Liquid - Solid transition : BCC lattice is the most stable one

As an example, we shall describe how to describe the liquid - solid transition using the Landau theory. In the Landau theory, the order parameters are n_G defined by

$$\langle \delta n(x) \rangle = \langle n(x) \rangle - n_0 = \sum_G n_G e^{i\vec{G}\cdot\vec{x}}$$

$n_G \neq 0$ for crystals.

There are infinite many G's, thus infinite many n_G's.

Near the transition, we can expand the free energy

$$\frac{F(D,T,n(r))}{V} = f_0 + f_1 + f_2 + f_3 + \cdots \quad (1)$$

where f_0 = Free energy of liquid

and $f_n (n \neq 0)$ contains terms with $n_{G_1} n_{G_2} n_{G_3} \cdots n_{G_n}$

with $G_1 + G_2 + G_3 + \cdots + G_n = 0 \quad (2)$

So that f_n is invariant under $\vec{r} \to \vec{r} + \vec{R}$:

$$n_{G_1} \cdots n_{G_n} \longrightarrow n_{G_1} n_{G_2} \cdots n_{G_n} e^{i(G_1 + G_2 + \cdots + G_n)\cdot\vec{R}} = n_{G_1} \cdots n_{G_n}.$$

Clearly, for $n=1$, ② implies $G=0$

$\therefore f_1 = 0$

$n=2$, $G_1 = -G_2$ $\therefore$ $f_2 = \sum_G \Delta_G |n_G|^2$

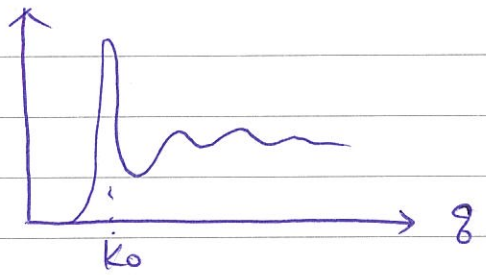
$(n_G = n_G^*)$

$n=3$, $f_3 = \sum_{G_1 G_2 G_3} B_{G_1 G_2 G_3} n_{G_1} n_{G_2} n_{G_3}$

$n=4$, $f_4 = \sum_{\substack{G_1 G_2 \\ G_3 G_4}} C_{G_1 G_2 G_3 G_4} n_{G_1} n_{G_2} n_{G_3} n_{G_4}$

...

The problem seems to intractable.
However, if we approach the crystal from the liquid side, as indicated by the structure factor,



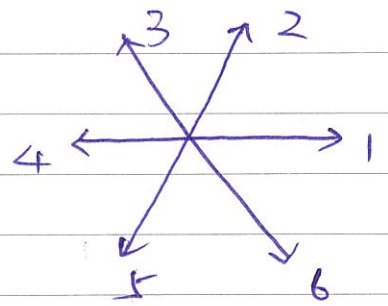
it would be reasonable to assume that only one length scale, i.e., one wave length for the density wave arises.
(Alexander & Mc Tague, Phys. Rev. Lett. 41, 702, 1978)

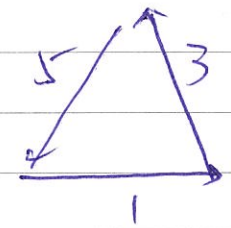
Therefore, we shall focus on $\vec{G}_i$ with the same magnitude G around k_0. The isotropy of liquid implies different directions of $\vec{G}$ are equivalent. Hence all A_G, $B_{G_1 G_2 G_3}$ & $C_{G_1 G_2 G_3 G_4}$ are the same!

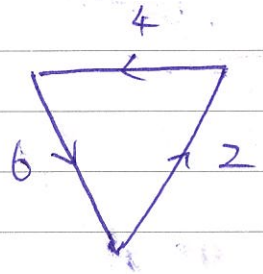
$\therefore$ we shall write $f_2 = r \sum_G |n_G|^2$

For $n=3$. Since $|\vec{G}_i| = G$, G_1, G_2, & G_3 must form an equilateral triangle. There are 3 possibilities if one collects all possible equilateral triangles:

(i) Six $\vec{G}_i$ $(i=1,2,3,4,5,6)$, # of $\vec{G}_i \equiv m = 6$.







$\Rightarrow$ crystals are hexagonal lattice

(ii) twelve $\vec{G}_i$, $m=12$ and they are edge vectors of an octahedron.

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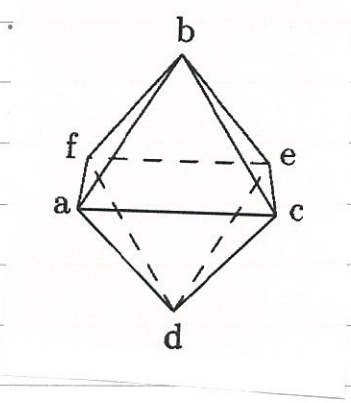
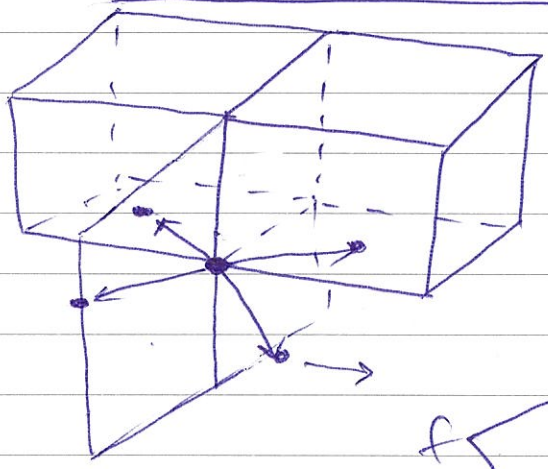
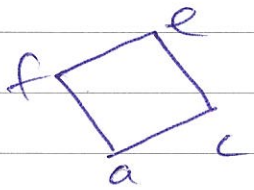


It's easy to see that acef, abcd & fbcd are 3 squares of a FCC crystal's nearest neighbouring vectors.
⇒ Crystals are BCC lattices!

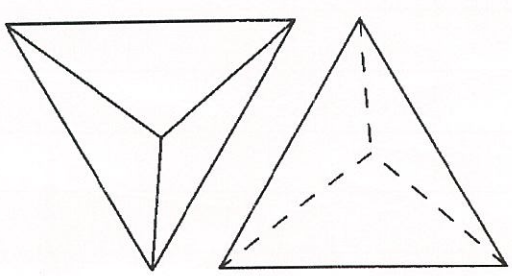




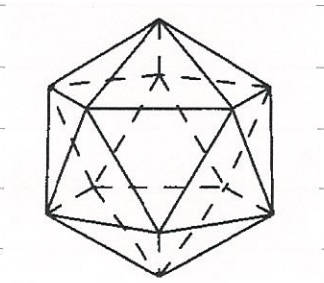
xy plane 4 neighbours
yz " "
zx " "

It's also possible to rearrangle the octahedron into two tetrahedrons:

$\begin{cases} \triangle abc, \text{ move } \bar{ce} \text{ to } b\ (d\to a),\ \bar{dc} \text{ to } a\ (d\to c),\ \bar{ad} \text{ to } c \\ \triangle dfe, \text{ move } \bar{af} \text{ to } d\ (b\to f),\ \bar{be} \text{ to } f\ (b\to e),\ \bar{fb} \text{ to } e \end{cases}$



(iii) m=30, they are edge vectors of an icosahedron.



For (iii), a solid with a reciprocal lattice generated by the edge vectors of an icosahedron is an <u>icosahedral quasi-crystal</u>!

