Ionization Equilibrium and Equation of State of Hydrogen Plasmas in Strong Magnetic Fields

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Abstract

We study hydrogen plasmas at magnetic fields $B \sim 10^{12} - 10^{13}$ G, densities $\rho \sim 10^{-3} - 10^{3}$ g cm$^{-3}$ and temperatures $T \sim 10^{5.5} - 10^{6.5}$ K, typical of photospheres of middle-aged cooling neutron stars. We construct an analytical free energy model of the partially ionized plasma, including into consideration the decentred atomic states, which arise due to the thermal motion across the strong field. We show that these states, neglected in previous studies, may contribute appreciably into thermodynamics of the outer atmospheric layers at $\rho \lesssim 1$ g cm$^{-3}$ and typical $B$ and $T$. We take into account Coulomb non-ideality of the ionized component of the plasma affected by intense magnetic field. Ionization degree, occupancies and equation of state are calculated, and their dependences on the temperature, density and magnetic field are studied.

1 Introduction

Magnetic fields $B \sim 10^{12} - 10^{13}$ G typical of isolated neutron stars qualitatively modify many physical properties of matter [1, 2]. It was suggested that the outer layers of the neutron stars may be composed of hydrogen at temperatures $T \sim 10^{5.5} - 10^{6.5}$ K [3]. Thus the study of hydrogen plasmas at such $B$ and $T$ is of great practical importance for astrophysics. For studying the magnetized matter, Thomas-Fermi-like methods were used starting from 1970 (see ref. [4] for recent results and references). It is well known, however, that they are not well suited for light elements. Here we employ the free-energy minimization method.

The motion of charged particles in a magnetic field is quantized into Landau orbitals. The magnetic field is called strongly quantizing if the free electrons populate mostly the ground Landau level 1. This occurs when the electron cyclotron energy $\hbar \omega_c = \hbar eB/(m_e c)$ (where $\hbar, e, m_e$ and $c$ are the Planck constant, electron charge, electron mass and speed of light, respectively) exceeds both the thermal energy $k_B T$ and the electron Fermi energy $\epsilon_F$ — that is for temperatures $T \ll T_B$ and densities $\rho < \rho_B$, where

$$T_B = 3.16 \times 10^5 \gamma \, \text{K}, \quad \rho_B = 0.809 \gamma^{3/2} \, \text{g cm}^{-3} , \quad \gamma \equiv \frac{\hbar^3 B}{m_e^2 c^3} = \frac{B}{2.35 \times 10^9 \, \text{G}} .$$

The atom in a strong magnetic field $\gamma \gg 1$ is compressed in the transverse directions to the size of the “magnetic length”: $a_m = (\hbar e B)^{1/2} = a_0 \gamma^{-1/2}$, where $a_0 = \hbar^2/(m_e e^2)$ is the Bohr radius. The ground-state binding energy grows logarithmically with $B$ and exceeds the ground-state energy of the field-free atom by order of magnitude at $B \sim 10^{12}$ G [4]. Ionization equilibrium of atoms in strong magnetic fields has been first discussed in ref. [5]. However, that pioneering work neglected modifications of the atomic properties caused by the thermal motion of the atoms across the field. These motional modifications arise from the coupling between the centre-of-mass motion across the field and the relative electron-proton motion. These effects were appreciated by Ventura et al. [6], but quantum-mechanical calculations of binding energies and wave functions of hydrogen atoms in any states of motion in the strong magnetic fields have been carried out only recently [7].
Lai and Salpeter \[9\] (see references therein for earlier work) considered the ionization equilibrium of strongly magnetized hydrogen using a crude approximation for binding energies of moving atoms which missed the so-called \textit{decentred states} with a large electron-proton separation \[3\]. The same approximation was used in ref. \[10\], devoted to the low-density equation of state. Here we employ new fitting formulae to atomic energies and sizes \[11\] based on the previous study \[12\], valid for any state of atomic motion. We construct an analytic model of the plasma free energy and derive and solve a generalized Saha equation.

## 2 Free Energy Model and Generalized Saha Equation

We consider a plasma consisting of \(N_e\) electrons, \(N_p = N_e\) protons, and \(N_H\) hydrogen atoms in a volume \(V\), and write the Helmholtz free energy as \(F = F_{\text{id}} + F_{\text{ex}}\), where \(F_{\text{id}} = F_{\text{id}}^{(e)} + F_{\text{id}}^{(p)} + F_{\text{id}}^{\text{neu}}\) is the sum of the ideal-gas free energies of the electrons, protons, and neutral species, respectively, and \(F_{\text{ex}}\) is the \textit{excess} free energy.

