Lectures no. 6 & 7

Structural and Thermodynamic Properties of Nonideal Plasma by Monte Carlo method

Pair Correlation Functions (Radial Distribution Functions)

A pair correlation function (PCF) $g(r)$ plays an important role in investigation of structural and thermodynamic (equilibrium) properties of a plasma. This function measures the time-independent correlations between the particles. More precisely, $g(r)$ is the probability that a particle is found at a distance r from any given (test) particle. In the spherical symmetric case when the function $g(r)$ depends on distance $r = \left|\vec{r}_i - \vec{r}_j\right|$ between particles, this function is called a radial distribution function (RDF). The pair correlation function for ideal and weakly nonideal plasma is easily calculated using well known integral equation methods (BBGKI chain, Ornstein-Zernike equation etc.). In the case of nonideal (dense) plasma the approximative methods of theoretical physics are not effective due to the absence of small parameters in the system. Therefore the computer simulation by the Monte Carlo method is applied for investigation of structural and thermodynamic properties of a dense plasma.

Algorithm for calculation of $g(r)$.

1. For each particle its surrounding space is divided into spherical layers with thickness Δr. For simplicity $0 < r \le L/2$.
2. To calculate the number of particles $\Delta N(r)$ in each layer.
3. The averaging of obtained results by all particles in any configuration. In this case we use the normal (arithmetical mean) averaging.
4. The averaging of obtained results for all configurations of Markov's chain. In this case we use the weight function averaging with the Boltzmann factor.

5. Then the average number of particles $\overline{\Delta N}(r)$ situated at a distance between r and $r+\Delta r$ from a given particle can be calculated by the following formula:

$$\overline{\Delta N}(r)=\sum_{i=1}^{M}\frac{1}{N}\sum_{j=1}^{N}(\Delta N)_{ij}\cdot\exp\left\{-\frac{\bar{U}_i}{k_B T}\right\}\quad, \tag{1}$$

here $\bar{U}_i$ is the average potential energy of configuration; M is the number of equilibrium configurations from "stationary" part of MC computer simulation "control card".

6. Finally, the pair correlation function (radial distribution function) is defined by the following expression:

$$g(r)=\frac{V}{N}\cdot\frac{1}{4\pi r^2}\cdot\frac{\overline{\Delta N}(r)}{\Delta r} \tag{2}$$

It should be noted that for a plasma we have the set of pair correlation functions $g_{\alpha\beta}(r)$, where α,β are the sorts of particles.

Discussion of results for $g(r)$.

The results for radial distribution function of dense semiclassical hydrogen plasma obtained by Monte Carlo method are presented in Figures 1 – 5. At $\Gamma<1$ we have a monotonic (Debye-like) character of $g(r)$. Fluctuations of $g_{ee}(r)$ at $\Gamma=0{,}8$ do not have any physical meaning and are within the range of statistical errors (Fig.1).

In Figure 2 the electron-ion radial distribution functions $g_{ei}(r)$ at different values of coupling parameter are shown. Notice that the values of $g_{ei}(r)$ for $\Gamma=0{,}8$ are situated above than corresponding values at $\Gamma=0{,}5$ and $\Gamma=0{,}3$. From physical point of view this fact means that the probability of finding of an electron-ion pair at the intermediate distance increases with increasing of the coupling parameter (increase of plasma density). In other words with increase of plasma density the probability of formation of electron-ion pair (probability of recombination) rapidly increases at intermediate and small interparticle distances.

