Equation of state of dense hydrogen plasma

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Abstract. In this paper, dense non-ideal, non-isothermal plasma is considered. Effective screened interaction potentials taking into account the quantum-mechanical diffraction effect have been used. Pair correlation functions were studied in the exponential approximation. Thermodynamic properties for hydrogen plasma were calculated using the analytical expressions derived from these effective potentials.

1. Introduction
In the non-ideal plasma (in which the potential energy of interaction between the particles is comparable with or exceeds their kinetic energy), the interaction between the particles plays an important role. Such plasma is of a particular interest to many experimental and theoretical investigations. For instance the dense non-ideal plasma constitutes the cores of planets and stars [1]. In practical applications this type of plasma is produced in the inertial fusion reactors and analyzed by different experimental approaches [2–4]. 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 with the thermal de Broglie wavelength of particles, quantum-mechanical effects caused by the wave nature of the 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 plasma it is necessary to use a model of interparticle interactions taking into account the screening effect at large distances and the quantum-mechanical effects at small ones [5–8].

There are two methods used to determine a model of interactions between the different types of particles. In the first method generalized Poisson–Boltzmann equation obtained from Bogolyubov’s equations for the phase space distribution function [9] is solved. In this work the effective interaction potential is determined by the second method that is a method of dielectric response function [10].

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 [11] potential was used as a micro-potential:

$$\phi^{\text{Deutsch}}_{\alpha\beta}(r) = \frac{Z_{\alpha}Z_{\beta}e^2}{r}(1 - \exp(-\frac{r}{\lambda_{\alpha\beta}})),$$

(1)
where $\alpha$ and $\beta$ are the types of particles, $Z_\alpha, Z_\beta$ are the atomic numbers of $\alpha, \beta$ particles, $\lambda_{\alpha\beta} = \hbar / \sqrt{4\pi m_{\alpha\beta} k_BT_{\alpha\beta}}$ is the thermal wave length, $e$ is the electron charge, $a = (3/4\pi n_e)^{1/3}$ is the average distance between electrons, $n$ is number of density of particles in the system, $m_{\alpha\beta} = m_\alpha m_\beta / (m_\alpha + m_\beta)$ is the reduced mass, $T_{ee} = T_e, T_{ii} = T_i$ are the temperatures of the electron and ion subsystems. In [12] it has been 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 used the following expression for the effective interaction potential between charged particles [13, 14]:

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

(2)

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

$$
C_{\alpha\beta} = \frac{k_D^2 \lambda_{\alpha\beta}^2 - k_i^2 \lambda_{ee}^2}{\lambda_{ee}^2 / \lambda_{\alpha\beta}^2 - 1},
$$

$$
A^2 = \frac{\gamma^2}{2} \left( 1 + \sqrt{1 - \left( \frac{2k_D}{\lambda_{ee}\gamma} \right)^2} \right),
$$

$$
B^2 = \frac{\gamma^2}{2} \left( 1 - \sqrt{1 - \left( \frac{2k_D}{\lambda_{ee}\gamma} \right)^2} \right).
$$

Polarizability $\alpha_p$ of atoms was taken into account in effective potentials [15] for charge-atom interactions:

$$
\Phi(r) = \frac{e^2 \alpha_p}{2r^4} \sqrt{1 - 4\lambda_{\alpha\beta}^2 k_D^2} (e^{-B_1 r} (1 + B_1 r) - e^{-A_1 r} (1 + A_1 r)),
$$

(4)

where

$$
A_1^2 = \frac{1}{2\lambda_{\alpha\beta}^2} \left( 1 + \sqrt{1 - 4\lambda_{\alpha\beta}^2 k_D^2} \right),
$$

$$
B_1^2 = \frac{1}{2\lambda_{\alpha\beta}^2} \left( 1 - \sqrt{1 - 4\lambda_{\alpha\beta}^2 k_D^2} \right),
$$

for hydrogen plasma $\alpha_p = 4.5a_B^3$.

3. Structural properties

Pair correlation functions were calculated in the exponential approximation:

$$
g_{\alpha\beta}(r) = \exp(-\Phi_{\alpha\beta}(r)/k_BT),
$$

(5)

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

Pair correlation functions for different potentials and types of interaction are presented in figure 1. As one can see from left-hand figure the results for effective potential (2) are in good agreement with the results for semiclassical potential, which takes into account the screening
Figure 1. Pair correlation functions of a fully ionized hydrogen plasma for different potentials and types of interaction at $\Gamma = 0.3, r_s = 2$: on left-hand: solid line, effective potential (2); dashed line, Deutsch potential (1); dashed-dotted line, Debye potential; dot line, Coulomb potential.

