Active dumbbells

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Work in collaboration with

D. Loi & S. Mossa (Grenoble, France, 2007-2009) and

G. Gonnella, P. Di Gregorio, G.-L. Laghezza, A. Lamura, A. Mossa & A. Suma

(Bari & Trieste, Italia, 2013-2015)

Palma de Mallorca, España, 2017

Plan

5 lectures & 2 exercise sessions

1. Introduction
2. Active Brownian dumbbells
3. Effective temperatures
4. Two-dimensional equilibrium phases
5. Two-dimensional collective behaviour of active systems

Fourth lecture

Plan

5 lectures & 2 exercise sessions

1. Introduction
2. Active Brownian dumbbells
3. Effective temperatures
4. **Two-dimensional equilibrium phases**
5. Two-dimensional collective behaviour of active systems

Plan

4th & 5ft Lectures

- Peierls (1934), Mermin-Wagner (1966-68) results.
- Berenzinskii-Kosterlitz-Thouless-Halperin-Nelson-Young scenario
- 2d passive systems made of hard or soft disks in interaction
- Brand new Bernard & Krauth two step transition scenario
- $2d$ active systems made of soft (though rather hard) dumbbells
- Mobility induced phase transition for purely repulsive interactions *vs.*

  an extension of the Bernard & Krauth passive system scenario
- Revisiting displacements & effective temperatures

Plan

4th Lecture : equilibrium phases of $2d$ matter

- Peierls (1934), Mermin-Wagner (1966-68) results.
- Berenzinskii-Kosterlitz-Thouless-Halperin-Nelson-Young scenario
- 2d passive systems made of hard or soft disks in interaction
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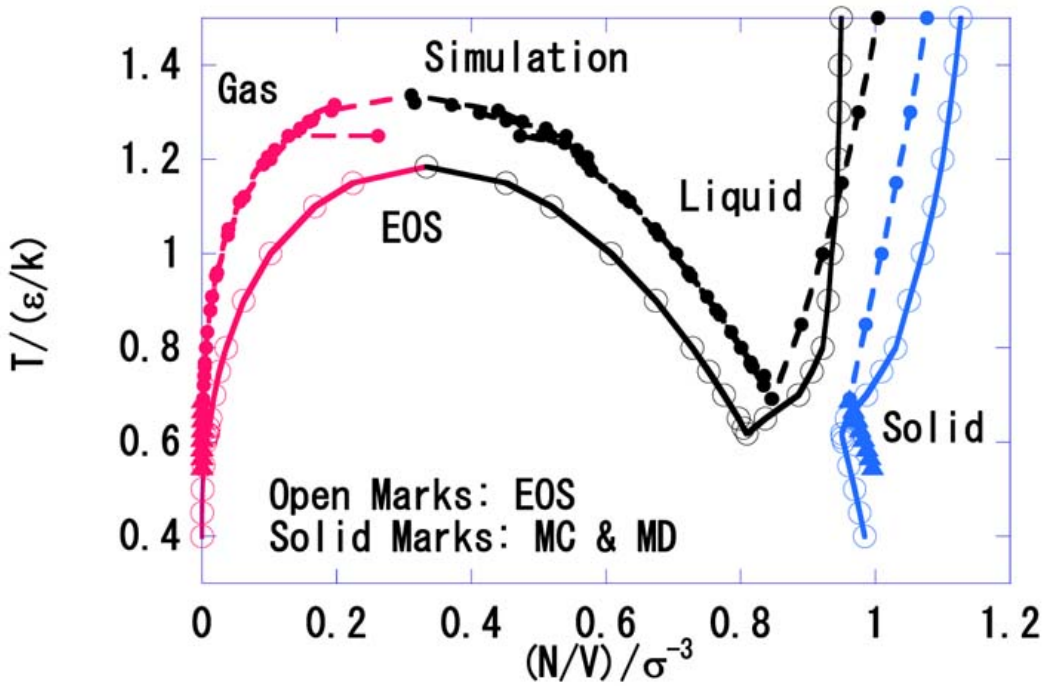
  an extension of the Bernard & Krauth passive system scenario
- Revisiting displacements & effective temperatures

