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Note: Melting criterion for soft particle systems in two dimensions

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According to the Berezinskii-Kosterlitz-Thouless-Halperin-Nelson-Young (BKTHNY) theory,[1] melting in two dimensions (2D) is a two-stage process. The crystal first melts by dislocation unbinding to an anisotropic hexatic fluid and then undergoes a continuous transition into an isotropic fluid. The dislocation unbinding occurs when the Young's modulus reaches the universal value of 16π,

$$\frac{4\mu(\mu+\lambda)}{2\mu+\lambda}\frac{b^2}{k_{\rm B}T} = 16\pi, \tag{1}$$

where μ, λ are the Lamé coefficients of the 2D solid, b is the lattice constant, and $k_{\rm B}T$ is the thermal energy. The Lamé coefficients to be substituted in Eq. (1) should be evaluated taking into account (i) *thermal softening* and (ii) *renormalization* due to dislocation-induced softening of the crystal.[2,3] Simplistic theoretical estimates using the elastic constants of an ideal crystalline lattice at $T = 0$ yield melting temperatures overestimated by a factor between $\simeq 1.5$ and $\simeq 2$ for various 2D systems.[3–6]

BKTHNY scenario has been confirmed experimentally, in particular, for systems with dipole-like interactions.[3,7,8] More recently, it has been reported that 2D melting scenario depends critically on the potential softness.[9] Only for sufficiently soft long-range interactions does melting proceed via the BKTHNY scenario. For steeper interactions, the hard-disk melting scenario with first order hexatic-liquid transition holds.[10–12]

The focus of this Note is on 2D soft particle systems. It is demonstrated that a melting criterion can be introduced, which states that the melting occurs when the ratio of the transverse sound velocity of an ideal crystalline lattice to the thermal velocity reaches a certain quasi-universal value.

The Lamé coefficients of an ideal 2D lattice can be expressed in terms of the longitudinal ($C_{\rm L}$) and transverse ($C_{\rm T}$) sound velocities as $\mu = m\rho C_{\rm T}^2$ and $\lambda = m\rho(C_{\rm L}^2 - 2C_{\rm T}^2)$, where m and ρ are the particle mass and number density.[5,13] Then condition (1) can be rewritten as

$$2\pi\sqrt{3}v_{\rm T}^2 = C_{\rm T}^2\left(1 - C_{\rm T}^2/C_{\rm L}^2\right), \tag{2}$$

where $v_{\rm T} = \sqrt{k_{\rm B}T/m}$ is the thermal velocity. For soft repulsive potentials, independent of space dimensionality, the following strong inequality, $C_{\rm L}^2/C_{\rm T}^2 \gg 1$, holds.[14–16] This implies that Eq. (2) can be further simplified to

$$C_{\rm T}/v_{\rm T} \simeq \text{const} \tag{3}$$

at melting. The value of the constant that follows from Eq. (2) is $\simeq 3.30$. However, this does not take into account thermal and dislocation induced softening. A working hypothesis to be verified is that a simple renormalization of the constant in Eq. (3) can account for these effects. In this case, Eq. (3) would be identified as a simple 2D universal melting rule for soft particle systems.

Let us verify whether the ratio $C_{\rm T}/v_{\rm T}$ does assume a universal value at melting. We consider three exemplary 2D systems with soft long-ranged repulsive interactions: one-component plasmas with logarithmic potential (OCP log),[17,19,20] 2D electron system with Coulomb $\propto 1/r$ potential (OCP $1/r$),[21,22] and dipole-like system with $\propto 1/r^3$ interaction.[7,8,18] The pair-wise interaction potential $\phi(r)$ can be written in a general form as

$$\phi(r)/k_{\rm B}T = \Gamma f(r/a),$$

where Γ is the coupling parameter and $a = 1/\sqrt{\pi\rho}$ is the 2D Wigner-Seitz radius. The system is usually referred to as strongly coupled when $\Gamma \gg 1$. The fluid-solid phase transition is characterized by a system-dependent critical coupling parameter $\Gamma_{\rm m}$ (the subscript "m" refers to melting). All systems considered here form hexagonal lattices in the crystalline phase (more complicated interactions and lattices should be considered separately).

The discussed soft-particle systems have been extensively studied in the literature and some relevant information is summarized in Table I. In particular, the last column lists the ratios $C_{\rm T}/v_{\rm T}$ at melting. The values presented indicate that as the potential steepness grows some weak increase of the ratio $C_{\rm T}/v_{\rm T}$ at melting is likely. At the same time, all the values are scattered in a relatively narrow range, 4.3 ± 0.3. This implies that Eq. (3) can be used as an approximate one-phase criterion of melting of 2D crystals with soft long-ranged interactions.

