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Equation of state for dense non-isothermal plasma

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Abstract. In this work the effective potentials taking into account screening effects at large distances and quantum-mechanical effects of diffraction at small distances were used as models of interaction between particles. Thermodynamic properties of dense non-ideal non-isothermal plasma were calculated using these potentials and obtained on their basis radial distribution functions (RDFs). The influence created by difference between temperatures of electrons and ions was also considered and found to be able to significantly influence the effects in such plasmas.

1. Introduction

In the non-ideal plasma – plasma, in which the potential energy of interaction between the particles is comparable to their kinetic energy or exceeds it, the interaction between the particles plays an important role. Such a plasma is of particular interest to many experimental and theoretical investigations. For example, dense non-ideal plasma constitutes cores of planets and stars [1,2]. In practical applications this type of plasma is produced in the inertial fusion reactors and analyzed by different experimental approaches [3–5]. It is important to note that plasma in these experiments is non-isothermal due to the difference between masses of ions and electrons hindering energy exchange. In dense plasmas, where the average distance between particles is comparable to the thermal de Broglie wavelength of particles, quantum-mechanical effects caused by the wave nature of particles colliding at small distances should be taken into consideration. In this work non-isothermal, weakly non-ideal, dense hydrogen plasmas are considered. To study properties of such a plasma it is necessary to use the model of interparticle interactions taking into account screening effect at large distances and quantum-mechanical effects at small distances.

There are two methods used to determine the model of interactions between different types of particles. In the first method generalized Poisson-Boltzmann equation obtained from Bogolyubov's equations for the phase space distribution function [6] is solved. In this work the effective interaction potentials determined by the second method – the method of dielectric response function [7] – are used.

2. Effective interaction potentials

The effective potentials taking into account both collective effects at large distances and quantum effects at small ones were obtained using the method of dielectric response function, where the



Deutsch [8] potential was used as a micro-potential:

$$\phi_{\alpha\beta}^{\text{Deutsch}}(r) = \frac{Z_{\alpha}Z_{\beta}e^2}{r}, \quad (1)$$

where α and β are types of particles, Z_{α}, Z_{β} are atomic numbers of α, β particles, $\lambda_{\alpha\beta} = \hbar/\sqrt{4\pi m_{\alpha\beta}K_B T_{\alpha\beta}}$ is the thermal wave length, e is the electron charge, $m_{\alpha\beta} = m_{\alpha}m_{\beta}/(m_{\alpha}+m_{\beta})$ is the reduced mass, $T_{ee} = T_e$, $T_{ii} = T_i$ are the temperatures of the electron and ion subsystems. In [9] it was shown that the electron-ion temperature is $T_{ei} = \sqrt{T_e T_i}$. It follows that $T_{\alpha\beta} = \sqrt{T_{\alpha} T_{\beta}}$.

We use such dimensionless parameters as the density parameter $r_s = a/a_B$ and coupling parameters $\Gamma_{ee}, \Gamma_{ii}, \Gamma_{ei}$:

$$\Gamma_{ee} = \frac{e^2}{ak_B T_e}, \quad \Gamma_{ii} = \frac{Z_i^2 e^2}{ak_B T_i} \left(\frac{n_i}{n_e} \right) = \Gamma_{ee} Z_i^{5/3} \left(\frac{T_e}{T_i} \right), \quad \Gamma_{ei} = \frac{Z_i e^2}{ak_B T_{ei}} = \Gamma_{ee} Z_i \sqrt{\frac{T_e}{T_i}}, \quad (2)$$

where $a = (3/4\pi n_e)^{1/3}$ is the average distance between electrons.