Depending on sets of G_i, we have different m.

For a given m, since each pair $G, -G$ is equivalent, we find

$$f_2 = \frac{1}{2} r m |hG|^2$$

$$= \frac{1}{2} r |hG|^2 \quad ---(3)$$

↑ rescale n_G by $\frac{n_G}{\sqrt{m}}$.

For n=3, one needs to count # of equilateral triangles.

Let <u>p</u> be the # of triangles that a given G_i belongs to.

$\therefore$ $\vec{G}_1$ has m choices, there are p ..... triangles including $\vec{G}_1$, $\vec{G}_2$ has two choices in each triangle, after $\vec{G}_1$ & $\vec{G}_2$ are chosen, $\vec{G}_3$ is fixed!

$\therefore$ f_3 can be written as

$$f_3 = \omega \cdot m \cdot 2p\, |n_G|^3\, e^{i(\theta_1+\theta_2+\theta_3)}$$

$\longrightarrow$ min at $\theta_1+\theta_2+\theta_3 = \pi$

rescale $|n_G| \to \frac{n_G}{\sqrt{m}}$

$$f_3 = -\frac{2\omega p}{\sqrt{m}} |n_G|^3 \qquad \omega = \text{a positive coefficient}$$

L -- (4)

To have a lower bound for F/V, one needs to include f_4. (otherwise f_3 can be arbitrarily negative).

There are two possible ways for summation of 4 vectors, $\vec{G}_1$, $\vec{G}_2$, $\vec{G}_3$ & $\vec{G}_4$ to zero

(i) $\vec{G}_1$, $\vec{G}_2$, $\vec{G}_3$ & $\vec{G}_4$ in the same plane (e.g. acef diamond) $\rightarrow$ two sets of opposite $\vec{G}_i$

(ii) ..... non-planar diamond (each vector belongs to 2 non-planar diamonds) (e.g. badc)

(C_2^4)

For (i), we have 6 ways to pair $n_{G_1} n_{G_2} n_{G_3} n_{G_3}$ into $n_G n_G n_{G'} n_{G'}$. $\because$ G, G' have m choices

This contributes $6u m^2 (n_G)^2$ ($|n_G|^2$, $|n_{G'}|^2$ are equivalent)

$\rightarrow 6u |n_G|^4$

rescale $n_G \rightarrow n_G/\sqrt{m}$ $\quad u$ = some positive constant

For (iii), m choices for $\vec{G}_1$, $\therefore$ there are g non-planar diamonds ($\vec{G}_1$ belongs to), and there are 3 choices of $\vec{G}_2$ for a given diamond.

$\therefore$ $3g$ choices for $\vec{G}_2$

2 choices for $\vec{G}_3$

1 " for $\vec{G}_4$

$\therefore$ $m \times 6g \times u |n_G|^4 \xrightarrow[\text{rescale}]{} \frac{6gu}{m} |n_G|^4$

$\therefore$ $f_4 = 6u\left(1+\frac{g}{m}\right)|n_G|^4$ ... (5)

$f = \frac{1}{2} r |n_G|^2 - \frac{zwp}{\sqrt{m}} |n_G|^3 + 6u\left(1+\frac{g}{m}\right)|n_G|^4$ ... (6)

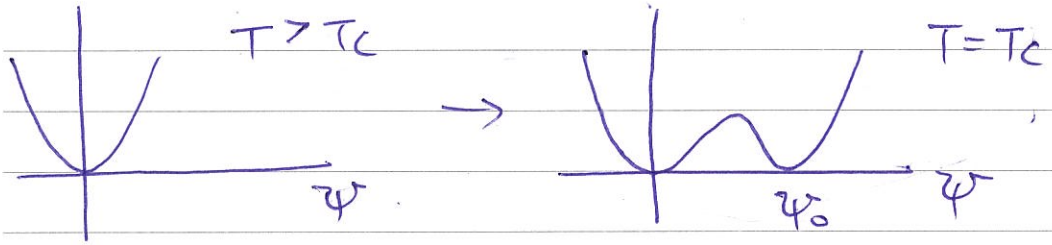
with $m=6$, $p=1$, $g=0$, for hexagonal lattice

$m=12$, $p=2$, $g=4$, for BCC

$m=30$, $p=2$, $g=4$, for icosahedral quasi crystal

Now, $r = \alpha(T - T_c^0)$ we can find transition temperature T_c by requiring

$$\begin{cases} \frac{df}{d\psi} = 0 \\ f(\psi=0, T_c) = f(\psi=\psi_0\neq 0, T_c) \end{cases} \qquad \psi = |M|$$



$$r\psi - \frac{6wp}{\sqrt{m}}\psi^2 + 24u\left(1+\frac{g}{m}\right)\psi^3 = 0$$

$$\psi = 0 \quad \text{or} \quad r - \frac{6wp}{\sqrt{m}}\psi_0 + 24u\left(1+\frac{g}{m}\right)\psi_0^2 = 0$$

$\because$ - ①

$f(\psi=0, T_c) = 0$

$$= f(\psi_0, T_c) = -\frac{1}{2}\psi_0^2\left[\alpha(T_c - T_c^0) - \frac{2wp}{\sqrt{m}}\psi_0 + 6u\left(1+\frac{g}{m}\right)\psi_0^2\right]$$

$$\therefore r - \frac{2wp}{\sqrt{m}}\psi_0 + 6u\left(1+\frac{g}{m}\right)\psi_0^2 = 0 \quad \cdots ②$$

$$① - ② \Rightarrow \psi_0\left[12u\left(1+\frac{g}{m}\right)\psi_0 - \frac{4wp}{\sqrt{m}}\right] = 0$$

$$\therefore \psi_0(T_c) = \frac{4wp}{\sqrt{m}\cdot 12u\left(1+\frac{g}{m}\right)}$$

Substituting it into eq. ②, we find

$$\alpha(T_c - T_c^0) = \frac{1}{2}\frac{(2wp)^2}{6u(m+g)} = \begin{cases} \frac{w^2}{18u} \text{ (hexagonal)} \\ \frac{w^2}{12u} \text{ (BCC)}, \quad \frac{2w^2}{5u} \text{ (Quasi crystal)} \end{cases}$$

It's clear that BCC crystal has highest T_c. Therefore, this analysis implies BCC lattice is the most stable one.

Indeed, a large # of materials crystallize from the melt into BCC (may assume some other structures in low temperatures)

In fact, 40 elements have high temperature BCC structures.

Of course, the above analysis does not explain why there are other high temperature structures.

To improve the theory, one needs to introduce a second $|\vec{G}'| \neq |\vec{G}|$ so that $\Delta f = \frac{r}{2} r_{G'} |h_{G'}|^2 - v |h_G|^2 |h_{G'}|$. Clearly, it leads to $|h_{G'}| = \frac{v}{r_{G'}} |h_G|^2$ so that $\Delta f = -\frac{v^2}{2 r_{G'}} |h_G|^4 < 0$. This would be the reason why other structures can be

also stablized. That would require more complicated analysis!

