Correlations and order in two dimensions

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Outline

- Order - disorder transitions in materials
- Symmetry breaking and phase transitions
- Ordering in two dimensions.
- Real life examples, experimental results

Order - disorder transitions

- Solid-liquid
- Ferromagnetic - paramagnetic
- Liquid crystal phases: nematic - smectic etc

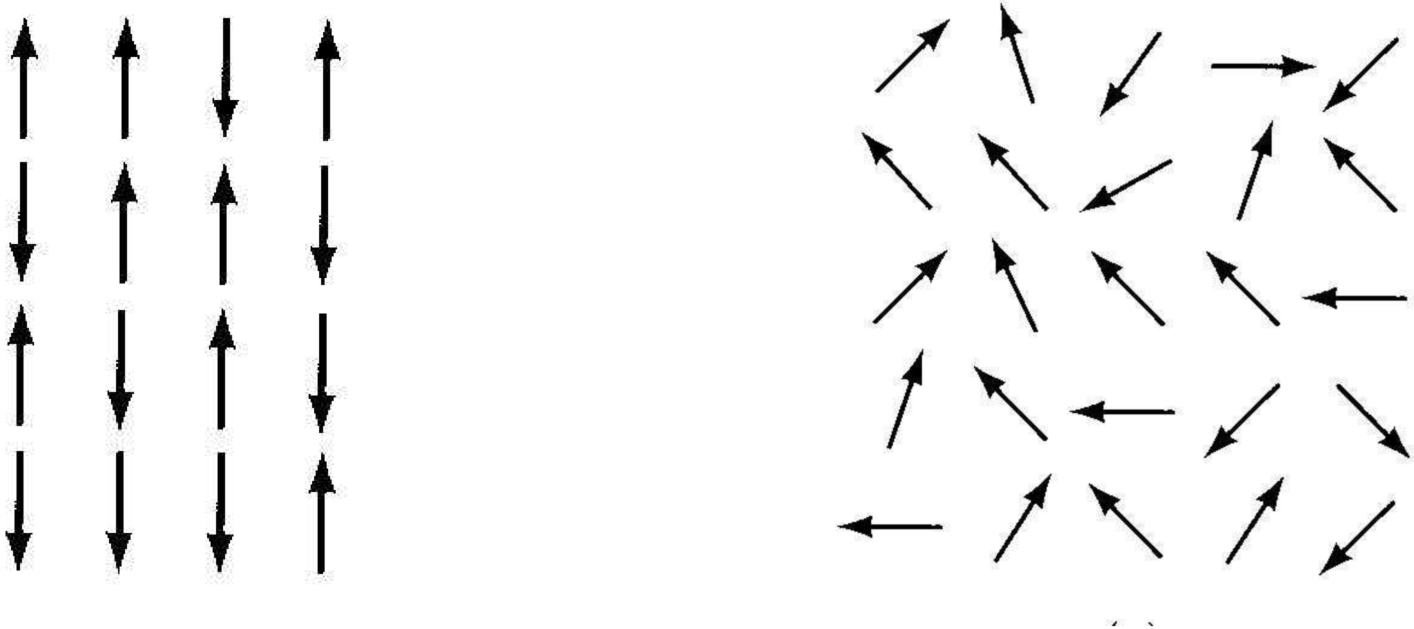
Ising model

- At Dimension $d > 1$ Ising model exhibits para- to ferro-magnetic transition
- $H = -J\Sigma S_i S_{i+1}$
- At $T < T_c$, $\langle S_i \rangle \neq 0$ (non-zero magnetisation)
- H is invariant under $S_i \to -S_i \Rightarrow$ discrete symmetry
- At $d = 1$ - no ordering at finite T
- Nothing special happens in $2d$
- In the ordered phase correlation function of the local order parameter goes to a constant in the large distance limit

Heisenberg/XY models

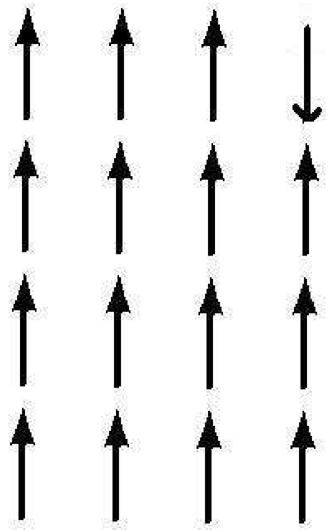
- $H = -J \Sigma \mathbf{S}_i \cdot \mathbf{S}_{i+1}$,
  $i = 1, 2$ for XY and $i = 1, 2, 3$ for Heisenberg
- H: Invariant under rotation of all spins by the same but *arbitrary* angle $\Rightarrow$ Invariance under a *continuous symmetry*
- Below T_c exhibit *long-range order* in the *broken symmetry phase* for $d > 2$
- $d = 2$ is the *lower critical dimension*

