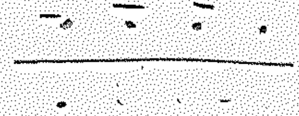
Commensurate - Incommensurate and Roughening transitions

How to make 2d solid?

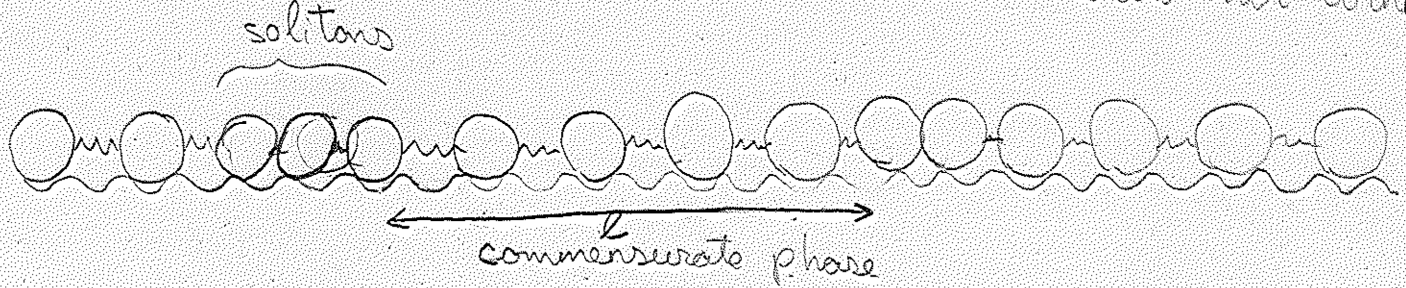
Put particles on the surface of ...

1) liquid $\Rightarrow$ electrons on He surface



2) Crystal - films on the crystal substrate - Nobel gases on graphite

Then one has a problem of interaction with the periodic potential of the substrate. In general periods of the 2d solid and substate should not coincide



C-I - transition, solitons

The simplest 1-d model is the Frenkel Kontorova model (1938)

$$H = \sum_n \frac{C(x_n - x_{n-1} - a)^2}{2} - V\cos\frac{2\pi x_n}{b}$$

b - period of the substrate, a - of the 2d lattice

In continuum approximation $x_n = bn + \frac{b\,u(x)}{2\pi}$, where u is a slow variable $x_n - x_{n-1} \Rightarrow b + \frac{b^2}{2\pi}\frac{du}{dx}$

Continuous hamiltonian is then:

$$H = \frac{1}{2} V \int dx \left[\frac{1}{2}\left(\xi \frac{\partial u}{\partial x} + \delta\right)^2 + (1-\cos u) \right], \quad \xi = \sqrt{\frac{c}{V}} \frac{b^2}{2\pi}$$

$$\delta = \sqrt{\frac{c}{V}} (b-a)$$

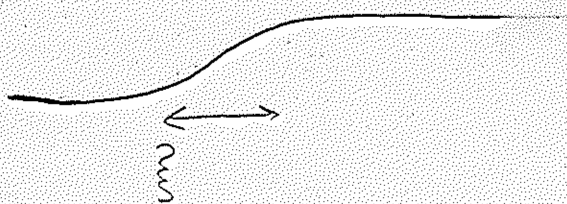
Equilibrium equation

$$\xi^2 u'' = \sin u \quad \Leftrightarrow \text{Sine Gordon equation}$$

$$\Downarrow$$

$$\frac{\xi^2 u'^2}{2} = 1 - \cos u \quad \Rightarrow \quad \frac{du}{\sqrt{2(1-\cos u)}} = \frac{dx}{\xi}$$

$$\boxed{u = \pm 4 \,\mathrm{arctg}\, \exp\left(\frac{x}{\xi}\right)}$$



Parameter δ changes the soliton energy

For $\delta = 0$ soliton energy is positive and the ground state — commensurate phase with $u=0$

for $\delta \to -\infty$ soliton energy ($u' > 0$) is negative

Problem: find δ_c where the soliton energy changes sign

Close to δ_c $E_s \propto (\delta - \delta_c)$

Two solitons of the same sign repel and of the opposite sign attract each other.

