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Criterions for Phase-Transitions in Yukawa systems (dusty plasma)

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Abstract. Phenomenological criteria for various phase transitions in the Yukawa system are considered including the melting of cubic lattices and the transitions between the *bcc*- and *fcc*-structures.

Weakly ionized dusty plasma can be considered as a dissipative system of macroparticles interacting with the screening Yukawa potential $\varphi = eZ\exp(-l/\lambda)/l$ (where eZ is the particle charge, and λ is the screening lengths). Under certain conditions, the dust immersed in plasma may form the stable structures similar to the liquid or the solid [1-5]. For analyses of phase state of dust systems the values of Coulomb coupling parameter are often used: $\Gamma = (eZ)^2/Td$, were T is the kinetic dust temperature in energy units, $d=n^{-1/3}$, and n is the dust concentration. In the case of Coulomb interactions the critical Γ_c value is about 106 at the line of fluid-solid transition. Nevertheless this rule is not suitable for Yukawa systems. Assumption of screening interactions ($\kappa = d/\lambda \neq 0$) leads to increasing of critical value Γ_c [6-9].

There are two known empirical rules for the first-order fluid-solid phase transition in three dimensions. The first one is the Hansen criterion for the freezing point, which determines the first maximum of the liquid structure factor as a value less than 2.85. The second rule is the Lindemann criterion, which determines the ratio of the root-mean-square displacement Δ_o of particle from its equilibrium position to the interparticle distance d on the melting line of the solid as a value close to 0.15. Thus the ratio $\delta_c = \sqrt{2}\Delta_o/d$ must be equal to ~ 0.21 on the melting line of system. It should be noted that the particle displacement $\Delta = \sqrt{2}\Delta_o$ from the center of mass of the system, measured in numerical simulations, is usually less than 0.2 d. Theoretical estimations show that the value of δ_c tends to 0.2 with increasing number of particles in the simulated systems [7]. The condition analogous to the Lindemann criterion can be obtained on the assumption that the average volume of thermal fluctuations $V_{tf} \cong 4\pi\Delta^3/3$ for the *bcc*-lattice should not exceed $(1-\pi\sqrt{2}/8)V \approx 0.32V$, where $V = n^{-1} \equiv (\alpha a_{W\text{-}S})^3$, $\alpha = (4\pi/3)^{1/3}$, and $a_{W\text{-}S} = (4\pi n/3)^{-1/3}$ is the Wigner-Seitz radius. For the stable *fcc*-structure to exist, it is necessary to satisfy the condition $V_{tf} < (1-\pi\sqrt{2}/6)V \approx 0.26V$ [10]. Taking into account the possibility of the counter displacement of grains, we find that the value of the ratio Δ/d must exceed either 0.211 ($\Delta_o/d > 0.15$) to melt the *bcc*-structure or 0.198 ($\Delta_o/d > 0.14$) to melt the *fcc*-lattice. The criterion for the transition

between *bcc*- and *fcc*-structure in Yukawa system can be obtained on the assumption that for the change of the *bcc*-symmetry of lattice, the interparticle distances should exceed λ (the intergrain interaction is in this case similar to that of "hard spheres" when formation of *fcc*-structures is possible):

$$2(1-\pi/(3\sqrt{2}))^{-1/3}\Delta_o \approx (a_{W\text{-}S} - \lambda). \quad (1)$$

Values of Δ_o/d for various phase transitions are presented in Fig. 1. We can see that the range of κ between 5.8 and 6.8 defines the region of the triple phase transition (*bcc-fcc*–liquid) and the values of Δ_o/d on the melting lines of *bcc*- and *fcc*- lattices are in accordance with the Lindemann Criterion.