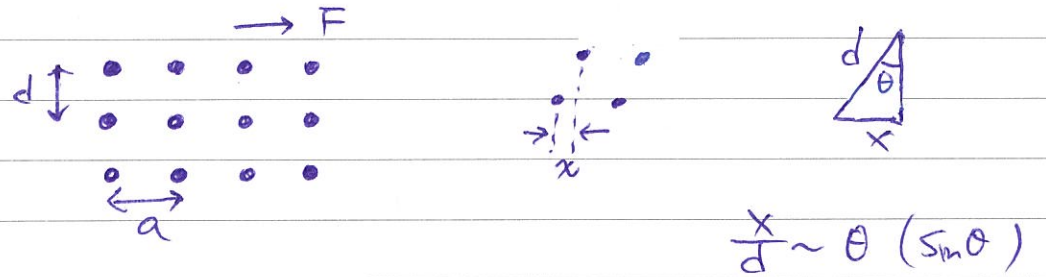
Defects and 2D melting

One can view the liquid-solid transition from the solid side. In this case, one sees that crystals become more & more deformed with defect proliferation and eventually melt.

Defects play an important role in the mechanical properties of a real crystal.

Why are real crystals much weaker than we thought?

Suppose we deform the crystal as follows:



$\frac{x}{d} \sim \theta \ (\sin\theta)$

u (elastic energy per unit volume)

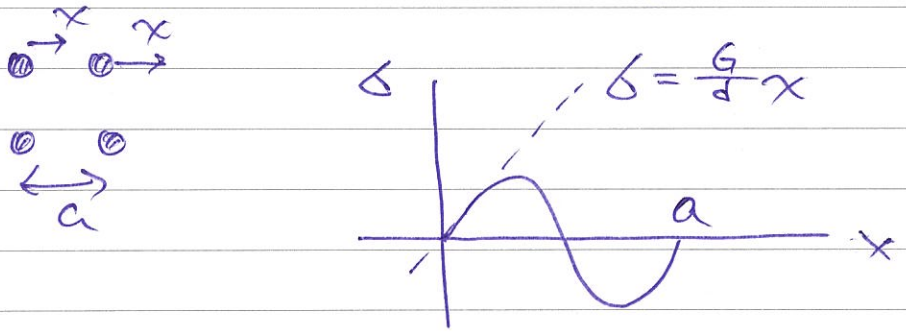
$= \frac{1}{2} G \left(\frac{x}{d}\right)^2$ $\quad G$ = shear modulus

This is valid only for small $\chi \ll 1$.

Experimentally, one can measure G in the regime $\chi \ll 1$ and find $G \sim 10^{11}-10^{12}$ dynes/cm^2

Now, we can extend the above to large χ. by noting that the stress $\sigma = G\frac{\chi}{d}$ (for ideal crystals, strain)

Since σ should be periodic in χ with period a (see the figure in below),



We can approximate σ by

$$\sigma = \frac{G}{d}\frac{a}{2\pi}\sin\frac{2\pi\chi}{a}$$

$$\max \sigma \equiv \sigma_c \text{ (critical shear stress)}$$

$$\simeq \frac{G}{d}\frac{a}{2\pi}$$

if $d \simeq a$, $\sigma \sim \frac{G}{2\pi} \sim 10^{11}$ dynes/cm^2

If we apply $\sigma > \sigma_c$, crystals undergo "slip", i.e. sliding one plane over the other!

From this, one can measure σ_c (expt.)

One finds Ag: $\sigma_c = 6 \times 10^6$ dynes/cm^2

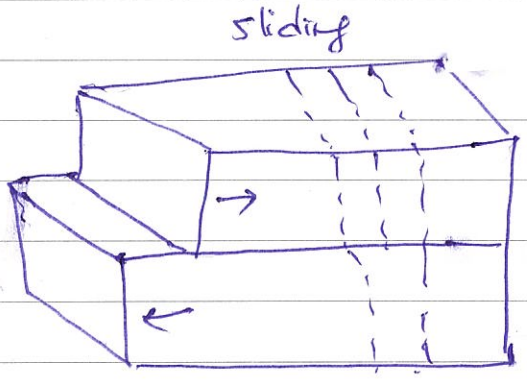
Al: $\sigma_c = 4 \times 10^6$ "

Which are 10^4 smaller than one expects!

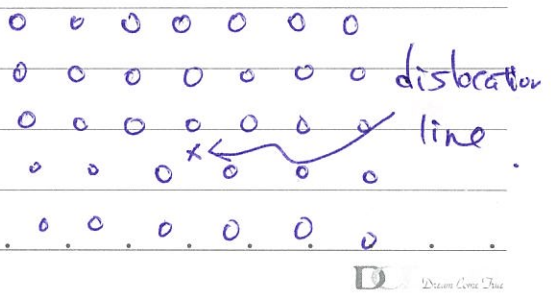
Therefore, real crystals are much weaker than we thought!

Why?

To explain the low yield stress, G.I. Taylor, Orowan & Polyanyi proposed that slip propagates by the motion of <u>dislocations</u> which were introduced earlier by Prandtl and Dehlinger. The dislocations proposed are <u>edge dislocations</u>:



It's equivalent to insert a half plane of atoms



notation: ⊥ ← extra plane ← slip plane ($\perp \hat{x}_1$)

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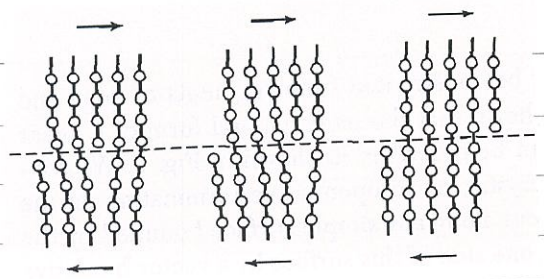
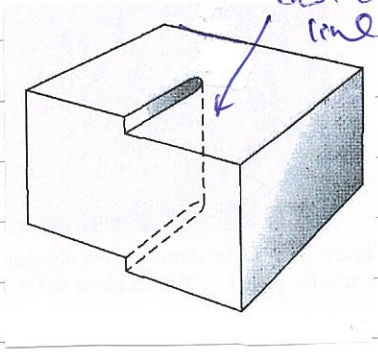


One can see that if there are edge dislocations, it's much easier to push/slide the crystal along x directions (see the left figure).

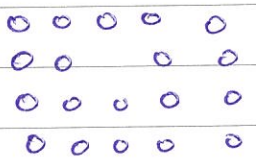
In addition to edge dislocations, there are also other possible defects.

Screw dislocations

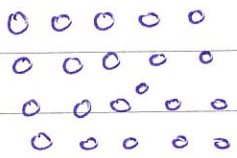


edge & screw dislocations are line defects.

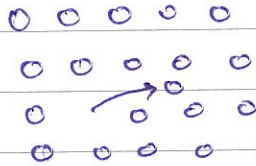
Point defects : Vacancies, interstitials



Vacancy (Schottky defect)



interstitials



Frenkel defect

n = # of point defects (Schottky) $\frac{n}{N-n} = e^{-\frac{E_U}{k_B T}}$ activation energy to remove one atom

if $n \ll N$ $\frac{n}{N} \sim e^{E_U/k_B T}$

$E_U \sim 1eV$, $T \sim 1000K$, $n/N \sim 10^{-5}$

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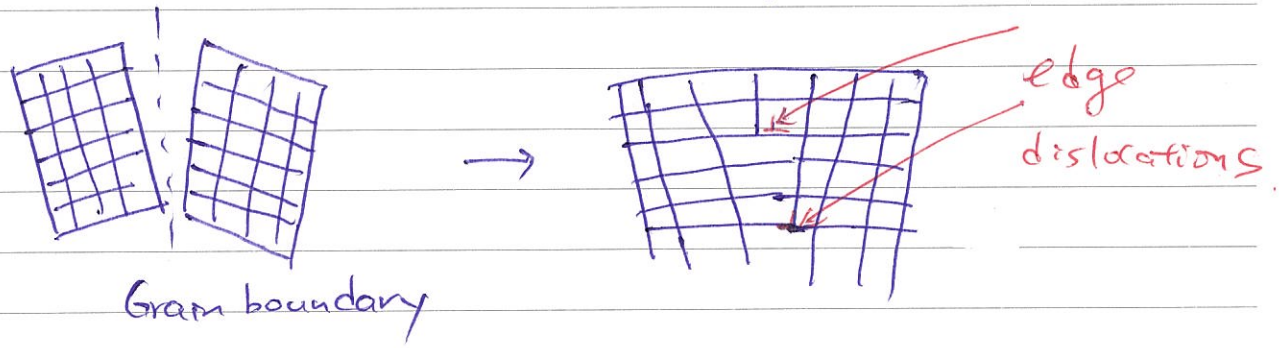
Surface defects

Grain boundary (low angle)

Can be viewed as a sequence of edge dislocations.