Phase diagram

Solid, liquid and gas equilibrium phases



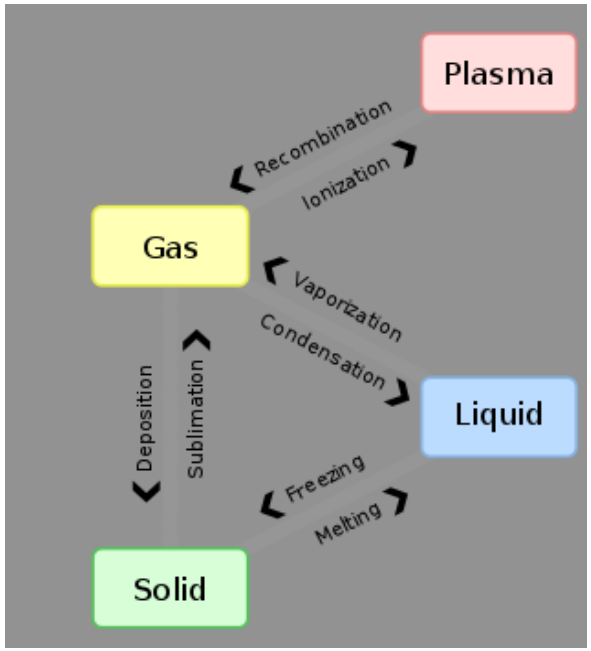
Typical (simple) (ϕ, T) phase diagram

Lennard-Jones model system for Argon in $3d$

Kataoka & Yamada, J. Comp. Chem. Jpn. 11, 81 (2012)

Phases and transitions

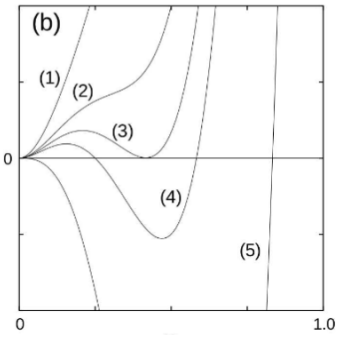
Names



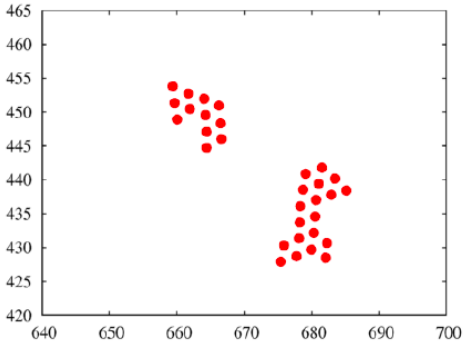
Focus on freezing/melting transition

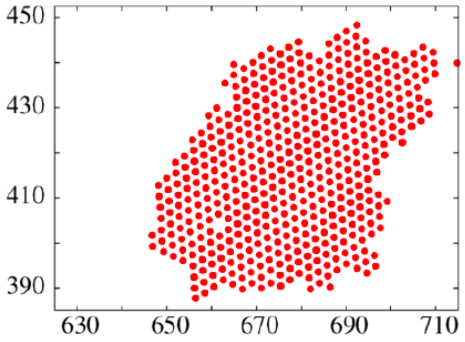
Freezing

First order route



Landau free-energy





Examples of two crystalline configurations

At $T > T_c$ the central minimum (liquid) is lower.

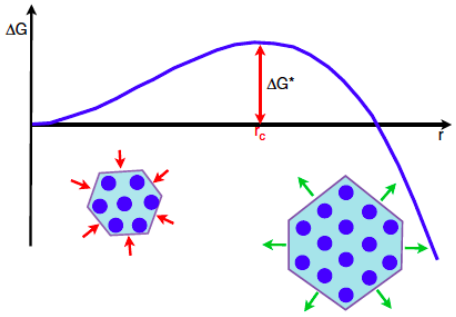
At $T = T_c$ the two minima are at the same level.

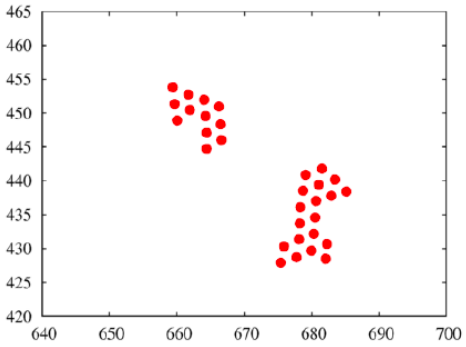
At $T < T_c$ the minimum at the right (solid) is lower.

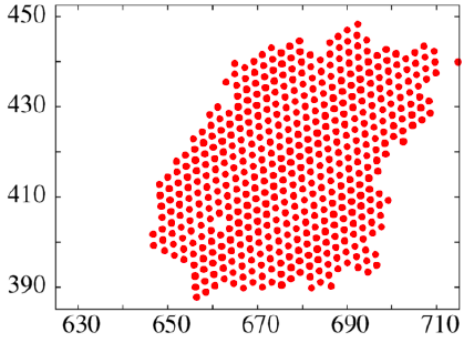
Metastability & hysteresis

Freezing

First order route: nucleation & growth







Nucleation barrier $\Delta F(R)$

Examples of two crystalline configurations

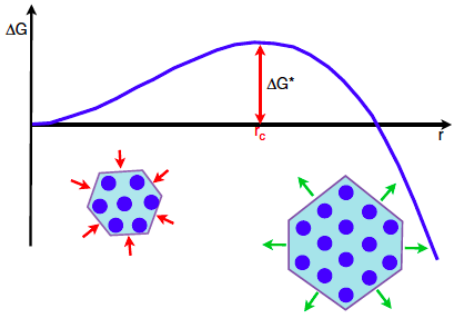
$$\Delta F(R) \equiv F_{\text{bubble}}(R) - F_{\text{no bubble}}(R) \approx -\delta f \, R^d + s \, R^{d-1}$$

