Thermodynamic stability of multicomponent nonideal plasmas

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Abstract The thermodynamic stability of a multicomponent nonideal plasma is studied. To find pair correlation functions and partial static structure factors, the OZ integral equations for a multicomponent fluid were used, which were closed using the HNC approximation. A procedure has been developed for the transition to the one-component approximation for the most nonideal plasma subsystem for the case of any number of plasma components. The thermodynamic potentials of a multicomponent plasma were determined: internal energy, pressure, free energy, chemical potentials and their derivatives. The data obtained in numerical calculations were used to determine the region of thermodynamic stability of a three-component nonideal dusty plasma.

1. Introduction

Plasmas which contain the so called condensed disperse phase or dusty plasmas are widely spread in nature and used in technology, therefore research of such complex systems is of considerable interest for both fundamental physics [1–5], and for a number of applications, for example, for the nanoparticle industry [6].

The present work, unlike the above papers, is dedicated to the description of electrostatic properties of dusty plasmas with the Coulomb pair interaction potential between charged plasma particles based on the multicomponent Ornstein-Zernike equation [7, 8].

2. OZ equations for a multicomponent plasma

We consider a three-component plasma with the interaction between charged particles described by the Coulomb potential:

$$V_{\nu\mu}\left(|\mathbf{r}_\nu-\mathbf{r}_\mu|\right)=\frac{e^2 z_\nu z_\mu}{|\mathbf{r}_\nu-\mathbf{r}_\mu|}. \tag{1}$$

The Ornstein-Zernike equation for a homogeneous multicomponent fluid has the form [7]:

$$h_{\nu\mu}(r)=C_{\nu\mu}(r)+\sum_\lambda n_\lambda\int C_{\nu\lambda}\left(|\mathbf{r}-\mathbf{r}'|\right)h_{\lambda\mu}(r')\,d\mathbf{r}',\qquad \nu=0,1,2,\ \mu=0,1,2, \tag{2}$$

where $h_{\nu\mu}=g_{\nu\mu}-1$ and $C_{\nu\mu}$ are the partial and the direct pair correlation functions, respectively; n_λ is the averaged number density of the λ-species particles, $n_\lambda=N_\lambda/V$, N_λ is their total number in the system of the volume V. Therefore, the total quasineutrality condition takes the following form:

$$\sum_{\nu=0}^{2} z_\nu n_\nu=0. \tag{3}$$

The three-dimensional Fourier transformation converts this system of integral equations into the system of algebraic equations:

$$\widetilde{h}_{\nu\mu}(k)=\widetilde{C}_{\nu\mu}(k)+\sum_\lambda n_\lambda\widetilde{C}_{\nu\lambda}(k)\,\widetilde{h}_{\lambda\mu}(k). \tag{4}$$

From (4) one gets

$$\widetilde{h}_{00}(k)=\widetilde{C}_{\mathit{eff}}(k)+n_0\widetilde{C}_{\mathit{eff}}(k)\,\widetilde{h}_{00}(k), \tag{5}$$

which involves the effective direct correlation function

$$\widetilde{C}_{\mathit{eff}}(k)=\widetilde{C}_{00}+\frac{1}{D(k)}\left[n_1\widetilde{C}_{01}^2\left(1-n_2\widetilde{C}_{22}\right)+n_2\widetilde{C}_{02}^2\left(1-n_1\widetilde{C}_{11}\right)+2n_1n_2\widetilde{C}_{01}\widetilde{C}_{02}\widetilde{C}_{12}\right], \tag{6}$$

where

$$D(k)=\left(1-n_1\widetilde{C}_{11}\right)\left(1-n_2\widetilde{C}_{22}\right)-n_1n_2\widetilde{C}_{12}^2.$$

One can see that Eq. (5) has the form of the OZ equation for a one-component liquid.

