Physics Letters A 378 (2014) 3475–3479

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Thermodynamics and phase transitions in two-dimensional Yukawa systems

O.S. Vaulina [a,b], X.G. Koss [a,b,*]

[a] Joint Institute for High Temperatures RAS, 125412, Izhorskaya st. 13 bd. 2, Moscow, Russia
[b] Moscow Institute of Physics and Technology, 117303, Kerchenskaya st. 1a-1, Moscow, Russia

ARTICLE INFO

Article history:
Received 4 June 2014
Received in revised form 18 August 2014
Accepted 1 October 2014
Available online 7 October 2014
Communicated by F. Porcelli

Keywords:
2D systems
Yukawa potential
Phase transitions
Numerical simulations
Hexatic phase

ABSTRACT

The results of numerical simulations of strongly-coupled two-dimensional dissipative Yukawa systems are presented. The thermodynamic characteristics of these systems were studied, namely the internal energy, the specific heat and the entropy. For the first time, it is discovered that the considered characteristics have two singular points on the melting line; one of these points corresponds to the first-order phase transition from crystal to the hexatic phase, and another point corresponds to the second-order phase transition from the hexatic phase to the isotropic liquid. The obtained results are compared to the existing numerical and analytical data.

Thermodynamic properties of the systems of interacting particles are of significant interest in various fields of science and technology, such as plasma physics, medical industry, physics of polymers and others [1–8]. Nowadays the special focus is on the study of the behavior of two-dimensional (2d) systems. The analysis of the physical characteristics of these systems has not only the fundamental scientific value, but is also vital in nano- and microtechnology, as well as for the development of new materials and coatings with tailored properties [5–8].

In thermodynamics of two-dimensional structures, their melting is of the greatest interest. At present, there are two main approaches describing the phase transitions in these systems, based on the analysis of formation of various topological defects. The first is KTHNY (Kosterlitz–Thouless–Halperin–Nelson–Young) theory, which predicts the two-stage transition from the crystal to the liquid state of the system via the intermediate hexatic phase [9–11]. The second is GBI (Grain-Boundary-Induced melting) theory, describing the melting of a 2d-system as the first-order transition from the crystal to the liquid without the formation of the intermediate phase [12,13].

The evidences for the KTHNY theory in 2d-systems with various interaction potentials were found both in numerical and experimental studies [14–23]. So, for example, the detailed analysis of the dynamics of the grains interacting via the screened Coulomb potential (of Yukawa type)

$$\phi(r) = (eZ)^2 \exp(-r/\lambda)/r, \tag{1}$$

where λ is the screening length, eZ is the charge of a grain, is presented in [21–23]. This model is of a special interest for the theoretical study of dusty plasma [5–8], and also is widely used for the numerical simulation of repulsion in the kinetics of interacting particles [1–8].

The numerical experiments in dissipative Yukawa systems with $\nu_{fr} \neq 0$ (where ν_{fr} is the friction coefficient of particles due to their collisions with the neutrals of surrounding gas) show that the physical characteristics (e.g. the maximum/minimum ratio of the pair correlation functions, the isothermal compressibility, the heat capacities, and the diffusion constants) of these systems have two singularities [21–23]. The first corresponds to the "liquid-hexatic" phase transition and is observed when the effective coupling parameter $\Gamma^* = \Gamma^*_h \approx 98 \pm 3$; the second singular point (when $\Gamma^* = \Gamma^*_c \approx 154 \pm 4$) is due to the transition from the hexatic phase to the "ideal" crystal, where the diffusion coefficient of the particles $D \to 0$. Here $\Gamma^* = 1.5\ (eZ)^2(1+\kappa+\kappa^2/2)\exp(-\kappa)/(Tr_p)$, where $\kappa = r_p/\lambda$, T is the temperature of the particles measured in energy units, and r_p is the mean interparticle distance. Note that Clark et al. [24] obtained similar values of Γ^* on the phase transitions lines for the Coulomb systems ($\kappa = 0$) in case of $\nu_{fr} = 0$ in classical limit of the problem, using the quantum Monte Carlo method.

* Corresponding author at: Joint Institute for High Temperatures RAS, 125412, Izhorskaya st. 13 bd. 2, Moscow, Russia. Tel.: +7 (495) 484 23 55.
E-mail address: Koss@gmail.com (X.G. Koss).

http://dx.doi.org/10.1016/j.physleta.2014.10.004
0375-9601/

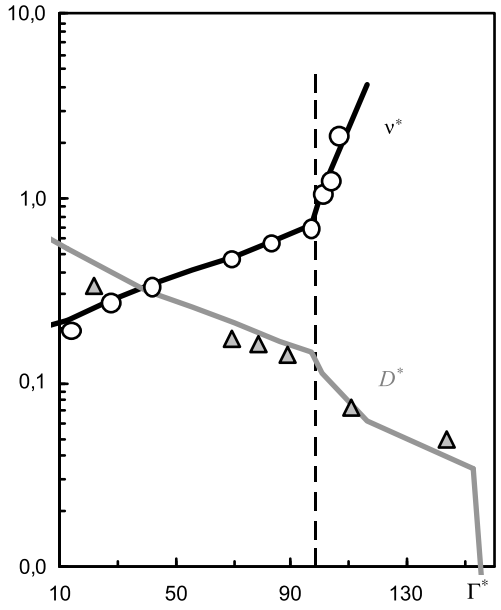

Fig. 1. The normalized values of the coefficients of diffusion D^* and viscosity ν^* for quasi-2d Yukawa systems [18] (solid lines). The symbols are the normalized data: (△) – for 2d-colloidal systems [25]; (○) – for 2d-disperse systems ($\nu_{fr} = 0$, $\xi \to \infty$, $\kappa = 0.56$) [33].