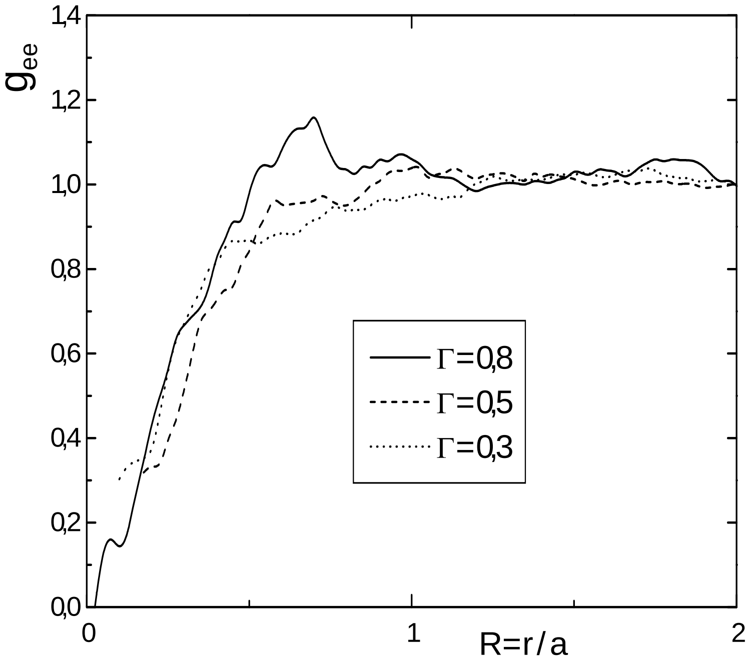

Figure 1. Electron-electron radial distribution functions for dense semiclassical plasma at $r_s = 1$.

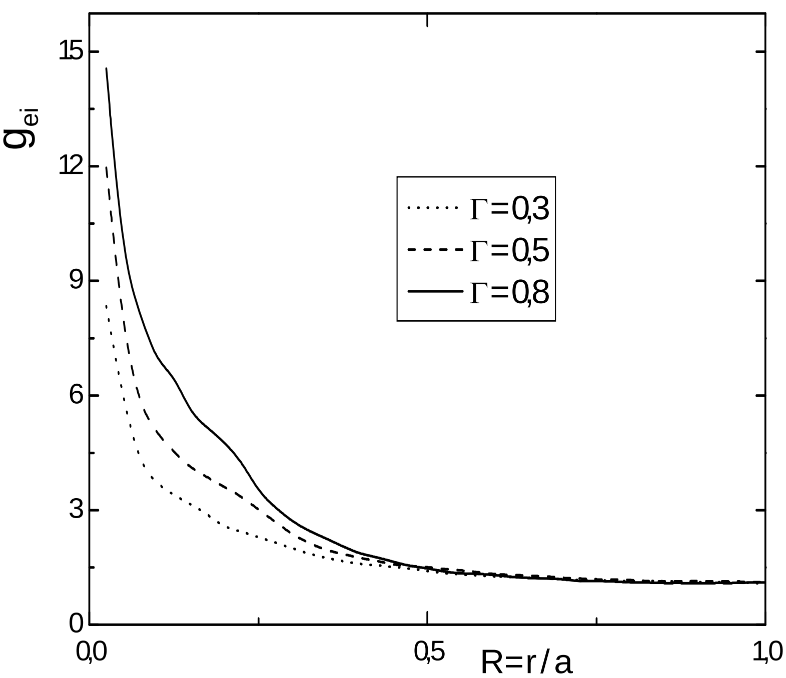

Figure 2. Electron-ion radial distribution functions for dense semiclassical plasma at $r_s = 1$.

It should be noted that we have the opposite situation for ion-ion correlation functions $g_{ii}(r)$ (see, Fig. 3). In this case the values of $g_{ii}(r)$ decrease with increasing of the coupling parameter (increasing of plasma density). This fact is connected with increasing of the probability of finding of like (repulsive) particles at increasing of plasma's density (or coupling parameter). It is seen from Fig.3 that the minimal nonzero probability of finding of ion-ion pair is observed at relatively large values of interparticle distances with increasing of Γ. This fact can be explained by relative increasing of average distances between ions (as a repulsive particles) with increasing of plasma density.