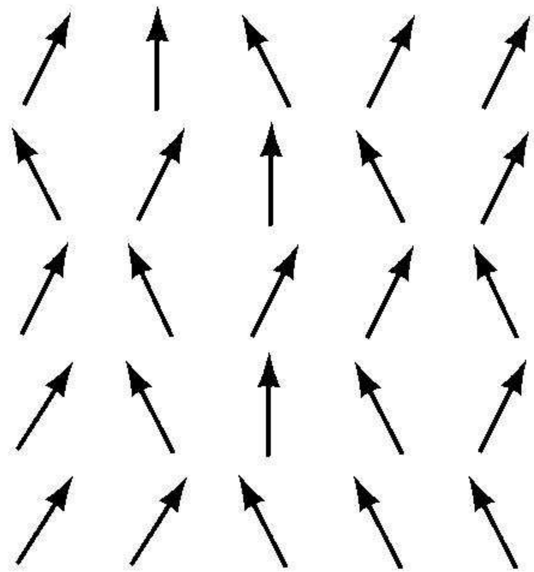
Paramagnetic states



left: Ising, right: XY/Heisenberg

Ferromagnetic states

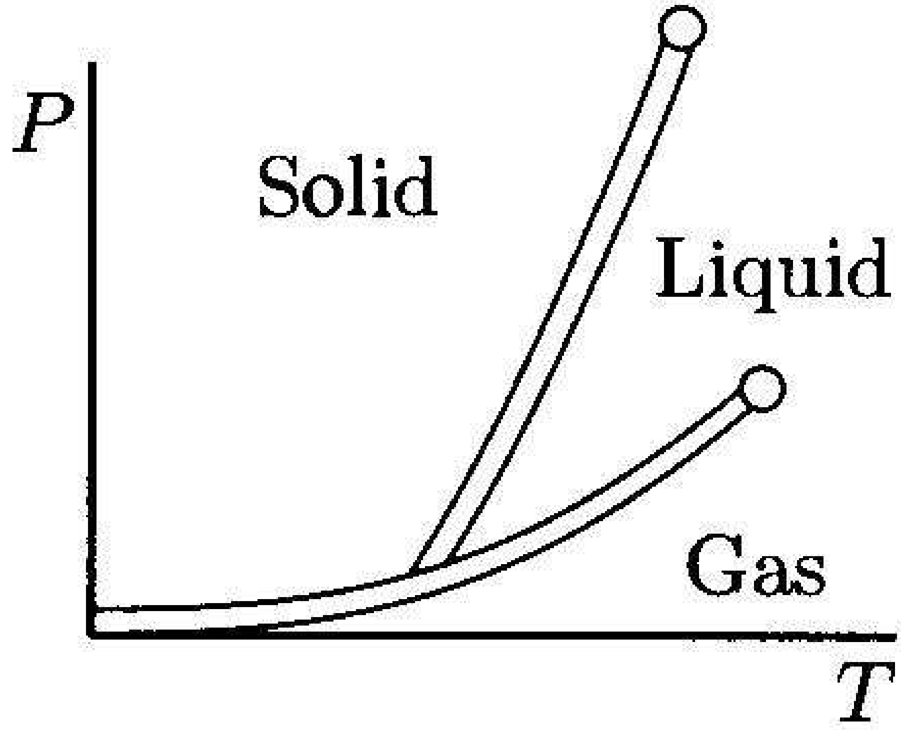




left: Ising, right: XY/Heisenberg

Melting of solids

Phase diagram



First order phase boundary in $3\mathrm{d}$

Broken symmetry variables

Breaking of continuous symmetries, e.g.,

- Broken translational invariances in liquid-to-solid $\Rightarrow$ complex order parameters $\rho_{\mathbf{G}}$
- Broken rotational invariances in para-to-ferromagnetic (Heisenberg/XY models) $\Rightarrow$ vector order parameter $\mathbf{m}$.
- Broken rotation invariances in liquid-to-nematic liquid crystal $\Rightarrow$ tensor order parameter Q_{ij}

Infinite number of (free energetically) equivalent ordered state, connected by a continuous variable (parameter) θ

