Structural Universalities in a Two-Dimensional Yukawa Fluid

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The structural properties of a two-dimensional fluid in a wide range of the screening parameter $\kappa$ are considered by example of a Debye–Hückel (Yukawa) system. The behavior of structural indicators appears universal and is independent of the screening parameter $\kappa$. This property makes it possible, in particular, to easily and noninvasively determine the key parameters of the interparticle interaction from the configuration of particles observed in experiments with complex (dusty) and colloidal plasmas.

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The behavior of strongly correlated two-dimensional systems is one of the most important problems of condensed matter physics. Such two-dimensional and quasi-two-dimensional systems have been intensively studied beginning with pioneering theoretical works [1–6], for which a Nobel Prize in physics was awarded recently. In those studies, the main attention was paid to the type and properties of a two-dimensional “crystal–liquid” transition. The physics of this transition is much richer than the physics of melting of three-dimensional systems, in particular, because of the existence of an intermediate hexatic phase, which is characterized by the presence of a quasi-long range orientational order [7–14]. The properties of a two-dimensional liquid (particularly, far from the melting curve) are much less studied. In this work, we consider the structural properties of a two-dimensional liquid using a model two-dimensional system with the Yukawa (Debye–Hückel) repulsive potential as an example. The pair interaction between particles in the Yukawa system is described by the potential

$$U(r) = (Q/r)\exp(-r/\lambda),$$

where $Q$ is the charge of a particle and $\lambda$ is the screening length. It is known that the phase state of this system is described by two parameters: coupling parameter $\Gamma = Q^2\exp(-\kappa)/(TD)$ and the screening parameter $\kappa = D/\lambda$, where $D$ is the average distance between particles in the system and $T$ is the temperature of particles. The Yukawa system is often used to describe experiments in a dusty (complex) plasma and in colloidal systems (see, e.g., [15, 16]). In this work, the main tool to obtain configurations of particles is the classical molecular dynamics method implemented for the canonical ($NVT$) ensemble with a Nosé–Hoover thermostat and periodic boundary conditions [17]. The typical number of microparticles in the system under study is $N \sim 10^5$.

The two-dimensional Yukawa system at zero temperature and any screening parameters $\kappa$ is a crystal with triangular (hexagonal lattice) and six nearest neighbors of each atom, which are located at the vertices of a regular hexagon. Defects in which the number of the nearest neighbors differs from six appear in this system at finite temperature. Dislocation pairs of five to seven defects (where one particle has five nearest neighbors and the other has seven nearest neighbors) and/or a dislocation quadruple consisting of four defects of different forms, which is the result of the fusion of pairs, usually dominate at low temperatures. The formation of single defects, disclinations (five or seven nearest neighbors), is also possible, but their concentration is usually much lower than the concentrations of dislocation pairs and quadruples because they create strong local elastic tension in the system at which their transformation to a dislocation is energetically favorable.

Figure 1 shows three phase states of the two-dimensional Yukawa system: (a) crystalline phase, (b) hexatic phase observed in the experiment with a colloidal plasma [18], and (c) equilibrium liquid near the melting curve. Defects are indicated in blue and red. Green color corresponds to crystal clusters with six nearest neighbors of the central particle. The inset of Fig. 1a demonstrates the images of dislocation pairs and quadruples, which are clusters of defects most widespread near the melting curve. The comparison of Figs. 1b and 1c indicates that it is difficult to visually distinguish the hexatic phase and melt, but the calculation of the two-dimensional structure factor (which is shown for each phase) allows one to do this easily because fine details of the angular distribution of the nearest neighbors disappear in the two-dimensional
The simplest characteristic of two-dimensional systems is the pair correlation function $g(r) = 1/N \left( \sum_{j \neq k} \delta(r - |r_j - r_k|) \right)$. Its parameters such as the first peak $g_{\text{max}}$ and the first nonzero minimum $g_{\text{min}}$ can be used to quantitatively describe the phase state of the ensemble of particles, as in the three-dimensional case (e.g., [21, 22]). Figure 2 shows the dependences of the parameters $g_{\text{max}}$ and $g_{\text{min}}$ of the two-dimensional liquid near the melting curve on the screening parameter $\kappa$. The inset of Fig. 2a shows typical functions $g(r)$ for the Yukawa system near the crystal–liquid transition line at different dimensionless temperatures $T^* = T/T_m$, where $T_m$ is the melting temperature of the system, which are indicated by colors shown in the legend: blue and red lines correspond to the crystalline and liquid states, respectively. The breaking of the translational order (disappearance of long-range correlations) under the melting of the system is clearly seen.