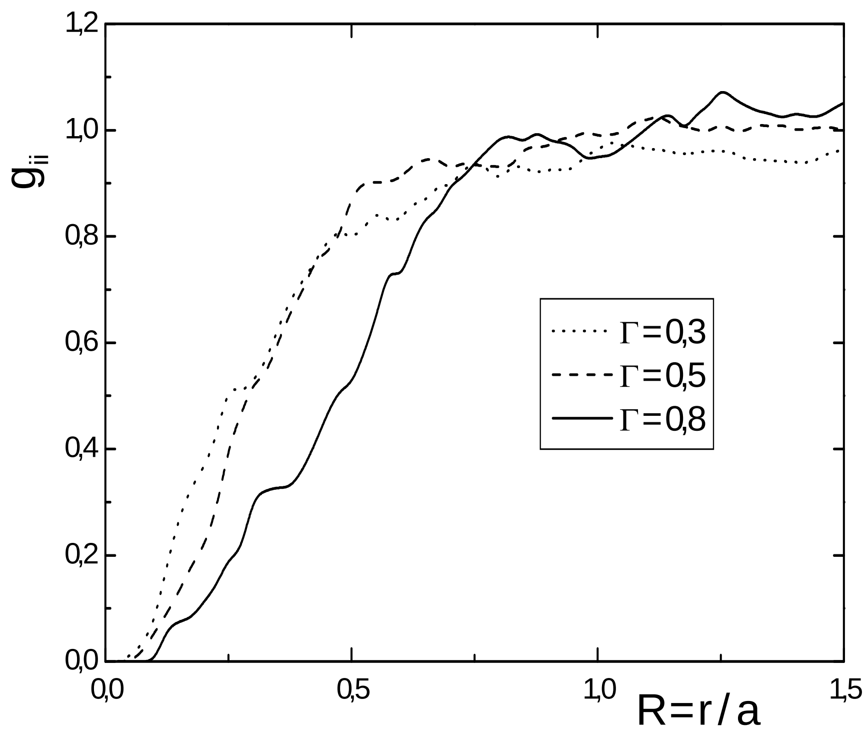

Figure 3. Ion-ion radial distribution functions for dense semiclassical plasma at $r_s = 1$.

Let us discuss the behavior of RDF at $\Gamma = (1 \div 10)$. For $\Gamma = 1$ we have the monotonic (Debye-like) character of $g_{ee}(r)$ (see, Fig. 4). It should be noted that at $\Gamma \geq 3$ $\lim_{r \to 0} g_{ee}(r)$ tends to the constant (nonzero!) value. This fact can be explained as follows. With increasing of coupling parameter it is necessary to take into account the interaction between electrons with anti-parallel spins due to the symmetry effect (the Pauli bloking principle). The extremums of $g_{ee}(r)$ are related with the formation of quazi-bound states in the dense plasma.

The ion-ion radial distribution functions are presented in Figure 5. It is seen that these functions have pronounced peaks at $\Gamma > 5$. This fact can be explained by formation of ordered structures in dense plasma (see, Fig.6).

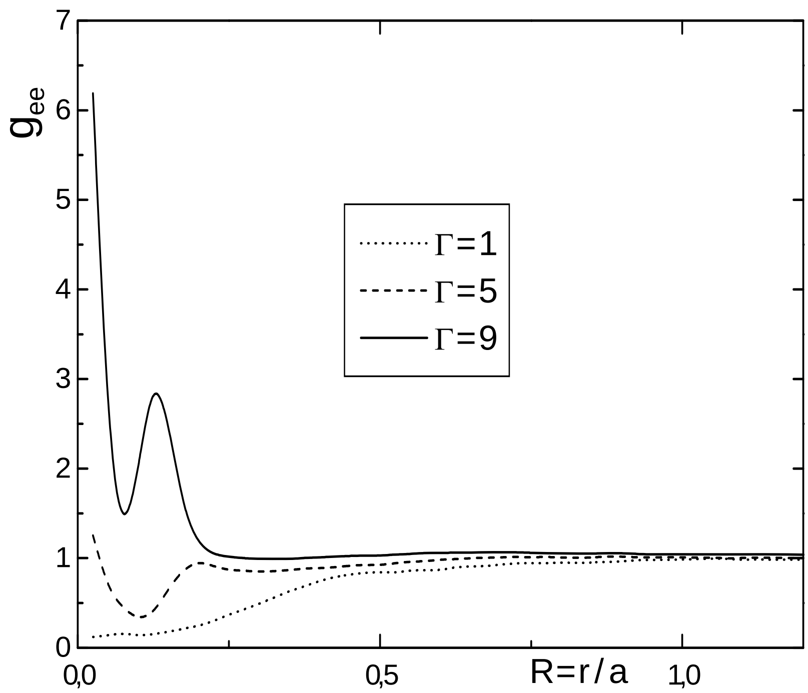

Figure 4. Electron-electron radial distribution functions for dense semiclassical plasma at $r_s = 1$.