At large distances $u \sim \exp\left(-\frac{x}{\xi}\right)$

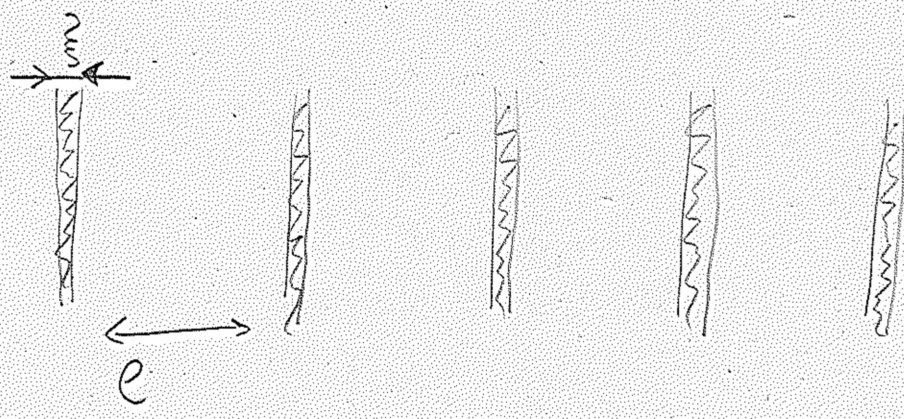
So the interaction of the solitons is exponentially weak $\Rightarrow$ the distance between the solitons ℓ can be found from

$$\exp\left(-\frac{\ell}{\xi}\right) \sim \frac{\delta_c - \delta}{\delta_c} \Rightarrow$$

$$\ell \sim \xi \ln\left(\frac{\delta_c}{\delta_c - \delta}\right)$$

Changing pressure one changes $\delta \Rightarrow$ C–I transition.

In the incommensurate (I) (floating) phase — soliton lattice with density $\propto \frac{1}{\ln\left(\frac{\delta_c}{\delta_c - \delta}\right)}$



Thermal effect on the C-I transitions

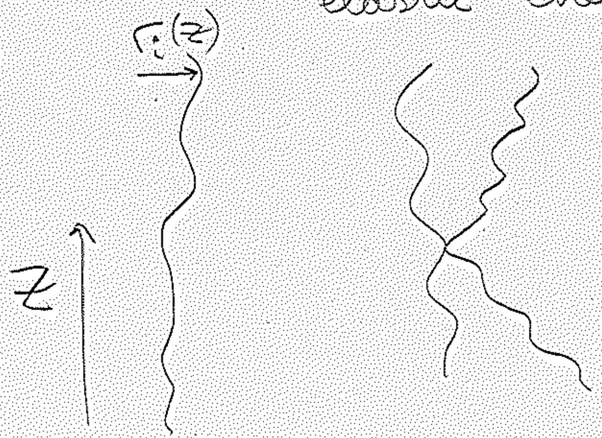
Pokrovskii & Talapov (79)

Solitons — line objects
for the weak interaction with the substrate $\xi \sim b^2 \sqrt{\frac{C}{V}} \gg b$. Then interaction of the solitons with the substrate is $\sim \exp\left(-\frac{c_1 \xi}{b}\right) \to 0$
So we neglect it and consider just interacting lines with line tension in 2d

$$H = \sum_{ij} \int \left(\frac{\varepsilon_e}{2} \left(\frac{\partial r_i(z)}{\partial z} \right)^2 + U(r_i(z) - r_j(z)) \right) dz$$

elastic energy

interaction which we assume to be repulsive



We should calculate partition function

$$Z = \int \mathcal{D} r_i \, e^{-\frac{H}{T}}$$

In quantum mechanics we usually calculate

$$W = \int \mathcal{D} r_i \, e^{i\frac{S}{\hbar}}$$ with

$$S = \sum_{ij} \int dt \left[m\left(\frac{dr_i}{dt}\right)^2 - V(r_i - r_j) \right]$$

Thus statistical mechanics of lines is equivalent to quantum mechanics in imaginary time (Feynman)

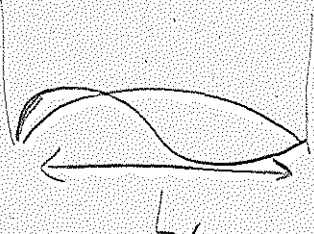
$$z \to it$$

$$T \to \hbar$$

$$\varepsilon_e \to m$$

For the hard core potential $V(r) = V_0 \delta(r)$ particles can be considered as spinless fermions

