Lecture 3 | 2-dimensional melting

Let us consider a 2d crystal.

Rigorously there should be no 2d crystals because the lattice order is destroyed by thermal fluctuations.

To see this, consider elastic Hamiltonian

$$H = \frac{1}{2}\int d^2k \left[\mu k^2 u^2 + (\mu+\lambda)(k\cdot u)^2\right] \qquad (1)$$

Average thermal displacement ($T/2$ per degree of freedom)

$$\langle |u_k|^2 \rangle = \frac{T}{\mu}\frac{(3\mu+\lambda)}{(2\mu+\lambda)k^2} \quad \Rightarrow$$

$$\langle [u(r)-u(0)]^2 \rangle = \int |u_k|^2 |e^{ikr}-1|^2 \frac{d^2k}{(2\pi)^2} = 2\int \langle |u_k|^2 \rangle (1-\cos kr)\frac{d^2k}{(2\pi)^2}$$

$$\langle [u(r)-u(0)]^2 \rangle = 2\frac{T(3\mu+\lambda)}{\mu(2\mu+\lambda)}\int \frac{d^2k}{(2\pi)^2}\frac{1-\cos kr}{k^2} = \frac{T}{\pi\mu}\frac{(3\mu+\lambda)}{(2\mu+\lambda)}\ln\frac{r}{a},$$

where a is a short distance cut off.

This logarithmic divergence of displacement field at large distances leads to a power law decay of the correlation function

$$C_{\vec{G}}(r) = \langle \rho_{\vec{G}}(r)\, \rho_{\vec{G}}(0) \rangle, \quad \text{with } \rho_{\vec{G}}(r) = e^{i\vec{G}\cdot\vec{u}(\vec{r})}$$

$$C_{\vec{G}}(r) = \langle e^{i\vec{G}\cdot[\vec{u}(r)-\vec{u}(0)]} \rangle = e^{-\frac{G^2\langle[u_x(r)-u_x(0)]^2\rangle}{2}} \sim$$

$$\sim r^{-\eta_G(T)} \quad \text{with } \eta_{\vec{G}} = \frac{T\, G^2 (3\mu+\lambda)}{4\pi\mu(2\mu+\lambda)} \Rightarrow$$

<u>No true long range order</u> (Peierls, Landau, Mermin, Wagner...)

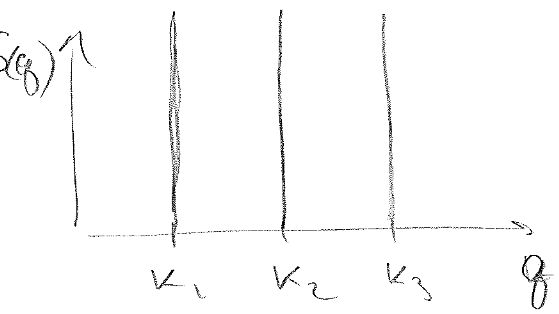
Let us consider structure factor

$$S(q) = \sum_r e^{i\vec{q}\vec{r}} \langle e^{iq\cdot[\vec{u}(r)-\vec{u}(0)]} \rangle$$

$$S(q) \sim \sum_{K_i} \frac{1}{|q-K_i|^{2-\eta_q}}$$

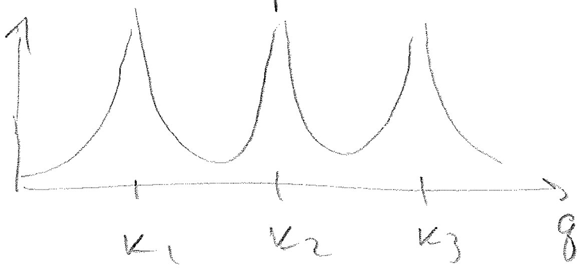
for real solid

$$S(q) = \sum \delta(q-K_i)$$



For the 2d solid one has power law singularities

<u>quasi solid</u>



This quasi solid with power law decay of the correlation function is very different from the liquid with $C(r) \sim e^{-r/\xi}$.

Thus there should be a phase transition — melting of quasi solid — BKT-transition

(V. Berezinskii 1971) (J. Kosterlitz & D. Thouless 1972,73)

If we treat $\vec{u}$ as a continuous variable, then, since Hamiltonian (1) is quadratic in $\vec{u}$, theory is Gaussian and there should be no phase transition — quasisolid would persist for any temperature.