Stacking fault:

ABC ABC AB ABC ABC ABC - -

↑ stacking fault

twin boundary : (hcp, fcc)

(High Tc materials such as YBCO have alot)

ABCABCABC BAC BAC BA

← · → mirror image

in hcp, A.B, C differ by in-plane positions.

∴ one can slip A → B, B → A

By sliping a planes, one can create twin

boundary : ABC ABC ABC AB C BAC BAC

↓ ↓

B A

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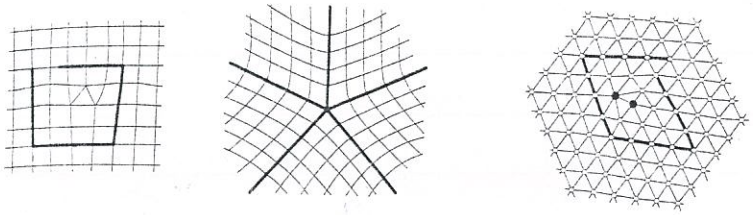
Defects-mediated melting

As we have seen, dislocations are the most important defects to explain the mechanical properties of real crystals.

In addiation to dislocations, there are also disclinations which are defects in orientation! (see left figures)



DISLOCATION DISCLINATION

It is known that two disclinations bounded are equivalent to a dislocation!

As we have learned, crystal order is not stable in 2D. Then, what is the state of a 2D solid?

Nelson & Halperin proposed that 2D solids are crystals with bound pairs of dislocations and disclinations. (Phys. Rev. 19, 2457, 1979) The theory represents the view of liquid-solid transition from the solid side.

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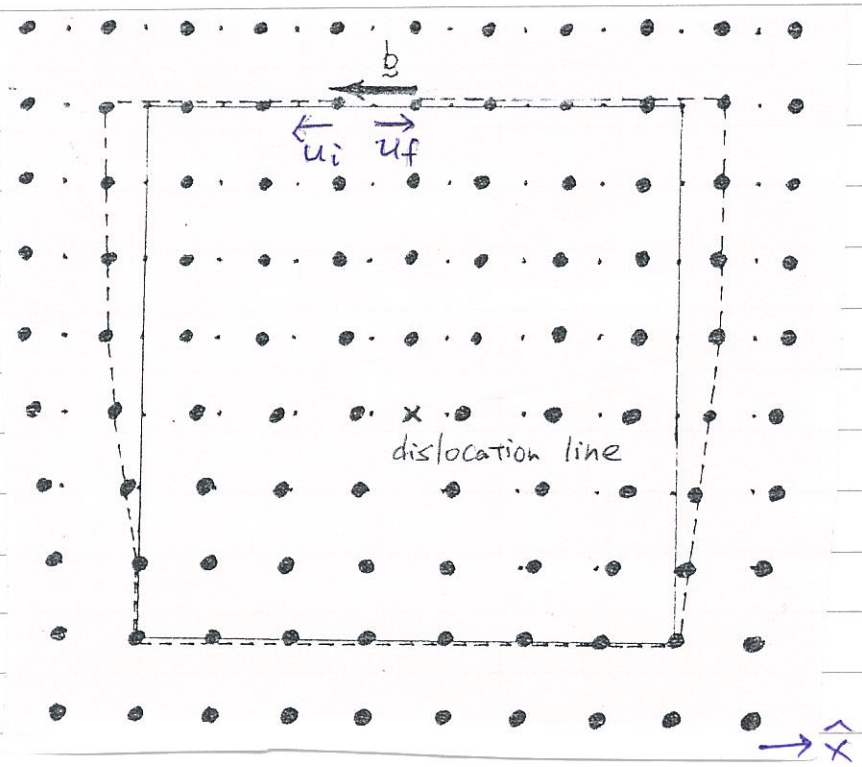
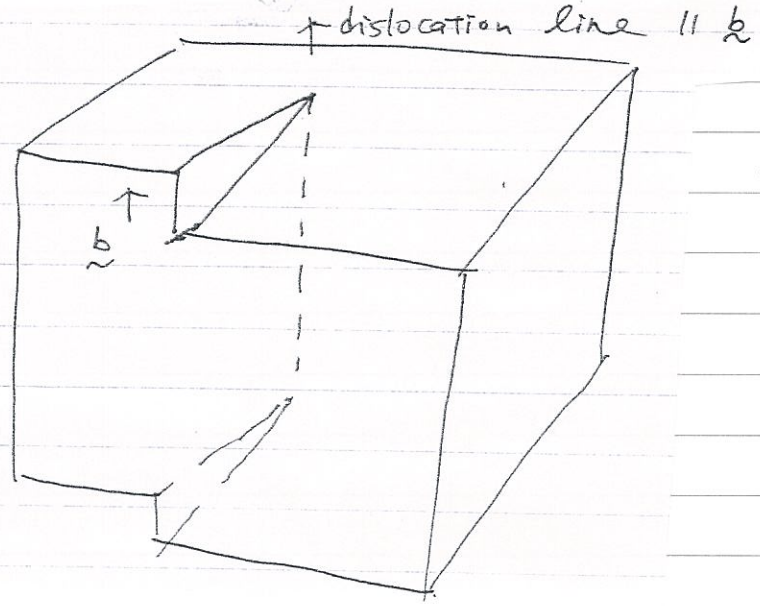
Burgers vector: To describe the melting from the 2D solid side, one needs to characterize the dislocations. Dislocations are characterized by the Burgers vector as shown below.



$\vec{b}$ = Burgers vector
= net displacement along a circle encircle the edge dislocation

$\vec{b} \perp$ dislocation line for edge dislocations

$$\oint d\vec{u} = \vec{u}_f - \vec{u}_i = +\vec{b} = -b\hat{x}$$



For screw dislocations as shown in the left figure,

$\vec{b} \parallel$ dislocation line

2D dislocations & their interactions

In 2D, one has edge dislocations.

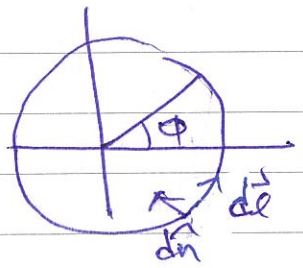
The displacement field $\vec{u}$ without any dislocation satisfies $\frac{\partial \sigma_{\alpha\beta}}{\partial x_\beta} = 0$, $\sigma_{\alpha\beta} = \lambda \delta_{\alpha\beta} \nabla\cdot\vec{u} + 2\mu \epsilon_{\alpha\beta}$

$$(\lambda+\mu)\vec{\nabla}(\vec{\nabla}\cdot\vec{u}) + \mu\nabla^2\vec{u} = 0 \quad \text{--- (9)}$$

in static situation.