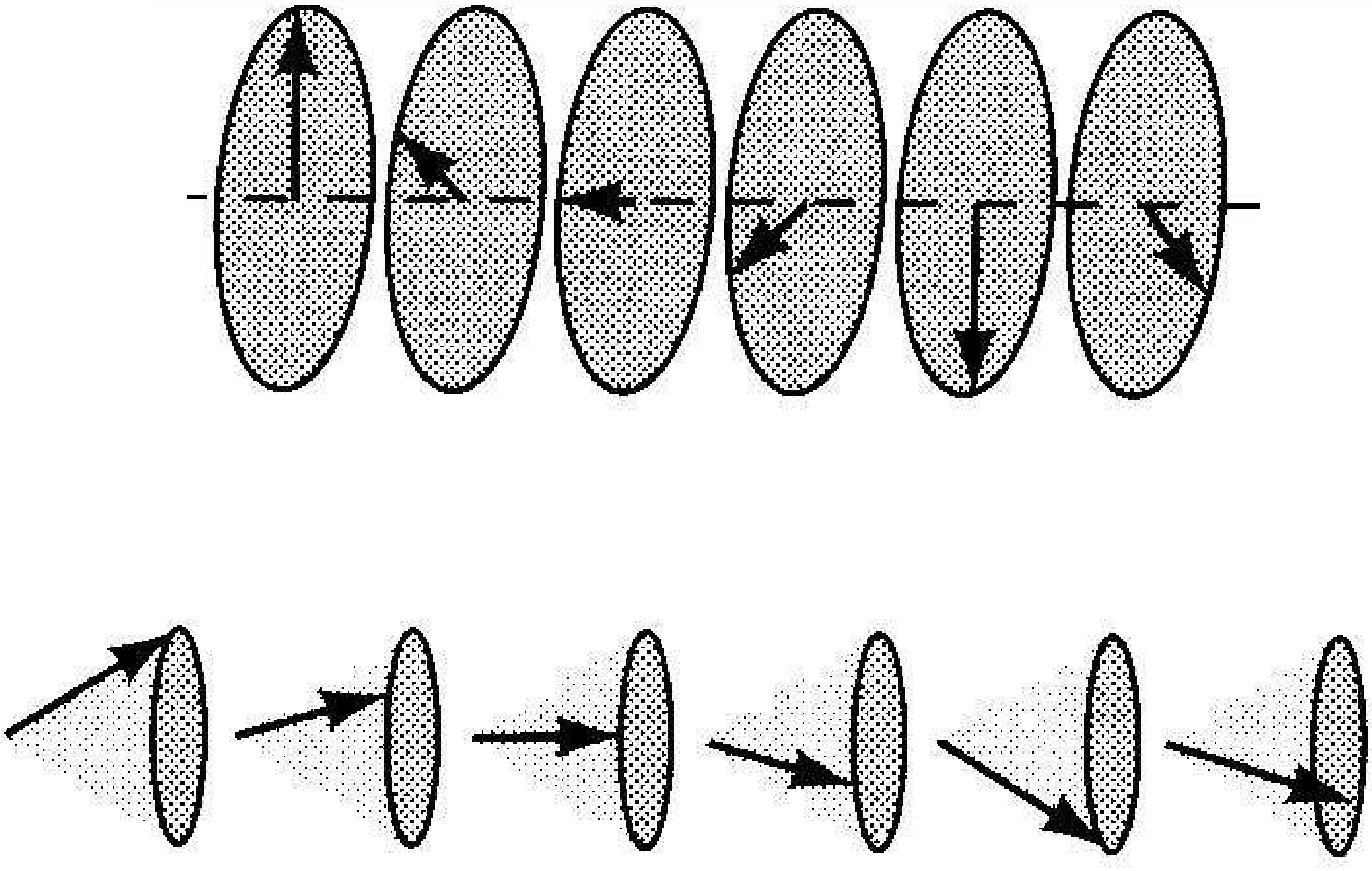
- $\theta \Rightarrow$ an angle for broken rotational invariance
- $\theta \Rightarrow$ a displacment (origin of the coordinate system) for broken translational symmetry

- Spatially uniform changes in θ connect different equivalent ordered states and do not cost any energy
- Spatially non-uniform changes $\theta = \theta(\mathbf{x})$ costs energy of the form $(\nabla\theta)^2$ for very slowly varying θ (*low energy excitations*)

Examples: Acoustic phonons (elastic waves) in a crystal,

Spin waves in a magnet

Spin wave



Elastic deformation energy in a solid

- Elasticity: Stress $= E$ Strain
- E is an elastic modulus
- Elastic energy $\sim$ stress $\times$ strain $\sim E$ (strain)^2
- Strain $\sim \Delta u / L \sim \nabla u$ in the continuum limit
- Elastic energy $E_{el} = E \int d^d x (\nabla u)^2 \Rightarrow$ similar to the XY Hamiltonian
- Phase transitions in the XY model should be similar to the melting of solids

Mean square fluctuations

To calculate $W = (1/2)\langle\theta(x)^2\rangle$ with a free energy

$F = (\kappa/2)\int d^dx(\nabla\theta)^2 = (\kappa/2)\int \frac{d^dq}{(2\pi)^d}q^2|\theta_q|^2$

Answer: $W = \frac{T}{2}\int \frac{d^dq}{(2\pi)^d}\frac{1}{\kappa q^2} \sim \int \frac{q^{d-1}dq}{q^2}$

- Lower limit: $\sim L^{-1}$ (system size), upper limit: $\sim Q_o$ (molecular cut off).
- Thermodynamic limit: $L \to \infty$
- $d = 1 \Rightarrow W \propto L$, L is the system size
- $d = 2 \Rightarrow W \propto \ln L$
- $d > 2 \Rightarrow W$ independent of system size