We must emphasize that one should perform the calculation of physical characteristics of 2d-systems (including spatial correlation functions) near the phase transition points and for the conditions corresponding to the hexatic phase with especial thoroughness, and the time of the simulation should be controlled for the results to be consistent [6,8,25]. This is particularly important for the systems with the small friction ($\nu_{fr} \to 0$). Thus, in [25] it was found that for the pure dispersive Yukawa systems with $\nu_{fr} = 0$ the hexatic phase is metastable and disappears in the limit of long times.

The most laboratory studies of the properties of two-dimensional systems is carried out in the colloids or in the weakly ionized gas discharge plasma, where the dissipation caused by the collisions of the charged grains with the neutral particles of the surrounding medium ($\nu_{fr} \neq 0$) can substantially affect the dynamics and the conditions of formation of the ordered dust structures. We should note that, unlike the experiments with colloidal systems, demonstrating the good agreement with the statements of KTHNY theory [16–19], the experiments with dusty structures in the laboratory radio-frequency discharge did not show the compelling evidence either of KTHNY or of GBI theories [26–29]. Nevertheless, the authors of the latest works [28,29] tend towards the GBI theory describing the melting scenario of the two-dimensional dusty structures forming in RF-discharge plasma.

It is usually assumed that in case of KTHNY scenario, both phase transitions in the system are of the second order [13,30]. Nevertheless, the results of some numerical and theoretical studies show that, depending on the type of pair interaction potential, both transitions could be of the first order, or one of them can be of the first, and the other – of the second order [24,25,31,32].

For the qualitative and quantitative analysis of the phase state of 2d-systems, the spatial correlation functions are usually used (pair $g(r)$ and orientational $g_6(r)$) [4–11,23,25,33]. It should be noted that in the work [23] the behavior of $g_6(r)$ function is presented, including the vicinity of the points of phase transitions. Also it is useful to study the behavior of various dynamical and structural properties of the system [21,22], for example, the diffusion and viscosity coefficients, which have the distinct singularity at Γ^* close to 98, which is much lower than the point of crystallization ($\Gamma_c^* \approx 154$), where $D \to 0$, see Fig. 1 [21,34,35].

Table 1
The energy, $U_0(\Gamma T)^{-1}$, for *hp*-lattices in Yukawa systems with various screening parameters, κ.

κ	$U_0(\Gamma T)^{-1}$
1	1.62532
1.5	7.59943×10^{-1}
2	3.93543×10^{-1}
3	1.19909×10^{-1}
4	3.91733×10^{-2}

Nevertheless, the analysis of these functions does not help to find out the character of the phase transitions observed. To know the order of the phase transition we should explore the behavior of various thermodynamic functions and characteristics, such as the specific entropy, the internal energy, the specific heat, the compressibility, etc. Thermodynamic characteristics of quasi-two-dimensional Yukawa systems (taking into account the displacements of particles perpendicular to the layer) close to the phase transitions were studied numerically in [22,36]. These works have confirmed the existence of two singularities near $\Gamma^* = 98$ and $\Gamma^* = 154$. However, the processed numerical data were not averaged, and were essentially discrete near the points of phase transitions, which is the reason the order of the observed phase transitions wasn't determined.

In the present work we show the results of the numerical study of thermodynamic properties of strongly coupled liquid and crystalline 2d-systems of particles which interact via the screened Coulomb (Yukawa) potential. The coupling parameter Γ^* was varied within the wide range, and its discretization interval was chosen to be small enough to disambiguate the behavior of the system close to the points of phase transitions.

In case of isotropic pair interactions (with the known interaction energy $\phi \equiv \phi(r)$) the physical properties of coupled systems, such as the energy density U, are determined by the particle 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 [4,36,37]:

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

where $m = 2, 3$ is the number of dimensions in the system, and $n = r_p^{-m}$. For a system with a constant number of particles, a lot of thermodynamic characteristics can be obtained from the calorific equation of state $U(T, n, \phi, g)$ and the basic formulas of thermodynamics – for example, the heat capacity, $C_V = (\partial U/\partial T)_V$, where V is the volume/surface area of the system, the pressure, the entropy, etc. [36].

In case of $T \to 0$ the value of U tends to U_0 – the energy density for the crystal lattice at $T = 0$. For any lattice of the known type the values of U_0 may be easily computed [36]. So, for the classical triangular lattice (*hp*-crystal) these values are as follows:

$$U_0 = \frac{1}{2}\sum_{i=1}\sum_{j=1}\phi(r_{ij}). \tag{3}$$

Here $r_{ij} = a\sqrt{i^2 + j^2 + ij}$, and $a = a_{hp} \equiv r_p(2/\sqrt{3})^{1/2}$ is the step (the lattice spacing) of *hp*-lattice. The normalized values of energy, $U_0(\Gamma T)^{-1}$, for *hp*-lattices in Yukawa systems with various screening parameters, κ, used in the numerical experiment, are shown in Table 1.

The numerical simulation was carried out by the Langevin molecular dynamics method (using the periodic boundary conditions in two chosen directions), based on the solution of the system of N_p ordinary differential equations, N_p being the number