We used the following expression for the effective interaction potential between charged particles [10, 11]:

$$\Phi_{\alpha\beta}(r) = \frac{Z_{\alpha}Z_{\beta}e^2}{r} \frac{1}{\gamma^2 \sqrt{1 - (2k_D/\lambda_{ee}\gamma^2)^2}} \left(\left(\frac{1/\lambda_{ee}^2 - B^2}{1 - B^2\lambda_{\alpha\beta}^2} \right) \exp(-Br) - \left(\frac{1/\lambda_{ee}^2 - A^2}{1 - A^2\lambda_{\alpha\beta}^2} \right) \exp(-Ar) \right) \frac{Z_{\alpha}Z_{\beta}e^2}{r} \frac{(1 - \delta_{\alpha\beta})}{1 + C_{\alpha\beta}} \exp(-r/\lambda_{\alpha\beta}), \quad (3)$$

where $(2k_D/\lambda_{ee}\gamma^2)^2 < 1$, $k_D^2 = k_e^2 + k_i^2$ is the screening parameter taking into account the contribution of electrons and ions, $\gamma^2 = k_i^2 + 1/\lambda_{ee}^2$, and

$$C_{\alpha\beta} = \frac{k_D^2 \lambda_{\alpha\beta}^2 - k_i^2 \lambda_{ee}^2}{\lambda_{ee}^2/\lambda_{\alpha\beta}^2 - 1}, \quad A^2 = \frac{\gamma^2}{2} \left(1 + \sqrt{1 - \left(\frac{2k_D}{\lambda_{ee}\gamma^2} \right)^2} \right), \quad B^2 = \frac{\gamma^2}{2} \left(1 - \sqrt{1 - \left(\frac{2k_D}{\lambda_{ee}\gamma^2} \right)^2} \right), \quad (4)$$

The interaction potentials for different values of ion and electron temperatures are presented in figure 1. The left-hand figure shows dependence of potential on relation between electron and ion temperatures at fixed values of ion temperatures. As one can see the results for effective potential (2) decrease with increasing electron temperature due to decrease of interaction between particles. The curves with lower ion temperatures are higher due to the increase in the non-ideality. The right-hand figure presents interaction potentials for different values of electron temperatures. Interaction between particles lessens with increase of ion temperature.

3. Thermodynamic properties

Pair correlation functions were calculated in the exponential approximation:

$$g_{\alpha\beta}(r) = \exp \left(-\frac{\Phi_{\alpha\beta}(r)}{k_B T} \right), \quad (5)$$

where $\Phi_{\alpha\beta}(r)$ is the effective interaction potential of α and β type particles.

Thermodynamic properties – internal energy $U = \sum_{\alpha} 3/2 N_{\alpha} k_B T_{\alpha} + U_N$, where the correlation energy of interaction is:

$$U_N = 2\pi V \int_0^{\infty} \sum_{\alpha, \beta} n_{\alpha} n_{\beta} \phi_{\alpha\beta}(r) g_{\alpha\beta}(r) r^2 dr, \quad (6)$$

