THERMODYNAMIC PROPERTIES OF HYDROGEN PLASMA

**Maratbek Gabdullin¹, Tlekkabul Ramazanov², Tomiris Ismagambetova³,
 Alexander Tikhonov⁴**

Abstract: In this paper dense hydrogen plasma, which is of considerable interest in both theoretical and practical areas such as non-ideal plasma encountered in thermonuclear reactors, is considered. The structural and thermodynamic properties of dense non-ideal hydrogen plasma were investigated. Potentials taking into account the quantum-mechanical effects of diffraction and symmetry have been used as a model of interaction. The symmetry effect was considered for the different directions of spin of electrons. Pair correlation functions have been obtained in the solution for the integral equation of the Ornstein-Zernike in hyper-netted chain approximation on the basis of the interaction potentials. Thermodynamic properties for hydrogen plasma were calculated using the interaction potentials and pair correlation functions. The quantum symmetry effect weakens the interaction between the charged particles leading to a decrease in the absolute value of the non-ideal part of the thermodynamic characteristics of the dense plasma. The symmetry effect is more pronounced for higher values of density.

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Introduction

One of the main problems of modern plasma physics is obtaining thermodynamic properties of a non-ideal plasma in a wide range of parameters.

In this paper, the model of interparticle interactions, which takes into account quantum-mechanical effects of diffraction and symmetry, was used to study properties of dense non-ideal hydrogen plasma (Moldabekov, 2012).

The quantum-mechanical effect of symmetry takes into account the Pauli principle, which prohibits the simultaneous presence of two identical particles with a half-integer spin (in this case, electrons) in the same state, hence reducing the probability of finding particles at a distance from each other.

Interaction potentials

In the work conducted by Moldabekov (2012), interaction potentials used in this paper that take into account quantum-mechanical effects of diffraction and symmetry were obtained:

$$u_{ab}(r) = \frac{e_a e_b}{r} \left\{ 1 - th \left(\sqrt{2} \frac{\lambda_{ab}^2}{a_0^2 + br^2} \right) e^{-th \left[\frac{\sqrt{2} \lambda_{ab}^2}{(a_0^2 + br^2)} \right]} \right\} \left(1 - e^{-r/\lambda_{ab}} \right) - \delta_{ae} \delta_{be} k_B T \ln \left(1 - \frac{1}{2} \exp \left(-\frac{r^2}{\lambda_{ee}^2} \right) \right). \quad (1)$$

where e_a , e_b are electrical charges of particles a and b, $m_{ab} = m_a m_b / (m_a + m_b)$,

$\lambda_{ab} = \hbar / \sqrt{2\pi m_{ab} k_B T}$ is the thermal de-Broglie wavelength,

$r_D = \left(k_B T / \left(4\pi e^2 \sum_j n_j Z_j^2 \right) \right)^{1/2}$ is the Debye radius, also dimensionless parameters such as

coupling parameter $\Gamma = \frac{(Ze)^2}{ak_B T}$ and density parameter $r_s = a/a_B$ were used, $a = (3/(4\pi n_e))^{1/3}$ is the

average distance between electrons. The first term in the formula (1) takes into account the diffraction effect, the second term - the symmetry effect.

The following formula was used to account for different electron spin directions instead of the second term in (1):

¹ al-Farabi Kazakh National University, gabdullin@physics.kz

² al-Farabi Kazakh National University, Tlekkabul.Ramazanov@kaznu.kz

³ al-Farabi Kazakh National University, miriael@mail.ru

⁴ Nazarbayev University, atikhonov@nu.edu.kz

$$U_{ee,0}^{S(T)}(r) = -k_B T \ln \left(1 \pm \exp \left(-\frac{r^2}{\lambda_{ee}^2} \right) \right), \quad (2)$$

where $S=1$ corresponds to parallel spins, $S=0$ – to antiparallel spins.

For interactions between ions, the effective potential from work by Ramazanov (2010) was used. Polarizability of atoms was taken into account in the effective potentials from work done by Ramazanov (2005).