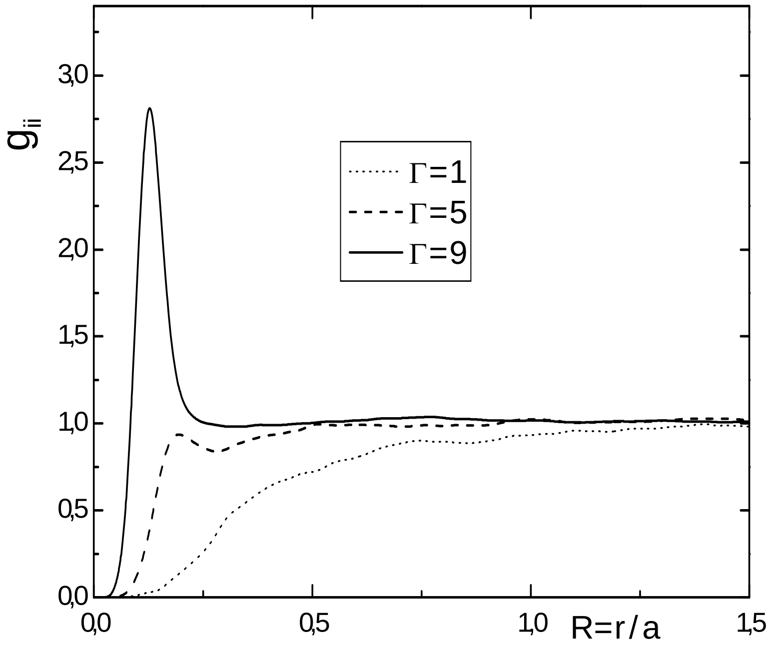

Figure 5. Ion-ion radial distribution functions for dense semiclassical plasma at $r_s = 1$.

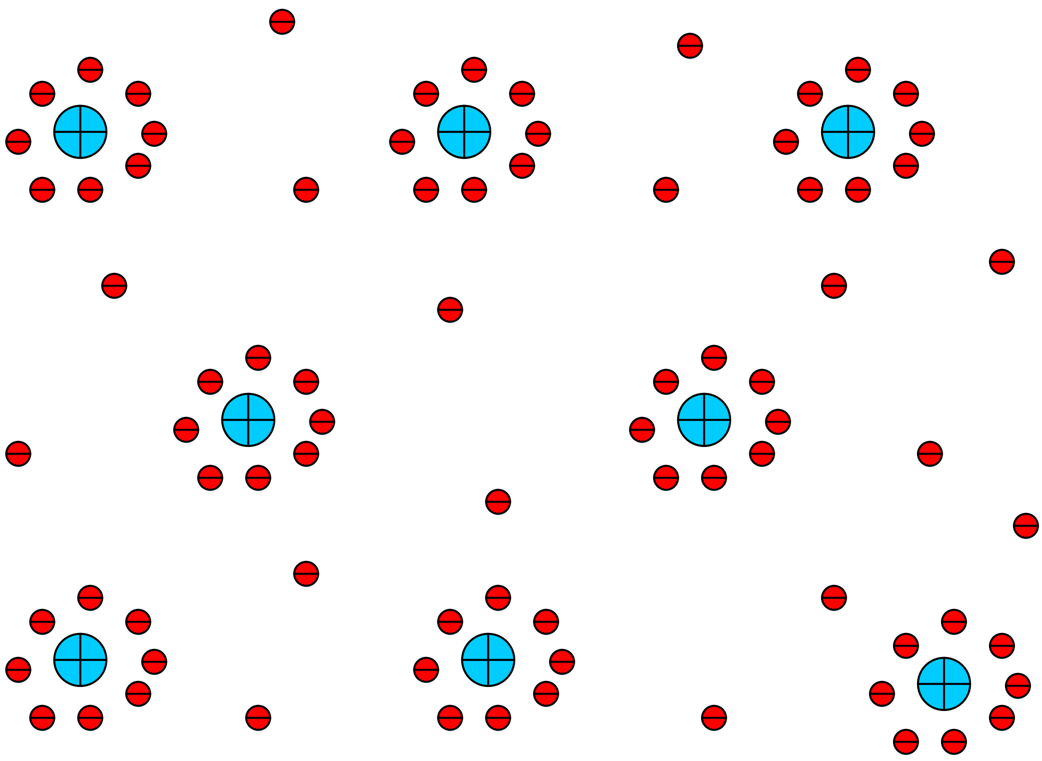

Figure 6. Formation of ordered structures in dense semiclassical plasma.

