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Modelling of dusty plasma properties by computer simulation methods

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Abstract
Computer simulation of dusty plasma properties is performed. The radial distribution functions, the diffusion coefficient are calculated on the basis of the Langevin dynamics. A comparison with the experimental data is made.

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Studies of dusty plasma properties are of interest for both applied and basic physics. Various structures that correspond to crystalline, liquid or gaseous state are known to occur in such plasma [1–4]. Therefore, the phase state of a system can be revealed with its structure characteristics such as the radial distribution function of particles; this can also be made by analysing the diffusion of macroparticles (grains).

A method of the Langevin dynamics can be used for studies of the dust plasma properties [5, 6]. Within this method, motion of macroparticles (due to their large dimensions compared to ion sizes) is considered in terms of a hydrodynamical approach [7, 8]. Below we give the list of forces, acting on a grain, considered within this approach:

(1) a force due to interaction with other grains $\vec{F}_{\rm int}(r)$
(2) friction $\vec{F}_{\rm fr}(t)$ due to motion of a grain in homogeneous media (η is the friction coefficient);
(3) random force $\vec{F}_{\rm br}(t)$ due to accidental influence of ions.

Therefore, the equation of motion for a macroparticle takes the form:

$$m_d \frac{{\rm d}^2\vec{r}_i}{{\rm d}t^2} = \sum_j F_{\rm int}(r)|_{r=|\vec{r}_i-\vec{r}_j|} \frac{\vec{r}_i-\vec{r}_j}{|\vec{r}_i-\vec{r}_j|} - m_d\eta\frac{{\rm d}\vec{r}}{{\rm d}t} + \vec{F}_{\rm br}(t), \tag{1}$$

where $F_{\rm int}(r) = -eZ_d\partial\Phi/\partial r, r = |\vec{r}_i - \vec{r}_j|$ is the distance between two grains, η is the friction coefficient determined by the frequency of collisions between a macroparticle and

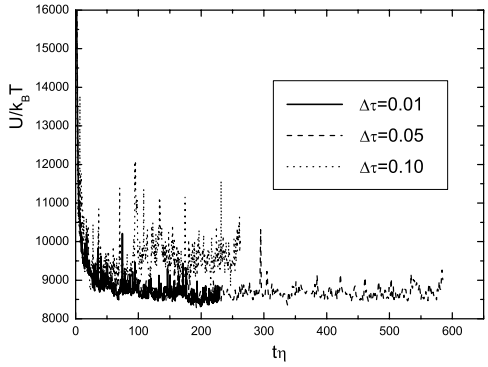

Figure 1. The time dependence of interaction energy for the method of the Langevin dynamics. $\theta = 0.45$, $\Gamma = 554$ and $\kappa = 4.84$.

plasma particles and m_d is the mass of a dust particle. We have used the Yukawa potential as the interaction potential between grains:

$$\Phi(R) = \frac{\Gamma}{R}\,\mathrm{e}^{-\kappa R}, \tag{2}$$

where $\Gamma = e^2/ak_BT$ is the coupling parameter, $\kappa = a/r_D$ is the screening parameter and $a = (3/(4\pi n_d))^{1/3}$ is the average distance between particles. Dimensionless time τ is taken in terms of the Langmuir frequency of dust component $\omega_d = (4\pi n_d e^2/m_d)^{1/2}$. The Brownian random force is taken in the form:

$$F_{\mathrm{br}}(\tau) = A\sqrt{2\theta}\xi(\tau), \tag{3}$$

where $\theta = \eta/\varpi_d$, $\xi(\tau)$ is the normally distributed random number within the range 0–1. The factor A is determined with the following condition. A value of factor A should be chosen which gives good agreement of the simulation data for the system without taking into account inter-particle interactions (i.e. without $\vec{F}_{\mathrm{int}}(r)$) with some well-known theoretical results.

The first step in the computer simulation is obtaining a correct time dependence of the interaction energy. It was calculated for different time steps and represented in figure 1. As one can see, the time dependence of the interaction energy has an equilibrium region and the amplitude of interaction energy oscillations depends on the chosen time step; therefore we chose the value $\Delta\tau = 0.01$ for calculations of the characteristics, since at this value the energy oscillations are comparatively small.