Structural properties

Pair correlation functions $g(r)$ were calculated on the basis of the integral equation of Ornstein-Zernike from work by Goodstein (2002):

$$h(\vec{r}) = C(\vec{r}) + n \int C(\vec{r}_3 - \vec{r}_1) h(|\vec{r}_3 - \vec{r}_2|) d\vec{r}_3, \quad (3)$$

which in HNC approximation can be written in the following form:

$$C_{HCA}(r) = h(r) - \ln g(r) - \frac{\Phi(r)}{k_B T}, \quad (4)$$

where $h(\vec{r}) = g(\vec{r}) - 1$ – full correlation function, $C(\vec{r})$ – direct correlation function, Φ is the interaction potential. The equations (3) and (4) were calculated by numerical schemes.

Thermodynamic Properties

Thermodynamic properties such as internal energy and the equation of state were calculated using interaction potentials (1-2) and were obtained on their basis pair correlation functions in approximation (4):

$$E = 3/2 N k_B T - \pi \sum_{\alpha=i,e} n_{\alpha} \sum_{\beta=i,e} n_{\beta} \int_0^{\infty} g^{\alpha\beta}(r) \Phi^{\alpha\beta}(r) r^2 dr, \quad (5)$$

$$P = n k_B T - \frac{2}{3} \pi \sum_{\alpha=i,e} n_{\alpha} \sum_{\beta=i,e} n_{\beta} \int_0^{\infty} \frac{\partial \Phi_{\alpha\beta}(r)}{\partial r} g_{\alpha\beta}(r) r^3 dr, \quad (6)$$

where N is the number of particles in the system (Ramazanov, 2014).

The interaction potentials for different models are presented in figure 1. Black, red, and green lines present the results based on the potential (1) with differences in the symmetry effect, the yellow line shows the results based on the Deutsch theory, and the blue line – on the Debye theory.

Pair correlation functions for different directions of spins are presented in Figure 2. The black lines represent results based on the potentials (1), the red lines represent the results for antiparallel spins, and the green lines represent the results for parallel spins. The results, denoted by a solid line, represent data for $r_s=1$. The results, indicated by the dashed line, represent data for $r_s=2$. The effect of symmetry takes into account the Pauli principle. The effect of the symmetry effect, as a quantum-mechanical effect, is more pronounced at short distances and for denser plasma.

Figures 3-4 show internal energy and the equation of state calculated in the present work in comparison with the results of other authors. It can be seen that for small values of the coupling parameter (up to $\Gamma=1$) the results of the present work are in good agreement with other results. With increasing value of the coupling parameter, the results of this work start to deviate due to the weakening of the interaction between the particles due to a change in the composition of the plasma.

Figure 1: Different potentials for $\Gamma=0.3$, $r_s=2$. Black line – potential (1), red line – potential (1) with antiparallel spins, green line – potential (1) with parallel spins, yellow line – Deutsch theory, blue line – Debye theory.

Source: Authors

Figure 2: Pair correlation functions for $\Gamma=0.3$. Black lines – potential (1), red lines – potential (1) with antiparallel spins, green lines – potential (1) with parallel spins. Solid lines – $r_s=1$, dashed lines – $r_s=2$.

Source: Authors

Figure 3: Internal energy for hydrogen plasma at $r_s=1$. Black line – Debye theory, circles – Izteleuov (2001), black triangles – Pierleoni (1996) and Magro (1996), green line – present work.

Source: Authors

Figure 4: Equation of state for hydrogen plasma at $r_s=1$. Solid line – Debye theory, dashed line – Ichimaru (1987), circles – Izteleuov (2001), black triangles – Pierleoni (1996) and Magro (1996), green line – present work.

Source: Authors

Conclusion

Thermodynamic properties of hydrogen plasma were calculated on the basis of the interaction potential taking into account the quantum-mechanical symmetry effect. Pair correlation functions were obtained through the solution of the integral equation of the Ornstein-Zernike in hyper-netted chain approximation. The quantum symmetry effect weakens the interaction between the charged particles, which leads to a decrease in the absolute value of the non-ideal part of the thermodynamic characteristics of the dense plasma. The symmetry effect is more pronounced for higher values of density. The results of this work are in a good agreement with the results of other authors.

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