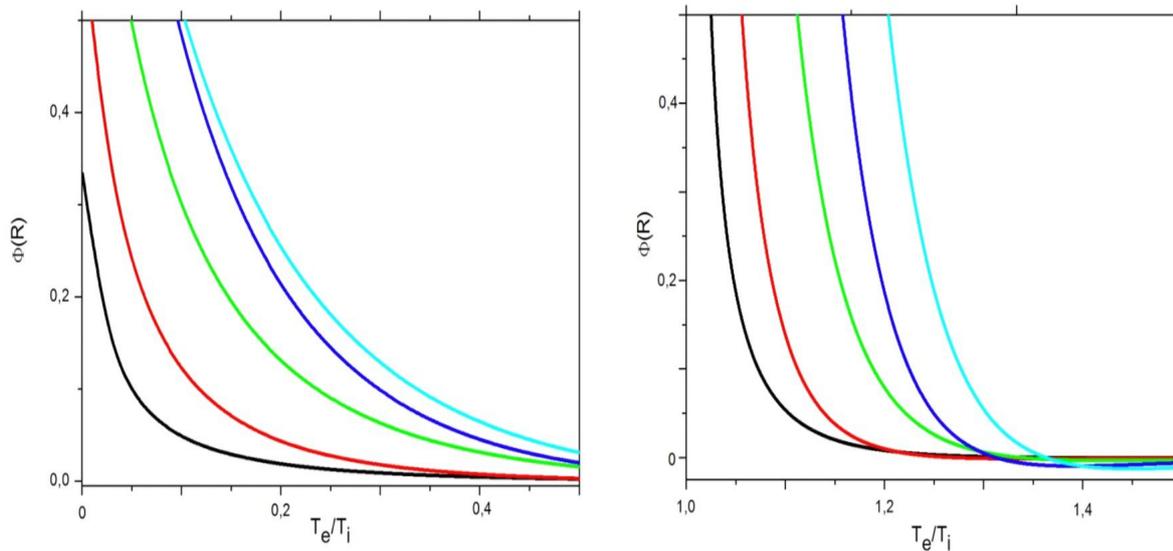


Figure 1. The interaction potential for different values of ion temperature on the left-hand and for different values of electron temperature on the right hand: black line – $T = 600000$ K, red line – $T = 300000$ K, green line – $T = 200000$ K, blue line – $T = 120000$ K, turquoise line – $T = 100000$ K.

and the equation of state is written as:

$$P = P_{id} - \frac{2\pi}{3} \int_0^{\infty} \sum_{\alpha,\beta} n_{\alpha} n_{\beta} \frac{\partial \phi_{\alpha\beta}(r)}{\partial r} g_{\alpha\beta}(r) r^3 dr, \quad (7)$$

where $P_{id} = n_e k_B T_e + n_i k_B T_i$ is the pressure of ideal plasma, N is the number of particles in the system.

In [10] using Deutsch potential (1) as the interaction micro-potential $\phi_{\alpha\beta}(r)$ and using the effective screened potentials without the diffraction effect (2), the analytical expressions for the correlation energy and for the equation of state were obtained.

Figures 2–3 show the results for the correlation energy and excess part of the equations of state. As one can see from the figures the results show that absolute values of the thermodynamic properties decrease with increasing electron temperatures (the left-hand figures in figure 2) and with increasing ion temperatures (the right-hand figures in figure 3) due to decrease of interaction between particles.

Obtained on the basis of effective potentials thermodynamic properties were used for solving the Hugoniot equation [12], which describes the relationship between thermodynamic properties on both sides of a shock wave:

$$H(V, P, E) = E - E_0 + 1/2(V - V_0)(P + P_0) = 0, \quad (8)$$

where $P_0 = 0$, $\rho_0 = 0.171 \text{ g/cm}^{-3}$, $E_0 = -13.6 \text{ eV/atom}$, V_0 – volume of gas, V – volume of plasma.

Shock adiabat or Hugoniot adiabat H binds the density and pressure of the plasma in front of and behind the shock front. The plasma is formed by compression, acceleration and heating of matter in front of the shock wave. Parameters of plasma change very rapidly and in a very narrow field with the passage through the shock wave.

Pressure of partially ionized hydrogen plasma is shown on figures 3 and 4. On figure 3 blue triangles are data from Dick and Kerley, green squares are from Nellis et al., and red circles are from T. Sano et. al. Solid line is theoretical predictions from the model EOS of Kerley,