To get a transition we should take into account that displacement of the crystal by its period doesn't change the structure. So we should consider $\vec{u}$ in some sense as a periodic variable. We should then take into account topological defects going around which displacement changes by the lattice period — dislocations. These dislocations produce the phase transition

Since energy of dislocation is $\propto \ln \frac{R}{a}$ at low temperatures there are no free dislocations – they are bound into small pairs $\perp$ $\top$. With temperature increase size of bound pairs increases and at some temperature T_m pairs dissociate and free dislocations appear. To find this temperature we can use **entropic** arguments due to **Kosterlitz** & Thouless (1973).

Energy of the single dislocation (edge)

$$E_d = \frac{\mu b^2}{8\pi(1-\sigma)} \ln \frac{R^2}{a^2}$$

Entropy $S_d = \ln \frac{R^2}{a^2}$ ($\frac{R^2}{a^2} \propto$ area = # of possible position of dislocation).

Free energy $E_d - TS_d = \left(\frac{\mu b^2}{8\pi(1-\sigma)} - T\right) \ln \frac{R^2}{a^2}$

It is favourable to have dislocation for

$$T > T_m = \frac{\mu b^2}{8\pi(1-\sigma)} \qquad (2)$$

Melting or dislocation unbinding temperature.

In a more formal way consider average size of the pair

$$\langle r^2 \rangle = \frac{\int d^2r \, r^2 \exp\left(-\frac{U_{pair}(r)}{T}\right)}{\int d^2r \, \exp\left(-\frac{U_{pair}(r)}{T}\right)}$$

with $U_{pair} = 2\, \mathcal{E}_d \ln \frac{r}{a}$, $\mathcal{E}_d = \frac{\mu b^2}{4\pi(1-\sigma)}$

Thus $\langle r^2 \rangle \propto \int d^2r \, r^2 \exp\left(-\frac{2\mathcal{E}_d}{T} \ln\frac{r}{a}\right) =$

$$\propto \int_a^\infty d^2r \, r^{\left(2 - \frac{2\mathcal{E}_d}{T}\right)}$$

For low temperatures

$$\langle r^2 \rangle \propto \frac{a^2}{\left(4 - \frac{2\mathcal{E}_d}{T}\right)} = \frac{a^2 T}{4\left(T - \frac{\mathcal{E}_d}{2}\right)}$$

With temperature increase $\langle r^2 \rangle$ grows and diverges at $T = \frac{\mathcal{E}_d}{2}$ which is just the melting temperature Eq. (2)

Problem: Show that for short range repulsive interaction $U \propto \exp\left(-\frac{r}{r_0}\right)$ minimal energy at fixed density corresponds to the triangular lattice

What is the phase above the melting temperature?

In the solid we have translational order $\rho_G(r) = \exp(i\vec{G}\cdot\vec{r})$

and orientational order $\psi_6(r) = e^{6i\theta(r)}$,

θ - bond angle for triangular lattice

Correlation function $C_6 = \langle \psi_6^*(r)\, \psi_6(0) \rangle$.

In the solid $\theta(r) = \frac{1}{2}\left(\frac{\partial u_y}{\partial x} - \frac{\partial u_x}{\partial y}\right)$

$$\langle \psi_6^*(r)\, \psi_6(0) \rangle = \langle e^{i6(\theta(r)-\theta(0))} \rangle = e^{-18\langle(\theta(r)-\theta(0))^2\rangle}$$

Since $\langle u^2 \rangle \sim \ln r$ and $\theta \sim \operatorname{rot} \vec{u}$ $\Rightarrow$

$\langle \theta^2 \rangle \sim \text{const}$ thus

Quasisolid has quasi longrange translational order but true orientational long range order.

Above the melting the shear modulus goes to zero but the orientational order may still exist.

$F_H = \frac{1}{2} K_H \int d^2r\, (\nabla\theta)^2$ — hexatic liquid crystal

Repeating calculations from the first page we obtain $\langle \psi^*(r)\, \psi(0) \rangle = r^{-\eta_6(T)}$ with