Figure 2. Pair correlation functions for hydrogen plasma for different values of $r_s$ and $\Gamma$: on left-hand figure for $\Gamma = 0.3$: dashed line, $r_s = 2$; solid line, $r_s = 5$; dot line, $r_s = 8$; on right-hand figure for $r_s = 3$: dashed line, $\Gamma = 0.2$; dot line, $\Gamma = 0.5$; solid line, $\Gamma = 0.6$.

effect (Debye potential) at large distances. The influence of quantum-mechanical diffraction effect is more pronounced at the small distances. Left-hand figure shows different types of interactions between particles. Pair correlation functions for different values of density and coupling parameters are presented in figure 2.

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

$$U_N = 2\pi V \int_0^\infty \sum_{\alpha,\beta} n_\alpha n_\beta \phi_{\alpha\beta}(r) g_{\alpha\beta}(r) r^2 dr,$$  \hspace{1cm} (6)
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 [13] 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:

\[
U_N = -2\pi V \sum_{\alpha,\beta} n_\alpha n_\beta e^2 e_\alpha e_\beta \frac{\lambda_{ee}}{2} \sqrt{1 - (2k_D/\lambda_{ee})^2} \times \left( \frac{1}{B(1 - B^2\lambda_{\alpha\beta})^2} - \frac{1}{A(1 - A^2\lambda_{\alpha\beta})^2} \right). + \quad (8) \\
+ 2\pi V e^2 \left( 2Z_i n_i n_e \lambda_{ei}^2 e_{ei} - n_e^2 \lambda_{ee} e_{ee} + \frac{Z_in_i n_e \lambda_{ei} e_{ei}}{k_B T_{ei}(1 - C_{ei})} \right),
\]

\[
P = P_{id} - \frac{2\pi}{3} \sum_{\alpha,\beta} n_\alpha n_\beta e^2 e_\alpha e_\beta \frac{\lambda_{ee}}{2} \sqrt{1 - (2k_D/\lambda_{ee})^2} \times \left( \frac{1}{B(1 - B^2\lambda_{\alpha\beta})^2} - \frac{1}{A(1 - A^2\lambda_{\alpha\beta})^2} \right) + \quad (9) \\
+ 2\pi e^2 \left( 2Z_i n_i n_e \lambda_{ei}^2 e_{ei} - n_e^2 \lambda_{ee} e_{ee} + \frac{Z_in_i n_e \lambda_{ei} e_{ei}}{12k_B T_{ei}(1 - C_{ei})} \right),
\]

The second term in (8)–(9) appears due to the quantum diffraction effect at the small distances.

The thermodynamic properties were calculated taking into account partial ionization.

At given values of the plasma parameters (temperature and density) the degree of ionization was calculated using the system of Saha equations [24]:

\[
\frac{n_0}{n_e n_i} = \frac{g_0}{g_e g_i} \exp \left( \frac{I - \Delta I}{k_B T} \right) \quad (10)
\]
Internal energy of H plasma at $T = 125000$ K: red circles, [16]; blue triangles, [17]; black circles, present work (partially ionized plasma).

Pressure of H plasma at $T = 100000$ K: red circles, [18]; green triangles, [19]; blue pentagons, [20]; black circles, present work (partially ionized plasma).

Correlation energy of H plasma: crossed triangles, [21]; triangles, [22]; solid line, Debye theory; black squares, present work (fully ionized plasma); black circles, present work (partially ionized plasma).

Excess part of equation of state for H plasma: red circles, $A_0 = 0$ [18]; green triangles, $A_0 = \pi/2$ [23]; black circles, present work (fully ionized plasma); black circles, present work (partially ionized plasma).

where $g_k$ is statistical weight, $\Delta I$ is the lowering of the ionization potential due to plasma polarization (plasma microfield) from [24, 25].

In figure 3, ionization of hydrogen for temperatures of $10^5$ K and 125000 K is shown. It can be seen that at high densities ($n > 10^{23}$ cm$^{-3}$) so-called Mott transition takes place and degree of ionization increases with increase in density.

Figures 4 and 6 show the comparison of present work's calculations with the results of other works obtained by the theoretical methods and computer simulation. As follows from analysis of figures 4 and 6, our results for the internal and correlation energy agree with the results of other authors. Increase of our curve at high densities and difference between our internal energy and the results of [21, 22] for large values of the coupling parameter can be attributed to the emergence of the concentration of the atomic component in the system. The results for
the equations of state are shown in figures 5 and 7. The figures show good agreement with the results of molecular dynamics simulations based on wave packets [18] and with the results of Monte Carlo simulation based on path integrals [19, 20]. The difference can be caused by influence of an atomic component.

5. Conclusion
The analytical expressions (8) and (9) for thermodynamic properties of dense non-ideal plasma obtained on the basis of effective screened potentials taking into account the quantum-mechanical effect of diffraction are shown. The internal energy and equation of state of partially ionized hydrogen plasma were calculated. The results of this work are in a good agreement with the results of other authors.

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