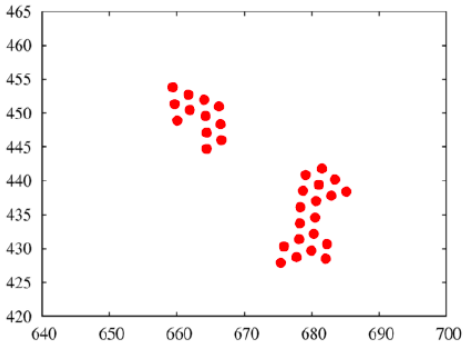
$$0 = \left. \frac{d\Delta F(R)}{dR} \right|_{R=R_c} \approx -\delta f \, R^{d-1} + s \, R^{d-2} \quad \Rightarrow \quad \boxed{R_c \approx \frac{s}{\delta f}}$$

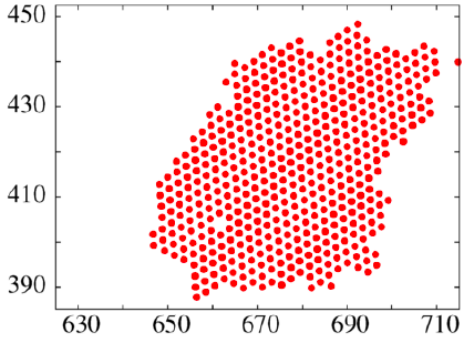
Left image from **Gasser, J. Phys. : Cond. Matt. 21, 203101 (2009)**

Freezing

First order route: nucleation & growth







Nucleation barrier $\Delta F(R)$

Examples of two crystalline configurations

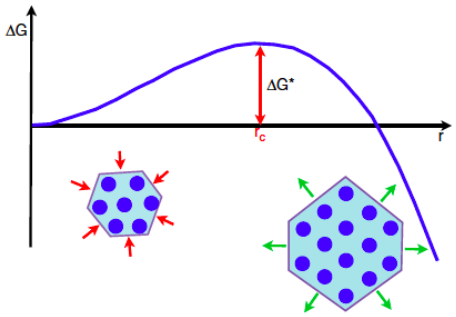
$$\Delta F(R) \equiv F_{\text{bubble}}(R) - F_{\text{no bubble}}(R) \approx -\delta f \, R^d + s \, R^{d-1}$$

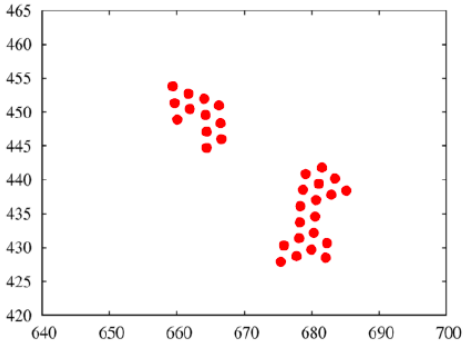
$$\Delta F(R_c) \approx \frac{s^d}{(\delta f)^{d-1}} \quad \text{and} \quad R_c \approx \frac{s}{\delta f} \quad \text{in} \quad d \geq 2$$

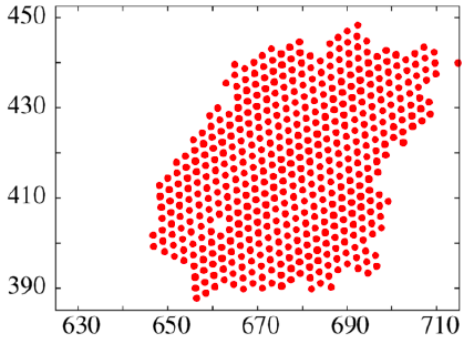
Left image from **Gasser, J. Phys. : Cond. Matt. 21, 203101 (2009)**

Freezing

First order route: nucleation & growth







Crossing point $\Delta F(R^*) = 0$

Examples of two crystalline configurations

$$\Delta F(R) \equiv F_{\text{bubble}}(R) - F_{\text{no bubble}}(R) \approx -\delta f \, R^d + s \, R^{d-1}$$

$$0 = \Delta F(R^*) \approx -\delta f \, R^{*d} + s \, R^{*d-1} \quad \Rightarrow \quad \boxed{R^* \approx \frac{s}{\delta f}}$$