This, however, is no longer true in presence of a dislocation. One expects source term with δ function would arise.

To get the equation for a single dislocation, we start by considering the integration of angle $\phi = \tan^{-1} y/x$



clearly $\oint \nabla\phi \cdot d\vec{\ell}$

$$= \oint d\phi = 2\pi$$

$\therefore$ if $\phi = \frac{\theta}{2\pi} \tan^{-1} y/x$

$$\oint \nabla\phi \cdot d\vec{\ell} = \theta \quad \text{--- (10)}$$

Now, $\tan^{-1} y/x$ is the imaginary part of $\ln z$ ....

with $z = x+iy$.

$$\ln z = \underbrace{\ln|z|}_{v} + i\phi$$

From complex analysis, we know $\frac{\partial v}{\partial x} = \frac{\partial \phi}{\partial y}$, $\frac{\partial v}{\partial y} = -\frac{\partial \phi}{\partial x}$

$$\therefore \nabla\phi \cdot d\vec{e} = \left(\frac{\partial \phi}{\partial x}, \frac{\partial \phi}{\partial y}\right)(dx, dy)$$

$$= \left(+\frac{\partial v}{\partial x}dy - \frac{\partial v}{\partial y}dx\right) = \left(\frac{\partial v}{\partial x}, \frac{\partial v}{\partial y}\right)\cdot(dy, -dx)$$

$$= \vec{\nabla} v \cdot d\vec{n}$$

Therefore, eq.(10) $\Rightarrow$ $\oint \vec{\nabla} v \cdot d\vec{n} = 8$

$$\int \nabla^2 v \, d^2\vec{r} = 8$$

We get the differential form of eq. (10)

$$\nabla^2 v = 8 f(\vec{r}) \qquad (11)$$

In terms of ϕ: $\frac{\partial^2 \phi}{\partial x \partial y} - \frac{\partial^2 \phi}{\partial y \partial x} = 8 f(\vec{r})$ ---

Now, for an edge dislocation with Burgers vector $\vec{b}$

$$\therefore \oint \nabla u^\alpha \cdot d\vec{e} = \oint du^\alpha = b^\alpha a_0 \qquad a_0 = \text{lattice constant}$$

we find $\frac{\partial^2 u^\alpha}{\partial x \partial y} - \frac{\partial^2 u^\alpha}{\partial y \partial x} = b^\alpha a_0 f(\vec{r})$

i.e.
$$\begin{cases} \frac{\partial^2 u^x}{\partial x \partial y} - \frac{\partial^2 u^x}{\partial y \partial x} = b^x a_0 f(\vec{r}) & \cdots (12) \\ \frac{\partial^2 u^y}{\partial x \partial y} - \frac{\partial^2 u^y}{\partial y \partial x} = b^y a_0 f(\vec{r}) & \cdots (13) \end{cases}$$

That is, differentiation with respect to x and y can not be exchanged.

In this case, $\frac{d\sigma_{\alpha\beta}}{dx_\beta}=0$ does not reduce to eq. (9).

Instead, $\because \frac{d\sigma_{\alpha\beta}}{dx_\beta}=\lambda\frac{d}{dx_\alpha}(\vec{\nabla}\cdot\vec{u})+2\mu\frac{d}{dx_\beta}e_{\alpha\beta}$

we find

$$\mu\frac{d}{dx_\beta}\left(\frac{du_\alpha}{dx_\beta}\right)+\mu\frac{d^2u_\beta}{dx_\beta dx_\alpha}+\lambda\frac{d}{dx_\alpha}(\vec{\nabla}\cdot\vec{u})=0$$

The term $\mu\frac{d^2u_\beta}{dx_\beta dx_\alpha}=\mu\frac{d^2u_x}{dxdx}+\mu\frac{d^2u_y}{dydx}$ for $\alpha=1$

↓ exchange $x\leftrightarrow y$

$$=\mu\frac{d^2u_x}{dxdx}+\mu\frac{d^2u_y}{dxdy}-b^y a_0\delta(\vec{r})$$

$$=\mu\frac{d}{dx}\nabla\cdot\vec{u}-b^y a_0\delta(\vec{r})$$

$\alpha=2$, $\mu\frac{d^2u_\beta}{dx_\beta dx_\alpha}=\mu\frac{d^2u_x}{dxdy}+\mu\frac{d^2u_y}{dy^2}$

$$=\mu\frac{d^2u_x}{dydx}+\mu\frac{d^2u_y}{dy^2}+b^x a_0\delta(\vec{r})$$

$$=\mu\frac{d}{dy}\vec{\nabla}\cdot\vec{u}+b^x a_0\delta(\vec{r})$$

$\therefore \mu\frac{d^2u_\beta}{dx_\beta dx_\alpha}=\nabla_x(\vec{\nabla}\cdot\vec{u})+b^\perp_\alpha a_0\delta(\vec{r})$, $\vec{b}^\perp=(-b^y,b^x)$

we get

$$\nabla^2\vec{u}+\frac{\lambda+\mu}{\mu}\nabla(\vec{\nabla}\cdot\vec{u})=-\vec{b}^\perp a_0\delta(\vec{r}) \quad \cdots (14)$$

It's important see that $\vec{u}(\vec{r})$ due to a dislocation is logarithmic.

For this purpose, we consider $\vec{u}^0$ such that

$\nabla \cdot \vec{u}^0 = 0$, then $\nabla^2 \vec{u}^0 = -\vec{b}^I a_0 f(\vec{r})$

$$\vec{u}^0 = \frac{-a_0 \vec{b}_\perp}{2\pi} \ln r/a_0 \qquad (\nabla^2 \ln r = 2\pi f(\vec{r}))$$

The energy for a single dislocation is then

$$E_e = \frac{1}{2}\int d^2r \left[2\mu \underbrace{e_{\alpha\beta}^2}_{\frac{\mu}{2}\left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha}\right)^2} + (\mu+\lambda)(\nabla \cancel{\vec{u}})^2\right]^0$$

$\frac{\partial u_\alpha}{\partial x_\beta}\frac{\partial u_\beta}{\partial x_\alpha}$ ↓ $\frac{\partial u_\alpha}{\partial x_\alpha}\frac{\partial u_\beta}{\partial x_\beta} \to 0$

$$= \frac{1}{2}\mu \int d^2\vec{r} \left(\frac{\partial u_\alpha}{\partial x_\beta}\right)^2$$

$$= \frac{1}{2}\mu \left(\frac{a_0}{2\pi}\right)^2 \cdot \sum_\alpha (b_\perp^\alpha)^2 \int d^2r \left(\nabla \ln \frac{r}{a_0}\right)^2$$

$$= \frac{1}{2}\mu \left(\frac{a_0}{2\pi}\right)^2 b_\perp^2 \int_{a_0}^{R} 2\pi r\, dr \left(\frac{1}{r}\right)^2$$

$$= \frac{1}{2}\mu \left(\frac{a_0 b_\perp}{2\pi}\right)^2 \times 2\pi \ln R/a_0 \quad \propto b^2 !$$

For two dislocations, $\nabla^2 \vec{u}^0 = -\vec{b}_1^I a_0 \times f(\vec{r}-\vec{r}_1) - \vec{b}_1^I a_0 f(\vec{r}-\vec{r}_2)$

$$\vec{u}^0 = \frac{a_0 \vec{b}_1^I}{2\pi} \ln\left|\frac{\vec{r}-\vec{r}_1}{a_0}\right| + \frac{a_0 \vec{b}_2^I}{2\pi} \ln\left|\frac{\vec{r}-\vec{r}_2}{a_0}\right|$$

$$E = \frac{1}{2}\mu \int d^2\vec{r} \left(\frac{\partial u_\alpha}{\partial x_\beta}\right)^2 = \frac{1}{2}\mu \int d^2\vec{r}\, \vec{u} \cdot \nabla^2 \vec{u}$$

$$\sim \vec{b}_1 \cdot \vec{b}_2^I \ln\left|\frac{\vec{r}_1-\vec{r}_2}{a_0}\right| \cdots$$

Hence, dislocations in 2D interact through $\ln\left|\frac{\vec{r}_1-\vec{r}_2}{a}\right|$ potential!