Static Structural Factors of the System

The static structural factor (SSF) also plays an important role in the investigation of microscopic properties of plasma. Knowing the radial distribution functions, SSF can be defined in the following form:

$$S_{\alpha\beta}(k) = 1 + n\int d\vec{r}\left[g_{\alpha\beta}(r) - 1\right]\exp(-i\vec{k}\cdot\vec{r}), \qquad (3)$$

where k is the wave vector; $n = n_e = n_i$ is the density number. As an example, SSF for dense semiclassical plasma is presented in Figure 7.

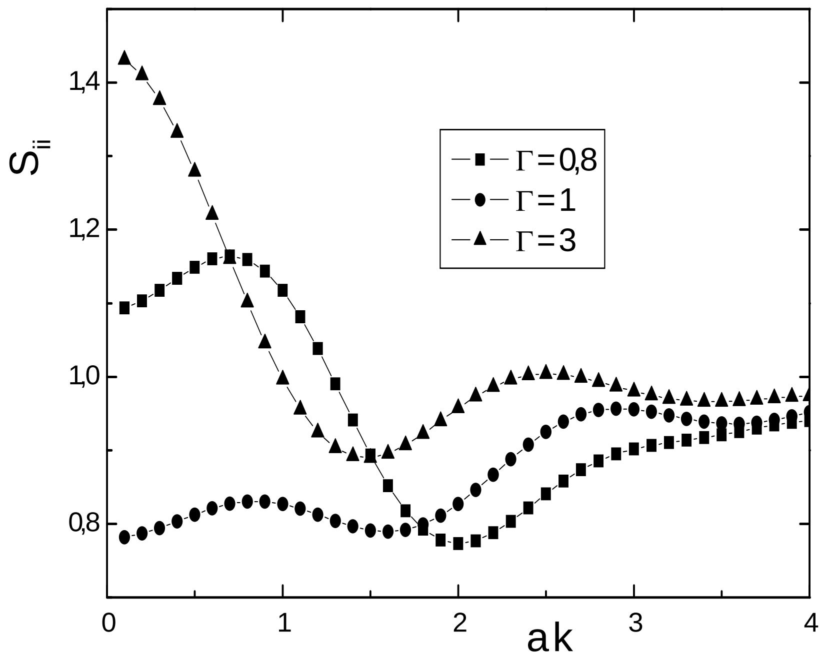

Figure 7. Static structural factors for a dense semiclassical plasma

Thermodynamic Properties of Plasma

We can define all thermodynamic properties of a plasma on the basis of the radial distribution functions. For instance, the equation of state $P = F(V,T) = f(\Gamma, r_s)$ can be calculated by the following formula:

$$P = nk_BT - \frac{2\pi}{3}n^2\sum_{\alpha,\beta}\int_0^\infty \frac{d\Phi_{\alpha\beta}(r)}{dr} g_{\alpha\beta}(r)r_{\alpha\beta}^3\, dr_{\alpha\beta} \qquad (4)$$

The internal energy is calculated as follows:

$$E = \frac{3}{2}Nk_BT + 2\pi n\sum_{\alpha,\beta}\int_0^\infty g_{\alpha\beta}(r)\Phi_{\alpha\beta}(r)r_{\alpha\beta}^2\, dr_{\alpha\beta} \quad . \qquad (5)$$

The excess part of the internal energy is given on the basis of the static structural factors by the following expression:

$$\frac{U_{\alpha\beta}}{Nk_BT} = \frac{1}{16\pi^3 k_BT}\int d\vec{k}\tilde{\Phi}_{\alpha\beta}(k)\left[S_{\alpha\beta}(k)-1\right] \quad , \qquad (6)$$

where $\tilde{\Phi}_{\alpha\beta}(k)$ is the Fourier transform of the potential.