For the ideal gas of electrons, the pressure and number density are

\[
P_e = \frac{k_B T}{\pi^{3/2} a_e^2 \lambda_e} \sum_{N=0}^{\infty} g_N I_{1/2} (\beta \mu_N), \quad n_e = \frac{1}{2\pi^{3/2} a_e^2 \lambda_e} \sum_{N=0}^{\infty} g_N I_{1/2} (\beta \mu_N),
\]

where \(I_p(x) = \int_0^\infty \rho \, dt / (e^{\rho t} - 1)\) is the Fermi integral, \(\mu_N \equiv m_e - N \hbar \omega_\text{cp}\), \(\mu_e\) is the chemical potential, \(\beta \equiv (k_BT)^{-1}\), \(\lambda_e \equiv \hbar / 2\pi \beta m_e\), \(g_{N=1} = 2\), and \(g_{N=0} = 1\). The free energy is given by \(F_{\text{id}}^{(e)} = \mu_e N_e - P_e V\), where \(\mu_e\) is found using an algorithm described in ref. \[12\].

In the strongly quantizing regime, the Fermi energy is \(\epsilon_F = \frac{2\pi^4}{3} (a_e^2 n_e^2 m_e)\), which differs from the non-magnetic case by a factor \((4/3)^{2/3}(\rho/\rho_B)^{4/3}\). Thus the degeneracy is strongly reduced at \(\rho \ll \rho_B\). Furthermore, in the non-degenerate regime \((k_BT \gg \epsilon_F)\), we have \(F_{\text{id}}^{(e)} = N_e k_BT \ln(2\pi a_e^2 \lambda_e n_e) - 1\).

For the protons, which are non-degenerate, we have

\[
\beta F_{\text{id}}^{(p)} / N_p = \ln(2\pi a_m^2 \lambda_p n_p) + \ln[1 - \exp(-\beta \omega_\text{cp})] - 1,
\]

where \(\omega_\text{cp} = (m_e / m_p) \omega_c\) is the proton cyclotron frequency. Here, for sake of brevity, we drop the zero-point energy \(\frac{1}{2} \hbar \omega_\text{cp}\) and the spin energy \(\pm \frac{1}{2} \hbar \omega_\text{sp}\), where \(\hbar = 5.858\) is the proton spin gyromagnetic factor. These terms are the same for free and bound protons. Taking them into account yields an additive contribution: \(\Delta F = N_0 \{\omega_\text{cp} / 2 - k_BT \ln[2 \cosh(\beta g_p \omega_\text{cp} / 4)]\}\), where \(N_0\) is the total number of protons (free and bound). \(\Delta F\) does not affect ionization equilibrium and pressure.

For the excess free energy of the ionized component, a general fitting formula in the non-magnetic case is given in ref. \[11\]. It is known that thermodynamics of \textit{classical} Coulomb plasmas is not affected by the magnetic field, which, however, affects the \textit{quantum-mechanical} contributions to \(F_{\text{ex}}\). These effects have been studied only in the low-temperature or low-density regimes (e.g., ref. \[10\] and references therein). Here we use a scaling \((r_s^{\text{id}} = s r_s)\) of the density parameter \(r_s = (4\pi n_e a_0^2 / 3)^{-1/3}\) at a fixed Coulomb parameter \(\Gamma = \beta e^2 / (\alpha q r_s)\) in the formulae of ref. \[13\]. The scaling is devised so as to reproduce the low-density, high-temperature results presented in ref. \[10\], as well as other known limiting cases. For the contribution of electron-electron and electron-ion interactions in \(F_{\text{ex}}\), the scaling factors are \(s_{ee} = (1 + \theta_m / \theta_0) / [1 + (\theta_m / \theta_0) \exp(-\theta_m^3 / 3)]\) and \(s_{ie} = 1 + f_1^2 / f_2^2\), where \(\theta_0 = 2 (9 \pi / 4)^{-2} r_s / \Gamma\) and \(\theta_m = 8 \gamma^2 r_s^3 (9 \pi / 4)^2\) are the non-magnetic and magnetic degeneracy parameters, respectively, and the factors \(f_1\) and \(f_2\) (depending on \(\beta \hbar \omega_c\)) are given in ref. \[10\].