$\eta_6(T) = \dfrac{18\,T}{\pi K_H}$ - quasi long range order in hexatic

Topological defects in hexatic

Disclinations

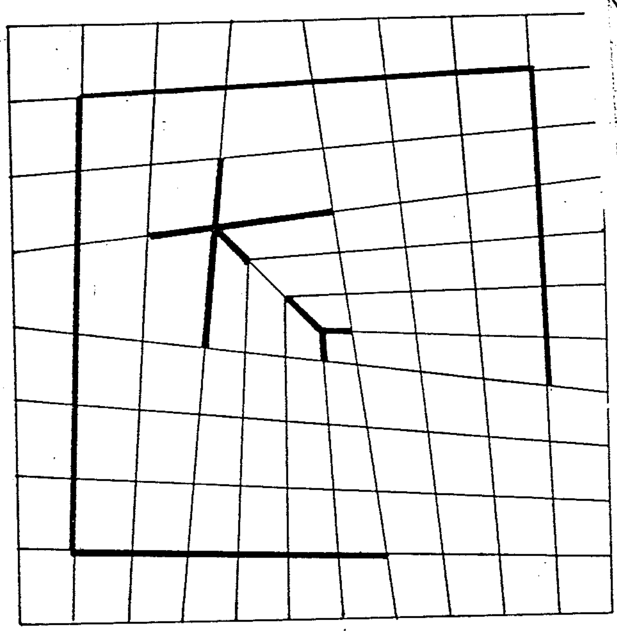


FIG. 5. Dislocation that may be viewed as a bound disclination pair. A path around the dislocation fails to close, as shown. The two disclinations, one having five nearest neighbors and one having three, are also shown.

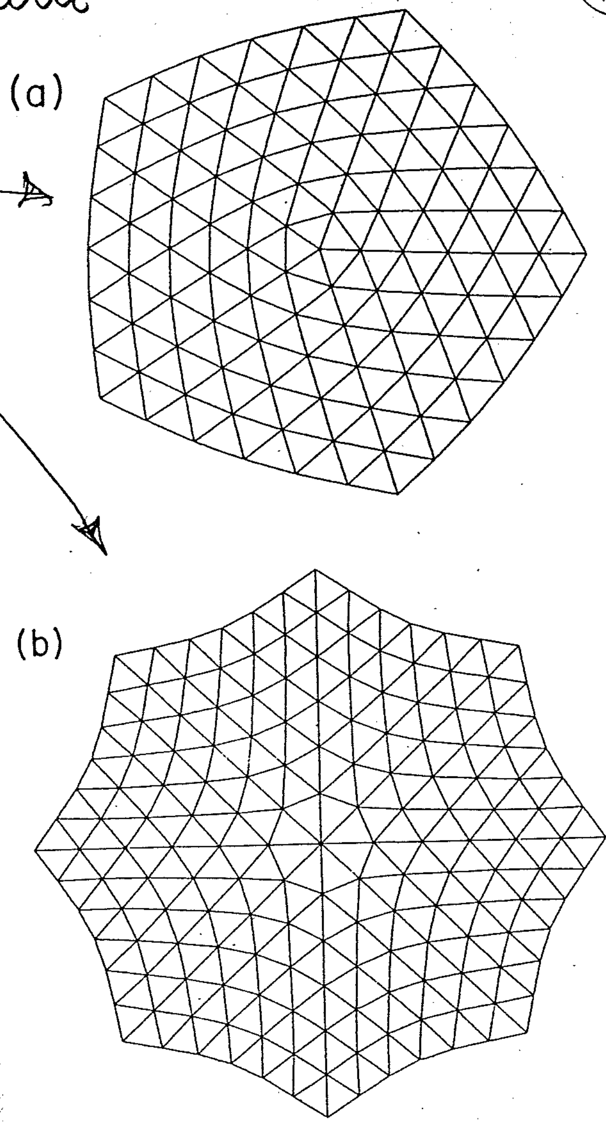


FIG. 4. Positive and negative disclinations in a triangular lattice. Note the rotation of the triangular cells by 60° (a) clockwise, and (b) counterclockwise, as a clockwise path around the disclination is traveled. Note that these disclinations may also be described as particles having (a) five, and (b) seven neighbors, respectively, rather than six.

In the solid phase energy of disclination pairs $\sim R^2$ they are bound.

1 dislocation = disclination pair, dislocation pair = disclination quartet

In Hexatic phase $H_{disc} = -\frac{\pi K_H}{36} \sum S(r) S(r') \ln \frac{|r-r'|}{r_0} + E_c \sum S^2(r)$

$\Rightarrow$ BKT transition - unbinding disclinations with

$K_H(T_d) = \frac{72}{\pi}$, correlation function $r^{-\eta_6(T)}$

$\eta_6(T_d) = \frac{1}{4}$