Lecture no.4

Thermodynamic Properties of Nonideal Plasmas

Introduction

There are several methods for investigation the thermodynamic properties of nonideal plasma. A perturbation theory can be applied at $\Gamma << 1$ for weakly nonideal plasma. For strongly coupled plasma ($\Gamma > 1$) we use a computer simulation Monte Carlo method. In order to apply the Monte Carlo method we have to know an interaction potential between particles in plasma. The thermodynamic properties of nonideal plasma at the moderate values of coupling parameter can be investigated by integral equation methods (BBGKI, Ornstein-Zernike etc.).

One Component Plasma (OCP)

Let us consider the simple and well-studied model of one component plasma (OCP). The one–component plasma (OCP) means a system of pointlike ions placed in a homogeneous medium of charges of opposite sign. The OCP-model is a good approximation for describing of the plasma at high pressures. Such plasma occurs in an inertial thermonuclear fusion and astrophysical objects (in the center of white dwarfs and giant planets). In these cases, matter is ionized under the effect of pressure and degenerate electrons have sufficient kinetic energy, i.e.

$$\bar{E}_{kin} \approx \left(3\pi^2 n_e\right)^{2/3} h^2 / 2m \quad , \qquad (1)$$

that means the degenerate electrons produce an almost uniform background density distribution. It should be noted that the kinetic energy of electrons is $\varepsilon_F >> k_B T$ due to the small electron mass at high density ($r_S \to 0$) and the pressure of electron component is much higher than the corresponding pressure of an ion subsystem. Consequently, we have two systems: the Coulomb system of pointlike nuclei described by the Boltzmann statistics, and the quantum electron fluid (see, the regions V,VI and VII in the lecture no. 2). Notice that interaction between these components is weak and most attention is concentrated on the analysis of the Coulomb internuclear (interionic) interaction. According to this

OCP model there are no bound states (of molecules, atoms, and ions). Because OCP model is the simplest, it has been studied in detail by theoretical and computer simulation methods for the wide range of coupling parameter.

Table 1. One–component plasma of astrophysical objects

Parameter	Jupiter	White dwarf	Neutron star
Z	1 (H)	6 (C)	26 (Fe)
n_{i}, cm^{-3}	$6 \cdot 10^{24}$	$5 \cdot 10^{30}$	10^{32}
T, K	10^4	10^8	10^8
γ	50	10–200	870
r_{s}, a_0	0.65	$0.4 \cdot 10^{-2}$	$0.8 \cdot 10^{-3}$

Duscussion of calculation results. The radial distribution functions are shown in the figure 1. Figure 2 represents the results for static structure factors.

