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Yu.V. Arkhipov[1], A. Askaruly[1], V.V. Voronkov[2], A.E. Davletov[1], A.B. Ashikbayeva[1], I. M. Tkachenko[3]

[1] Scientific-Research Institute of Experimental and Theoretical Physics, Al-Farabi Kazakh National University, Almaty, Kazakhstan

[2] Kazakh-British Technical University, Almaty, Kazakhstan

[3] Instituto de Matemática Pura y Aplicada, Universidad Politécnica de Valencia, Spain

Statical structural properties of nonideal plasma

Abstract. In this article radial distribution functions and static structure factors of nonideal plasma are investigated in the framework of Ornstein-Zernike equation with Percus-Yevick bridge function and Deutch micropotential. It is shown that short range symmetries appear in ionic subsystem of dense plasma and bridge contributions of electrons promote creation of symmetries in ionic subsystem of nonideal plasma.

Keywords: dense plasma, radial distribution function, bridge function.

Introduction

There exist a large variety of different methods for determining static properties of nonideal plasma. One of the most proved methods is usage of the hypernetted chain Ornstein-Zernike equation [1]. This approach needs long ranged, not screened potentials. Earlier works used long ranged classical Coulomb potential, but such a method does not allow a researcher to consider quantum effects which play significant role in a nonideal plasma. The importance of considering quantum effects for research of nonideal plasma properties was demonstrated in [2]. Here we use the Deutch potential [3] which considers quantum effects of diffraction at short distances, and coincides with the Coulomb potential at large distances.

Ornstein-Zernike equation in the hypernetted chain approximation with bridge functions and Deutch micropotential of interaction of particles

This work studies nonideal two component fully ionized nondegenerate hydrogen-like plasma which consists of electrons and ions of masses m and M respectively. Two dimensionless coupling and density parameters describe such plasma:

$$\Gamma = \frac{e^2}{a k_B T}, \tag{1}$$

$$r_s = \frac{a}{a_0} = \frac{a m e^2}{\hbar^2}, \tag{2}$$

here $a = \sqrt[3]{3/4\pi n}$ is the interionic radius, a_0 is the radius of the first Bohr orbit of electron in an atom, $\hbar$ is the Plank constant, all the other notations are standard.

The static correlation functions are found with the integral Ornstein-Zernike equation in the hypernetted chain approximation [1]. It follows from the formalism of density functional that complete correlation function

$$h_{ab}(r) = g_{ab}(r) - 1, \tag{3}$$

is connected with direct correlation function $C_{ab}(r)$ through the following relation of Ornstein-Zernike:

* Corresponding author e-mail: voronkov.v@hotmail.com.

$$h_{ab}(r) = c_{ab}(r) + \sum_d n_d \int d\mathbf{r}' h_{ad}(|\mathbf{r}-\mathbf{r}'|)\, c_{db}(r'). \quad (4)$$

The hypernetted chain approximation determines the radial distribution function in the following form:

$$g_{ab}(r) = \exp\left(-\beta\varphi_{ab}(r) + h_{ab}(r) - c_{ab}(r)\right). \quad (5)$$

Equations (3)-(5) forms a closed system of equations and can be calculated numerically till the necessary accuracy.

In a case when there exist experimental data of computer simulation a researcher can use bridge functions to improve the results of numerical solution of the Ornstein-Zernike equation (3) – (5). That is a more precise expression for radial distribution function must be used:

$$g_{ab} = \exp\left(-\beta\phi_{ab} + N_{ab}(r) + B_{ab}(r)\right). \quad (6)$$

Here $N_{ab}(r)$ is the sum of nodal diagrams and $B_{ee}(r)$ is the bridge function which is found via computer simulations in [4]:

$$B_{ee}(r) = -g(r) + 1 + \ln g(r) + C(r) + \beta\varphi_{ee}(r) \quad (7)$$

Then we can rewrite the numerical scheme for solution of Ornstein-Zernike equation (3) – (4) in order to consider the correlation functions with respect to the bridge function in the following form:

$$\tilde{N}_s = \frac{\tilde{C}}{(1-\rho\tilde{C})} - \tilde{C}, \quad (8)$$

$$g(r) = \exp[B(r) + N_s(r) - u_s(r)], \quad (9)$$

$$C_s(r) = g(r) - 1 - N_s(r), \quad (10)$$

where

$$u_s(r) = u(r) - u_l(r), \quad (11)$$

$$C_s(r) = C(r) + u_l(r), \quad (12)$$

$$N_s(r) = N(r) - u_l(r). \quad (13)$$

Equations (11) – (13) are auxiliary functions which help to decrease the number of iterations. Meanwhile $N(r)$ is the sum of nodal diagrams.