Left image from **Gasser, J. Phys. : Cond. Matt. 21, 203101 (2009)**

Freezing

but, this is not the route to freezing in $2d$

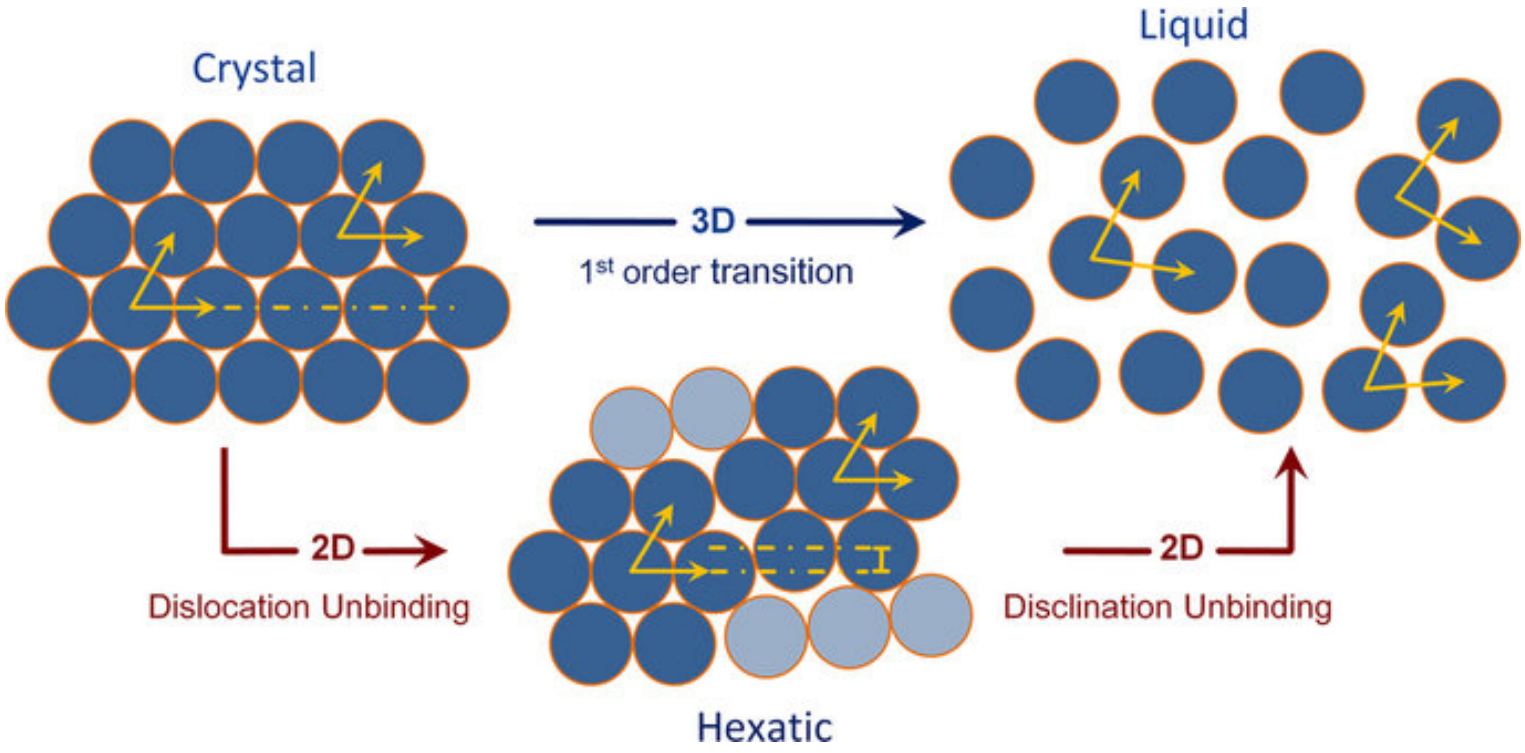


Image from **Pal, Kamal & Raghunathan, Sc. Rep. 6, 32313 (2016)**

Freezing