The ideal-gas contribution of the magnetized atoms reads

\[
\beta F_{\text{id}}^{(H)} = \sum_{s\nu} \int d^2 k_{\perp} N_{s\nu} (K_{\perp}) \left\{ \ln \left[ n_H \lambda_H^2 (2 \omega_{\text{sw}} (K_{\perp}) / Z_w - 1 \right] \right\},
\]
where $s$ and $\nu$ relate to electronic excitations, $N_{\text{st}} = (\lambda_H/2\pi\hbar)^2 N_H w_{\text{st}} e^{2\chi_{\text{st}}}/Z_w$ are the atomic occupancies per unit phase space of the transverse component $K_\perp$ of the pseudo-momentum $\textbf{K}$ which characterizes the atomic motion in the magnetic field, $w_{\text{st}}(K_\perp)$ and $\chi_{\text{st}}(K_\perp)$ are the occupation probabilities and binding energies of the moving atom, and $Z_w = (\lambda_H/2\pi\hbar)^2 \int d^2K_\perp w_{\text{st}}(K_\perp) \exp[\beta \chi_{\text{st}}(K_\perp)]$ is the internal partition function.

The contribution of atoms in the nonideal part $F_{\text{ex}}$ of the free energy is calculated in the hard-sphere approximation using the van der Waals one-fluid model by analogy with ref. [14]. Its straightforward generalization to the magnetic case involves the composite quantum number $\kappa = (s\nu K_\perp)$, so that $\Sigma_\kappa$ includes now integration over $K_\perp$. The hard-sphere diameters are set equal to the effective atomic sizes $l_{\kappa}$ given in [11]. The occupation probabilities are then given by formulae derived in ref. [14], extended to the magnetic case.

Our model is valid as long as the formation of molecules may be neglected. In order to quantify the range of validity, we estimate the abundance of $\text{H}_2$ molecules following ref. [9], but with inclusion of the non-ideal effects.

Minimization of the free energy yields the ionization equilibrium (generalized Saha) equation:

$$n_H = n_p n_e (\lambda_p \lambda_e/\lambda_H^2)(2\pi a_m^2)^2 \left[ 1 - \exp(-\beta \hbar \omega_{cp}) \right] Z_w \exp(\Lambda),$$

where $\Lambda = \beta \mu_e - \ln(2\pi a_m^2 \lambda_p n_e) + \beta \partial \mu_e/\partial \ln n_e - \partial P_e/\partial n_e$ takes into account effects of electron degeneracy and population of excited Landau levels.

### 3 Results and Discussion

Figure 1 shows selected results obtained for $B = 10^{12}$ G. The left panel shows the neutral fraction of atoms $f_H = N_H/N_0$ and molecules $f_{\text{H}_2} = 2N_{\text{H}_2}/N_0$ at $T = 10^6$ K. For comparison, we plot the fraction of atoms in the centred states, $f_H$ according to ref. [9] and $f_{\text{IT}}$ in the non-magnetic case. Long dashes display the fraction of atoms that satisfy the Inglis–Teller (IT) criterion and thus can be identified in optical spectra of the plasma. The IT fraction is estimated according to the formula $n_{\kappa}^\text{IT} \sim n_\kappa \exp[-n_p(4\lambda_\kappa)^3]$ (cf. Eq. (31) of ref. [14]). We can see that (a) the strong magnetic field increases the non-ionized fraction and shifts the region of pressure ionization to much higher $\rho$ (compare the solid line and triangles in the left panel of Fig. 1), (b) the approximation of ref. [9] reproduces only the abundance of the centred atoms at low density and fails at high density where the pressure-ionization effects are important, and (c) at the low density, the decentred atomic states are significantly populated.

The right panel demonstrates the equation of state, which is seen to be much softer than (a) in the non-magnetic case (mainly because of the electron degeneracy “taken away” by the strongly quantizing field, but also due to the increased neutral fraction) and (b) in the magnetic but ideal proton-electron plasma (because the Coulomb interactions yield negative contribution to the pressure).

The obtained results are used for modelling neutron-star atmospheres. In particular, the IT fraction of atoms, multiplied by the absorption cross sections calculated in ref. [13], determines an atomic contribution to atmospheric opacities. Preliminary calculations of the opacities, carried out with a simplified $F_{\text{ex}}$, were presented in ref. [10]. The more elaborated model of the plasma described here confirms qualitative results of that work. An important conclusion is that the bound species contribute significantly to the absorption at $B = 10^{12} - 10^{13}$ G, even at relatively high $T \sim 10^6$ K.

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Figure 1: Left panel: Non-ionized fraction of atoms in any states (solid line), atoms in the centred states (short-dashed line), molecules (dash-dot line), and the weakly perturbed atoms contributing to the optics (long-dashed line), compared with the non-magnetic case (triangles) and the approximation [9] (dotted line). Right panel: Pressure isotherms of magnetized hydrogen plasma (solid lines) at $\lg T[K] = 5.5, 6.0$ and $6.5$, compared with the non-magnetic case (dashed lines) and with the ideal magnetized plasma (dotted lines).

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