$$N(r) = h(r) - C(r), \quad (14)$$

ρ is the number density of particles, by sign «~» above the quantities the Fourier images of these quantities are noted. For example this is the expression of the direct correlation function:

$$\tilde{c}_{\alpha\beta}(k) = 4\pi n \int_0^\infty \frac{\sin kr}{kr} c(r) r^2 dr. \quad (15)$$

If the auxiliary function $u_l(r)$ is chosen correctly then the given system of equations is numerically solved till any necessary accuracy. The difficulty of the given method is to obtain converging solution for large values of the coupling parameter Γ (1). Thus, for building a more stable iterative scheme, the function $C_s(r)$ must ensure the convergence of the transition into the Fourier space. When the coupling parameter Γ increases the initial values of the direct correlation function are determined on the basis of values of direct correlation functions for smaller Γ by using linear extrapolation. The following condition defines obtaining solution of good accuracy:

$$C_{rms} \equiv \left\{ \int \left| C^{(out)}(r) - C^{(in)}(r) \right|^2 dr \right\}^{1/2} < 10^{-10}\Gamma \quad (16)$$

The effective potential considering quantum effects was proposed by Deutch and co-authors in work [3]:

$$\phi_{ab}(r) = \frac{e_a e_b}{r}\left[1 - \exp\left(-\frac{r}{\lambda_{ab}}\right)\right], \quad (17)$$

where $\lambda_{ab} = \hbar/(2\pi\mu_{ab}k_B T)^{1/2}$ refers to the thermal de Broglie wavelength of relative motion of this two particles a and b, $\mu_{ab} = m_a m_b/(m_a + m_b)$ is the reduced mass of interacting particles, $T_{ab} = (m_a T_b + m_b T_a)/(m_a + m_b)$ is the temperature of the media in the case of anisothermal plasma. In expression (17) the exponential term with the thermal de Broglie wavelength accounts for the quantum effects of diffraction. It is worthwhile to notice that if expressed in plasma parameters, the thermal de Broglie wavelength is $\lambda_{ab}/a \sim (\Gamma/r_s)^{1/2}$ thus, the less value of the parameter r_s is chosen, the more influential quantum effects upon potential (17) are, that is the more dense plasma, the more significant role quantum effects play in such a plasma media. One can see that considering quantum effects in potential (17) leads to decrease in forces, acting between particles (decrease in electron-electron and ion-ion repulsion and electron-ion attraction), that is plasma becomes less "elastic".

Static structure properties of nonideal plasma

The electron-electron, electron-ion and ion-ion radial distribution functions g_{ee}, g_{ei}, g_{ii} can be obtained by solving the numerical scheme (8) – (10) for Ornstein-Zernike equation with Deutch micropotential (17). Then we can calculate the static structure factors with the following formula:

$$S_{\alpha\beta}(k) = \delta_{\alpha\beta} + n\int d\vec{r}\left[g_{\alpha\beta}(r) - 1\right]\exp(-i\vec{k}\cdot\vec{r}), \quad (18)$$

$\delta_{\alpha\beta}$ is the Kroneker symbol. Below are pictures for radial distribution functions and statical structure factors for various values of the coupling parameter Γ (1) and density parameter r_s (2).

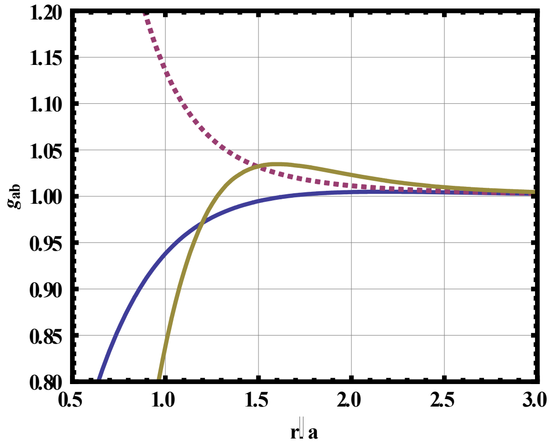

Figure 1 – Radial distribution functions of a two component hydrogen-like plasma at Γ=3, r_s= 2. Solid blue line - g_{ee}, dotted red line – g_{ei}, solid grey green line - g_{ii}.