In general, if one does not restrict to $\nabla\cdot\vec{u}=0$, one finds

$$\frac{F}{K_BT} = -\frac{1}{2\pi}\sum_{r\neq r'} K_1\,\vec{b}(r)\cdot\vec{b}(r')\ln\left|\frac{\vec{r}-\vec{r}'}{a_0}\right| - K_2\frac{[\vec{b}(r)\cdot(\vec{r}-\vec{r}')][\vec{b}(r')\cdot(\vec{r}-\vec{r}')]}{|\vec{r}-\vec{r}'|^2} + \frac{E_c}{K_BT}\cdot\sum_r |b(r)|^2 \quad \cdots (15)$$

(Nelson & Halperin)

E_c = creation energy for a unit dislocation

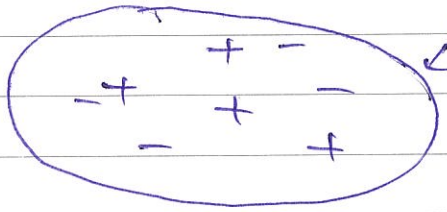
Since large b is large, we can restrict ourself to small b, i.e., dislocations with unit Burgers vector $\pm\vec{a}_0$

Furthermore, we require $\sum_r \vec{b}(r)=0$ because there is no overall slip of the crystal.

The dominant interaction for 2D dislocations is log-range log interaction. This is also known as 2D Coulomb gas with

$$H' = \frac{-1}{2} \sum_{i \neq j} q_i q_j \ln \frac{|\vec{r}_i - \vec{r}_j|}{a} \qquad q_i = \pm q$$

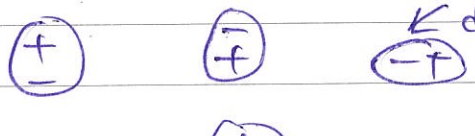
$$\sum_i q_i = 0 \quad \text{(neutral)}$$

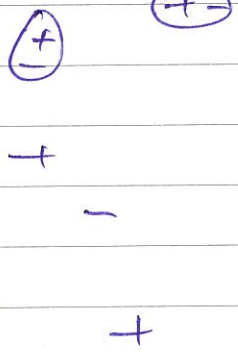


Kosterlitz & Thouless

(J. Phys. C 5, L124, 1972, C6, 1181, 1973)

solved this system by using so-called renormalization group method and found that it is binding-unbinding transition:

$T < T_c$  (+ −) form dipoles

$T > T_c$  This is known as KT transition

To estimate T_c, we define

$$\Phi = -q \ln \left| \frac{\vec{r}}{a} \right| \quad \therefore \nabla^2 \Phi = -2\pi q \delta(\vec{r})$$

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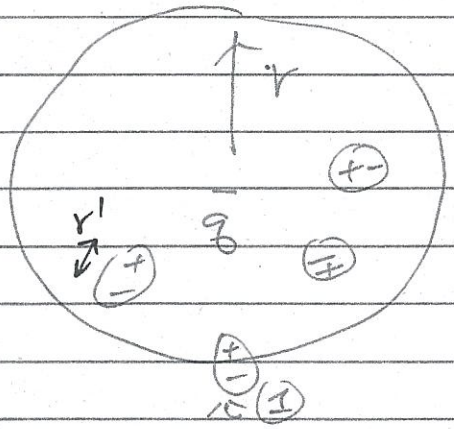
if $r \to \infty$, after screening, we expect

$$\phi = -\frac{q}{\varepsilon} \ln r/a \qquad \varepsilon(r \to \infty) \neq 0$$

$\Rightarrow$ (+−) bond together ∵ still strongly interacting attraction!

if $\frac{1}{\varepsilon} \to 0$. free vortices!

Let us look at one vortex:



if (+−) < r

total charge inside r $(-\frac{q}{\varepsilon})$ is almost the same as q

Only dipoles such as (I) contribute to charge total charge. but this finite!

∴ To create screening, (+−) has to > r!

(size of)

Suppose, we have picked up the 1st charge, the probability distribution (per area) for picking up

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the other partner $P(r') \propto e^{-\frac{q^2}{K_B T} \ln \frac{r'}{a'}} = (r'/a')^{-q^2/K_B T}$

2nd

∴ total probability per unit area for charge's location

$$= \int_r^\infty dr' \, 2\pi r' \, P(r')$$

∴ # of dipoles with one charge $< r$ the other charge $> r$

$$\propto (\pi r^2) \int_r^\infty 2\pi r' dr' \left(\frac{r'}{a'}\right)^{-q^2/K_B T}$$

(πr^2): probability for picking up the 1st charge

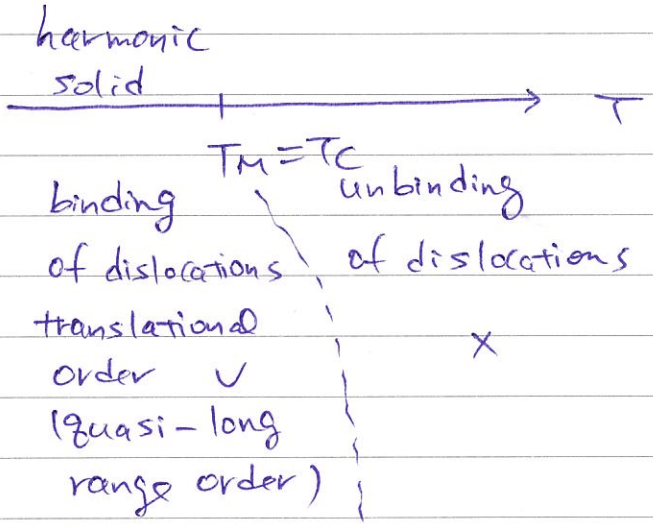
$$\propto r^{4 - \frac{q^2}{K_B T}}$$

∴ $T < T_c \cong \frac{q^2}{4K_B} \sim \frac{b^2}{4K_B}$ → 0 as $r \to \infty$

∴ dipoles combined!

Otherwise, $T > T_c$, dipoles dissociate!

Because disolocations are associated with additional half row of atoms, they are quite effective at breaking up translational order. Hence binding – unbinding of dislocations describes transition of translational order!



$T < T_c$, dislocations bind

Above $T_M = T_c$, dislocations unbinds

$\langle (\vec{u}_i - \vec{u}_j)^2 \rangle$ $\ln |\vec{r}_i - \vec{r}_j|$ is no longer true!

