Lecture 4) Dislocation - mediated melting II

Coulomb gas analogy

Let us consider system similar to dislocations in 2d - systems of charges in 2d with

$$H = \frac{1}{2}\sum_{i\neq j} V(r_i - r_j) \ ,$$ where

$$V(|r_i - r_j|) = -2 q_i q_j \ln\left|\frac{r_i - r_j}{a}\right| + 2E_c \quad \text{at } r > a$$

$$V = 0 \quad \text{at } r < a$$

$2E_c$ is the energy for creation of a pair at short distances (core energy)

Average size of the pairs (+ -)

$$\langle r^2 \rangle = \frac{\int d^2r\, r^2 \exp(-2\frac{q^2}{T}\ln r/a)}{\int d^2r \exp(-2\frac{q^2}{T}\ln\frac{r}{a})} = a^2 \frac{q^2 - T}{q^2 - 2T}$$

average distance between the pairs

$$\frac{1}{d^2} \sim \frac{1}{a^4}\int \exp\left(-2\frac{E_c}{T} - \frac{2q^2}{T}\ln\frac{r}{a}\right) d^2r$$

$$\frac{1}{d^2} \sim \frac{Te^{-2\frac{E_c}{T}}}{a^2(q^2 - T)} \Rightarrow \left\langle\left(\frac{r}{d}\right)^2\right\rangle \sim \frac{Te^{-2E_c/T}}{q^2 - 2T}$$

Thus pairs start to overlap for $T \to \frac{q^2}{2}$

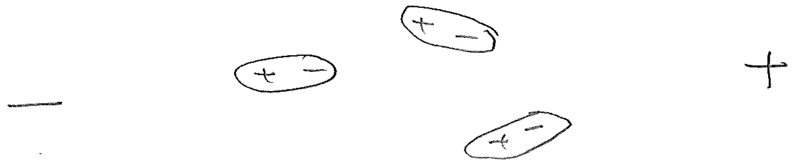
This is the BKT transition temperature

If core energy is large there are few pairs away from the transition temperature

$y_0 = e^{-E_c/T}$ fugacity $\ll 1$

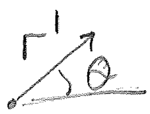
In this case one can build a selfconsistent theory of the phase transition.

Within the range of a large pair $r \gg a$ there would be small pairs which renormalise interaction between the charges producing



effective dielectric constant $\varepsilon(r)$

$$\varepsilon(r) = 1 + 4\pi P(r), \quad \text{with } P(r) = \int_a^r n(r', \theta)\,\alpha(r')\, r'dr'd\theta \qquad (1)$$

where $n(r', \theta')$ density of pairs with 

and $\alpha(r')$ - polarizability of the single dipole

$$\alpha(r) = q\frac{\partial}{\partial E}\langle r\cos\theta\rangle\Big|_{E=0} = q\int \frac{\partial}{\partial E} e^{-\frac{H_0(r)}{T} + \frac{E q r\cos\theta}{T}}\, r\cos\theta\, d\theta\Big|_{E=0}$$

$$\Rightarrow \alpha(r) = \frac{q^2 r^2 \langle\cos^2\theta\rangle}{T} = \frac{q^2 r^2}{T\,2} \qquad (2)$$

Let us denote $\pi K_0 = \frac{q^2}{T}$

Energy (over T) of interaction is modified from $2\pi K_0 \ln r/a$ because of the screening effect of smaller pairs. To get it we integrate force and denoting this energy as $2\pi \mho(r') \ln\left(\frac{r'}{a}\right)$ we obtain

$$2\pi \mho(r') \ln \frac{r'}{a} = 2\pi K_0 \int_{\ln a}^{\ln r'} \frac{d \ln r''}{\varepsilon(r'')}$$

Density of $\overbrace{\text{dipoles}}^{\text{with sizes between } \vec{r}' \text{ and } \vec{r}'+d\vec{r}'}$ is given by (see page 1)

$$n(r', \theta) = \left(\frac{y_0}{a^2}\right)^2 \left(\frac{r'}{a}\right)^{-2\pi \mho(r')} \qquad (3)$$

and combining everything together [(2),(3) → (1)] we obtain

$$\varepsilon(r) = 1 + 4\pi^3 y_0^2 K_0 \int_a^r \left(\frac{r'}{a}\right)^{4 - 2\pi \mho(r')} \frac{dr'}{r'}$$

This is a self-consistent equation for $\varepsilon(r)$

Let us define $K(r) = \frac{K_0}{\varepsilon(r)}$ and $l = \ln \frac{r}{a}$

Then we get

$$K^{-1} = K_0^{-1} + 4\pi^3 y_0^2 \int_0^l \exp\left(4l' - 2\pi \int_0^{l'} K(l'') dl''\right) dl' \qquad (4)$$

It is useful to replace double integral by the system of differential equations.