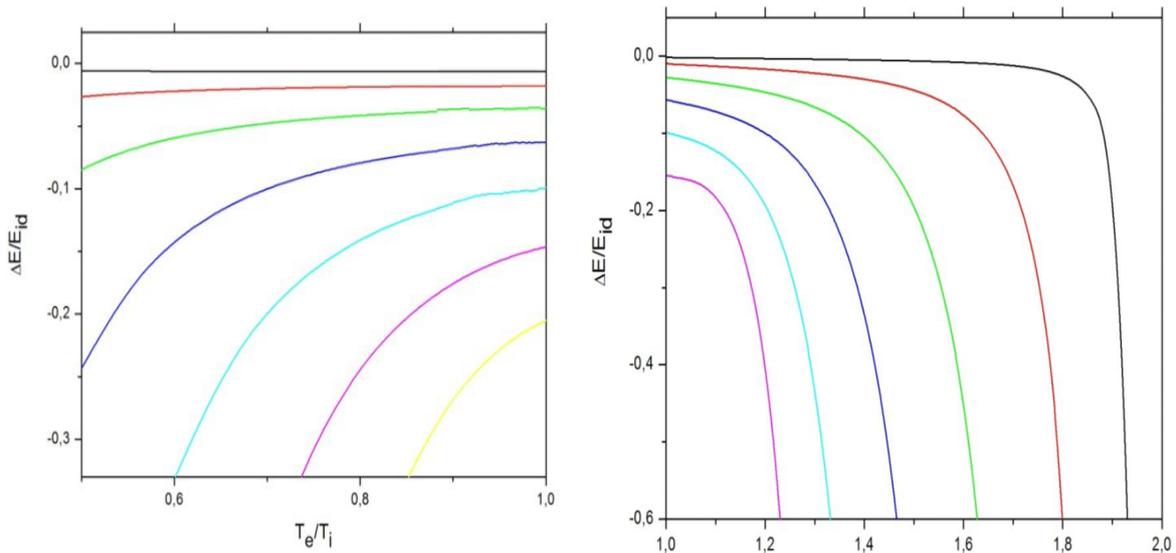


Figure 2. Correlation energy for hydrogen plasma for different values of ion temperatures (black line – $T = 300000$ K, red line – $T = 200000$ K, green line – $T = 160000$ K, blue line – $T = 120000$ K, turquoise line – $T = 100000$ K, violet line – $T = 90000$ K, yellow line – $T = 80000$ K) in the left-hand figure at $n = 1.2 \cdot 10^{22} \text{ cm}^{-3}$ and for different values of electron temperatures (black line – $T = 600000$ K, red line – $T = 300000$ K, green line – $T = 200000$ K, blue line – $T = 160000$ K, turquoise line – $T = 120000$ K, violet line – $T = 100000$ K) in the right-hand figure at $n = 2 \cdot 10^{23} \text{ cm}^{-3}$.