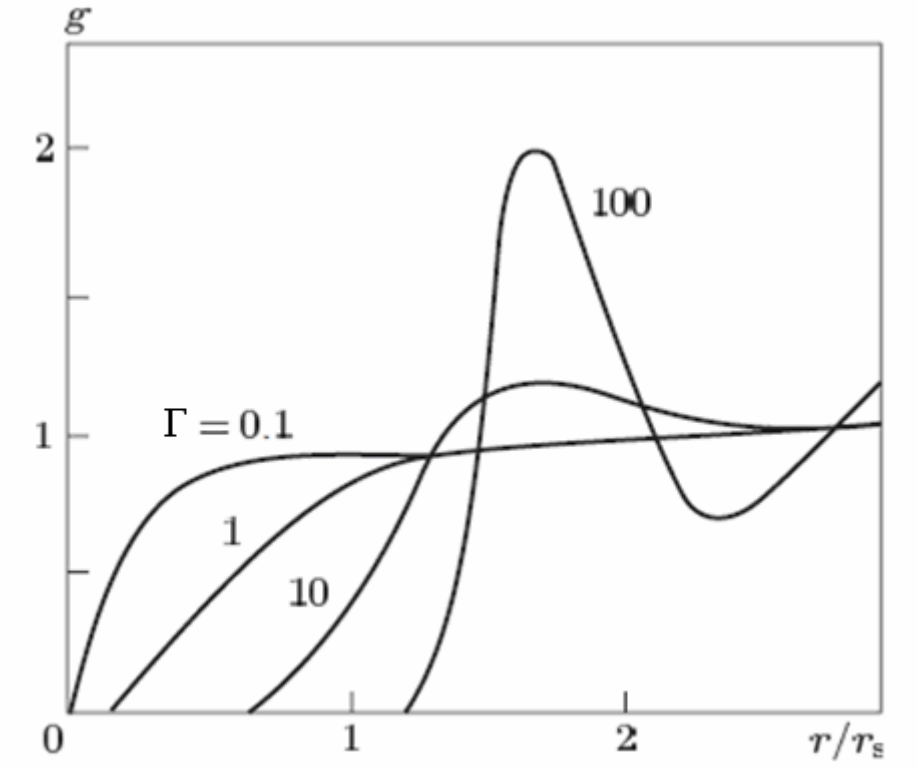

Figure 1. The radial distribution function of the OCP for different values of the coupling parameter Γ .

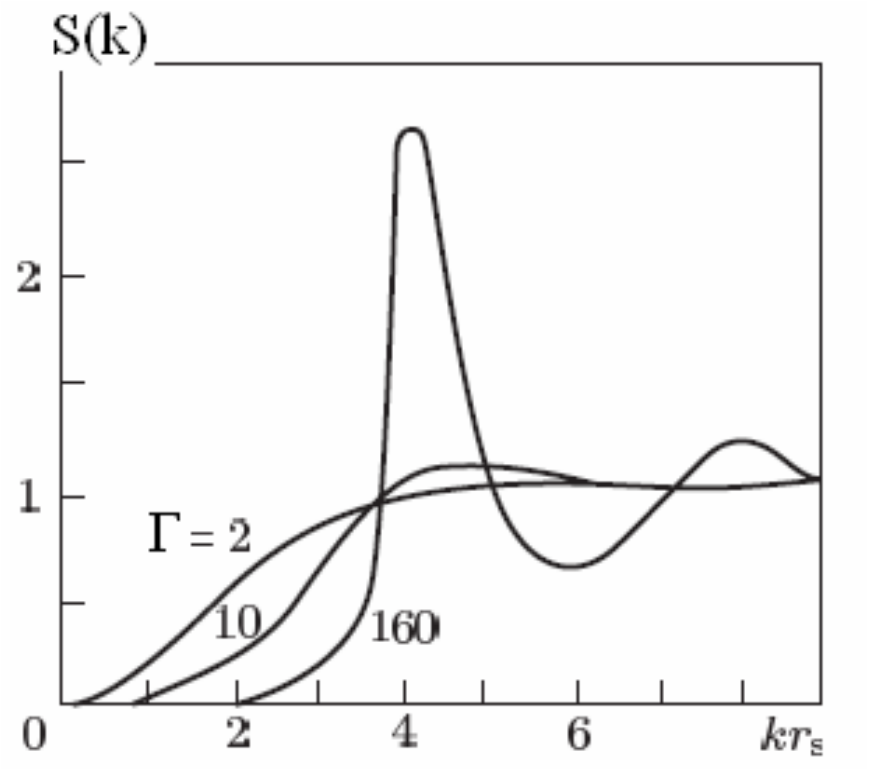

Figure 2. The static structure factors of the OCP for different values of the coupling parameter Γ .