Defining an auxiliary variable

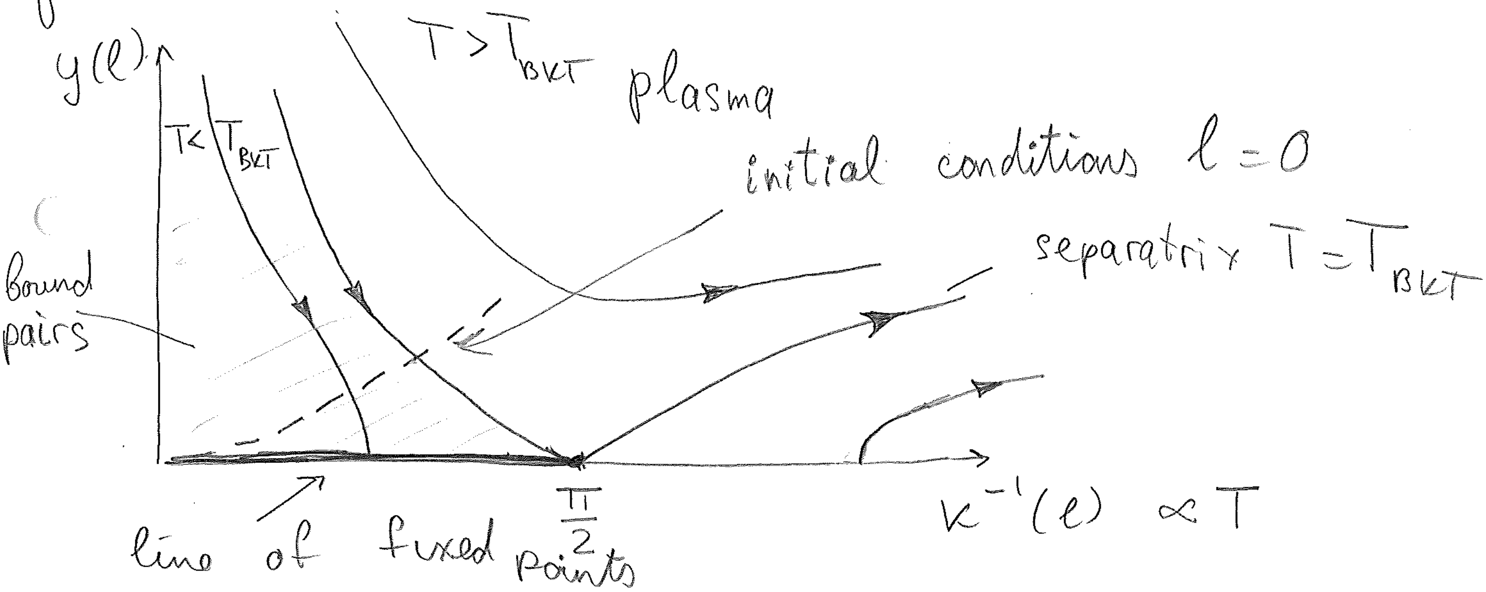
$$y(\ell) = y_0 \exp\left(2\ell - \pi \int_0^\ell K(\ell')\,d\ell'\right)$$

we rewrite Eq. (1) as

$$\begin{cases} \dfrac{dK^{-1}}{d\ell} = 4\pi^3 y^2 \\ \dfrac{dy}{d\ell} = (2 - \pi K)\, y \end{cases}$$

Kosterlitz recursion relations (1974)

The renormalization group flow given by these equations



For the dashed region at $\ell \to \infty$ $y \to 0$, $K^{-1} \to$ const $\Rightarrow$

$\varepsilon < \infty$ this is the dielectric phase

Above T_{BKT} at $l \to \infty$, $y, K^{-1} \to \infty$ and $\varepsilon \to \infty$

$\Rightarrow$ dissociation of pairs and at T_{BKT} we have transition from a gas of dipoles to a plasma.