Here we present a new empirical rules which determine the normalized coupling parameter $\Gamma_n = K_n \exp(-\kappa)\ \Gamma$ as a values close to the constants C_p at the line of different phase transitions (including the melting of cubic lattices and the transitions between the *bcc*- and *fcc*- structures): $\Gamma_n = K_n \exp(-\kappa)\ \Gamma \equiv C_p \approx$ const. The values of normalized coefficients K_n and constants C_p can be obtained from the relationship for the harmonic oscillator:

$$\Delta_o^2 = 3T/m_p\omega_c^2, \quad (2)$$

where m_p is the mass of the dust particle, and ω_c is the characteristic grain oscillation frequencies in lattices of different types. The value of $\omega_c = \omega_{bcc}$ in the *bcc*-lattice can be obtained from expression $F = (eZ)^2 \exp(-l/\lambda)(1+ l/\lambda)/l^2$ for the intergrain force assuming that the electric fields of all particles except the nearest ones are fully compensated [9]: $\omega_{bcc} = eZ(4n/\pi m_p)^{1/2} (1+\kappa+\kappa^2/2)^{1/2} \exp(-\kappa/2)$. Substitution of ω_{bcc} in Eq. (2) gives

$$\Gamma_n = \Gamma^* \equiv (1+\kappa+\kappa^2/2) \exp(-\kappa)\ \Gamma \quad (3)$$

and $C_p \cong 3\pi/(2\ \delta_c^{\,2}) \approx$106 n accordance with [9,11], here $\delta_c \equiv \sqrt{2}\Delta_o/d = (1-\pi\sqrt{2}/8)^{1/3} /2\alpha \approx 0.211$ at the melting line of *bcc*- structure.

Under the assumption that the characteristic frequency for the *fcc*–structure $\omega_c = \omega_{fcc} \propto dF/dl$, the value of the parameter Γ^* on the crystallization line for lattices of both types should be constant which contradicts to the results of numerical simulations, see Fig. 2. Suitable approximation $\omega_{fcc}^{\,2} \approx 2\alpha^3\, n\, (eZ)^2 \exp(-\kappa)(\kappa-\alpha)/m_p$ for the characteristic grain frequency in the *fcc*–structure can be obtain for the homogeneous system, where the gradient dF_Σ/dl of the sum F_Σ of the electrical forces can be estimated as $dF_\Sigma/dl \propto n\ (eZ)^2 \exp(-\kappa)(\kappa-\alpha)$. Thus, assuming that $\delta_c = (1-\pi\sqrt{2}/6)^{1/3} /2\alpha$ on the melting line of the *fcc*–lattice, we determine from Eq. 2:

$$\Gamma_n = (\kappa-\alpha) \exp(-\kappa)\ \Gamma,\ C_p \cong 6/(2\alpha^3\delta_c^{\,2}) \approx 18.5,$$

and the parameter Γ^* for this phase transition as

$$\Gamma^* \approx 18.5\ (\kappa\text{-}\alpha)^{-1}(1+\kappa+\kappa^2/2). \qquad (4)$$

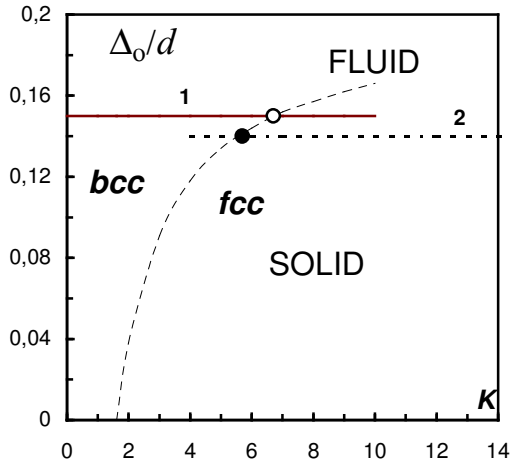

FIGURE 1. Dependencies of Δ_o/d on κ for different phase transitions:
1 –*bcc*→ fluid, **2** - *fcc*→ fluid; **3** - *bcc* ↔*fcc*;
● - κ = 5.8; O- κ =6.8

