Equation of state of a dense plasma: Analytical results on the basis of quantum pair interaction potentials in the random phase approximation

Zh A Moldabekov, T S Ramazanov and M T Gabdullin
Research Institute of Experimental and Theoretical Physics of the Al-Farabi Kazakh National University, al-Farabi Avenue 71, Almaty 050040, Kazakhstan
E-mail: zhandos@physics.kz

Abstract. In this work, using recently obtained expansion of the dielectric function in the long wave length limit by Moldabekov et al (2015 Phys. Plasmas 22 102104), we extended previously obtained formulas for the equation of state of the semiclassical dense plasma from Ramazanov et al (2015 Phys. Rev. E 92 023104) to the quantum case. Inner energy and contribution to the pressure due to plasma non-ideality derived for both Coulomb pair interaction and quantum pair interaction potentials. Obtained analytical result for the equation of state reproduces the Montroll–Ward contribution, which corresponds to the quantum ring sum. It was shown that the obtained results are consistent with the Thomas–Fermi approximation with the first order gradient correction. Additionally, the generalization of the quantum Deutsch potential to the case of the degenerate electrons is discussed. Obtained results will be useful for understanding of the physics of dense plasmas as well as for further development of the dense plasma simulation on the basis of the quantum potentials.

1. Introduction

Nowadays, many experimental and theoretical investigations aim at a better understanding of dense plasmas. This is due to the importance of understanding the evolution of planets and stars [1]. Moreover, many expectations are associated with the use of plasma in inertial fusion reactors. Experimentally, dense nonideal plasmas are analyzed by the shock wave compression method [2], using high-power lasers [3] and ion accelerators [4]. To describe such a type of plasma it is necessary to take into account collective as well as quantum effects.

The problem of calculating the equation of state for dense nonideal plasmas taking into account quantum effects was studied by a number of authors [5]. For example, Vorberger et al [6, 7] considered this problem using the Green’s function method. In [10] quantum effects in dense plasma were studied using quantum molecular dynamics. However, these models require a vast number of calculations. Therefore, to calculate the static properties of plasma in various fields of physics and astrophysics [8,9] it is necessary to have a simple analytical approach. Such a simple self-consistent analytical model, which can be used for the calculation of thermodynamic and structural characteristics of semiclassical dense weakly coupled plasmas, has been developed recently [10]. Here we extend the results of our previous work to the case of the quantum plasma.

In the next section it is shown that the second order result of the long wavelength expansion of the Lindhard dielectric function and dielectric function obtained using quantum Deutsch
potential in combination with the classical polarization function are similar to each other. In the third section, this fact is used to generalize our previous results for the thermodynamic properties of a dense semiclassical plasma to the case of a quantum plasma. The obtained results are discussed in the last section.

2. Wavenumber expansion of the inverse dielectric function

We start with the lowest order many-body approximation for the dielectric function

$$\epsilon(\mathbf{k}, 0) = 1 - \frac{4\pi e^2}{k^2} \Pi_{RPA}(k) - \frac{4\pi Z^2 e^2}{k^2} \Pi_{ion},$$  \hspace{1cm} (1)$$

where $\Pi_{ion}$ is the polarization function of point like classical ions, and $\Pi_{RPA}(k)$ is the polarization function of quantum electrons in the random phase approximation (RPA) for an arbitrary temperature [11]:

$$\Pi_{RPA}(k, \omega) = -\frac{k^2 \chi_0}{16\pi e^2 Z^2} [g_3(u + z) - g_3(u - z)],$$  \hspace{1cm} (2)$$

where $u = \omega/(k\nu_F)$, $z = k/(2k_F)$, $\chi_0 = 3/16 (\hbar\omega_p/E_F)^2 = 1/(\pi k_F a_B)$, $k_F = (3\pi^2 n)^{1/3}$, $\omega_p = 4\pi n e^2/m$, $a_B = \hbar^2/m e^2$ is the Bohr radius, $\nu_F$ is Fermi velocity, and

$$g_3(x) = -g_3(-x) = \int \frac{y dy}{\exp(y^2/\theta - \eta) + 1} \ln \frac{x + y}{x - y},$$  \hspace{1cm} (3)$$

where $\theta = k_B T/E_F$, and $\eta = \mu/k_B T$ is the ratio of the chemical potential to thermal energy. The parameter $\eta$ depends on the density via relation $2/3\theta^{-3/2} = I_{1/2}(\eta)$.

