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The influence of electron degeneracy on the contribution of bound states to the non-ideal hydrogen plasma EOS

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Abstract
An equation of state for a weakly non-ideal hydrogen plasma was developed to account for the influence of degenerate electrons on the contribution of bound states. Asymptotic expressions for the contribution were derived and compared. In this work, the reduced model EOS includes the ideal gas contribution with degenerate electrons and relativistic corrections, bound states contribution and the Coulomb interaction in the Debye–Hückel approximation. The influence of the electron degeneracy on the adiabatic exponent and the total pressure is shown.

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For conditions of solar plasma and interior of denser stars the influence of electron degeneracy (ED) may be significant. Some models (for example, SAHA-S [1]) include the contribution of free degenerate electrons. But it is also necessary to take into account the effect of degeneracy on the bound states (BS) contribution. In this work, we estimate the influence for a weakly non-ideal hydrogen plasma in the approximation of low occupation numbers.

For the non-degenerate case the BS pressure may be written in the form [2–5]

$$\delta P^{\mathrm{BS}} = \zeta_{\mathrm{e}}\zeta_{\mathrm{p}} T \lambda_{\mathrm{ep}}^{3} \Sigma^{\mathrm{BS}}. \tag{1}$$

Here $\zeta_{\mathrm{e}}, \zeta_{\mathrm{p}}$ are the activities of electrons and protons, T is the temperature, $\lambda_{\mathrm{ep}} = [2\pi\hbar^2/(\mu_{\mathrm{ep}}T)]^{1/2}$, $\mu_{\mathrm{ep}} = m_{\mathrm{e}}m_{\mathrm{p}}/(m_{\mathrm{e}} + m_{\mathrm{p}})$ is the reduced mass. As was shown in [3] for the case without taking account of the atomic states broadening after all integrations one can obtain the series on the principal quantum number n ($u_n = \alpha^2/n^2, \alpha = \sqrt{\mathrm{Ry}/T}$)

$$\Sigma^{\mathrm{BS}} = \Sigma^{\mathrm{BS}}_{\mathrm{SRM}} = \sum_{n=1}^{\infty} n^2 \mathrm{e}^{u_n} F(u_n), \tag{2}$$

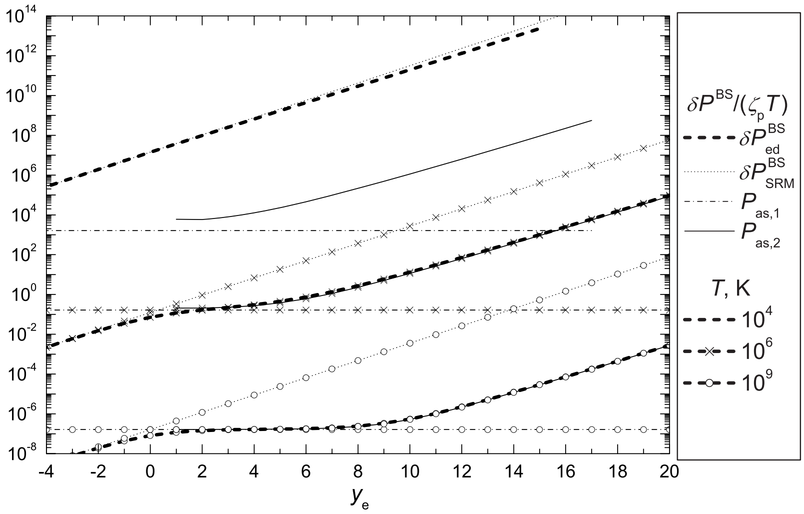

Figure 1. BS contribution (thick dash line) with account of ED and asymptotics (thin lines) divided by $\zeta_p T$ for $T = 10^4, 10^6, 10^9$ K.

where $F(u) = 1 - e^{-u}\left(4 - \frac{6}{\sqrt{\pi}}u^{1/2} + \frac{4}{\sqrt{\pi}}u^{3/2}\right) + (3 - 4u + 4u^2)\,\mathrm{erfc}\,\sqrt{u}$. This expression can be calculated as a sum of series on α (see [3, 5]).