Hence W diverges in the thermodynamic limit $L \to \infty$ at

XY model

$$H = -J\Sigma \mathbf{s}_i \cdot \mathbf{s}_{i+1} = -J\Sigma_{\langle l,l'\rangle} \cos(\theta_l - \theta_{l'}) = \frac{1}{2}\int d^d x \kappa (\nabla\theta(\mathbf{x}))^2$$

Let $\langle \mathbf{s} \rangle = \langle s \rangle e_x$. Then

$$\frac{\langle \mathbf{s} \rangle}{s_o} = \langle \cos\theta \rangle \equiv e^{-W} = \Re\left(\frac{1}{Z}\int \mathcal{D}\theta e^{-\beta H} e^{i\theta}\right) \equiv e^{-W}$$

where $W = \frac{1}{2}\langle \theta^2(\mathbf{x}) \rangle = \frac{T}{2}\int \frac{d^2 q}{(2\pi)^2}\frac{1}{\kappa q^2}$

Debye-waller factor

Fluctuations work against ordering...

$$W = \frac{T}{2}\int \frac{d^2 q}{(2\pi)^2}\frac{1}{\kappa q^2} \sim \int \frac{q^{d-1}\,dq}{q^2}$$

- Lower limit: $\sim L^{-1}$ (system size), upper limit: $\sim Q_o$ (molecular cut off).
- Thermodynamic limit: $L \to \infty$
- $W \sim \int dq$ does not diverge in the thermodynamic limit at $d = 3$
- W diverges as ln L at $d = 2$
- W diverges as L at $d = 1$

- (e^{-2W} suppression of the order parameter due to thermal fluctuations $\rightarrow$ *Debye-Waller factor*
- $Rightarrow$ order is destroyed for $\mathrm{d} = 1$!
- What happens in $2\mathrm{d}$?

Correlation function
$C(\mathbf{x}) = \langle \mathbf{s}(\mathbf{x}) \cdot \mathbf{s}(0) \rangle = s_o^2 \langle \cos[\theta(\mathbf{x}) - \theta(0)] \rangle = s_o^2 e^{-g(\mathbf{x})}$ which for $|\mathbf{x}| \to \infty$ yields

- $g(\mathbf{x}) = 2W$ for $d = 3$: LR (long range) order,
- $g(\mathbf{x}) = \frac{T}{2\pi\kappa} \ln(\Lambda|\mathbf{x}|)$ at $d = 2$: QLR (quasi long range) order (Λ is a high momentum cut-off) and
- $g(x) = \frac{T}{2\kappa}|x|$ for $d = 1$: SR (short range) order.

- Clearly $C(\mathbf{x})$ finite for large $\mathbf{x}$ in $3d$ and $C(x)$ decays exponentially for large $|x|$ in $1d$
- In $2d$ $C(\mathbf{x})$ decays *algebraically* to 0 for large $|\mathbf{x}| \Rightarrow C(\mathbf{x}) = s_0^2(\Lambda|\mathbf{x}|)^{-\eta}$ for T/κ finite, similar to its form at a critical point in $3d$
- $T = 0 \Rightarrow C(\mathbf{x})$ is a constant for large $|\ bfx| \Rightarrow$ long range order at $T = 0$ (expected)
- $\kappa \to 0 \Rightarrow T/\kappa \to \infty \Rightarrow C(\mathbf{x}) \to 0$ much faster than algebraically for large $|\mathbf{x}| \Rightarrow$ possibility of a QLRO-disorder transition

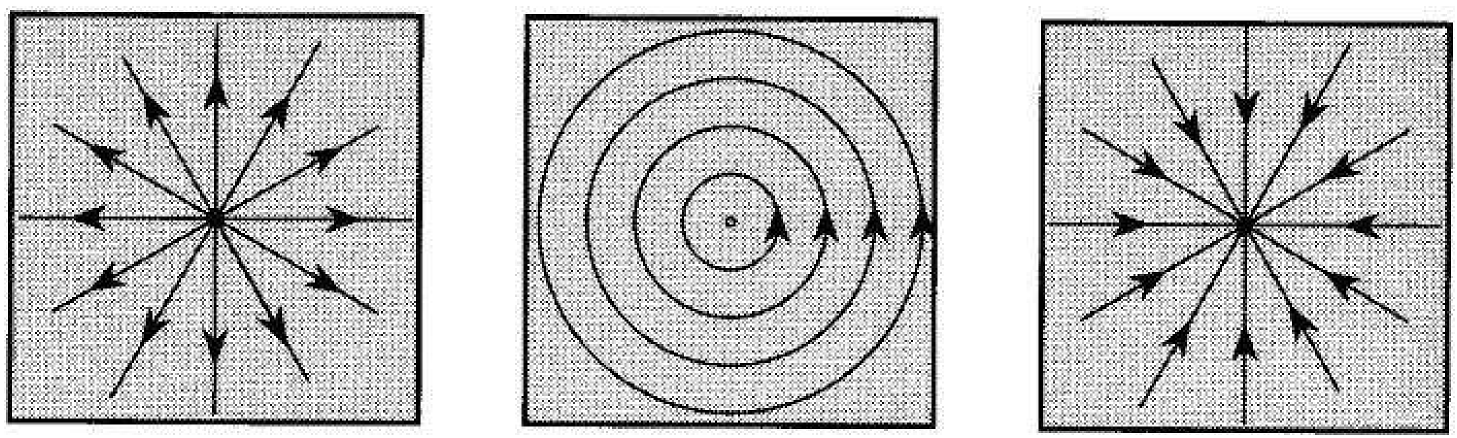
Vortex excitations

What sort of excitations are responsible for a QLRO - SR transition?
Creation of a vortex
Assumptions made so far:

- The angle variable $\theta(\mathbf{x})$ was continuous everywhere
- The magnitude $\langle s(\mathbf{x})\rangle$ of the order parameter was everywhere non-zero

$\langle \mathbf{s}(\mathbf{x})\rangle = s(\cos\theta(\mathbf{x}), \sin\theta(\mathbf{x}))$ is a periodic function of $\theta(\mathbf{x}) \Rightarrow$ it is possible to have situations when $\langle \mathbf{s}(\mathbf{x})\rangle$ is continuous everywhere in $2\mathrm{d}$ except for isolated points $\Rightarrow$ *Topological defects*

Example: At $d = 2, \ \ \theta(\mathbf{x}) = \phi + \theta_o$,
where θ_o is a constant, $\mathbf{x} = (r, \phi)$ in polar coordinates, then $\langle \mathbf{s}(\mathbf{x}) \rangle$ is continuous and $\nabla\theta = 1/r$ is finite everywhere except at $r = 0$



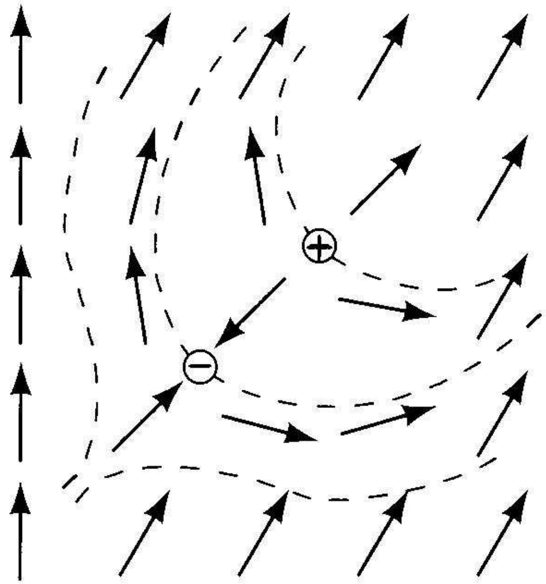
(a) (b) (c)

Vortex configuration with $\theta_o = 0$, $\theta_o = \pi/2$, $\theta_o = \pi$

Ill-defined at the origin

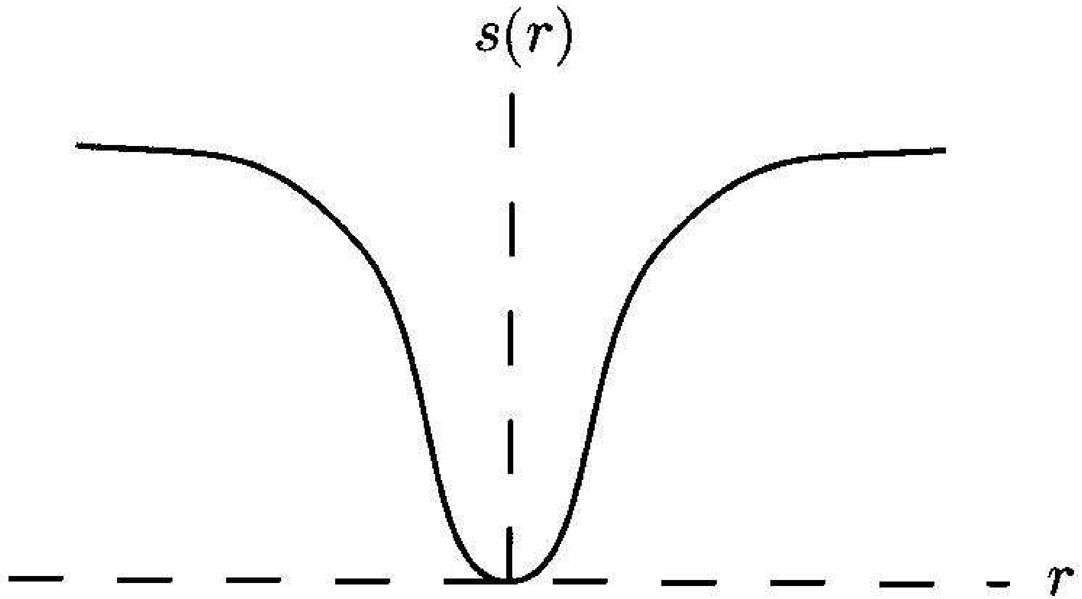
Vortex-antivortex

In general $\theta = k\phi + \theta_o$, $k = \pm 1, \pm 2, .., \; k$ is the *charge* of the vortex