As an example of the application of the proposed criterion, the melting curve of a 2D Yukawa crystal has been calculated. The Yukawa potential is characterized by $f(x) = \exp(-\kappa x)/x$, where κ is the screening parameter (ratio of the mean interparticle separation a to the screening length). This potential is used as a reasonable first approximation to describe actual interactions in colloidal suspensions and complex (dusty)

TABLE I. Selected properties of 2D one-component plasma with logarithmic (OCP log) and Coulomb (OCP $1/r$) interactions and of the 2D system with the dipole-like interaction. Here C_T is the transverse sound velocity of an ideal triangular lattice, v_T is the thermal velocity, and Γ_m is the coupling parameter at melting.

System	$f(x)$	C_T/v_T [a]	Γ_m [b]	$C_T/v_T\|_{\Gamma_m}$
OCP log	$-\ln x$	$\sqrt{\Gamma/8}$	$\simeq 130 \div 140$	$\simeq 4.0 \div 4.2$
OCP $1/r$	$1/x$	$0.372\sqrt{\Gamma}$	$\simeq 120 \div 140$	$\simeq 4.1 \div 4.4$
Dipole	$1/x^3$	$0.547\sqrt{\Gamma}$	$\simeq 60 \div 70$	$\simeq 4.2 \div 4.6$

[a]See, e.g., Ref. 17 for OCP log, Ref. 5 for OCP $1/r$, and Ref. 18 for the dipole system.
[b]See Refs. 19 and 20 for OCP log; Refs. 21 and 22 for OCP $1/r$, and Refs. 7 and 18 for the dipole system.

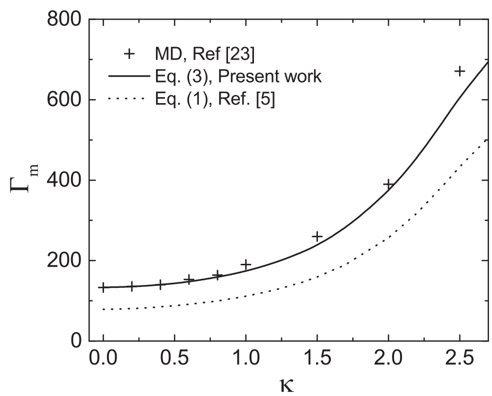

FIG. 1. Melting curve of a 2D Yukawa crystal in the (κ, Γ) plane. The solid curve corresponds to the condition $C_T = 4.3v_T$. The symbols correspond to the results of the numerical melting "experiment."[23] The dotted line corresponds to the solution of Eq. (1) with the asymptotic $T = 0$ values of elastic constants.[5]

plasmas.[24–27] In the latter case, the screening is normally weak,[28,29] $\kappa \lesssim 1$, which corresponds to the soft interaction limit. Thermodynamics and dynamics of 2D Yukawa systems are well understood;[23,30,31] simple practical expressions for thermodynamic functions[32] and sound velocities[16,33] have been derived. In particular, the transverse sound velocity of an ideal Yukawa lattice can be expressed using the Madelung constant $M(\kappa)$ as[16]

$$C_T^2 = \frac{v_T^2}{8}\left(\kappa^2\frac{\partial^2 M}{\partial \kappa^2} + \kappa\frac{\partial M}{\partial \kappa} - M\right),$$

where the product $M\Gamma$ defines the lattice energy per particle in units of temperature (reduced lattice sum). Using condition (3) with an "average" const = 4.3, the dependence $\Gamma_m(\kappa)$ for the triangular lattice has been calculated. The resulting melting line (solid curve) appears in Fig. 1. The agreement with the numerical melting "experiment"[23] is satisfactory in the weakly screened regime. An early attempt to estimate the location of the melting curve by using Eq. (1) with the asymptotic $T = 0$ values of elastic constants[5] is depicted by the dotted curve. A significant improvement is documented.

To conclude, a simple criterion for melting of two-dimensional crystals with soft long-ranged interactions has been proposed. It states that the ratio of the transverse sound velocity of an ideal crystalline lattice to the thermal velocity is a quasi-universal number close to 4.3 at melting. Application of these criteria allows estimating melting lines in a simple yet relatively accurate manner. Two-dimensional weakly screened Yukawa systems represent just one relevant example.

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