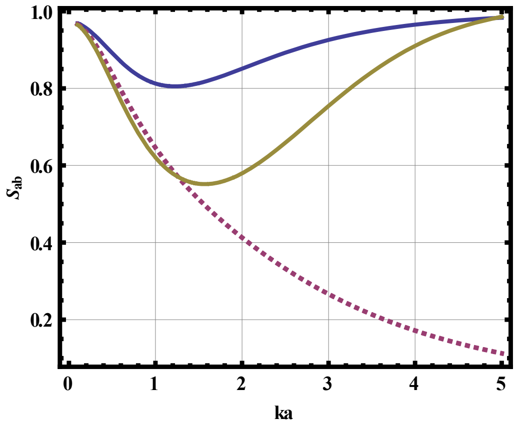

Figure 2 – Static structure factors of a two component hydrogen-like plasma at Γ=3, r_s= 2. Solid blue line - g_{ee}, dotted red line – g_{ei}, solid grey green line - g_{ii}.

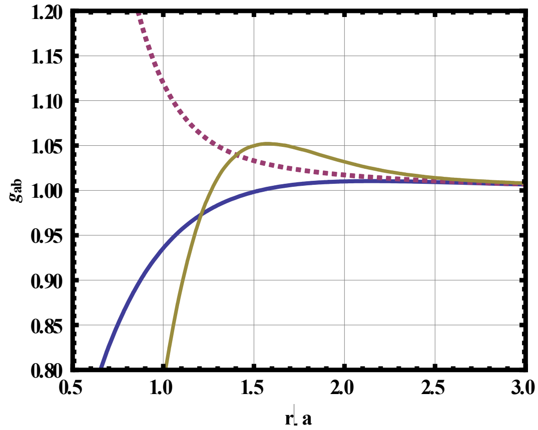

Figure 3 – Radial distribution functions of a two component hydrogen-like plasma at Γ=4, r_s= 2. Solid blue line - g_{ee}, dotted red line – g_{ei}, solid grey green line - g_{ii}.

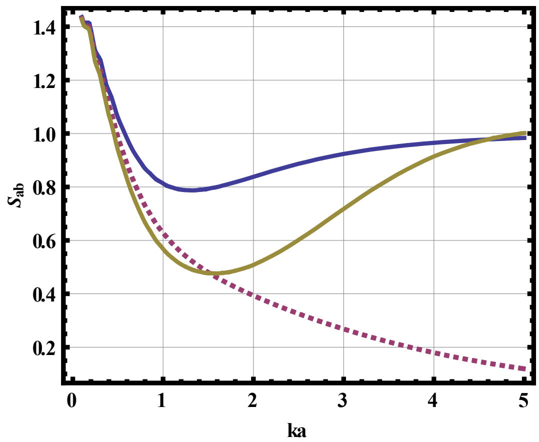

Figure 4 – Static structure factors of a two component hydrogen-like plasma at Γ=4, r_s= 2. Solid blue line - g_{ee}, dotted red line – g_{ei}, solid grey green line - g_{ii}.

As it follows from figures (1) – (4), the proposed model predicts creation of short range symmetries in ionic system of dense plasma. Moreover, comparing results for different parameters we found that the larger the coupling parameter Γ the more explicit this symmetry. This is in good agreement with the fact that the coupling parameter describes the ratio of the average potential energy of ions to their thermal energy.

Contribution of bridge function to radial distribution functions

Our study of contribution of bridge function (7) to shape of radial distribution functions shows that mostly it increases with decreasing r_s (see Fig. 5 - 8). What can be explained by the fact that increasing number density of plasma particles makes bridge contributions of electrons to be more manifested. Also our study shows that bridge contributions of electrons makes symmetry peaks in ion-ion radial distribution function more explicit (see Fig. 7, 8). It means that a researcher must take into account bridge contributions of electrons because they promote creation of symmetries in ionic subsystem of nonideal plasma.