In the box with N particles



states with

$K_m = \frac{\pi m}{L}$ and $\Rightarrow$ Fermi momentum

$$K_F = \frac{\pi N}{L} = \pi n \text{ — density of solitons}$$

Kinetic energy is $\sum^{K_F} \frac{K_i^2}{2m} = \frac{K_F^3}{6\pi m} = \frac{\pi^2 n^3}{6m}$

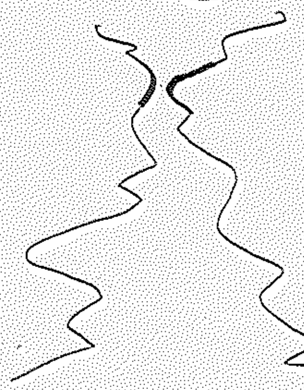
Thus the total energy close to C-I transition

$$F(n) \sim C_1(\delta - \delta_c) n + C_2 e^{-\frac{B}{n}} + C_3 n^3 \Rightarrow$$

$$n \propto \sqrt{\delta_c - \delta} \text{ rather than } \ln \frac{\delta_c}{\delta_c - \delta}$$

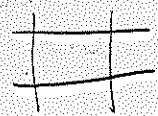
This term in energy $\propto n^3$ is called steric or entropic repulsion.
It corresponds to $\frac{1}{\ell^2}$ repulsion between solitons.
One can get it without mapping to quantum mechanics.
Since solitons cannot cross each other their collisions reduce entropy.

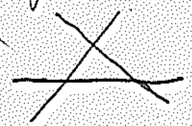
- Between the collisions – diffusive motion $r^2 \propto z$ thus average length between the collisions $\propto \ell^2 \Rightarrow$



$$\mho \sim \frac{1}{\ell^2}$$

- Up to now we consider all solitons to be parallel. In general there may be several easy directions for solitons (2 for square lattice and 3 for hexagonal one).

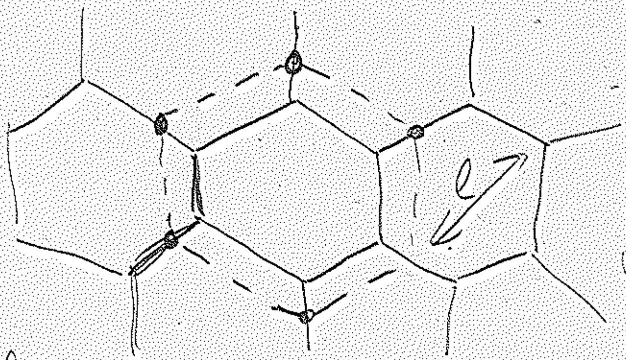




Crossing energy depends on interatomic <u>interaction</u> and may be of any sign. For positive crossing energy $\Rightarrow$ solitons are parallel

as described above.

For negative crossing energy number of intersections should be as large as possible $\Rightarrow$ Hexagonal lattice $\Rightarrow$ honeycomb network



The length of the walls does not change under the deformation of the hexagon $\Rightarrow$ the network at $T=0$ can be stabilised only by the exponential repulsion, which may be neglected if l is large. In this case walls form an irregular network.

Since any of the $\nu \propto \frac{1}{l^2}$ hexagons can be deformed without energy change there are ν "soft" degrees of freedom. Maximal deformation $\sim l \Rightarrow$

Entropy $\quad S \simeq k_B \nu \ln l \simeq \frac{k_B}{l^2} \ln l$

Free energy

$$F(n) \simeq c_1(\delta-\delta_c)n - c_2 n^2 \ln\frac{1}{n} + c_3 n^3 + c_4 e^{-\frac{\beta}{n}}$$

$\Downarrow$

First order transition

(Villain 1980)

How does the substrate potential influences 2 d melting?

Commensurate phase is pinned $\Rightarrow$ real 2d solid with true long range order.