At the transition $K(T_{BKT}) = \frac{2}{\pi}$ - universal ratio $\Rightarrow$

$$\underline{\varepsilon(T_{BKT}) = \frac{q^2}{2T_{BKT}}} \qquad (2)$$

This result we could obtain from the Kosterlitz-Thouless entropic arguments

Energy of the charge is

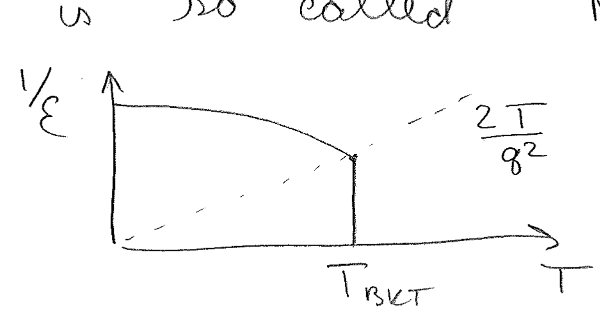
$$\frac{q^2}{\varepsilon} \ln \frac{R}{a}$$

Free energy $E - TS = \frac{q^2}{2\varepsilon} \ln \frac{R^2}{a^2} - T \ln \frac{R^2}{a^2}$

changes sign at $T_{BKT} = \frac{q^2}{2\varepsilon}$

Although ε is space and temperature dependent its longwave value at T_{BKT} is universal

This is so called Nelson-Kosterlitz jump



Behaviour close to T_{BKT}

Close to $K = \frac{2}{\pi}$ we introduce $x_\ell = 2 - \pi K(\ell) \ll 1$

and $y_\ell = 4\pi y_\ell$ => Kosterlitz equations can be rewritten as

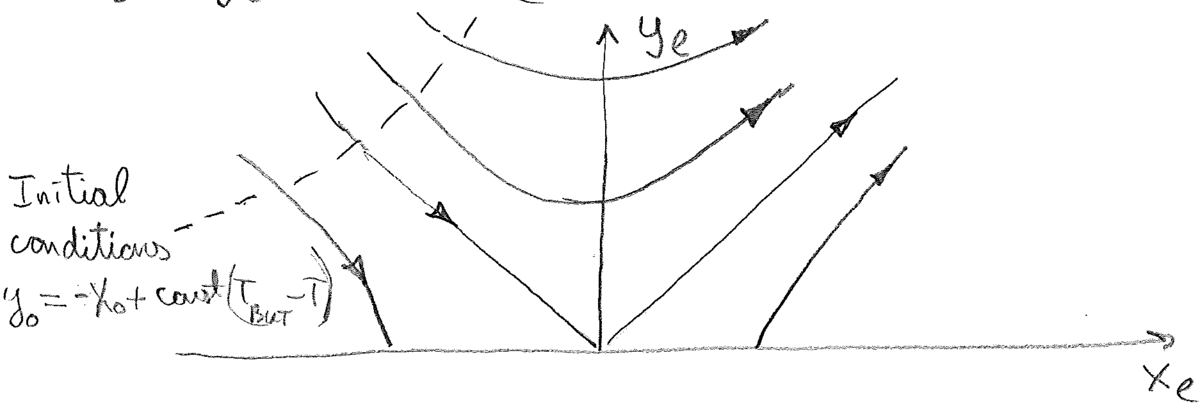
$$\begin{cases} \dfrac{dx_\ell}{d\ell} = y_\ell^2 \\[2ex] \dfrac{dy_\ell}{d\ell} = x_\ell y_\ell \end{cases}$$

Solution is hyperbola

$$\frac{d}{d\ell}\left(x_\ell^2 - y_\ell^2\right) = 0 \Rightarrow$$

$$x_\ell^2 - y_\ell^2 = C \propto (T_{BKT} - T)$$

Separatrix is $y_\ell = \pm x_\ell$



Correlation radius.

Below T_c $(C > 0)$ fixed points will be reached at $\ell \to \infty$ and $\underline{\xi = \infty}$

Above T_c $(C < 0)$ $y_\ell^2 = x_\ell^2 + C_0^2$,

$$\frac{dx}{d\ell} = x_\ell^2 + C_0^2 \Rightarrow \ell \sim \int_{x_0}^{\infty} \frac{dx}{x^2 + C_0^2} \sim \frac{1}{C_0} \sim \frac{1}{\sqrt{T - T_{BKT}}}$$

It takes $\ell \sim \dfrac{1}{\sqrt{T - T_{BKT}}}$ to go from initial (short scale) value of ξ to diverging ξ

at large scales. Since real length is $r = a e^{l}$ then we naturally obtain a correlation length above the transition point

$$\xi_+ = a e^{l} \sim e^{\frac{b T_{BKT}}{\sqrt{T - T_{BKT}}}}$$

Constant b is nonuniversal – it depends on properties on short distances (how close were initial conditions to the separatrix)

Note, that although there is ξ_+, $\xi_- = \infty$

Below T_{BKT} correlation function is power law and there is no characteristic length.