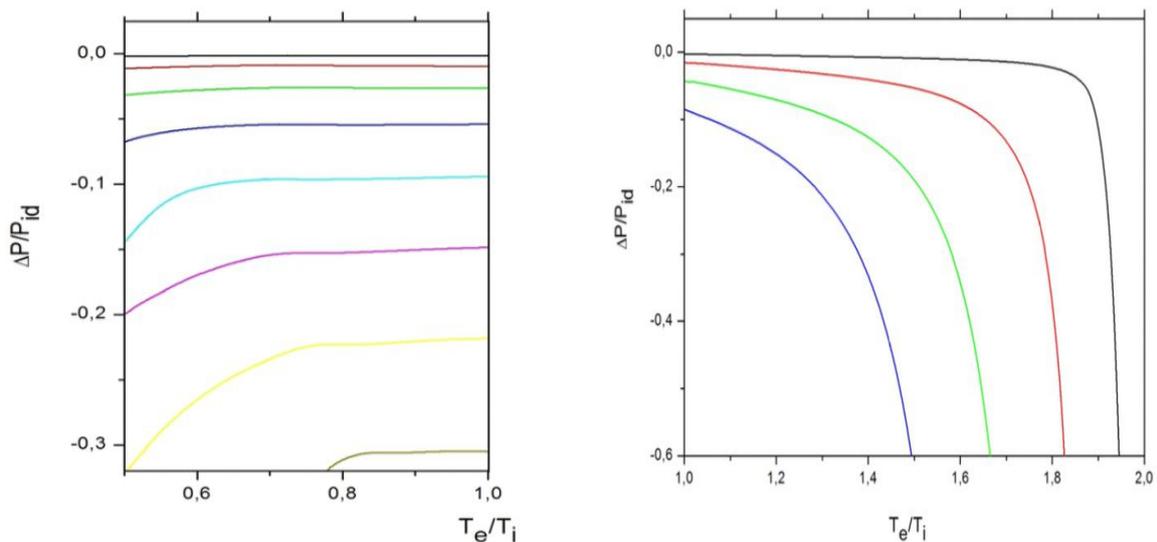


Figure 3. Excess part of equation of state for H plasma for different values of ion temperatures (black line – $T = 600000$ K, red line – $T = 300000$ K, green line – $T = 200000$ K, blue line – $T = 160000$ K, turquoise line – $T = 120000$ K, violet line – $T = 100000$ K, yellow line – $T = 90000$ K, brown line – $T = 80000$ K) in the left-hand figure at $n = 1.2 \cdot 10^{22} \text{ cm}^{-3}$ and for different values of electron temperatures (black line – $T = 600000$ K, red line – $T = 300000$ K, green line – $T = 200000$ K, blue line – $T = 160000$ K) in the right-hand figure at $n = 2 \cdot 10^{23} \text{ cm}^{-3}$.

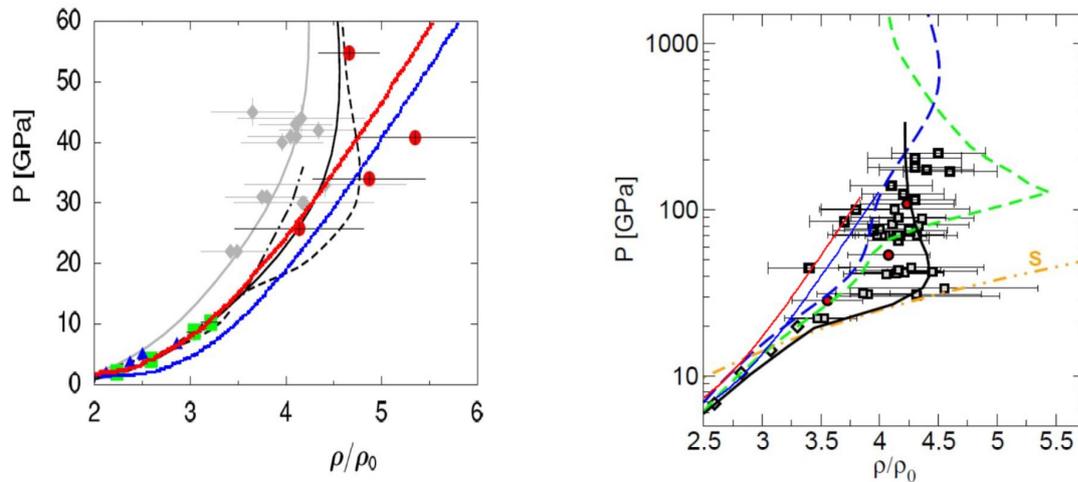


Figure 4. Pressure of partially ionized hydrogen plasma: left-hand figure: blue triangles – [15], green squares and diamonds – [16], red circles – [17], dashed black line – [18], dash-dotted black line – [19], a straight black line – [20]; right-hand figure: solid black line – [21], dash green line – [22], dash blue line – [23], grey filled squares – [24], open squares – [25], circles – [26]; red line – this work ($T_e < T_i$), blue line – this work ($T_e > T_i$).

dashed line is quantum molecular dynamics simulations, and dot-dashed line is the linear mixing model. For reference, the Hugoniot data for liquid deuterium are shown by gray diamonds, and gray curve is the EOS model for deuterium. In figure 4 theoretical hydrogen Hugoniot curves are shown as a solid black line – H-REOS.2, a dash green line – H-SCvH-I, and a dash blue line – Sesame – 5251. Experimental data are given as grey filled squares – SNL Z-pinch, open squares – modified omega laser, circles – explosives, diamonds – gas gun. A dot-dashed orange curve (5) shows part of the Saturn adiabat from [13], a solid olive line – data from [14]. Red and blue lines are the result of this work: red line is the pressure for the case, when electron temperature is higher than ion temperature, blue line – when electron temperature is lower than ion temperature. The difference between these results are due to decrease of absolute values of correlation energy and excess part of equation of state with decrease of interaction between particles.

4. Conclusion

The internal energy and the equation of state of partially ionized hydrogen plasma were calculated. Thermodynamic expressions calculated on the basis of the effective interaction potential taking into account collective as well as quantum-mechanical effects were used to obtain Hugoniot adiabat. The results of this work coincide with the results of other authors.

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