Recently, the following formula for the wavenumber expansion of the inverse polarization function was derived [12]:

$$\frac{1}{2\Pi(k)} = \tilde{a}_0 + \tilde{a}_2 k^2 + \tilde{a}_4 k^4 + \ldots.$$  \hspace{1cm} (4)$$

Substituting the second order result of equation (4) into (1) and taking classical long wavelength limit of the ions' polarization function in the random phase approximation $\Pi_{ion}(k) = -n_i/(k_B T_i)$, we have:

$$\epsilon_2(k)^{-1} = \frac{k^2 \left(1 + \frac{2\tilde{a}_2}{\tilde{a}_0} k^2\right)}{k^2 (1 + \frac{\tilde{a}_2}{\tilde{a}_0} k^2) + k^2_D + \frac{\tilde{a}_4}{\tilde{a}_0} k^4},$$  \hspace{1cm} (5)$$

where $k^2_D = k^2_0 + k^2_i$, and $k^2_i = 4\pi n_i Z^2 e^2/k_B T_i$.

The result for $\tilde{a}_2/\tilde{a}_0$ is

$$\tilde{a}_2/\tilde{a}_0 = \frac{I_{-3/2}(\eta)}{12\theta k_F^2 I_{-1/2}(\eta)}. $$  \hspace{1cm} (6)$$

here $I_{\nu} = \int_0^\infty x^\nu/(1 + \exp(x - \eta)) dx$ is the Fermi-Dirac function of order $\nu$, $k_F^2 = k_F^2 T^2 \theta^{1/2} L^{-1/2}/I_{-1/2}(\eta)/2$ is the screening length which interpolates between Debye and Thomas-Fermi expansions. Further the electrons density is characterized by the density parameter $r_S = a/a_B$, where $a = (4/3\pi n)^{-1/3}$.

The similar formula for $\epsilon(k)^{-1}$ was obtained in [10] using the classical polarization function of electrons $\Pi(k) = -n_i/(k_B T_i)$ and the quantum (Deutsch) [13] potential for the electron-electron interaction $\varphi_{ee}^{Deutsch} = \frac{e^2}{r} (1 - \exp(-r/\lambda_{ee}))$ instead of the Coulomb interaction:

$$\epsilon(k)^{-1} = \frac{k^2 \left(1 + \lambda_{ee}^2 k^2\right)}{k^2 (1 + \lambda_{ee}^2 k^2) + k^2_D + \lambda_{ee}^2 k^4},$$  \hspace{1cm} (7)$$
where $k_D^2 = k_e^2 + k_i^2$, $k_e^2 = 4\pi n_e e^2/k_B T_e$, and $\lambda_{ee} = \hbar/\sqrt{\pi m_e k_B T}$.

Originally the Deutsch potential was not designed to describe plasma with degenerate electrons. From comparison of the equations (6) and (5) we see that the description of the plasma on the basis of the quantum potential can be generalized to the quantum case replacing $\lambda_{ee}^2$ and $k_e$ by $\tilde{a}_2/\bar{a}_0$ and $k_Y$, respectively.

3. Thermodynamic properties of a weakly coupled dense plasma at any degeneracy parameter

To study the thermodynamic properties of the plasma we used a method based on particle pair correlation function:

$$g_{\alpha\beta}(r) \simeq 1 + \frac{\Phi_{\alpha\beta}(r)}{k_B T}.$$  \hspace{1cm} (8)

The key of this approach is to absorb the screening and quantum diffraction effects into an effective screened potential $\Phi$:

$$\Phi_{\alpha\beta}(\vec{r}) = \int \frac{d^3k}{2\pi^2} \frac{\phi_{\alpha\beta}(r)}{\epsilon(k, \omega = 0)} e^{i\vec{k} \cdot \vec{r}},$$  \hspace{1cm} (9)

where $\phi_{\alpha\beta}(r)$ is the pair interaction potential, and for $\epsilon(k, \omega = 0)^{-1}$ the second order result $\epsilon_2(k)^{-1}$ was used.