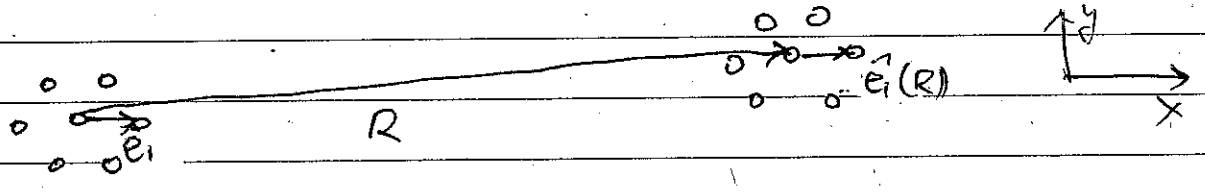
Screening leads to $\langle \rho_G(r) \rho_G(0) \rangle \sim e^{-r/\xi_s}$

$\therefore$ translational order is broken.

However, as pointed by Nelson & Halperin, this is not the end of the story.

The location of G reflects the translational invariance of crystals. Therefore, when it disappears, it means only the translational order is broken!

Nelson & Halperin points that if one calculates the orientational order, it still persists:



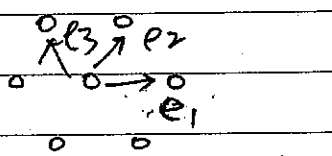
it could happen

$\vec{R} \neq m\vec{a} + n\vec{b}$ (lattice)

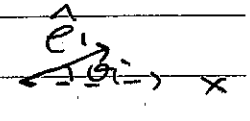
... but $\hat{e}_1(R) \parallel \hat{e}_1$

To see if $\hat{e}_1(R) \parallel \hat{e}_1$, one realizes

$$\hat{e}_1 = \underbrace{(R_i^0 + u_{i+\hat{e}_1})}_{\vec{R}_{i+\hat{e}_1}} - \underbrace{(R_i^0 + u_i)}_{\vec{R}_i}$$



$$= \hat{e}_1^0 + (u_{i+\hat{e}_1} - u_i)$$



if $\hat{e}_1^0 \parallel \vec{x}$, then $\sin\theta_{i,1} = u^y_{i+\hat{e}_1} - u^y_i$

For small u_i, $\theta_{i,1} = u^y_{i+\hat{e}_1} - u^y_i = \hat{e}_{1\perp} \cdot (u_{i+\hat{e}_1} - u_i)$

Similarly, $\theta_{i,n} = \hat{e}_{n\perp} \cdot (u_{i+\hat{e}_n} - u_i)$ ...

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The average deviation of hexagon can be represented by $\theta_i = \frac{1}{6}\sum_{n=1}^{6}\theta_{in}$

$$= \frac{1}{6}\sum_{n=1}^{6}\hat{e}_n^{\perp}\cdot(\vec{u}_{i+\hat{e}_n}-\vec{u}_i)$$

$$= \frac{1}{6}\sum_{n=1}^{6}\hat{e}_n^{\perp}[(\hat{e}_n\cdot\vec{\nabla})\vec{u}_i]$$

$$\frac{1}{6}\sum_{n=1}^{6}(\hat{e}_n^{\perp})_\alpha(\hat{e}_n)_\beta = \frac{1}{2}\epsilon_{\alpha\beta} = \frac{1}{2}\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$$

$\hat{e}_n^{\perp} = \hat{z}\times\hat{e}_n$

$$\hat{z}\times\frac{1}{6}\sum_{n=1}^{6}(\hat{e}_n)_\alpha(\hat{e}_n)_\beta = \frac{\hat{z}}{6}\times 3\overleftrightarrow{I} = \frac{1}{2}\hat{z}\times\overleftrightarrow{I} \Rightarrow \frac{1}{2}\epsilon_{\alpha\beta}$$

$\hat{z}\times(\hat{x}\hat{x}) = \hat{y}\hat{x}$, $\hat{z}\times(\hat{y}\hat{y}) = -\hat{x}\hat{y}$

$$\therefore\ \theta(R) = \frac{1}{2}\sum_{\alpha\beta}\varepsilon^{\alpha\beta}\partial_\beta u^\alpha = \frac{1}{2}\left(\frac{\partial u^y}{\partial x}-\frac{\partial u^x}{\partial y}\right)$$

$$= \frac{1}{2}(\nabla\times\vec{u})\cdot\hat{z}$$

$\because\ \theta(R) \to \theta(R)+\frac{2\pi}{6} \Rightarrow$ same orientation,

$\therefore$ the order parameter can be defined

$$\psi_6(R) = e^{6i\theta(R)}$$

(bond orientational order)

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Its correlation can be defined as

$$g_6(R) = \langle \psi_6(R)\, \psi_6^*(0) \rangle$$

$$= \langle e^{i6(\theta(R)-\theta(0))} \rangle$$

Obviously, because $\theta \sim \nabla \times u$, $\therefore$ θ has a dimension higher than u. As a result, when $T > T_M$, $g_6(R) \to$ const as $R \to \infty$:

$$g_6(R) = e^{-36\frac{1}{2}\langle(\theta(R)-\theta(0))^2\rangle}$$

$$\frac{1}{2}\langle(\theta(R)-\theta(0))^2\rangle$$

$$= \frac{1}{8}\langle(\nabla\times u(R) - \nabla\times u(0))^2\rangle$$

$$= \frac{1}{8}\varepsilon^{\mu\alpha}\varepsilon^{\nu\beta}\partial_\mu\partial_\nu\langle(u^\alpha(R)-u^\alpha(0))(u^\beta(R)-u^\beta(0))\rangle$$

$$= \frac{1}{8}\varepsilon^{\mu\alpha}\varepsilon^{\nu\beta}\partial_\mu\partial_\nu\int_K(1-e^{iK\cdot R})\langle u^\alpha(K)\,u^\beta(-K)\rangle$$

↗ eq. ④

$$= \frac{1}{8}\varepsilon^{\mu\alpha}\varepsilon^{\nu\beta}\int_K K^\mu K^\nu(1-e^{iK\cdot R})\langle u^\alpha(K)\,u^\beta(-K)\rangle$$

$$= \frac{1}{8}\varepsilon^{\mu\alpha}\varepsilon^{\nu\beta}\int_K \frac{k_BT(1-e^{iK\cdot R})}{K^2}\left[\frac{P_T^{\alpha\beta}}{C_{66}} + \frac{P_L^{\alpha\beta}}{C_{11}}\right]K^\mu K^\nu$$

$\because \varepsilon^{\mu\alpha}K^\mu K^\alpha = (\vec{K}\times\vec{K})\cdot\hat{z} = 0$ $\therefore \varepsilon^{\mu\alpha}\varepsilon^{\nu\beta}\delta^{\alpha\beta}K^\mu K^\nu = |K|^2$ ∎

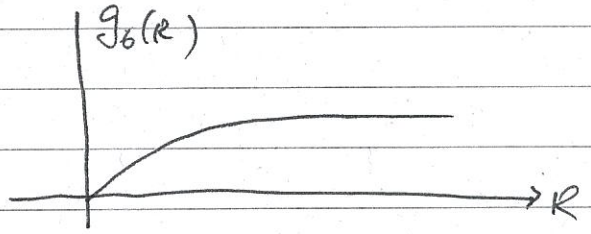
$$\therefore \frac{1}{2}\langle(\theta(R)-\theta(0))^2\rangle$$

$$= \frac{1}{8}\int_K \frac{k_BT}{C^2}\left(1-e^{iK\cdot R}\right)$$

$$= \frac{k_BT}{8C^2}\left(1-\delta_{R,0}\right)\times(2\pi)^3$$

$\therefore R\to\infty \quad \frac{1}{2}\langle(\theta(R)-\theta(0))^2\rangle = \text{const}$

