

Thermal fluctuations of the pair-interaction forces in two-dimensional fluid Yukawa systems

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Abstract. In the paper, the particle dynamics in two-dimensional (2D) Yukawa systems were studied numerically. New data on a density of the thermal fluctuations of pair-interaction forces have been obtained for non-ideal systems in a wide range of their parameters. Comparisons of these thermal fluctuations with the internal energy density were performed. For the first time we have found, that for strongly correlated fluid 2D Yukawa systems the dielectric constant is inversely proportional to the second derivative of a pair potential at the mean inter-particle distance.

The study of physical properties in non-ideal systems is of significant interest from the basic point of view and, at present, it is a subject of an intensive theoretical and experimental research in various areas of physics [1–6]. The main problem involved in the studies of these systems is associated with the absence of analytical theory of liquid. To predict the physical properties of non-ideal systems the various semi-empirical approaches and computer simulations with the help of numerical techniques (Monte-Carlo or molecular dynamics methods) are commonly used [1–6]. So, for an analysis of the thermodynamic properties of liquids (such, as the thermal coefficients of pressure, the heat capacities, the isothermal compressibility, etc.) the equations of state can be used [5–8]. In case of isotropic pair interactions (with the interaction energy $\phi(r)$) the physical properties of non-ideal systems, such as the energy density, and the pressure are determined by the temperature T , the concentration, n , and the pair correlation function, $g(r)$, which can be measured experimentally or may be found from the computer simulations [5–8]. So, the internal energy density U per a particle of a system (*calorific* equation of state) may be written as

$$U = \frac{m}{2}T + (m-1)\pi n \int_0^{\infty} \phi(r)g(r)r^{m-1}dr, \quad (1)$$

here $m = 2, 3$ is the number of dimensions in the system and $n = r_p^{-m}$, where r_p is the mean inter-particle distance. In the scope of a classical electrostatics the energy density, U , in the non-ideal quasi-equilibrium three-dimensional systems (with an accuracy of constant not dependent on T) may be presented as [9, 10]

$$U \cong \frac{m}{2}T + U_0 + \frac{\langle \delta E^2 \rangle}{8\pi n} \left(\epsilon + T \frac{\partial \epsilon}{\partial T} \right), \quad (2)$$



where ϵ is the dielectric constant ($\partial\epsilon/\partial T = 0$ for monatomic non-polar fluids), and $\langle\delta E^2\rangle$ is the mean square of electric field fluctuations, which result from the small thermal perturbations of particles' concentration and can produce the fluctuations of the of electric current density [9–11] and U_0 is the energy density for the crystal lattice at $T = 0$. For any lattice of known type, for example, for the fcc, bcc or hp lattices, the values of U_0 may be easily computed [8].

The simple semi-empirical approximation for the energy densities in the two-dimensional ($m = 2$), and three-dimensional ($m = 3$) strongly non-ideal liquids was proposed in [8]. The thermal component ($U - U_0 - mT/2$) of the potential part of U may be written as [8]

$$\delta U = \frac{U - U_0 - mT/2}{T} \cong \frac{4\gamma}{1 + \exp(\gamma)}, \quad (3)$$

where $\gamma = 0.5 + (m - 0.5)\Gamma^*/\Gamma_c^*$, $\Gamma^* = r_p^2\phi^{(2)}/(2T)$ is the effective coupling parameter, $\phi^{(2)}$ is the second derivative of a pair potential $\phi(r)$ at the point of $r = r_p$, Γ_c^* is the value of Γ^* in the melting line of solid ($\Gamma_c^* \cong 104.5 \pm 5$ for the body-center cubic (bcc) lattice; $\Gamma_c^* \cong 102.5 \pm 5$ for the hexagonal primitive (hp) lattice [8, 12]).

Here we present the results of numerical studies of the thermal fluctuations of pair forces for the two-dimensional (2D) systems of particles interacting with the energy

$$\phi(r) = (eZ)^2 \exp(-r/\lambda)/r, \quad (4)$$

where eZ is the particle charge, r is the distance between particles, λ is the screening length. This type of potential is widely used within the framework of physical kinetics for the description of the interaction in various systems, e.g. in physics and chemistry of polymers, in medicine, biology, complex plasma [1–6]. Note that the model of screened Yukawa potential (4) has been successfully applied to the analysis of results of various experiments [1, 4].

For the Yukawa systems, $\Gamma^* = \Gamma(1 + \kappa + \kappa^2/2)\exp(-\kappa)$, where $\Gamma = (eZ)^2/(r_p T)$ is the Coulomb coupling parameter, $\kappa \equiv r_p/\lambda$ is the screening parameter. The numerical simulation was carried out by the Langevin molecular dynamics method based on the solution of the system of N_p ordinary differential equations, where N_p is the number of the independent particles in computational cell. The stochastic character of motion of the particles with the given kinetic temperature T was determined by the Langevin force F_{ran} . The simulation technique is detailed in [1].