The dependences of the parameters $g_{\text{max}}$ and $g_{\text{min}}$ on the screening parameter $\kappa$ demonstrate an interesting effect for Yukawa melts: the maximum of the pair correlation function $g_{\text{max}}$ increases with the stiffness of the interparticle interaction (i.e., with the screening parameter $\kappa$), whereas the parameter $g_{\text{min}}$ hardly changes on the melting curve in the considered screening parameter range and at $g_{\text{min}} \approx 0.27$ (for $\kappa \approx 0–8$). We note that such a behavior of the parameters $g_{\text{max}}$ and $g_{\text{min}}$ as functions of the stiffness of the pair interaction was also observed for three-dimensional melts of the system with the inverse power-law repulsion [22]. Therefore, the parameters $g_{\text{max}}$ and $g_{\text{min}}$ are important characteristics of the two-dimensional liquid; the parameter $g_{\text{max}}$ can be used as a quasi-universal indicator of melting for a wide class of systems, at least, for two-dimensional Yukawa and Coulomb systems.
In addition, the parameters $g_{\text{max}}$ and $g_{\text{min}}$ make it possible to easily and noninvasively determine the key parameters of the pair interaction in two-dimensional experiments with melts of complex and colloidal plasmas: the parameter $g_{\text{min}}$ indicates that the liquid under study is a melt, and the stiffness of the interaction (the screening parameter $\kappa$) is determined from the parameter $g_{\text{max}}$. A single configuration with $N \sim 10^3–10^4$ particles in the system is sufficient for such a determination. These $N$ values are easily achievable in experiments with two-dimensional colloidal (see, e.g., [11]) and complex plasmas (e.g., [23, 24]). It can be shown that the parameter $g_{\text{min}}$ for the two-dimensional Yukawa liquid at $T/T_m > 1$ depends only on the dimensionless temperature $T^*$. These dependences $g_{\text{min}}(T^*)$ for several screening parameters $\kappa$ are shown in Fig. 3. It is clearly seen that $g_{\text{min}}(T^*)$ hardly depends on $\kappa$ in a wide range $\kappa \approx 0–8$ and $T^* \approx 1–2.5$. For this reason, the parameter $g_{\text{min}}$ is a simple and convenient indicator, which (together with $g_{\text{max}}$) allows one to determine the location of the studied two-dimensional liquid on the phase diagram even if this liquid is far from the...
melting curve. Such a universality for three-dimensional Yukawa systems was revealed in [25].

We note that the integral characteristics of the pair correlation function, such as the pair entropy $s_2$ [26] and the cumulative pair entropy $C_{s_2}$, can also be used to characterize the two-dimensional liquid [27–30]. The functions $s_2$ and $C_{s_2}$ are defined as

$$s_2 = \frac{n}{2} \int_0^\infty [g(r) \ln g(r) - g(r) + 1] dr,$$

$$C_{s_2}(r) = -\pi \int_0^r [g(x) \ln g(x) - g(x) + 1] dx,$$

where $n$ is the density of particles. It can be shown [27] that $s_2$ for two-dimensional systems diverges for crystalline and hexatic phases and converges for the liquid phase. The cumulative function $C_{s_2}$ is a characteristic of this convergence (because $C_{s_2}(\infty) \equiv s_2$) and allows one to easily distinguish the liquid phase from the other aforementioned phases of the two-dimensional material. Figure 4 shows the dependence of $s_2$ on the dimensionless temperature of the system $T^* = T/T_m$ for two values of the parameter $\kappa$. The inset of Fig. 4 illustrates the behavior of the cumulative pair entropy $C_{s_2}(r)$ for various $T^*$ values and various phase states of matter and, in particular, its divergence for the solid phase. It is seen that $s_2$ is defined only for the liquid and only a part of the line with $T^* > 1$ in Fig. 4 has a physical meaning. The quasi-universality of $s_2$ for the liquid near the melting curve is demonstrated for two $\kappa$ values, but the parameter $g_{\min}$ is favorable in practice.