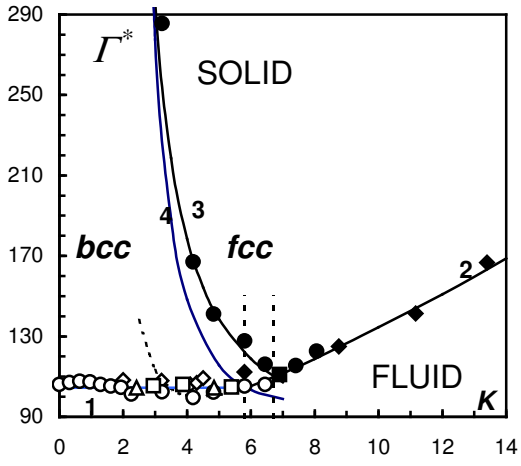

FIGURE 2. Dependencies of Γ^* on κ for different phase transitions:
O - [6]; ❑ - [7]; ◇- [8]; ∇ - [9]
1 – Γ^* =106 (*bcc*→ fluid) (Eq. 3), **2** - *fcc*→ fluid (Eq. 4); **3** – *bcc* →*fcc* (Eq. 5); **4** – *fcc* → *bcc* (Eq. 6).

The use of the modified parameter Γ^* Eq.(2) allows us to illustrate the behavior of the melting curves for the transitions *fcc*–lattice – liquid and *bcc*–lattice – liquid for the linear (not logarithmic) scale, Fig. 2. The difference between condition (4) and previous results [7,11] of modeling the *fcc*-lattice -liquid phase transition does not exceed 2% for κ>6.8.

Normalized coupling parameter Γ_n and modified parameter Γ^* at the line of transition of system from *bcc*- to *fcc*-structure can be obtain from Eqs. 1-2 with $\omega_c = \omega_{bcc}$

$$\Gamma^* \approx 64\ \kappa^2(\kappa\text{-}\alpha)^{-2}. \qquad (5)$$

Suitability of condition (5) as a criterion for the *bcc-fcc*-transition was checked using data of Ref. [6]. We obtained that deviation of the calculated values of Γ^* for the *bcc-fcc*-transition from Eq. (5) is within the limits ±2%, as illustrated on Fig. 3 (curve 3). Taking into account that the possibility of the reverse transition from the *fcc*- to *bcc*-structure is defined by the frequency ω_{fcc}, as a criterion for this transition we can consider the expression

$$\Gamma^* \approx 9.8\ \kappa^2\ (\kappa\text{-}\alpha)^{-3}(1+\kappa+\kappa^2/2) \qquad (6)$$

Note that condition (6) depends on the approximation of the frequency ω_{fcc} and therefore can be incorrect for small values of $\kappa \to \alpha$. However, calculations on the basis of expressions (5)-(6) (curves 3 and 4 on Fig. 2) fully determine the region of the triple phase transition (κ=5.8-6.8) and agree with the results of calculation of Δ_o/d (see Fig. 1). We add also that the difference in the positions of curves described by Eqs. (5) - (6) is capable to explain disagreements of the results of numerical simulations on finding the position of the triple point of system in Refs. [6,7].

To conclude, we considered the existent and proposed new phenomenological criteria for various phase transitions in the Yukawa system. Algorithm presented for the calculations of phase diagrams may be used for the systems with the another types of lattices or intergrain interactions in the case of $T>>\theta_d$, where θ_d is the Debye temperature. The values of characteristic frequencies ω_c can be obtained by the direct calculations, the estimations of gradients of intergrain interaction forces and also by the analytical approximations of the numerical simulation results or the experimental data. Presented results are independent on viscosity of surrounding gas (a friction produced by impacts of the gas atoms or molecules) and can be applied for analysis of particle dynamics in binary colloidal systems of different types, for example, in solutions of viruses, or for studies of diffusion controlled processes in physics of polymers, where Yukawa-type potentials are used extensively.

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