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,

$$\frac{4\mu(\mu + \lambda)}{2\mu + \lambda} \frac{b^2}{k_B T} = 16\pi, \quad (1)$$

where \(\mu, \lambda\) are the Lamé coefficients of the 2D solid, \(b\) is the lattice constant, and \(k_B T\) 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

Simplest theoretical estimates using the elastic constants of an ideal crystalline lattice at \(T = 0\) yield melting temperatures overestimated by a factor between \(\approx 1.5\) and \(\approx 2\) 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 \((C_L)\) and transverse \((C_T)\) sound velocities as \(\mu = m\rho C_L^2\) and \(\lambda = m\rho(C_L^2 - 2C_T^2)\), where \(m\) and \(\rho\) are the particle mass and number density.3,13 Then condition (1) can be rewritten as

$$2\pi \sqrt{3} v_T^2 = C_T^2 \left(1 - \frac{C_L^2}{C_T^2}\right), \quad (2)$$

where \(v_T = \sqrt{k_B T/m}\) is the thermal velocity. For soft repulsive potentials, independent of space dimensionality, the following strong inequality, \(C_L^2/C_T^2 \gg 1\), holds.14–16 This implies that Eq. (2) can be further simplified to

$$C_T/v_T \approx \text{const} \quad (3)$$

at melting. The value of the constant that follows from Eq. (2) is \(\approx 3.30\). 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 \(C_T/v_T\) 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 \((\text{OCP log})\),17,19,20 2D electron system with Coulomb \(\propto 1/r\) potential \((\text{OCP 1/r})\),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

$$\phi(r)/k_B T = \Gamma f(r/a),$$

where \(\Gamma\) is the coupling parameter and \(a = 1/\sqrt{4\pi\rho}\) 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 \(\Gamma_m\) (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 \(C_T/v_T\) at melting. The values presented indicate that as the potential steepness grows some weak increase of the ratio \(C_T/v_T\) at melting is likely. At the same time, all the values are scattered in a relatively narrow range, \(4.3 \pm 0.3\). 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 \(f(\kappa) = \exp(-\kappa x)/\kappa\), where \(\kappa\) is the screening parameter (ratio of the mean inter-particle 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, $\nu_T$ is the thermal velocity, and $\Gamma_m$ is the coupling parameter at melting.

<table>
<thead>
<tr>
<th>System</th>
<th>$f(\chi)$</th>
<th>$C_T/\nu_T^4$</th>
<th>$\Gamma_m$</th>
<th>$C_T/\nu_T V_m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>OCP log</td>
<td>$-\ln x$</td>
<td>$\sqrt{\Gamma/\pi}$</td>
<td>$\approx 130 \div 140$</td>
<td>$4.0 \div 4.2$</td>
</tr>
<tr>
<td>OCP 1/r</td>
<td>$1/\chi^2$</td>
<td>$0.372\sqrt{\Gamma}$</td>
<td>$\approx 120 \div 140$</td>
<td>$4.1 \div 4.4$</td>
</tr>
<tr>
<td>Dipole</td>
<td>$1/\chi^3$</td>
<td>$0.547\sqrt{\Gamma}$</td>
<td>$\approx 60 \div 70$</td>
<td>$4.2 \div 4.6$</td>
</tr>
</tbody>
</table>

$^{a}$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.

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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