$\xi_+(T)$ can be associated as the average distance between the free charges.

$$n_{\text{free charges}} \simeq \xi_+^{-2}$$

Heat capacity $C \propto \xi_+^{-2} \propto \exp\left(2b \frac{T}{\sqrt{T - T_{BKT}}}\right)$ and has very weak singularity.

What should we change for dislocations?

(B. Halperin & D. Nelson, A.P. Young 1978, 79)

We have vector Coulomb gas with Hamiltonian

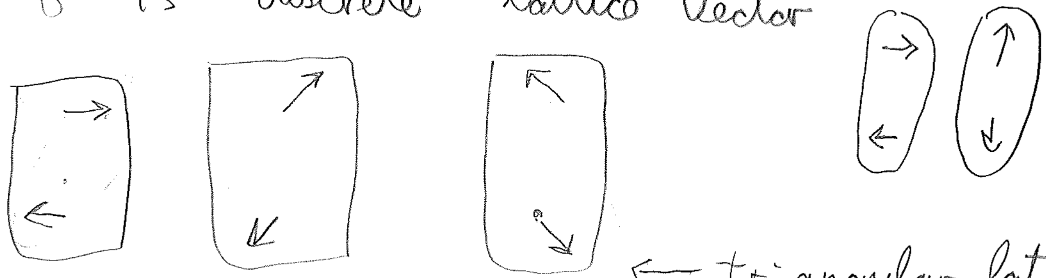
$$\frac{H}{T} = 2\pi \sum_{ij}\left[K(\vec{b}_i\cdot\vec{b}_j)\ln\frac{r_{ij}}{a} - K\,\frac{(\vec{b}_i\cdot\vec{r}_{ij})(\vec{b}_j\cdot\vec{r}_{ij})}{r_{ij}^2}\right] + \frac{E_c}{T}\sum \vec{b}(r)^2$$

<u>Problem</u> derive ↗

$\vec{b}_i$ - Burgers vectors and $K = \dfrac{\mu b^2}{4\pi^2(1-\sigma)T}$

1. $\vec{b}$ is discrete lattice vector

and



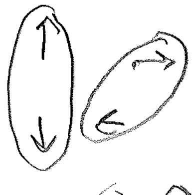
square lattice

← triangular lattice

polarizability $\alpha(r') = \frac{\pi K_0}{2}\, r'^2 \left(1 - \frac{1}{2}\langle \cos 2\theta\rangle_{ang}\right)$

where θ is an angle between the displacement vector of the pair and the Burgers vector

$$n(r',\theta) = 2\left(\frac{y_0}{a^2}\right)^2 \exp[\pi K(r')\cos 2\theta)\left(\frac{r'}{a}\right)^{-2\pi\upsilon(r')}$$

factor 2 is for square lattice (2 species of dislocation pairs with opposite Burgers vectors )

For triangular lattice 2 is replaced by 3 

Substituting this relations and performing the angular integration we obtain for the square lattice

$$\begin{cases} \dfrac{dK^{-1}}{dl} = 8\pi^3 y^2 \left[I_0(\pi K) - \frac{1}{2} I_1(\pi K) \right] \\ \\ \dfrac{dy}{dl} = (2 - \pi K)\, y \end{cases}$$

For the triangulare lattice $8 \to 12$ in the first equation.

2. Another less trivial change for the triangular lattice is due to the fact that two dislocations with Burgers' vectors produce also dislocation

$\nearrow + \searrow = \rightarrow$

Since we replace the pair of dislocations with separation $r' < r$ by a continuous medium we should also ignore structure in the pair $\nearrow \searrow$ if their separation $r' < r$

$\rightarrow = \rightarrow + \nearrow \searrow$

Thus we should replace y_0 by $\bar{y}(r')$, where $\bar{y}(r')$ is y_0 + probability to have their a pair of type $\nearrow \searrow$ with separation $r'' < r'$

$$\Rightarrow \;=\; \rightarrow \;+\; \nearrow \searrow$$

$$\bar{y}(r') = y_0 + y_0^2 \int_a^{r'} \left(\frac{r''}{a}\right)^{2-\pi U(r'')} \exp[\pi K(r'')\cos 2\theta]\, d\theta \frac{dr''}{r''}$$

$$\Downarrow$$

$$\bar{y}(\ell) = y_0 + 2\pi \int_0^{\ell} \bar{y}^2(\ell')\, I_0(\pi K)\, \exp\left(2\ell' - \pi \int_0^{\ell'} K(\ell'')\,d\ell''\right) d\ell'$$