although the $2d$ mechanism is not so clear yet

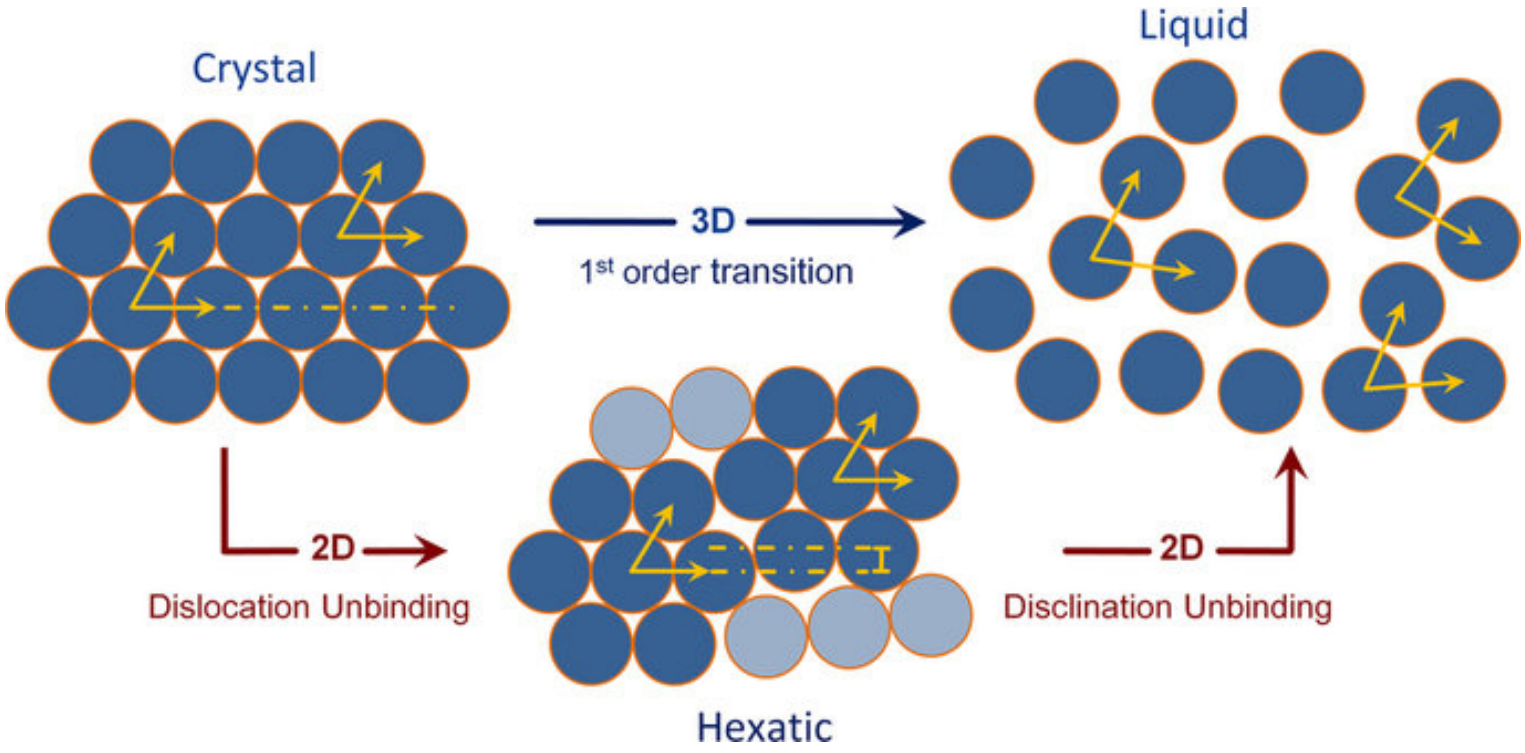
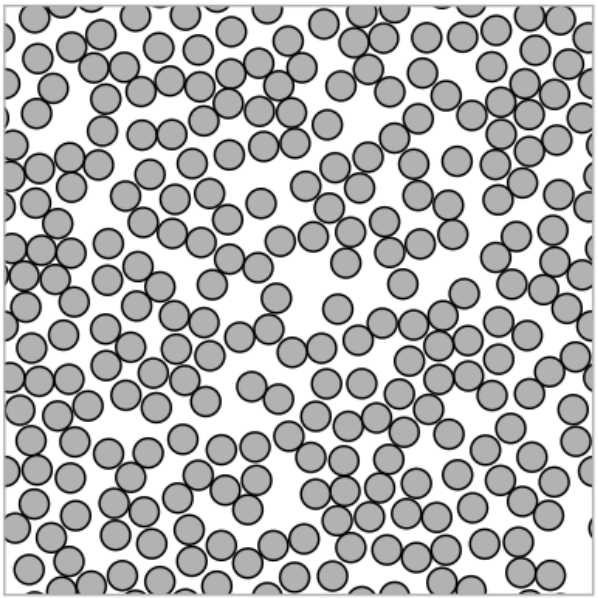


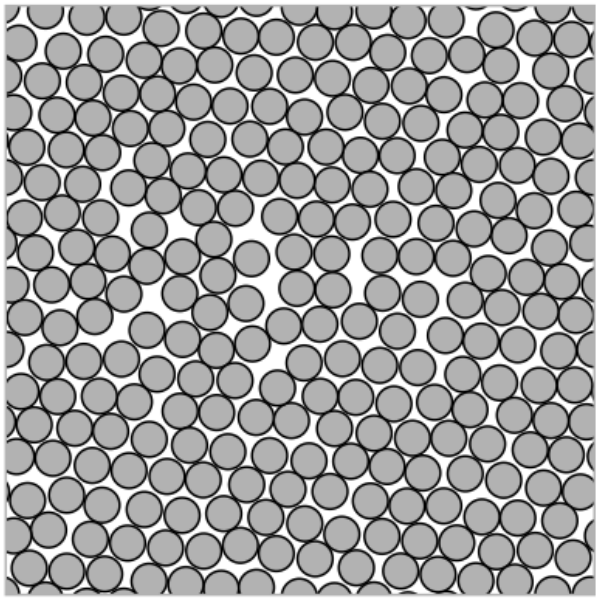
Image from **Pal, Kamal & Raghunathan, Sc. Rep. 6, 32313 (2016)**