In the case coupling parameters is small for all subsystems besides the dusty subsystem

$$\widetilde{C}_{\nu\mu}(k)=-\frac{4\pi e^2 z_\nu z_\mu\beta}{k^2},\qquad \nu=0,1,2;\ \mu=1,2. \tag{7}$$

Here β is the inverse temperature: $\beta=1/T$. From Eq. (6),

$$\widetilde{C}_{\mathit{eff}}(k)=\widetilde{C}_{00}(k)+\frac{4\pi e^2 z_0^2\beta k_{ei}^2}{k^2\left(k^2+k_{ei}^2\right)}, \tag{8}$$

where $k_{ei}^2=k_1^2+k_2^2$, with the electron, k_1, and ion, k_2, screening constants defined by relations

$$k_1^2=4\pi e^2 n_1\beta,\quad k_2^2=4\pi e^2 z_2^2 n_2\beta. \tag{9}$$

The solution for h_{00} will not change if the effective Debye potential

$$V_{\mathit{eff}}(r)=\frac{e^2z_0^2}{r}e^{-k_{ei}r} \tag{10}$$

is introduced. It is important that the screening constant in this case is determined only by electrons and ions whose number densities are related to that of the dust particles by the total quasineutrality condition (3). Therefore, when the charge or number density of dust particles varies, the screening constant k_{ei} also changes.

In the HNC approximation, the bridge functional is assumed to be zero: $B_{\nu\mu}(r)=0$ and for the closure of the OZ equation (5) the equation

$$h_{00}(\mathbf{r})=e^{-\beta V_{\mathit{eff}}(\mathbf{r})+h_{00}(\mathbf{r})-C_{\mathit{eff}}(\mathbf{r})}-1 \tag{11}$$

can be employed.

The pair interaction potential of charged particles in the plasma remains the Coulomb one. In general, V_{eff} is defined by the expression

$$V_{\mathit{eff}}(r)=V_{00}-\frac{1}{2\pi^2\beta r}\int_0^\infty\frac{1}{D(k)}\left[n_1\widetilde{C}_{01}^2\left(1-n_2\widetilde{C}_{22}\right)+n_2\widetilde{C}_{02}^2\left(1-n_1\widetilde{C}_{11}\right)+2n_1n_2\widetilde{C}_{01}\widetilde{C}_{02}\widetilde{C}_{12}\right]k\sin(kr)\,dk. \tag{12}$$

3. Pressure and internal energy

The interaction-associated part of the internal energy in a homogeneous plasma is defined as [7]

$$\Delta U=\tfrac{1}{2}\sum_\nu\sum_\mu n_\nu n_\mu\int V_{\nu\mu}(r)\,g_{\nu\mu}(r)\,d\mathbf{r}, \tag{13}$$

and the pressure as [7]

$$P=\frac{n}{\beta}-\frac{1}{6}\sum_\nu\sum_\mu n_\nu n_\mu\int\mathbf{r}\frac{\partial V_{\nu\mu}(r)}{\partial\mathbf{r}}g_{\nu\mu}(r)\,d\mathbf{r}. \tag{14}$$

Hence, for the Coulomb interaction potential (1), taking into account the condition of total quasineutrality (3) one finds:

$$\Delta U=2\pi e^2\sum_\nu\sum_\mu n_\nu n_\mu z_\nu z_\mu\int_0^\infty h_{\nu\mu}(r)\,r\,dr, \tag{15}$$

$$P=\frac{n}{\beta}+\frac{2\pi e^2}{3}\sum_\nu\sum_\mu n_\nu n_\mu z_\nu z_\mu\int_0^\infty h_{\nu\mu}(r)\,r\,dr=\frac{n}{\beta}+\frac{1}{3}\Delta U. \tag{16}$$

4. Numerical simulations and discussion of results

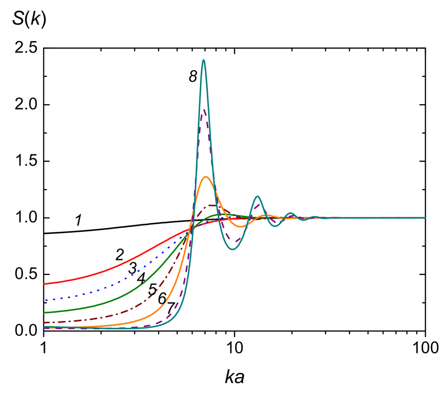

Figure 1: *The structure factor of the dust component found from the OZ equation in the HNC approximation for different coupling parameter values: curve 1 corresponds to $\Gamma=0.1$ and curves 2, 3, 4, 5, 6, 7, and 8 correspond, respectively, to $\Gamma=1, 2, 4, 10, 30, 100$, and 155.*