Defining $y(\ell) = \bar{y}(\ell)\exp\left(2\ell - \pi\int_0^{\ell} K(\ell')\,d\ell'\right)$

we arrive at the following equations for the triangular lattice

$$\begin{cases} \dfrac{dK^{-1}}{d\ell} = 12\pi^3 y^2 \left[I_0(\pi K) - \frac{1}{2} I_1(\pi K)\right] \\[2ex] \dfrac{dy}{d\ell} = (2 - \pi K)\,y + 2\pi I_0(\pi K)\, y^2 \end{cases}$$

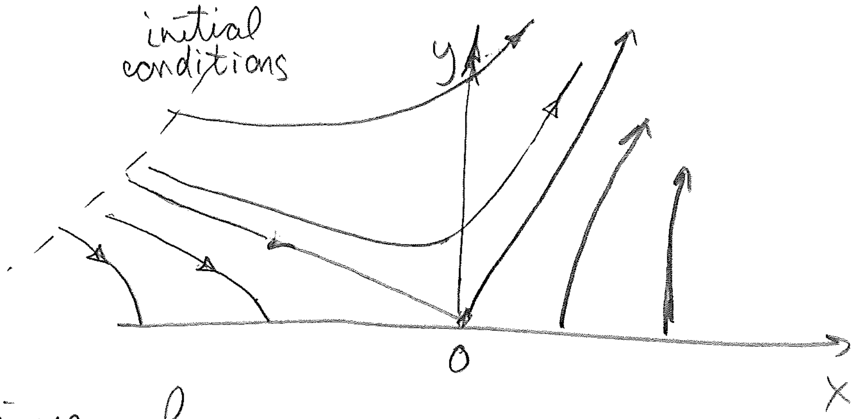
Close to T_m

$x = 2 - \pi K$, $\tilde{y} = \pi y \frac{I_0(2)}{\alpha}$, where $\alpha^2 = \frac{I_0(2)}{48}\left(1 - \frac{I_1(2)}{2 I_0(2)}\right)^{-1} \approx$

≈ 0.073

For $x, \tilde{y} \ll 1$ (dropping $\sim$ in $\tilde{y}$) we obtain

$$\begin{cases} \frac{dx}{dl} = y^2 \\ \frac{dy}{dl} = xy + 2\alpha y^2 \end{cases}$$



Separatrices are given by $y = m \cdot x \Rightarrow$

$\Rightarrow m^2 - 2\alpha m - 1 = 0 \Rightarrow$

$m = \alpha \pm \sqrt{\alpha^2 + 1}$,

We are interesting with negative slope with $m = \alpha - \sqrt{\alpha^2 + 1} < 0$

On this separatrix $\frac{dx}{dl} = m^2 x^2 \Rightarrow$

$\Rightarrow x(l) = \frac{-1}{m^2 (l + l_0)}$, $y = -\frac{1}{m} \frac{1}{l + l_0}$

If we are just above T_m we can write

$y(l) = m\,x(l) + D(l)$

Substituting this to the recursion relations in first order in D we obtain

$$\frac{dD}{dl} = -x D \Rightarrow D(l) = D(0) \exp \int_0^l |x(l')| \, dl'$$

using $x(l) = \frac{-1}{m^2 (l + l_0)}$ we get

$$D(l) = D(0) \, (l + l_0)^{1/m^2}$$

We could use this result to integrate recursion relations to a value l^* where the trajectory starts to deviate substantially from the separatrix.

Then $D(l^*) \sim y(l^*) \Rightarrow$

$$D(0) \, (l^* + l_0)^{1/m^2} \sim \frac{-1}{m (l^* + l_0)}.$$ As for Coulomb gas

$$D(0) \propto (T - T_m) \Rightarrow l^* \sim (T - T_m)^{-\nu}$$

with $\nu = \frac{m^2}{1 + m^2} = 0.3696$

Since $l^* \sim \ln \frac{\xi^*_+}{a}$ we obtain correlation radius (distance between free dislocations)

$$\xi_+ \propto e^{\frac{\text{const}}{(T - T_m)^\nu}}$$