Freezing

Disks in two dimensions



Low density liquid

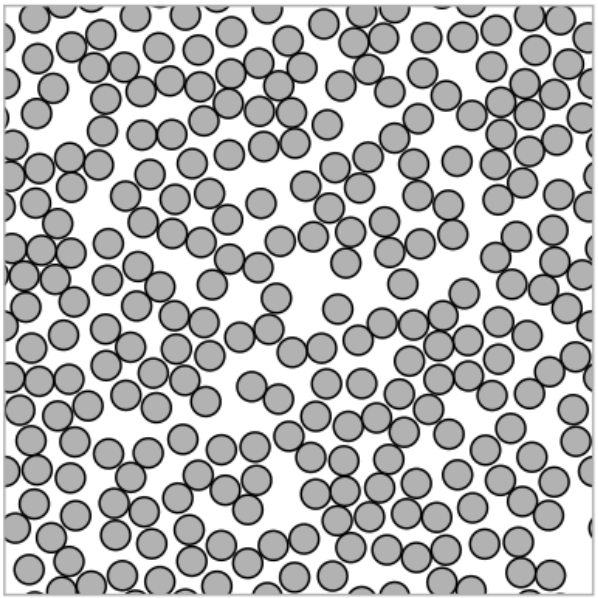


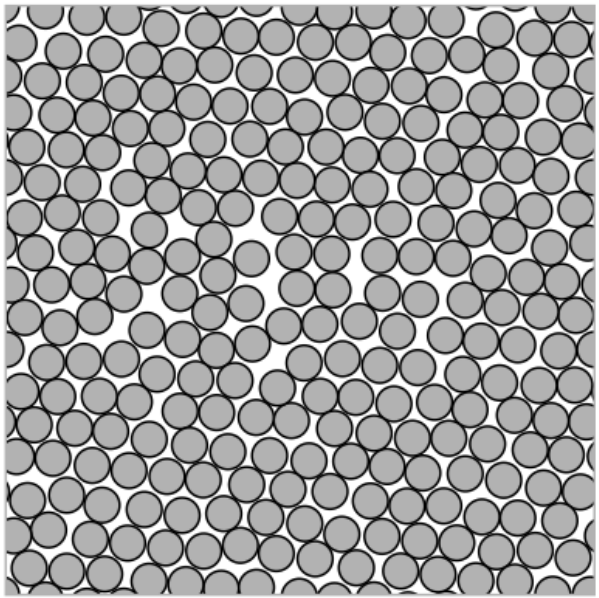
High density, which phase ?

(Many) Figure(s) from **E. Bernard, PhD Thesis, UPMC**

Freezing

Disks in two dimensions





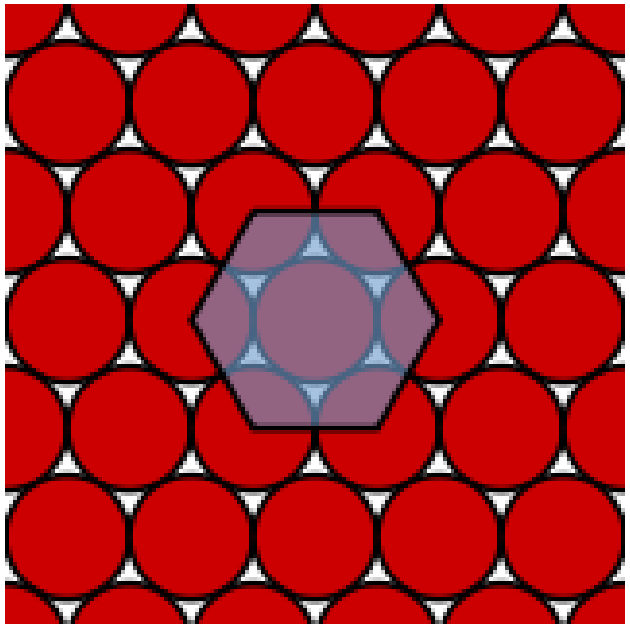
Low density liquid

$\phi_{\mathrm{RCP}} \approx 0.82$

The Random Close Packing (RCP) is the maximum volume fraction of solid objects packed randomly

Freezing

Disks in two dimensions



$\phi_{\mathrm{hex}} \approx 0.91$

Crystalline triangular lattice ordering

Observables

Positional order

The (fluctuating) local particle number density

$$\rho(\boldsymbol{r}_0) = \sum_{i=1}^{N} \delta(\boldsymbol{r}_0 - \boldsymbol{r}_i)$$

with normalisation $\int d^d\boldsymbol{r}_0\, \rho(\boldsymbol{r}_0) = N$. In a homogeneous system $\rho(\boldsymbol{r}_0) = N/V$.