The correlation energy is determined by the formula:

$$U_N = 2\pi V \sum n_\alpha n_\beta \phi_{\alpha\beta}(r) g_{\alpha\beta}(r) r^2 dr.$$  \hspace{1cm} (10)

The plasma equation of state is written as:

$$P = P_{\text{ideal}} + \frac{2\pi}{3} \sum n_\alpha n_\beta \frac{d\phi_{\alpha\beta}(r)}{dr} g_{\alpha\beta}(r) r^3 dr,$$  \hspace{1cm} (11)

where $P_{\text{ideal}}$ is the pressure of ideal plasma.

3.1. Thermodynamic properties on the basis of the quantum potential

First, we use the quantum Deutsch potential as the pair interaction potential in equations (9-11). For the correlation energy we obtained:

$$U_N = -2\pi V \sum \frac{n_\alpha n_\beta e_{\alpha\beta}^2}{k_B T \gamma^2 \sqrt{1 - (2k_D/\lambda_{ee} \gamma)^2}} \left[ \frac{1/\lambda_{ee}^2 - B^2}{B \left(1 - B^2 \lambda_{ee}^2 \right)} - \frac{1/\lambda_{ee}^2 - A^2}{A \left(1 - A^2 \lambda_{ee}^2 \right)} \right] + U_\lambda,$$  \hspace{1cm} (12)

where the second term

$$U_\lambda = 2\pi V e^2 \left[ 2Z_i n_i n_e \lambda_{ei}^2 - n_e^2 \lambda_{ee}^2 + Z_i n_i n_e \lambda_{ei} e^2 / (k_B T (1 + C_{ei})) \right]$$

is due to the quantum diffraction effect at small distance, $\lambda_{ei} = \lambda_{ee}/\sqrt{2}$, $\gamma^2 = k_i^2 + 1/\lambda_{ee}^2$ and $C_{ei} = (k_D \lambda_{ei}^2 - k_i \lambda_{ee}^2) / (\lambda_{ei}^2 / \lambda_{ei}^2 - 1)$,

$$A^2 = \gamma^2 / \left(1 + \sqrt{1 - (2k_D/\lambda_{ee} \gamma)^2}\right), \quad B^2 = \gamma^2 / \left(1 - \sqrt{1 - (2k_D/\lambda_{ee} \gamma)^2}\right).$$  \hspace{1cm} (13)
For the equation of state we have:

$$P = P_{\text{ideal}} - \frac{2\pi}{3} \sum \frac{n_\alpha n_\beta c_\alpha^2 c_\beta^2}{k_B T \gamma^2 \sqrt{1 - (2k_D/\lambda_{ee} \gamma)^2}} \left[ \frac{1/\lambda_{ee}^2 - B^2}{B \left(1 - B^2 \lambda_{\alpha \beta}^2\right)} \right] + P_\lambda,$$

(14)

here the second term $P_\lambda = 2\pi e^2 \left[ 2Z_i n_i n_e \lambda_{ee}^2 - n_e^2 \lambda_{ee}^2 + Z_i n_i n_e \lambda_{ee}^2 e^2 / (12k_B T (1 + C_{ei})) \right]$.