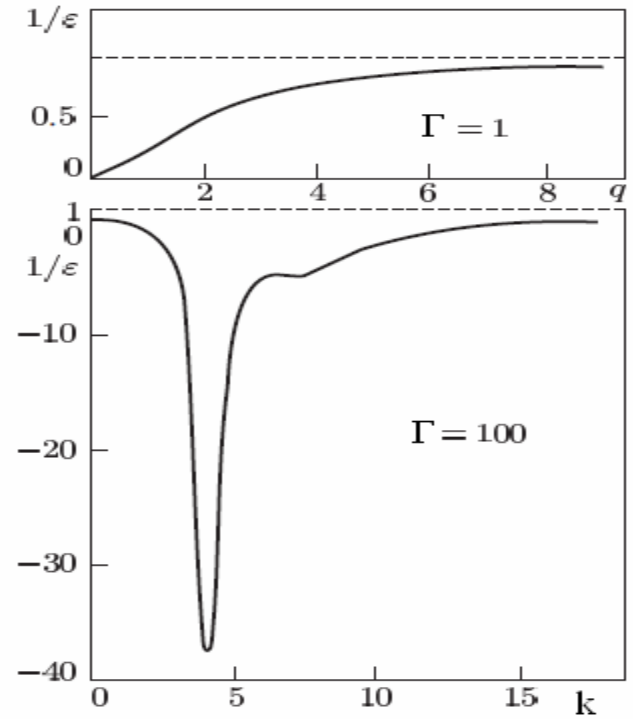

Figure 3. The static dielectric function of the OCP for different values of the coupling parameter Γ .

Knowing static structure factors the static dielectric permeability $\varepsilon(k,0)$ can be determined as follows:

$$\varepsilon(k,0)=\left[1-\kappa_D^2/k^2S(k)\right]^{-1}, \quad (2)$$

where $\kappa_D^2=4\pi n_i(Ze)^2/k_BT$. In the case of the almost ideal plasma ($\Gamma<<1$) these functions are monotonic and are described by the linearized Debye approximation:

$$S_D=k^2\left(k^2+\kappa_D^2\right)^{-1} \quad (3)$$

$$\varepsilon(k,0)=\left(k^2+\kappa_D^2\right)/k^2 \quad . \quad (4)$$

The radial distribution (pair correlation) functions are monotonic up to $\Gamma\approx 3$ and can be described by the linearized Debye approximation:

$$g(r)=1-\frac{\gamma}{r}\cdot r_D\cdot\exp\left(-r/r_D\right), \quad (5)$$

where $\gamma=(eZ)^2/(r_Dk_BT)$ is the nonideality parameter and $r_D=(4\pi Z^2e^2n_i/k_BT)^{-1/2}$ is the Debye radius of screening. At $\Gamma\geq 3$ functions $g(r)$ have oscillations due to the formation of short-range ordered structures. It means that the system changes from the ideal gas to a liquid state. With increasing of Γ, the oscillations increase and an effective hard core is formed.

Knowing the pair correlation functions and static structure factors the thermodynamic properties can be calculated. Here we will briefly discuss these results. Let us consider the regions of weak ($\Gamma<<1$) and moderate ($0{,}1\leq\Gamma\leq 1$) nonideality. On the basis of Mayer's diagrams for excess part of free energy we have the following expression:

$$\frac{F_{ex}}{Nk_BT}=-\frac{\sqrt{3}}{3}\Gamma^{3/2}+S_2(\Gamma)+S_3(\Gamma)+\ldots, \quad (6)$$

here the first term corresponds to a summation of the "ring" diagrams (the Debye approximation), $S_2(\Gamma)$ and $S_3(\Gamma)$ are contributions to the free energy on the basis of the screened Coulomb potential:

$$\Phi(r) = \frac{e^2}{r}\exp\left(-r/r_{TF}\right), \tag{7}$$

where r_{TF} is the Tomas-Fermi radius. The expression for $S_2(\Gamma)$ is given by

$$S_2 = \frac{N}{2}\int\left[e^{-\Phi(r)/k_BT} - 1 + \Phi(r)/k_BT - \frac{1}{2}(\Phi(r)/k_BT)^2 \ldots\right]d\vec{r} \tag{8}$$

and has the value $O(\Gamma^3 \ln\Gamma)$ at $\Gamma \to 0$. On the basis of the relations between thermodynamic functions we can write the following expressions for the internal energy and thermal capacity:

$$\frac{U_{ex}}{Nk_BT} = -\frac{\sqrt{3}}{2}\Gamma^{3/2} + \frac{3}{2}\Gamma\frac{d}{d\Gamma}\left[S_2(\Gamma) + S_3(\Gamma) + \ldots\right] \tag{9}$$

$$\frac{c_V}{Nk_BT} = \frac{\sqrt{3}}{4}\Gamma^{3/2} - \frac{3}{2}\Gamma^2\frac{d^2}{d\Gamma^2}\left[S_2(\Gamma) + S_3(\Gamma) + \ldots\right]. \tag{10}$$

For the case of weakly nonideal regime $(\Gamma << 1)$ we have the following simple relations according to the well-known Debye theory:

$$\frac{F_{ex}}{Nk_BT} = -\frac{1}{3}E; \qquad \frac{U_{ex}}{Nk_BT} = -\frac{1}{2}E;$$
$$\frac{c_V}{Nk_BT} = \frac{1}{4}E; \qquad E = \sqrt{3}\Gamma^{3/2}. \tag{11}$$

In the opposite case $(\Gamma >> 1)$ the asymptotic expression for internal energy can be written as:

$$\frac{U_{ex}}{Nk_BT} = -\frac{9}{10}\Gamma \quad . \tag{12}$$

In order to obtain the formula for wide range of the coupling parameter we have to approximate the computer simulation Monte Carlo data:

$$\frac{U_{ex}}{Nk_BT} = a\Gamma + b\Gamma^{1/4} + c\Gamma^{-1/4} + d \quad , \tag{13}$$

where $a = -0{,}897; b = 0{,}945; c = 0{,}179; d = -0{,}801$ and expression (13) describes the internal energy of OCP at $1 \le \Gamma \le 160$.

Multicomponent Plasma (MCP)

It is known that OCP model does not take into account the structure of opposite compensating background and basic quantum mechanical effects. The neglecting of quantum–mechanical features can lead to major difficulties with the classical description of the particle motion at small distances (at $a \sim \lambda_e$). It should be noted that taking into account of quantum mechanical effects leads to the formation of bound states (that is, molecules, atoms, and ions). These quantum mechanical effects should be taken into account on the basis of the Boltzmann factor and the Slater sum (see, lecture no.1).

Confined atom model (V.Fortov and V.Gryaznov, 1980).

Let us consider a three–component plasma consisting of atoms, single-charged ions and electrons. We assume that the atoms are spheres with variable radius r_c. For simplicity the sizes of electrons and ions are ignored. We will consider the subsystem of finite–size atoms as a set of hard spheres which do not interact when the distance between them exceeds $2r_c$. In this case it is necessary to take into account plasma action on discrete spectrum of atoms and ions in dense plasma. These effects can be described in the framework of the confined atom model:

$$\Phi(r) = \begin{cases} -\dfrac{Ze^2}{r}, & r < r_c \\ \infty \ , & r > r_c \end{cases} . \qquad (14)$$

The free energy of such model can be written as:

$$F(N_a, N_i, N_e, V, T) = F_{id} + F_{hs} + \Delta F_{coul} , \qquad (15)$$

here the first term is the free energy of the ideal plasma, but the atomic partition function depends on the radius, the second term is the contribution of the hard sphere repulsion which also depends on r_c. In order to include this contribution, the computer simulation molecular dynamic results for the hard-sphere systems are used:

$$\Delta F_{hs} = n_a k_B T \frac{3y-4}{(y-1)^2} y \quad , \qquad (16)$$

where $y = n_a(4\pi r_c^3/3)$. An equilibrium value of atomic radius can be determined from the condition of the minimum of the free energy:

$$\frac{\partial F}{\partial r_c} = 0 \quad . \qquad (17)$$

In order to determine the dependencies of partition functions on atomic radius r_c, it is necessary to numerically solve the set of nonlinear integro-differential equations according to the Hartree-Fock method.