The computer simulation data provided us with various characteristics of the system, for instance the radial distribution functions of particles. As stated above, their form corresponds to the phase state of the system. Figure 2 presents the radial distribution functions for gaseous and crystalline states as well as corresponding images that visualize the location of particles obtained with the same numerical simulation method. The developed code enables a feature to generate simultaneously a form of basic cell and a corresponding radial distribution function, so one can observe changes in the structure and characteristics of the system.

The results were compared with the experimental data obtained in the Institute for High Energy Densities in Russia. On the determination of dusty plasma parameters it was revealed that it is as yet impossible to determine unambiguously the values of the parameters Γ and κ while only the parameter $\Gamma^* = \Gamma(1 + \kappa + \kappa^2/2)\exp(-\kappa)$ can be determined. Therefore, for a fixed value of Γ^* one can choose various pairs of the values Γ and κ. The calculations

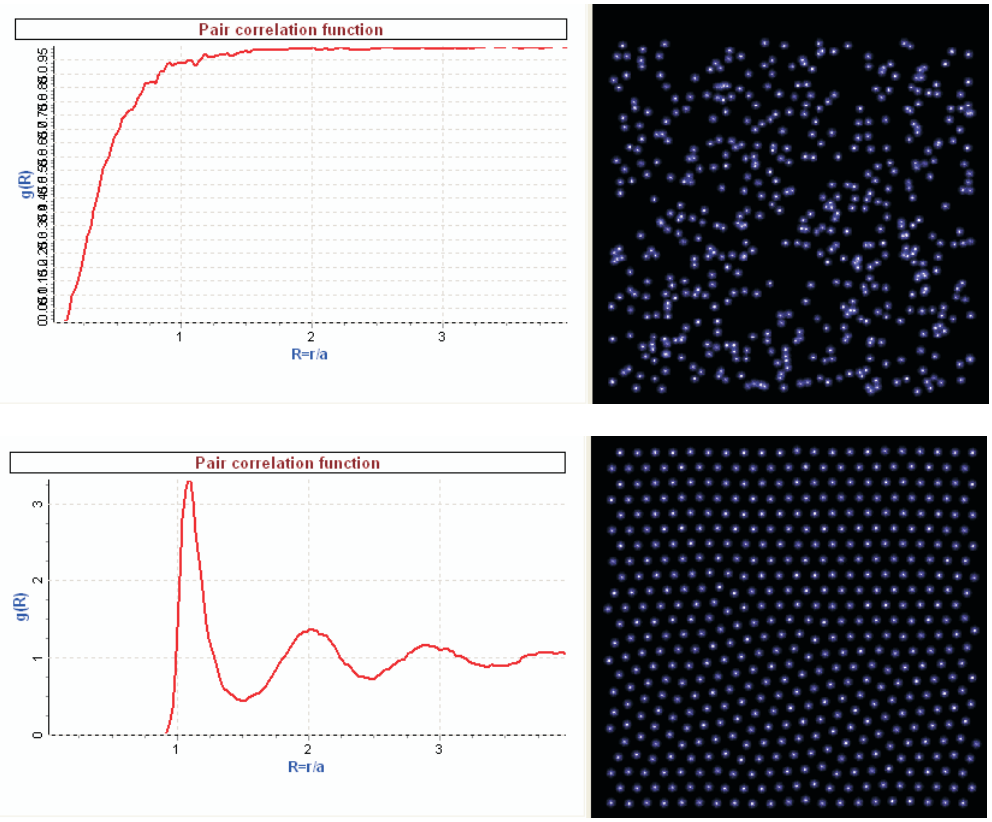

Figure 2. Radial distribution function and 2D representation of a basic cell in gaseous and crystalline states, respectively.

showed that the radial distribution functions obtained for these pairs coincided within the allowable errors. The experiment has been performed with plastic monodisperse particles of $a_d = 1.9\,\mu$m at a pressure of the argon buffer gas $P = 5$ Pa and an electron temperature of about 2 eV. At such parameters $\eta = 30,17\,\mathrm{s}^{-1}$ and $\theta = 0.64$. Figure 3 presents the radial distribution functions for particles; these functions were obtained for two combinations of Γ and κ that correspond to $\Gamma^* = 5$. Also, the experimental data obtained at $\Gamma^* = 5$ are presented. All the curves simultaneously reach an uncorrelated region and have maximum and minimum that correspond within the allowable error. It should be noted that for such small values of Γ^*, the experimental error exceeds 50%.