The density-density correlation function $C(\boldsymbol{r} + \boldsymbol{r}_0, \boldsymbol{r}_0) = \langle \rho(\boldsymbol{r} + \boldsymbol{r}_0)\rho(\boldsymbol{r}_0) \rangle$ that, for homogeneous (independence of $\boldsymbol{r}_0$) and isotropic ($\boldsymbol{r} \mapsto |\boldsymbol{r}| = r$) cases, is simply $C(\boldsymbol{r} + \boldsymbol{r}_0, \boldsymbol{r}_0) = C(r)$.

The double sum in $C(\boldsymbol{r} + \boldsymbol{r}_0, \boldsymbol{r}_0) = \langle \sum_{ij} \delta(\boldsymbol{r} - \boldsymbol{r}_i)\delta(\boldsymbol{r}_0 - \boldsymbol{r}_j) \rangle$ has contributions from $i = j$ and $i \neq j$: $C_{\text{equal}} + C_{\text{diff}}$

Observables

Positional order

The density-density correlation function

$$C(\boldsymbol{r}+\boldsymbol{r}_0,\boldsymbol{r}_0)=\langle\rho(\boldsymbol{r}+\boldsymbol{r}_0)\rho(\boldsymbol{r}_0)\rangle=\sum_{ij}\langle\delta(\boldsymbol{r}+\boldsymbol{r}_0-\boldsymbol{r}_i)\delta(\boldsymbol{r}_0-\boldsymbol{r}_i)\rangle$$

is linked to the structure factor

$$S(\boldsymbol{q})\equiv N^{-1}\langle\tilde{\rho}(\boldsymbol{q})\tilde{\rho}(-\boldsymbol{q})\rangle=\frac{1}{N}\langle\sum_{i=1}^{N}\sum_{j=1}^{N}e^{-\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)}\rangle$$

by

$$N\,S(\boldsymbol{q})\;=\;\int d^d\boldsymbol{r}_1\int d^d\boldsymbol{r}_2\,C(\boldsymbol{r}_1,\boldsymbol{r}_2)\,e^{-\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)}$$

Observables

Positional order

In isotropic cases, i.e. liquid phases, the pair correlation function

$\frac{N}{V}\, g(r) =$ average number of particles at distance r

from a tagged particle at $\boldsymbol{r}_0$

is linked to the structure factor

$$S(\boldsymbol{q}) = \frac{1}{N}\langle \sum_{i=1}^{N}\sum_{j=1}^{N} e^{-\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)} \rangle$$

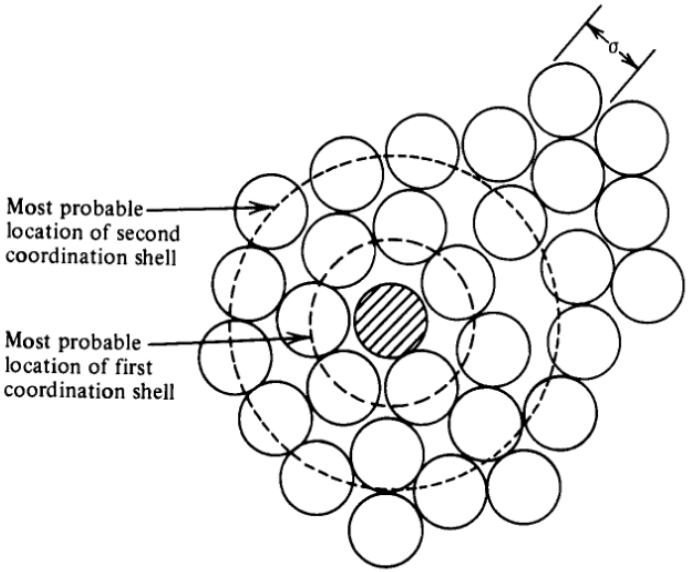
by

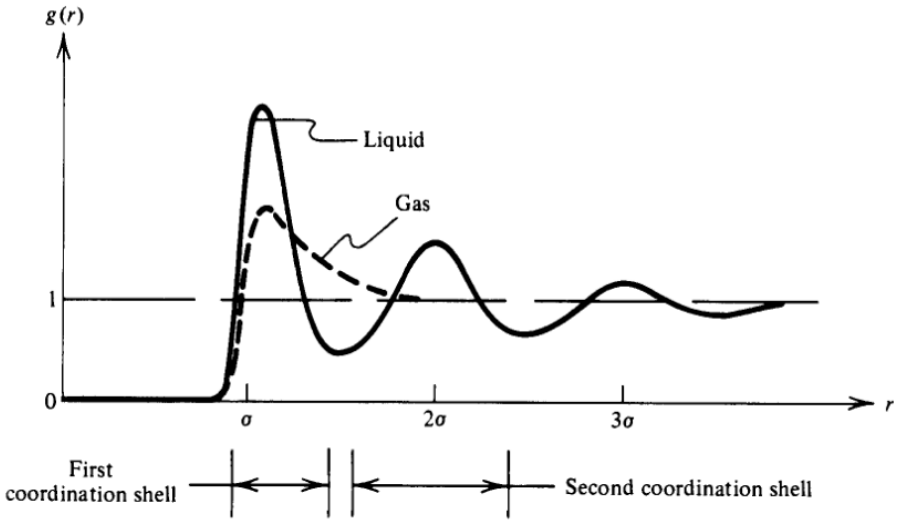
$$S(\boldsymbol{q}) = 1 + \frac{N}{V}\int d^d\boldsymbol{r}\; g(r) e^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}$$