3.2. Thermodynamic properties on the basis of Coulomb potential

Second, we use Coulomb potential as the pair interaction potential in equations (9-11). For the correlation energy we derived:

$$U_N = -2\pi V \sum \frac{n_\alpha n_\beta c_\alpha^2 c_\beta^2}{k_B T \gamma^2 \sqrt{1 - (2k_D/\lambda_{ee} \gamma)^2}} \left[ \frac{1/\lambda_{ee}^2 - B^2}{B \left(1 - B^2 \lambda_{\alpha \beta}^2\right)} \right] + 2\pi V \frac{Z_i n_i n_e \lambda_{ei} e^4}{k_B T (1 + C_{ei})} +$$

$$+ 2\pi V \frac{Z_i n_i n_e \lambda_{ei} e^4}{k_B T (1 + C_{ei})} +$$

(15)

The equation of state has the following form:

$$P = P_{\text{ideal}} - \frac{2\pi}{3} \sum \frac{n_\alpha n_\beta c_\alpha^2 c_\beta^2}{k_B T \gamma^2 \sqrt{1 - (2k_D/\lambda_{ee} \gamma)^2}} \left[ \frac{1/\lambda_{ee}^2 - B^2}{B \left(1 - B^2 \lambda_{\alpha \beta}^2\right)} \right]$$

$$- \frac{1/\lambda_{ee}^2 - A^2}{A \left(1 - A^2 \lambda_{\alpha \beta}^2\right)} \right] + \frac{2\pi}{3} \frac{Z_i n_i n_e \lambda_{ei} e^4}{k_B T (1 + C_{ei})}.$$

(16)

4. Summary and discussions

The formulas for correlation energy (12), (15) and for equation of state (14), (16) were derived in our previous work [10] for the semi-classical plasma using the dielectric function (7). The comparison with the results of the simulations and other theoretical works has shown that the obtained formulas correctly describe a weakly coupled dense plasma. Additionally, it was revealed that the equation of state (14), obtained using the quantum Deutsch potential, reproduces the Montroll–Ward contribution in the limit $(\lambda_{ee} k_D) \ll 1$, whereas the equation of state (16), obtained using Coulomb potential, fails to reproduce this term. Above, we generalized these formulas to the case of any degeneracy. This was possible due to identity of the dielectric functions (5) and (7) to each other. In [12] it was demonstrated that the term with $\tilde{a}_2$ in the second order result of the polarization function expansion (4) is related to the first order gradient correction to the kinetic energy of the non-interacting fermion gas and that the dielectric function (5) gives description at the same level as the finite temperature Thomas-Fermi theory with the first order gradient correction.

To conclude, the presented here formulas (12) and (14), for the description of the thermodynamic properties of a dense plasma, take into account quantum effect of the electrons degeneracy and the effect of the weakly non-ideality within quantum ring sum. Additionally, it is shown that the quantum potential in the form of the Deutsch potential can be used for the description of the weakly non-ideal plasma at small degeneracy parameters $\theta < 1$ if the $\lambda_{ee}$ is replaced by $\sqrt{\tilde{a}_2 / \tilde{a}_0}$. 


Acknowledgments
This work has been supported by the Ministry of Education and Science of Kazakhstan.

References
[1] French M et al 2012 Astrophys. J., Suppl. Ser. 202 5
[2] Fortov V E and Yakubov I N 1999 Physics of Nonideal Plasma (Singapore: World Scientific)
[3] Lower T et al 1994 Phys. Rev. Lett. 72 3186
[4] Tahir N A et al 2011 Phys. Plasmas 18 032704
[5] Reinholz H, Redmer R and Nagel S 1995 Phys. Rev. E 52 5368
[6] Vorberger J, Schlanges M and Kraeft W D 2004 Phys. Rev. E 69 046407
[7] Vorberger J, Gericke D O and Kraeft W D 2013 High Energy Density Phys. 9 448
[8] Khrapak S A, Khrapak A G, Ivlev A V and Morfill G E 2014 Phys. Rev. E 89 023102
[9] Potekhin A Y, Chabrier G and Rogers F J 2009 Phys. Rev. E 79 016411
[10] Ramazanov T S, Moldabekov Z A and Gabdullin M T 2015 Phys. Rev. E 92 023104
[11] Arista N R and Brandt W 1984 Phys. Rev. A 29 1471
[12] Moldabekov Z A, Schoof T, Ludwig P, Bonitz M and Ramazanov T 2015 Phys. Plasmas 22 102104
[13] Deutsch C 1977 Phys. Lett. A 60 317