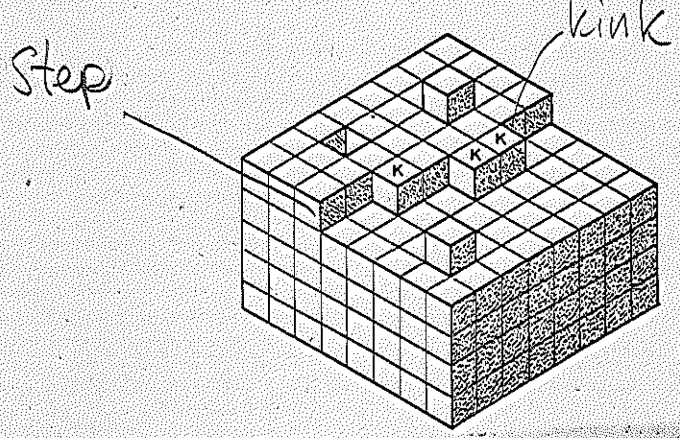
For the substrate period $b = \frac{a}{p}$ with large $p > 4$ at first one has depinning $\Leftrightarrow$ roughening transition (see later) at $T_R < T_m$ and then melting of quasi solid. However, there is angular term in $H \sim \theta^2$ even in the liquid $\Rightarrow$ true long range orientational order $\Rightarrow$ No disclination unbinding.

For $p = 1$; $T_R > T_m$ one has roughening transition to a liquid phase, no "floating" solid

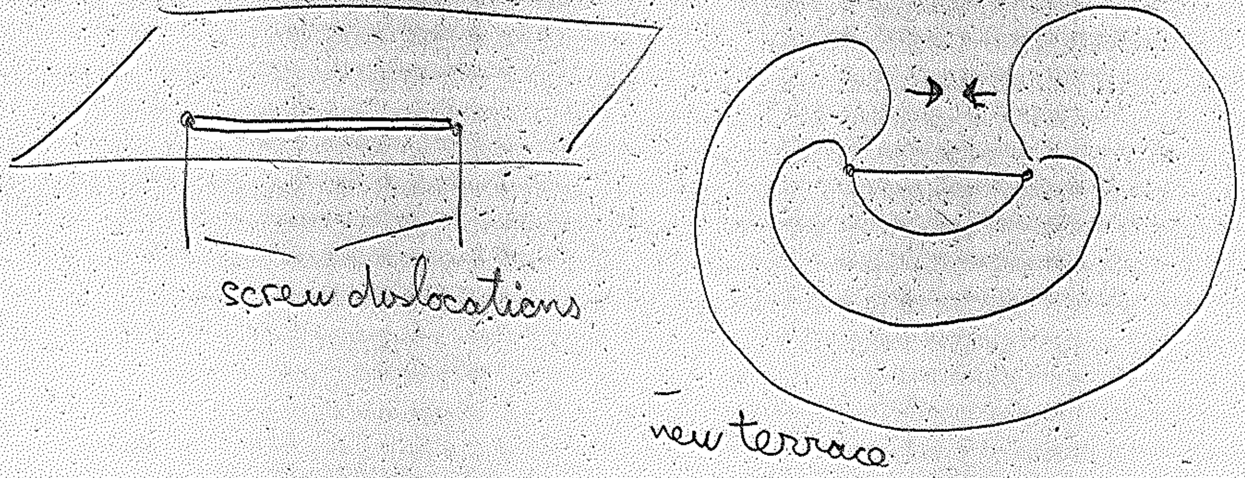
(Below roughening transition interaction between dislocations is not $\log(R)$ but $\sim R$ so they do not unbind.)

Roughening transition

Surface growth



Creation of steps – Frank-Read source



Interaction between steps – steric repulsion $\sim \frac{1}{\ell^2}$

but usual elastic interaction also goes $\sim \frac{1}{\ell^2}$

Fluctuations of the interface

In continuum approximation $E = \int \frac{\sigma}{2}(\nabla h)^2 d^d s$

$$\langle (h(R) - h(0))^2 \rangle \sim T \int \frac{(1-\cos kR)}{\sigma k^2} d^d k$$

for $d > 2$ interface has finite thickness

$\lim_{R\to\infty} (h(R) - h(0))^2 = \text{const} < \infty$ - surface is flat

for $d < 2$ $\langle (h(R) - h(0))^2 \rangle \sim R^{2-d}$ - surface is rough

for $d = 2$ (surface of real crystal) $\langle h^2 \rangle = \frac{T}{2\pi\sigma} \ln\left(\frac{R}{\Delta}\right)$

But steps are discrete. Possible model is

$$H = \int \left(\frac{\sigma(\nabla h)^2}{2} + V\left(1 - \cos\left(\frac{2\pi h}{a}\right)\right)\right) d^2 r$$