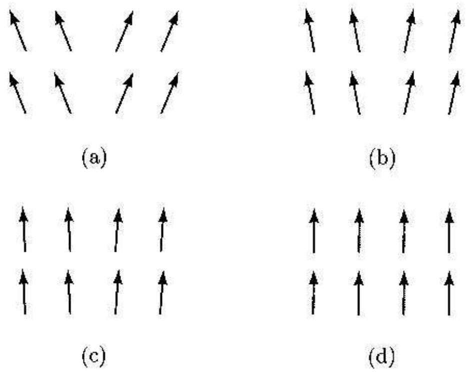
Singularities

- Singularities can be removed by *defining* the order parameter magnitude to go to 0 at the singularity and to rise to its equilibrium value at a radius ζ_o which is the *size of the defect*



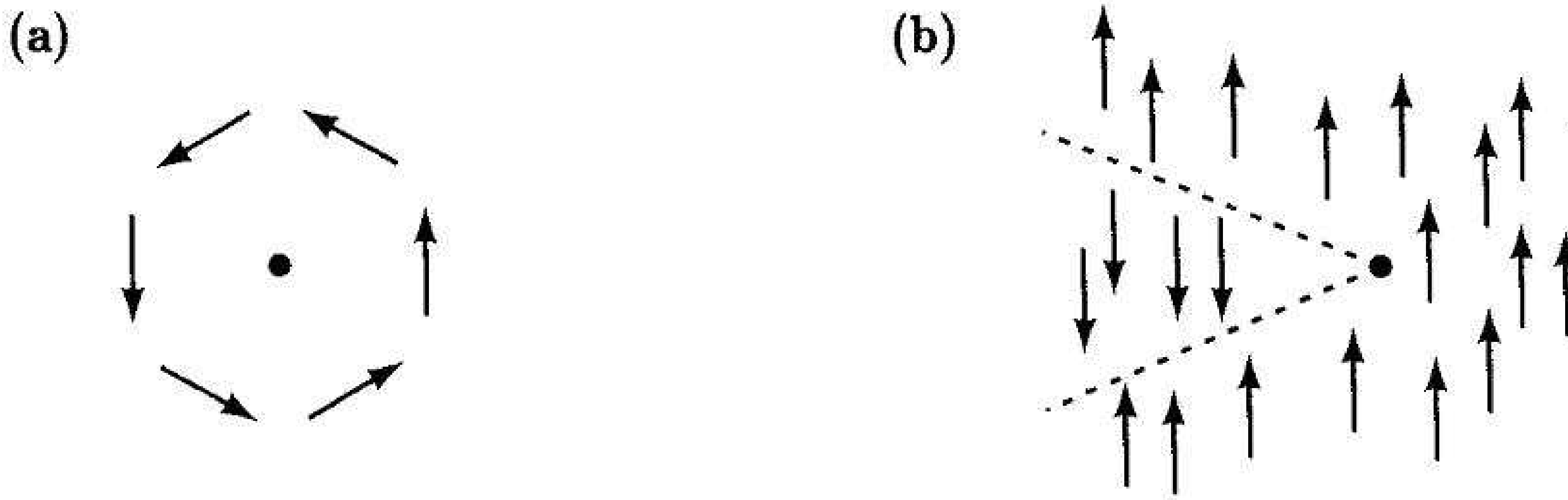
A *Vortex-antivortex* pair

Stability of a vortex



Sequence of continuous distortions form a singularity free excited state (spin wave type excitations) to uniform alignment

In contrast....



Attempt to align spins by a continuous distortion creates boundaries across which spin changes rapidly - energetically expensive - hence stable

KT *transition*

- A single vortex has an energy $E = \kappa \ln(R/a)$ where R, a are the linear size of the system and size of the defect
- Entropy of a single vortex of size a in a $2d$ box of linear size R is $2k_B \ln(R/a)$
- Hence free energy $F = (\kappa - 2k_B T) \ln(R/a)$
- $\Rightarrow$ F reduces at high T if a vortex is produced
  $\Rightarrow T_c = \kappa/(2k_B)$

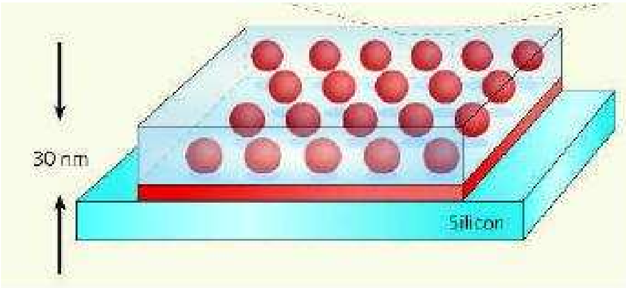
Rigorous analyses

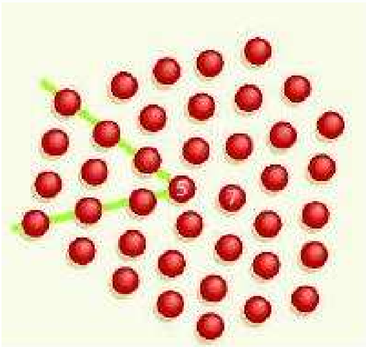
- Vortices in $2d$ are like charged particles with both signs, form a $2d$ Coulomb gas and interact via a $\ln r$-type potential
- At low T they remain in vortex-antivortex pairs (like dipoles)
- At high T we have a plasma of vortex and antivortex (like free charges)
- Transition between these two is the *KT transition*