In the non-degenerate case $\zeta_i = 2\lambda_i^{-3}\exp(y_i)$, $\lambda_i = [2\pi\hbar^2/(m_i T)]^{1/2}$, $y_i = \mu_i/T$ ($i = \mathrm{e, p}$). The activity of degenerate electrons in the Fermi statistics is calculated as

$$\zeta_e = \frac{2}{\lambda_e^3}\frac{2}{\sqrt{\pi}}\int_0^\infty \frac{x^{1/2}\,dx}{\exp(x - y_e) + 1}. \tag{3}$$

The bound states contribution, taking into account ED in the approximation of low occupation numbers can be obtained as follows ($m_e \ll m_p$):

$$\delta P_{\mathrm{ed}}^{\mathrm{BS}} = \zeta_p \frac{32}{\pi}\,\mathrm{Ry}\sum_{n=1}^{\infty} 2\int_0^1 \lambda\,d\lambda \int_0^\infty \frac{t^2\,dt}{(1+t^2)^3}\,\frac{\exp\left(\lambda^2 u_n^2(1+t^2)\right) - 1}{\exp\left(\lambda^2 u_n^2 t^2 - y_e\right) + 1}. \tag{4}$$

This expression has been derived without taking account of the Pauli blocking in the calculation of the scattering amplitude using techniques of Galitskii [6].

At moderate y_e it seems that for large $T \gg \mathrm{Ry}$ the integral grows slowly on y_e: $\delta P_{\mathrm{ed}}^{\mathrm{BS}} \to P_{\mathrm{as},1} = \zeta_p T(2\pi^2/3)(\mathrm{Ry}/T)^2$, but for large y_e it can be derived that the contribution grows sub-exponentially (see figure 1):

$$\delta P_{\mathrm{ed}}^{\mathrm{BS}} \to P_{\mathrm{as},2} = \zeta_p T\left(\frac{2\pi^2}{3}\left(\frac{\mathrm{Ry}}{T}\right)^2 + \frac{64\,\zeta(3)}{15\pi}\left(\frac{\mathrm{Ry}}{T}\right)^{5/2}\frac{\exp(y_e)}{y_e^{3/2}}\right). \tag{5}$$

Really, due to the influence of ion microfields the partition function Σ^{BS} must be limited to the first n_l states with the dimensionless ionization potential u_n greater than the similar characteristic energy $\tilde{B}_n = B_n\mathcal{E}_0\hbar/T$, where B_n is the effective Stark constant for the state, $\mathcal{E}_0$ is the field characteristic value (see [7, 22]): $B_n = B_0(n^2 - 1)$ for $n > 1$, $B_1 = B_0$, $B_0 = (3/8)^{2/3}\hbar/(m_e e)$; $\mathcal{E}_0 = 2\pi(4/15)^{2/3} e N^{2/3}$, $N = \rho N_A/\mu_H$.

Below in calculations the number of states is limited by a decreasing weight factor w_n: $\Sigma_w^{\mathrm{BS}} = \sum_n w_n G_n$, where $w_n = 1/(1+\tau^2)$, $\tau = \tilde{B}_n/u_n - 1$ if $\tau > 0$, $w_n = 1$ if $\tau < 0$.

The HEOS code for the simulation of a weakly non-ideal hydrogen plasma thermodynamics was developed previously in [3–5]. The model is based on the assumptions

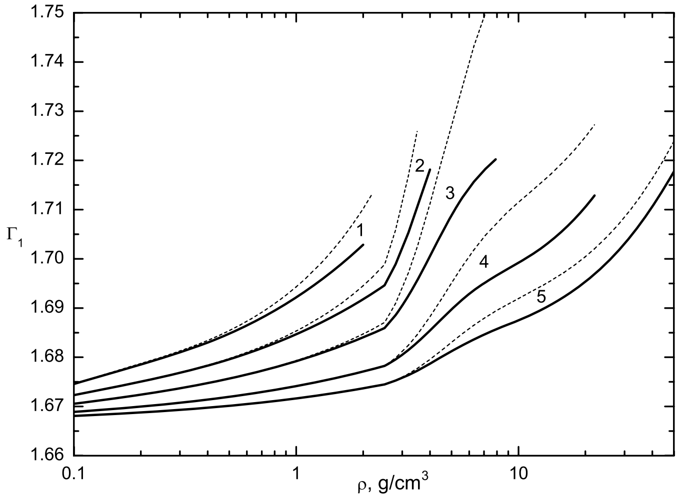

Figure 2. Adiabatic exponent versus density at different temperatures for the models with and without ED in BS contribution (where $\Gamma_D < 1$): BS contribution: solid lines—with ED, dash lines—without ED; T (K): 1—4.5×10^5, 2—5.6×10^5, 3—7.1×10^5, 4—1.0×10^6, 5—1.3×10^6.