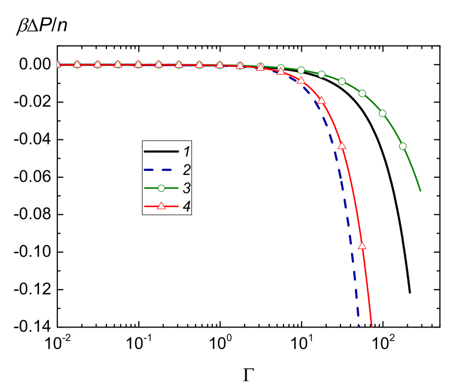

Figure 2: *Pressure corrections due to the Coulomb interaction in a multicomponent dusty plasma vs the coupling parameter. The curves 1 and 2 are for $n_0=10^5$ cm^{-3}, $n_2=10^8$ cm^{-3}, $\overline{T}=300$ K, and $z_0<0$; 3 and 4 are for $n_0=10^7$ cm^{-3}, $n_2=10^{10}$ cm^{-3}, $\overline{T}=2000$ K, and $z_0>0$. Curves 1 and 3 are the pressure corrections (16) obtained by the numerical solution of the OZ equation in the HNC approximation, 2,4 are the pressure corrections within the Debye approximation.*

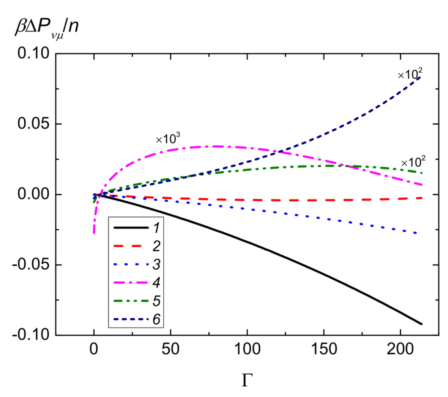

Figure 3: *Partial corrections to the pressure due to the Coulomb interaction in a multicomponent dusty plasma vs the coupling parameter for $n_0=10^5$ cm^{-3}, $n_2=10^8$ cm^{-3}, $\overline{T}=300$ K, and $z_0<0$, found on the basis of the solution of the OZ equation in the HNC approximation. Curves 1, 2, 3, 4, 5 and 6 display, respectively, P_{00}, $2P_{01}$, $2P_{02}$, P_{11}, $2P_{12}$, and P_{22}.*

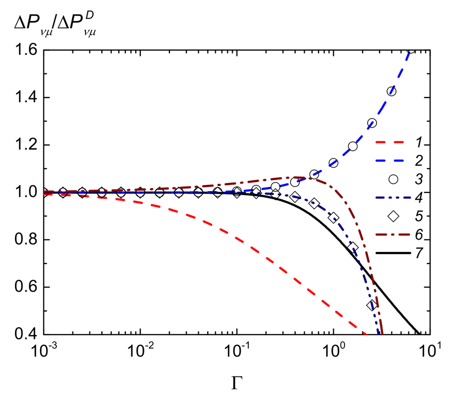

Figure 4: *The partial (curves 1-6, reduced to the partial Debye pressure correction, see Fig. 3) and the full pressure correction (curve 7) vs the coupling parameter for $n_0=10^5$ cm^{-3}, $n_2=10^8$ cm^{-3}, $\overline{T}=300$ K, and $z_0<0$.*