Experimental realisation

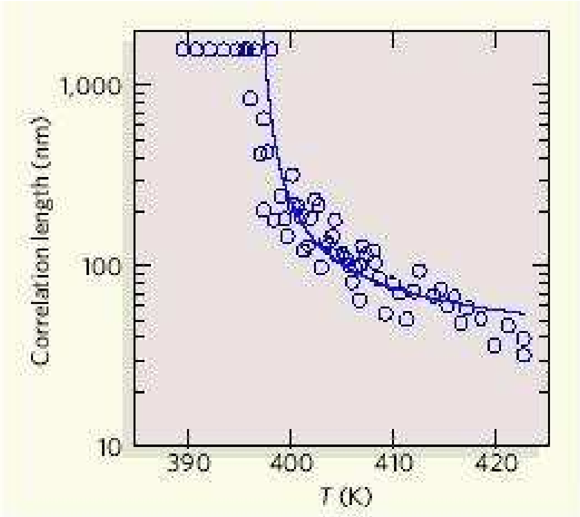
- Free standing liquid crystal films
- Electrons on the surface of liquid helium
- Rare gases absorbed on the surface of graphite
- Colloids or polyballs

An example





[E. Kramer, *Nature*, 2005]

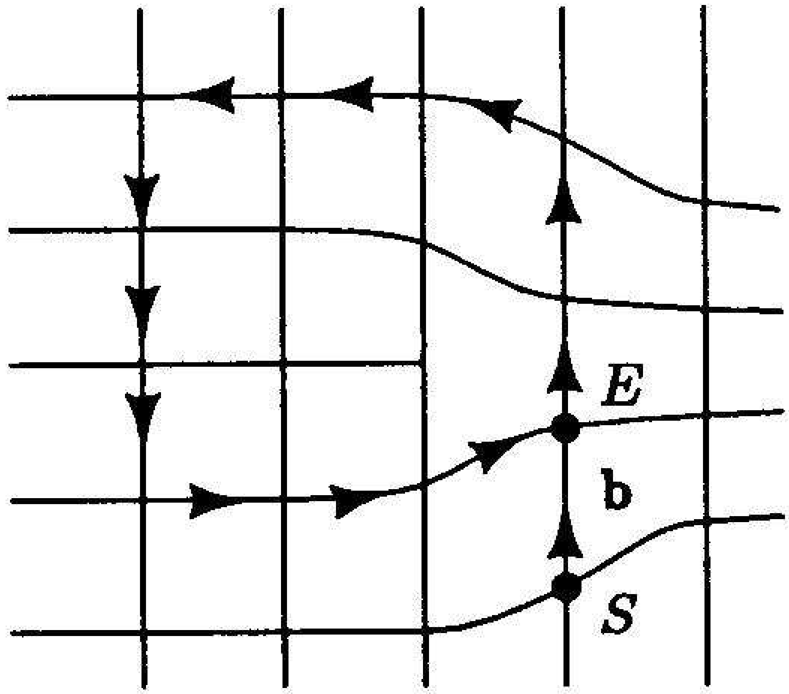


Correlation function in a $2d$ array of polyballs

KT theory: $C(\mathbf{x}) \sim \frac{\ln^{1/8}(|\mathbf{x}|/a)}{|\mathbf{x}|^{1/4}},$

Correlation length $\zeta(T)/a \sim e^{b/|T-T_c|^{1/2}} \Rightarrow$ *essential singularity at* T_c