For $T \to 0$ cos term is important, expanding

$$H = \int \frac{\sigma(\nabla h)^2}{2} + \frac{\alpha h^2}{2} d^2 r \Rightarrow$$

$$h^2 \sim T \int \frac{d^2 k}{\alpha + \sigma k^2} \sim \frac{T}{\sigma} \ln\left(\frac{\alpha}{\alpha_0}\right) = \text{const} \Rightarrow$$

surface is flat

But thermal fluctuations also renormalize the value of the potential

Self consistent approximation

Let us average potential

using $\left\langle \cos \frac{2\pi h}{a} \right\rangle = \exp\left(-\frac{2\pi^2 \langle h^2 \rangle}{a^2}\right)$

we obtain that the total interaction energy

$\langle E_p \rangle \sim V R^2 \exp\left(-\frac{2\pi^2 \langle h^2 \rangle}{a^2}\right)$, R^2 - area

using $h^2 = \frac{T}{2\pi\sigma} \ln \frac{R}{\Lambda}$ we obtain

$\langle E_p \rangle \sim V R^2 \frac{1}{(R/\Lambda)^{\pi T/\sigma a^2}}$

if $T > T_R = \frac{2\sigma a^2}{\pi}$ then $\langle E_p \rangle \xrightarrow[R\to\infty]{} 0$ and the surface is free (rough)

for $T < T_R$ $\langle E_p \rangle \xrightarrow[R\to\infty]{} \infty \Rightarrow$ interface is locked on a macroscopical scale (flat)

$\Downarrow$

Roughening transition at $\underline{T = T_R = \frac{2\sigma a^2}{\pi}}$

belongs to BKT universality class $\Rightarrow$ universal relation between the surface tension and T_R

Solid on solid models (SOS)

$H = \sum V(h_i - h_j)$ where h_i – discrete variable

simplest example – discrete Gaussian model

$$H = \frac{J}{2} \sum_{j,\delta} (h_j - h_{j+\delta})^2 = \frac{J}{2} \sum_{i,j} h_i G^{-1}(i,j) h_j =$$

nearest neighbours

$$= \frac{J}{2} \sum |h_q|^2 G^{-1}(q) \quad \text{where } h_q = \frac{1}{\sqrt{N}} \sum_j h_j e^{iqj}$$

$$G^{-1}(q) = 4 - 2(\cos q_x + \cos q_y)$$

for discrete h_j it can be mapped to Coulomb gas problem

(Chui & Weeks 76)

Partition function for discrete model

$$Z = \int \mathcal{D} h_j \prod_j W(h_j) \exp\left(-\frac{H}{T}\right) \quad \text{with}$$

$$W = \sum_{n_j=-\infty}^{\infty} \delta(h_j - n_j) = \sum_{k_j=-\infty}^{\infty} \exp(i k_j h_j 2\pi)$$

$$Z = \int \mathcal{D} h_j \mathcal{D} k_j \exp\left(i 2\pi k_j h_j - \frac{J}{2T} \sum_{ij} h_i G^{-1}(i,j) h_j\right)$$

we can perform Gaussian integral over h_i field then for the dual field k_i we get

$$Z = \int \mathcal{D} k_i \exp\left[-\frac{2\pi^2 T}{J} k_i G_{ij} k_j\right]$$

with $G(ij) = \int \frac{d^2q}{(2\pi)^2} \frac{e^{iq(i-j)}}{G^{-1}(q)} =$

$$= \frac{1}{4} \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dq_x \int_{-\pi}^{\pi} dq_y \frac{e^{iq(i-j)}}{1 - \frac{1}{2}(\cos q_x + \cos q_y)}$$

for $(i-j) \to \infty$ effective q are small and we can expand $\cos q_x \Rightarrow$

$$\int d^2q \frac{e^{iq(i-j)}}{q^2} \sim \ln(i-j) \Rightarrow$$

$$G(ij) = \frac{1}{2\pi} \ln|i-j| \Rightarrow$$

we reduce discrete Gaussian model to Coulomb gas model $\Rightarrow$ BKT transition

Note, that in this dual model temperature is inverse temperature of the original model

Plasma of "dual charges" $\Leftrightarrow$ flat surface