5. Thermodynamic stability of dusty plasmas

Consider the system as a solution: dust particles are particles of a substance dissolved in an electron-ion plasma, while electrons and ions are particles of a solvent. In this case, the following conditions must be satisfied for the TDS of a dusty plasma [9, 10]:

$$C_V=\left(\frac{\partial U}{\partial T}\right)_{V,N_0,N_1,N_2}>0,\quad K_T=-\frac{1}{V}\left[\left(\frac{dP}{dV}\right)_{T,N_0,N_1,N_2}\right]^{-1}>0, \tag{17}$$

$$\mu_{00}>0,\quad \mu_{11}>0,\quad \mu_{00}\mu_{11}-\mu_{01}\mu_{10}>0. \tag{18}$$

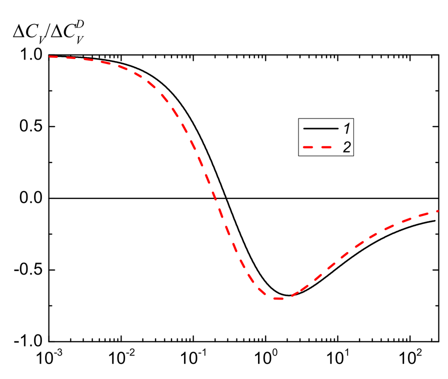

Figure 5: *The interaction correction to the ideal isochoric heat capacity reduced to the Debye one for a multicomponent dusty plasma vs the coupling parameter. Curve 1 corresponds to $n_0=10^5$ cm^{-3}, $n_2=10^8$ cm^{-3}, $\overline{T}=300$ K, and $z_0<0$; 2 is for $n_0=10^7$ cm^{-3}, $n_2=10^{10}$ cm^{-3}, $\overline{T}=2000$ K, and $z_0>0$.*

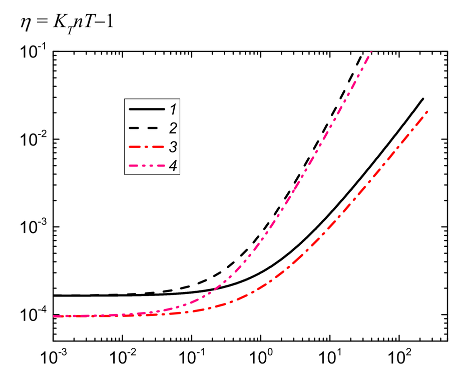

Figure 6: *Isothermal compressibility of a multicomponent dusty plasma as a function of coupling parameter. Curves 1 and 2 are for $n_0=10^5$ cm^{-3}, $n_2=10^8$ cm^{-3}, $\overline{T}=300$ K, and $z_0<0$; 3 and 4 are for $n_0=10^7$ cm^{-3}, $n_2=10^{10}$ cm^{-3}, $\overline{T}=2000$ K, and $z_0>0$. Curves 1,3 were calculated from the solution of the OZ equation in the HNC approximation, 2, 4 were calculated in the Debye approximation.*

Figure 5 shows the values of the isothermal compressibility of a dusty plasma: The thermodynamic stability of the dusty plasma is determined by the sign of the dimensionless parameters ζ_ν, $\nu=0,1$, defined as

$$\zeta_\nu=\frac{N_\nu}{T}\mu_{\nu\nu}=\left(1-\frac{\beta e^2z_\nu^2k_D^2}{4k_D}\right)-\frac{n_\nu}{8n}\frac{\left(4-\beta z_\nu^2k_De^2\right)^2}{\left(3P\beta/n-1\right)}, \tag{19}$$

and by the sign of the dimensionless parameter ζ_{01} defined as

$$\zeta_{01}=\frac{2N_0N_1}{T^2}\left(\mu_{00}\mu_{11}-\mu_{01}\mu_{10}\right)=\frac{2n_2}{n}\left(1-\frac{k_D^3}{16\pi n}\right)^{-1}\left(1-\frac{e^2k_D}{4T}\frac{\sum_\nu n_\nu z_\nu^4}{\sum_\nu n_\nu z_\nu^2}\right). \tag{20}$$

Norman and Starostin observed in [11] that the third condition (18) can be reduced to the requirement of stability of a non-ideal subsystem without taking into account the ideal subsystems, for which the isothermal compressibility must be positive:

$$K_{T,00}=-\frac{1}{V}\left[\left(\frac{\partial P_{00}}{\partial V}\right)_T\right]^{-1}. \tag{21}$$

It is the positivity condition of $K_{T,00}$ that is employed to determine the thermodynamic stability in the one-component approximation.