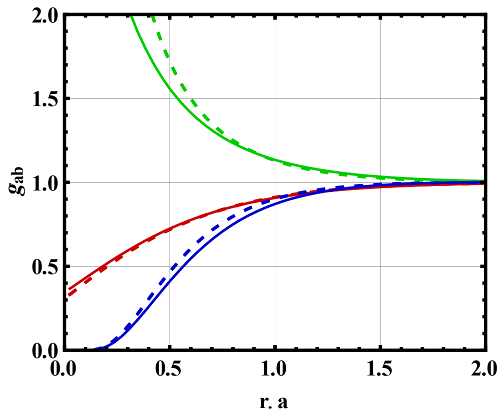

Figure 5 – Radial distribution functions of a two component hydrogen-like plasma at Γ=1, r_s= 1. Red lines - g_{ee}, green lines – g_{ei} , blue lines - g_{ii}, solid lines – calculations with bridge function (7), dotted line – without bridge function.

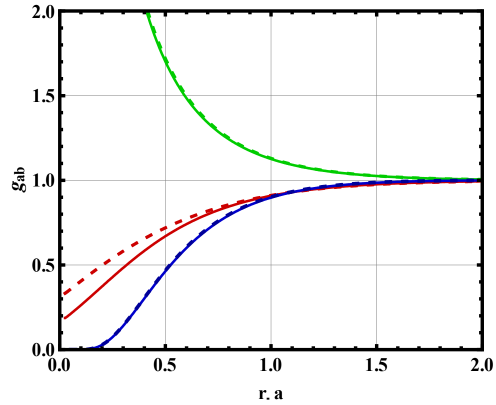

Figure 6 – Radial distribution functions of a two component hydrogen-like plasma at Γ=1, r_s= 2. Red lines - g_{ee}, green lines – g_{ei} , blue lines - g_{ii}, solid lines – calculations with bridge function (7), dotted line – without bridge function.

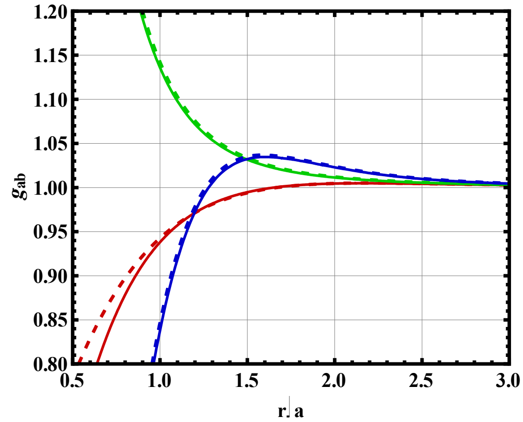

Figure 7 – Radial distribution functions of a two component hydrogen-like plasma at Γ=3, r_s= 2. Red lines - g_{ee}, green lines – g_{ei} , blue lines - g_{ii}, solid lines – calculations with bridge function (7), dotted line – without bridge function.

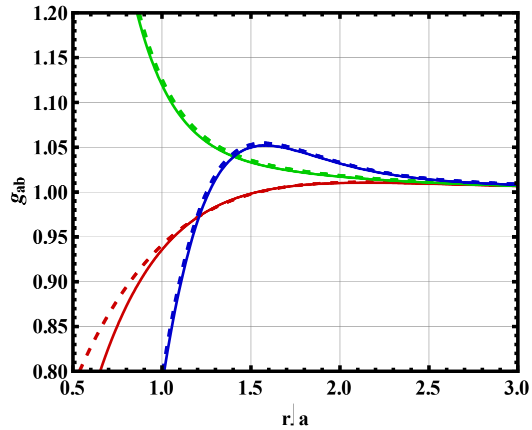

Figure 8 – Radial distribution functions of a two component hydrogen-like plasma at Γ=4, r_s= 2. Red lines - g_{ee}, green lines – g_{ei} , blue lines - g_{ii}, solid lines – calculations with bridge function (7), dotted line – without bridge function.

Conclusions

In this work radial distribution functions and static structure factors were calculated with the aid of Deutch potential and Ornstein-Zernike equation in the hypernetted chain approximation with Percus-Yevick bridge function. It is shown that short range symmetries appear in dense plasma. Additionally it is found that the greatest importance for development of the symmetry in plasma has the value of the coupling parameter Γ. Our research shows that as a rule increasing number density of plasma particles makes bridge contributions of electrons to be more manifested. Also it is found that bridge contributions of electrons promote creation of symmetries in ionic subsystem of nonideal plasma.

In general, these results expand the scope of applicability of the hypernetted chain approximation for different interaction potentials in a wide range of plasma parameters.

Acknowledgements

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