of the perturbation theory and includes terms right up to the 2nd virial coefficient. In this model, the total pressure includes additive contributions of the ideal gas of protons and electrons taking into account ED and relativistic corrections, the Debye–Hückel, logarithmic, diffraction and exchange corrections, the contributions of bound states and scattering states from e–e, p–p, e–p interactions, and the radiation pressure. Each contribution can be altered and some of them were described in different forms. For example, the BS pressure can be calculated using expressions: Saha, Planck–Larkin, SRM, and taking account of the atomic states broadening [5]. The partition functions (SRM and with account of broadening) may be modified with a weight limitation of the atomic states number. The HEOS code solves the system of two equations: $\sum_{i=\mathrm{e,p}} \partial(\Omega V^{-1})/\partial\mu_i = -2N$ and the neutrality condition $\zeta_e = \zeta_p$ [4] for independent variables y_e, y_p. The results obtained with the HEOS code for different simplified hydrogen EOS models were compared to those obtained with the SAHA-S code and had shown almost a perfect agreement. New expressions of the BS pressure taking account of the ED (the original unlimited partition function and the weight-limited one) were introduced to the code.

A physical model EOS taking account of the ED in all contributions including the ideal gas pressure, the Coulomb correction and the BS contribution has been modeled using the HEOS code. Dependences $\Gamma_1(\rho)$ were calculated for models with BS contribution with and without taking account of ED at different temperatures. The degeneracy gives maximal effect at the point $\rho = \rho_0 \approx 8$ g cm^{-3} with $\Gamma_D(\rho_0) \approx 1$ for $T \approx 7 \times 10^5$ K. The half-maximum range on temperature is about 5×10^5–10^6 K. The effect decreases rapidly outside the range. Dependences $\Gamma_1(\rho)$ are shown in figure 2 at some characteristic temperatures. However, it should be noted that at the $\Gamma_D \approx 0.1$ level the difference introduced by taking account of ED in this model is negligible. Figure 3 shows the ratio of the total pressure to the ideal gas one of free non-degenerate electrons and protons ($P_{\mathrm{tot}}\mu_H/(2\rho RT)$) at the same temperatures as in figure 2.

It can be concluded that the estimate of the BS contribution decreases by orders of magnitude due to taking account of the electrons degeneracy in the case of large T ($>10^5$ K) and strong degeneracy ($y_e \gg 1$). Numerical simulations show that the adiabatic exponent

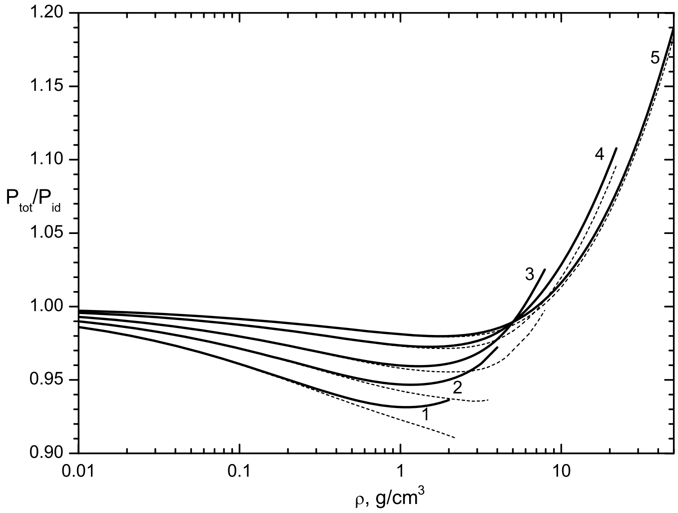

Figure 3. Ratio $P_{tot}\mu_H/(2\rho RT)$ versus density at different temperatures in the same notations as in figure 2.

value can differ significantly from the ideal gas value $\Gamma_1 = 5/3$ even for a moderate nonideality ($\Gamma_1 \sim 1.75$ for $\Gamma_D \sim 1$). For hydrogen plasma and conditions of the interior of the Sun taking account of degeneracy in the BS contribution leads to correction of sound speed $<10^{-4}$ in comparison to the model with the SRM partition function. The usage of a truncated partition function gives maximal relative correction of sound speed $\sim 2.5 \times 10^{-3}$.

There exists extensive work concerning the influence of electron degeneracy on the equation of state, see, for example, [8, 9]. Our consideration differs in focusing on the EOS for conditions of stars' interior. The influence of bound states on the adiabatic exponent is significant, even if the BS contribution is not large. Even a small correction may be important and we have concentrated on the second virial coefficient that is of interest to astrophysics.

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