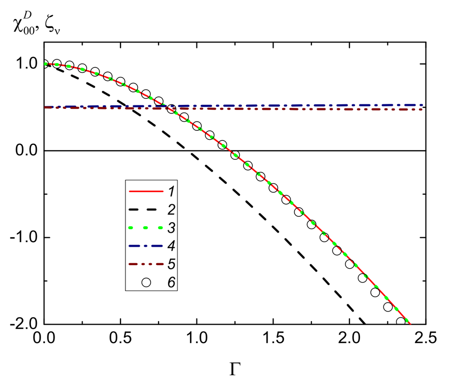

Figure 7: *Inverse isothermal compressibility $\chi_{00}^D=\left(K_{T,00}^Dn_0T\right)^{-1}$, the derivatives of the chemical potential ζ_ν (19) and ζ_{01} (20) in the Debye approximation vs the coupling parameter for $n_0=10^5$ cm^{-3}, $n_2=10^8$ cm^{-3}, $\overline{T}=300$ K, and $z_0<0$ with the curves 1, 2, 3 ,4, 5 and 6 standing for $\eta=K_{T,00}n_0T$, $\eta=K_{T,0}n_0T$, ζ_0, ζ_1, ζ_2, and ζ_{01}, respectively.*

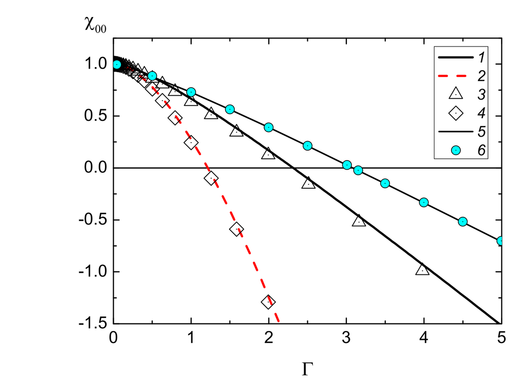

Figure 8: *Inverse isothermal compressibility of the plasma dust component $\chi_{00}=\left(K_{T,00}n_0T\right)^{-1}$ as a function of the coupling parameter: 1 and 2 are for $n_0=10^5$ cm^{-3}, $n_2=10^8$ cm^{-3}, $\overline{T}=300$ K, and $z_0<0$; 3 and 4 are for $n_0=10^7$ cm^{-3}, $n_2=10^{10}$ cm^{-3}, $\overline{T}=2000$ K, and $z_0>0$; 1 and 3 are from the solution of the OZ equation in the HNC approximation, 2,4 are in the Debye approximation, 5 is calculated from $\chi_{00}=1+\frac{4}{9}a\Gamma+\frac{13}{36}b\Gamma^{1/4}+\frac{1}{3}c$ valid at $\Gamma\geq 1$ with $a=-0.89643$, $b=0.86185$, $c=-0.5551$ obtained by a least square fit to the MD data over the entire fluid range $1\leq\Gamma\leq 160$ in [12], 6 are calculated using the OCP equation of state obtained by numerical simulation of the OZ equation in the HNC approximation in [13].*

6. Conclusions

In the present work, on the basis of the OZ equation for a multicomponent plasma, a transition is described to the OCP approximation with an effective pseudopotential and in order to calculate the dust-dust pair correlation function. It was established that in the case when all subsystems except the dust one are ideal the effective pseudopotential becomes the Debye potential with the screening constant which should be determined without the contribution of the dust subsystem but taking into account the condition of the total plasma quasineutrality. If the non-dust components are not ideal the above effective potential might deviate from the Debye form. In other words, we do not initially model the dusty plasma as a Yukawa one-component system applicable only when all components are weakly coupled.

It has been shown also that the isothermal compressibility of dusty nonideal subsystem becomes negative at $\Gamma\approx 2$ both in dusty plasmas (in thermal equilibrium) with negative and positive charges.

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