In Figures 8 and 9 the results for excess internal energy and equation of state of dense semiclassical plasma are presented. The MC simulation results have a reasonable agreement with the Debye's asymptotic theory at $\Gamma \ll 1$ and the data of Ishimaru et al., and Pierleoni et al. at another values of coupling parameter.

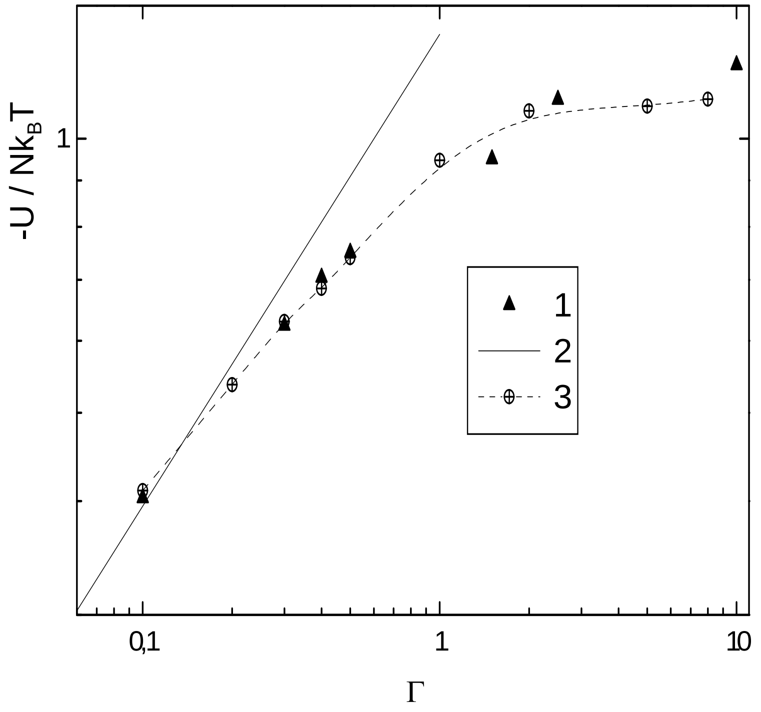

Figure 8. Excess internal energy of a dense semiclassical plasma. 1 – Pierleoni et al.; 2 – the Debye's asymptotic dependence; 3- MC simulation of Ramazanov et al.

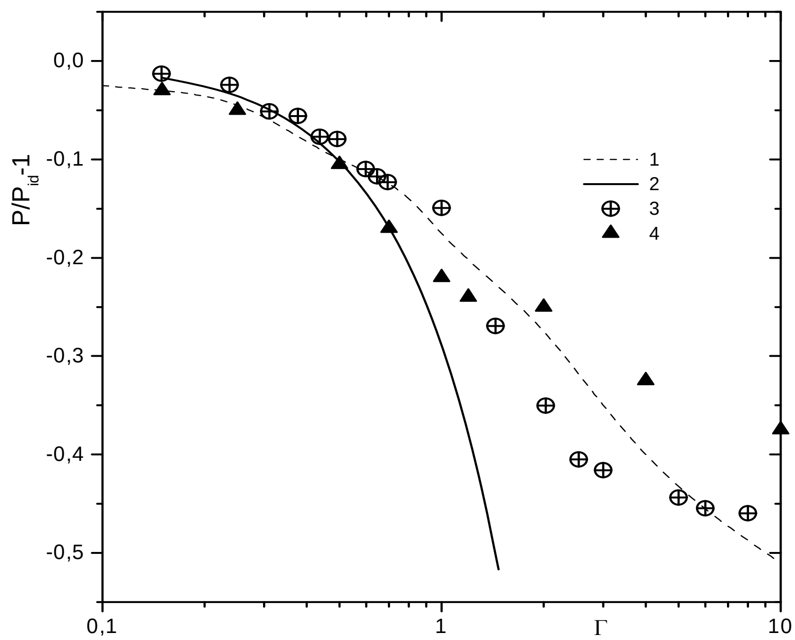

Figure 9. Equation of state of a dense semiclassical plasma. 1 – interpolation formula of Ishimaru et al.; 2 – the Debye's asymptotic dependence; 3- MC simulation of Ramazanov e.a.; 4 - Pierleoni et al.