The calculations were performed for 2D monolayer of grains with periodical boundary conditions for the Yukawa systems with the screening parameters κ from 1.5 to 5. The number of independent particles, N_p , in the central computational cell was varied from 256 to 4096. Depending on the number of particles the cut-off length of potential r_{cut} was changed from $5r_p$ to $25r_p$ (where $r_p = \sqrt{N_p/S}$, and S is the area of the computational cell). The majority of data were obtained for $N_p = 1024$ independent particles and $r_{\text{cut}} = 12r_p$.

The equations of motion were solved for various values of effective parameters: the coupling parameter Γ^* and the scaling parameter $\xi = \omega/\nu_{\text{fr}}$, where ν_{fr} is the friction coefficient,

$$\omega = \sqrt{\phi^{(2)}/(2M)} \equiv \sqrt{(eZ)^2(1 + \kappa + \kappa^2/2)\exp(-\kappa)},$$

and M is the mass of the particle. The value of scaling parameter was varied from $\xi \approx 0.4$ to $\xi \approx 4$, that is typical, for example, for the grains in weakly ionized plasma, where the friction of particles is determined by their collisions with the neutrals of surrounding gas [1, 4]. The value of effective coupling parameter Γ^* was varied in the range from 4 to 120.

We have calculated the magnitude of the thermal fluctuations of pair forces $\langle\delta F^2\rangle = eZ^2\langle\delta E^2\rangle$ (and the fluctuations of the electric field $\langle\delta E\rangle$, correspondingly) acting on the separate particle of the simulated systems. The normalized values $\langle\delta F^2\rangle^* = \langle\delta F^2\rangle/(C_n M T \omega^2)$ vs. Γ^* (where

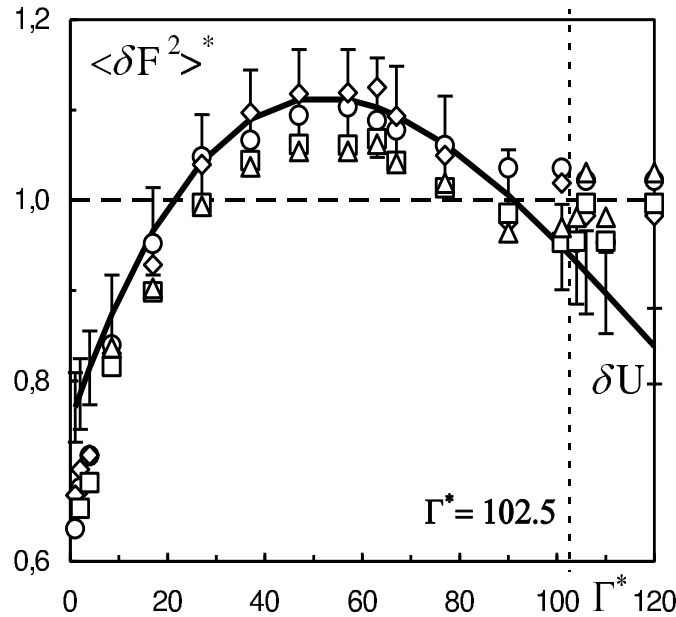


Figure 1. The value of $\langle \delta F^2 \rangle^* = \langle \delta F^2 \rangle / C_n M T \omega^2$ vs. Γ^* for 2D Yukawa systems with various κ : ($\diamond$)—1.5; ($\circ$)—2; ($\square$)—3; ($\triangle$)—5. Solid lines are the approximations of δU , see (3); bars denote the deviation $\pm 5\%$ from the equation (3).

$C_n = 3.44$) is presented in figure 1. It is easy to see a good agreement between the analytical and numerical data; the difference between them doesn't exceed $\sim 3 - 5\%$; with the exception of data for $\Gamma^* > \Gamma_c^* \approx 102.5$, and for $\Gamma^* < 5$, where the deviation from analytical curve was $\sim 10 - 25\%$, see figure 1. (We emphasize that the results of the simulation practically didn't depend on the values of ξ ; the difference between the measured quantity and its average value didn't exceed the numerical error of $\pm 3\%$.) Because $\langle \delta E^2 \rangle \propto U$, the results of the presented studies allow to assume, that for strongly correlated fluid 2D systems ($5 < \Gamma^* < \Gamma_c^*$) the dielectric constant $\epsilon \propto \omega^{-2} \propto 1/\phi^{(2)}$ and $\partial\epsilon/\partial T \cong 0$.

To conclude, the particle dynamics in 2D Yukawa systems were studied numerically. New data on a density of the thermal fluctuations of pair forces have been obtained for fluid systems in a wide range of their parameters. Comparisons of these thermal fluctuations with the internal energy density were performed. For the first time we have found, that for strongly correlated fluid 2D Yukawa systems the value of dielectric constant is proportional to the second derivative of a pair potential at the mean interparticle distance.

Finally we have to note that the scope of presented results is not limited by 2D Yukawa systems, and these results may be easily adapted for a wide range of 2D and 3D systems with various isotropic repulsive potentials.

Acknowledgments

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