} together with the condition of chemical equilibrium, and found a phase transition, with a critical point defined by $P_c = 0.40$ MBar, $T_c = 16500$K, $\rho_c = 0.30$ g cm^{-3}. The Jupiter adiabat goes through the phase transition line(*cf.* Fig. 1), but substellar objects may be too hot for this plasma phase transition to occur.

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3) CONCLUSION

We have developed a new EOS for hydrogen in a temperature and density domain relevant to low mass stars, giant planets, and the outer layers of DA white dwarfs, using the most sophisticated tools presently available in statistical physics. We believe that this EOS incorporates significant improvements over existing equations of state, especially in the intermediate density regime ($-3 < \log \rho < 0$) and the partial ionization zone (Saumon, Chabrier and Van Horn 1988). Using two sophisticated free energy models, we calculated a critical transition line and a critical point and found that a plasma phase transition might occur in the interior of giant planets (Saumon and Chabrier 1988).

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