The concentration of defects $n_d$ and the geometric properties of clusters of defects are very important characteristics of two-dimensional systems [31]. Defects for the triangular lattice are easily determined by the Voronoi diagram of the region occupied by particles (e.g., [31–33]). In this diagram, each particle of the system corresponds to a convex polygon with the number of sides equal to the number of nearest neighbors $n_{nn}$. Particles with $n_{nn} \neq 6$ are treated as defects and their number in the system is $n_d$. A cluster of defects is defined as an assembly of defect particles that are nearest neighbors (for details, see [31]).

Here, we consider the dependences of the concentration of defects $n_d$ only near the melting curve on the dimensionless temperature $T^*$ for several values of the screening parameter $\kappa$, which are shown in Fig. 5. A sharp increase in $n_d$ at $T^* \approx 1$ corresponds to the melting of the system. The further behavior of the function $n_d(T^*)$ at $T^* > 1$ is quasi-universal and is almost independent of the screening parameter $\kappa$ at least to temperatures $T/T_m \approx 10$. An important feature of the two-dimensional liquid is that the concentration of defects increases slowly (logarithmically) with the temperature; e.g., only half of all atoms are defects at $T/T_m \approx 10$. This is illustrated in the inset of Fig. 5, where the distribution of defects in the two-dimensional Yukawa
liquid at $T/T_m \approx 5$ is shown. Particles with five, six, and seven nearest neighbors are shown in blue, green, and red, respectively. A significant number of crystalline clusters are seen. On the melting curve, $n_d \approx 0.25$ for all considered $\kappa$ values, which means, in particular, that the two-dimensional Yukawa melt consists mainly of crystallites (clusters of particles with six nearest neighbors). This property fundamentally distinguishes two-dimensional systems from three-dimensional ones (where the melt includes almost no crystalline clusters).

In this work, the structural properties of a two-dimensional liquid have been considered by example of a Yukawa system. It has been shown that simple parameters of the pair correlation function $g(r)$ such as its first maximum $g_{\text{max}}$ and the first nonzero minimum $g_{\text{min}}$, are important parameters characterizing two-dimensional systems. In particular, it has been found that the parameter $g_{\text{min}}$ for two-dimensional Yukawa melts is quasi-universal in a wide range of stiffness of the interparticle interaction (i.e., screening parameter $\kappa$), which makes the parameter $g_{\text{min}}$ a simple indicator of two-dimensional melting and allows one to easily identify the melt of such a system. The indicated quasi-universality of the parameter $g_{\text{min}}$ apparently reflects the universality of melts of all two-dimensional close-packed systems such as Yukawa systems, Coulomb systems, and soft spheres (systems with inverse power-law repulsion).

A monotonic increase in the parameter $g_{\text{max}}$ with the parameter $\kappa$ and the quasi-universality of the indicator $g_{\text{min}}$ allow one to easily and noninvasively determine the key parameters of the interparticle interaction in experiments with melts of complex (dusty) and colloidal plasmas, which previously required significant efforts. It has been established that the relative concentration of defects $n_d$ in two-dimensional Yukawa liquid is universal: in a wide $\kappa$ range, it depends only on the dimensionless temperature $T^* = T/T_m$. Finally, two-dimensional melts consist primarily (75%) of crystallites, which fundamentally distinguishes two-dimensional systems from three-dimensional ones.

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**CONFLICT OF INTEREST**

The author declares that he has no conflicts of interest.

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