The diffusion coefficient was calculated on the basis of numerical simulations according to the formula:

$$D(t) = \langle \vec{r}(t) - \vec{r}(0) \rangle^2 / 6t, \tag{4}$$

where $\langle \vec{r}(t) - \vec{r}(0) \rangle^2$ is the mean-square displacement; we considered the diffusion coefficient as the value expression (4) tends to at $t \to \infty$. In order to calculate the diffusion coefficient along one coordinate axis (x, for instance) one can use a formula:

$$D_x(t) = \langle \vec{x}(t) - \vec{x}(0) \rangle^2 / 2t. \tag{5}$$

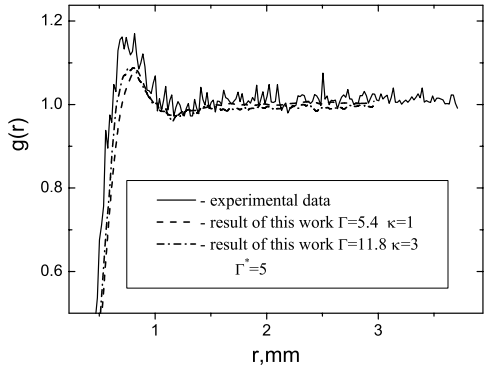

Figure 3. Comparison of the calculated radial distribution functions with experimental results (IHED RAS).

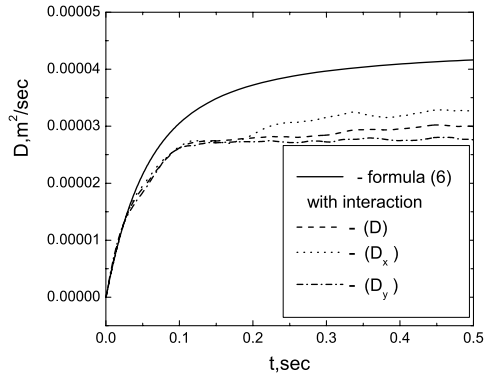

Figure 4. Diffusion coefficient of dusty plasma.

When the interaction force is neglected, equation (1) has an analytical solution in the form:

$$D(t)/D_0 = 1 - [1 - \exp(-\eta t)]/\eta t, \tag{6}$$

where $D_0 = k_B T_d/(\eta m_d)$.

Figure 4 presents a diffusion curve when interaction was not taken into account (6); there are also 3D and 1D diffusion coefficients calculated by taking into account the interactions at the same parameters of the experiment: $\Gamma^* = 5, \theta = 0.64$. The 3D diffusion coefficient is equal to about 4.2×10^{-5} m^2 s^{-1}, and the 1D one to 2.8×10^{-5} m^2 s^{-1} which agrees well with the experiment. The diffusion coefficient obtained by the computer simulation without taking into account the inter-particle interaction coincides with the theoretical curve (6). Besides, the diffusion coefficient can be calculated on the basis of the velocity autocorrelation function using the formula:

$$D = \frac{1}{3}\int_0^\infty \langle \vec{v}(0)\vec{v}(t)\rangle \, \mathrm{d}t, \tag{7}$$

where $\langle \cdots \rangle$ means ensemble averaging. Calculations made with formula (7) provided us with the same result.

Conclusions

The computer simulation data of the radial distribution functions and the diffusion coefficient are in good agreement with the corresponding experimental results. The method of Langevin dynamics can be used for the adequate investigation of the properties of the dusty plasma.

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