2d *Melting* - defect mediated



Defects in a solid - *dislocations*

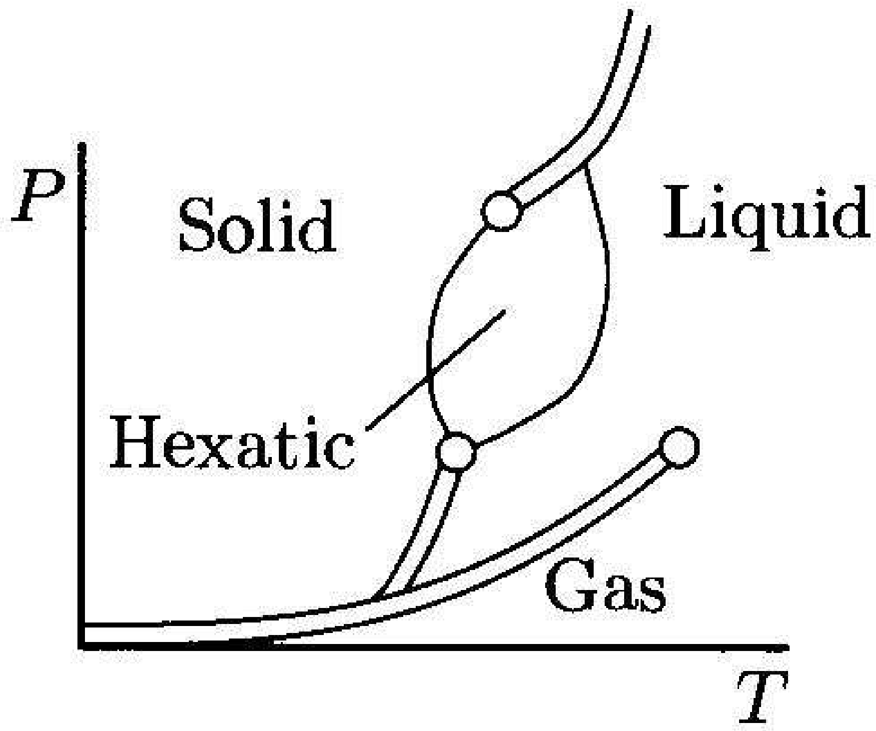
Characterised by *vector charges - Burgers vector*

$2d$ ***melting***

As you raise T

- Step I: The QLR positional order of a $2d$ crystal is destroyed by *free dislocations* to produce the *hexatic phase*
- Step II: The QLR orientational order of the hexatic phase is destroyed by *free disclinations* to produce isotropic liquids

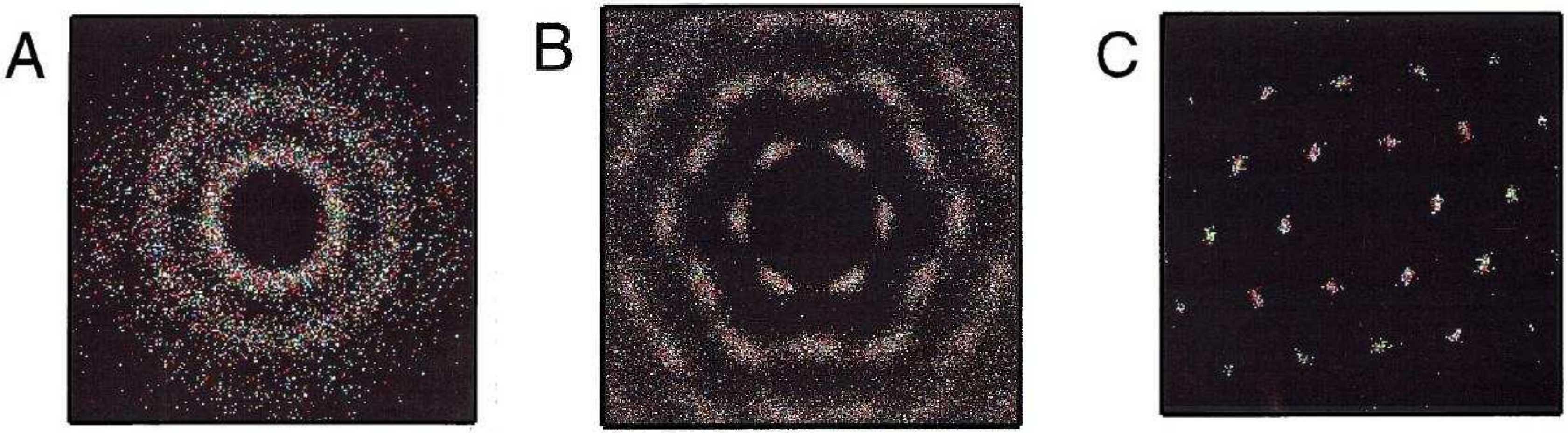
2d ***Melting phase diagram***



Second order phase boundaries! *Hexatic phase* $\Rightarrow$ only orientational order but no translational order.

2d *Solid-liquid transition*

Hexatic order - 6-fold orientational order



A:- liquid phase (isotropic), B:- hexatic phase (orientational order), C:- crystalline solid - second order liquid - solid transition!

[A. H. Markus et al, *PRE* (1997)]

Applications and Future directions

- Applications: Industrial (thin film and monolayer making, lithography), experimental ($2\mathrm{d}$ experiments on confined colloids) and theoretical (stat-mech, field theory)
- Future: Driven $2\mathrm{d}$ samples (industrial and biological), e.g., sheared $2\mathrm{d}$ colloidal crystals, ordering in a cell membrane

References

- D. R. Nelson, in Phase Transitions and Critical Phenomena, edited by C. Domb and J. L. Lebowitz Academic, London, 1983, p. 1
- K. J. Strandburg, Reviews of Modern Physics, **60**, 161 (1988)
- P. Chaikin and T. C. Lubensky, Principles of Condensed Matter Physics Cambridge University Press, Cambridge, 1995