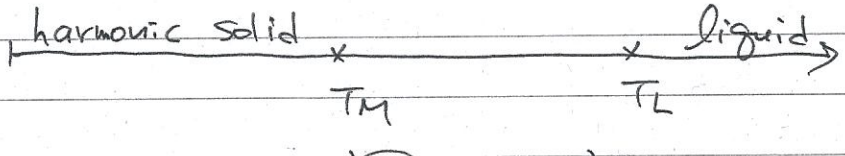
$g_6(R)\to \text{const}$



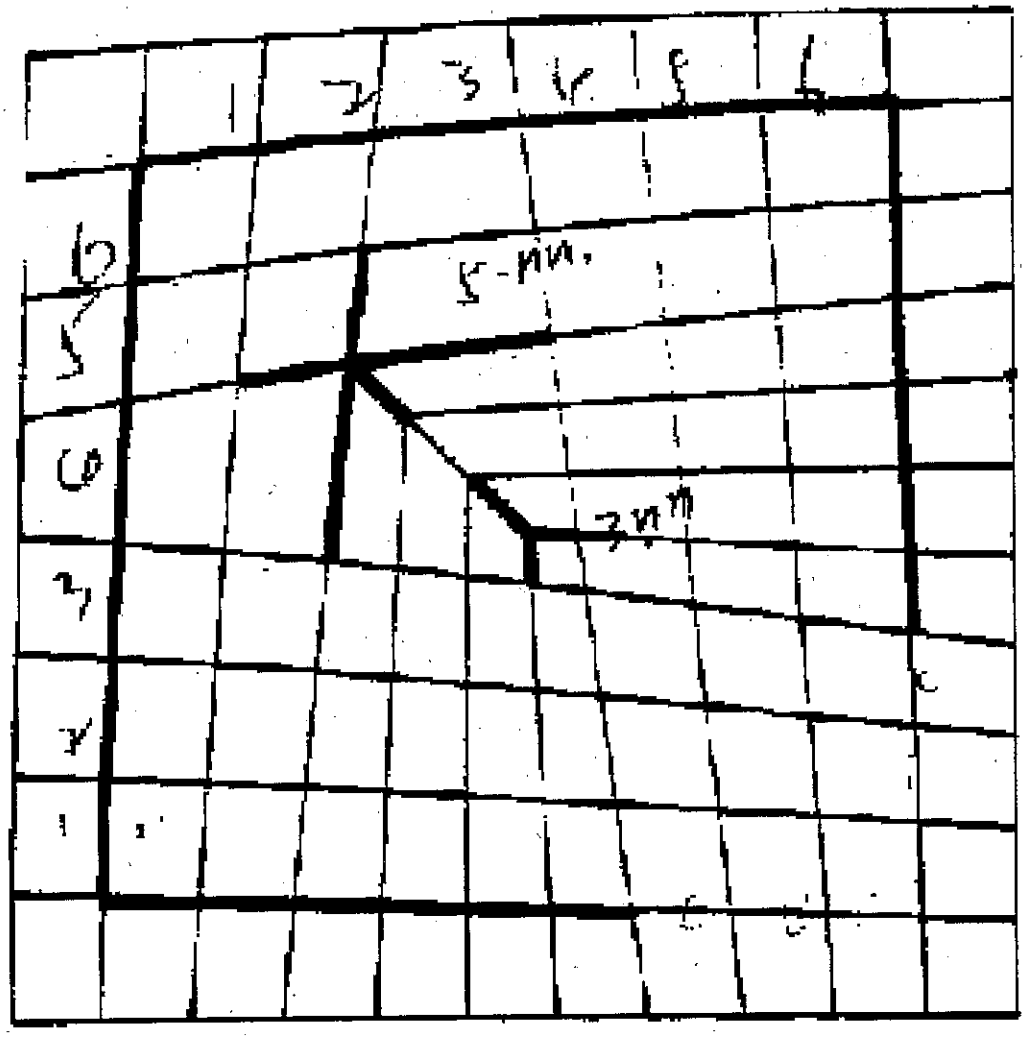
$\therefore$ It still possess long-range orientational order if F is given by the harmonic approximation (eq. ②) !

Nelson & Halperin pointed out that this is because even though dislocations are free for $T>T_M$, each dislocation actually contains a pair of bound disclinations. (see Fig in the next page 7-30)

What will happen is :



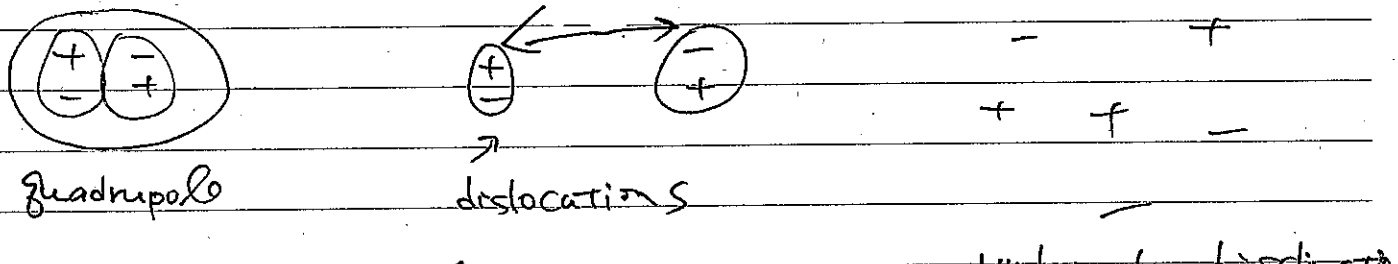
exist an intermediate phase called hexatic phase



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

$T > T_L$, orientational order breaks down. When bound disclinations are free (see Fig 3.), if we use $\pm$ to present two disclinations, one gets the following picture:

Solid | Hexatic | Liquid



quadrupole | dislocations | unbound disclination

$\langle \rho_G(r)\rho_G(0)\rangle \sim \frac{1}{r^{\eta_G}}$ | $\langle \rho_G(r)\rho_G(0)\rangle \sim e^{-r/\xi_+(T)}$

$\langle \psi_6(R)\psi_6^*(0)\rangle \sim \frac{1}{r^{\eta_6}}$ | $\langle \psi_6(R)\psi_6^*(0)\rangle \sim e^{-r/\xi'}$ $(\xi' = \xi_+^2)$

$$F_D/k_BT = \frac{-K}{8\pi}\sum_{r\neq r'}\left[\vec{b}(\vec{r})\cdot\vec{b}(\vec{r}')\ln\frac{|\vec{r}-\vec{r}'|}{a} - \frac{\vec{b}(\vec{r})\cdot(\vec{r}-\vec{r}')\,\vec{b}(\vec{r}')\cdot(\vec{r}-\vec{r}')}{|\vec{r}-\vec{r}'|^2}\right] + \frac{E_c}{k_BT}\sum_r |\vec{b}(\vec{r})|^2$$

based on the existance of long-range order of θ

$$\Rightarrow F \propto \int \frac{1}{2} K_A \, d\vec{r}\,(\nabla\theta)^2$$

singularity of θ $\Rightarrow$ disclination

$\therefore$ logarithmic interaction too!

$$F_{dis} = \frac{1}{2}K_A\int d^2r\,(\nabla\theta)^2 = -\frac{\pi K_A}{36}\sum_{r\neq r'} s(r)\,s(r')\ln\frac{|\vec{r}-\vec{r}'|}{a} + E_c\sum_r s(r)$$