Peaks in $g(r)$ are related to peaks in $S(q)$. The first peak in $S(q)$ is at $q_0 = 2\pi/\Delta r$ where Δr is the distance between peaks in $g(r)$ (that is close to the inter particle distance as well).

Observables

Liquid

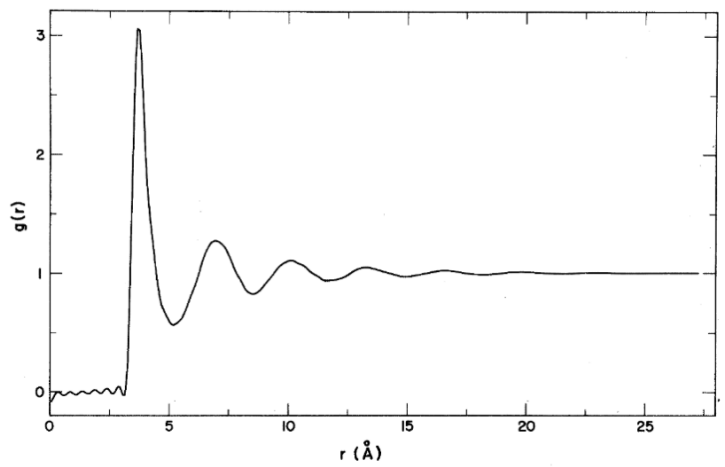


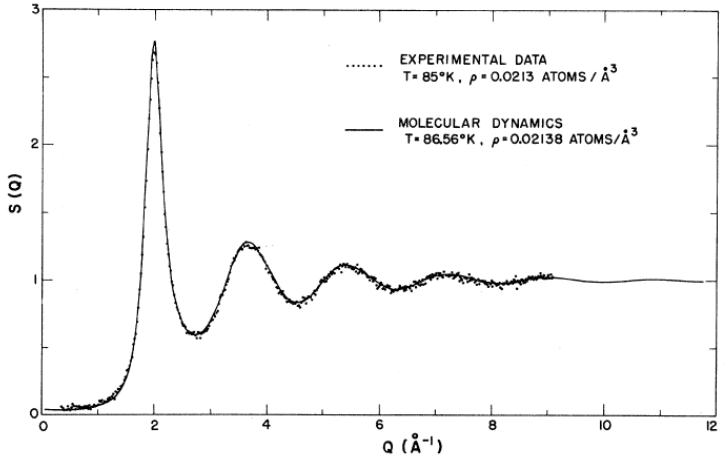


"Introduction to Modern Statistical Mechanics", **Chandler** (OUP)

Observables

Experiments & simulations of liquids





Inter-peak distance between the peaks in $g(r)$ is $\Delta r \simeq \sigma \simeq 3$Å

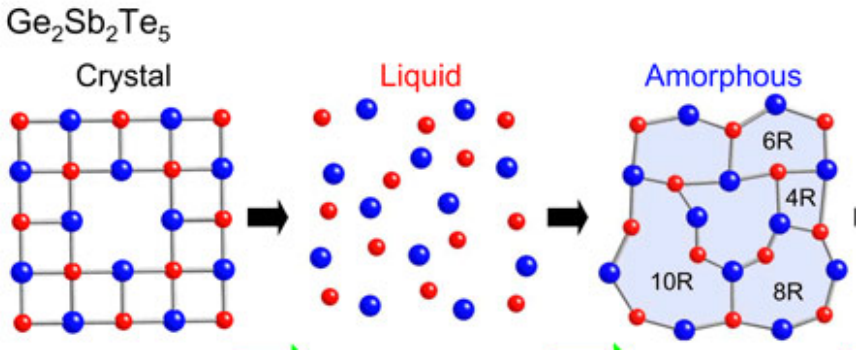
Position of the first peak in $S(q)$ is at $q_0 \simeq 2\pi/\Delta r \simeq 2$ Å^{-1}

"Structure Factor and Radial Distribution Function for Liquid Argon at 85K",

Yarnell, Katz, Wenzel & König, Phys. Rev. Lett. 7, 2130 (1973)

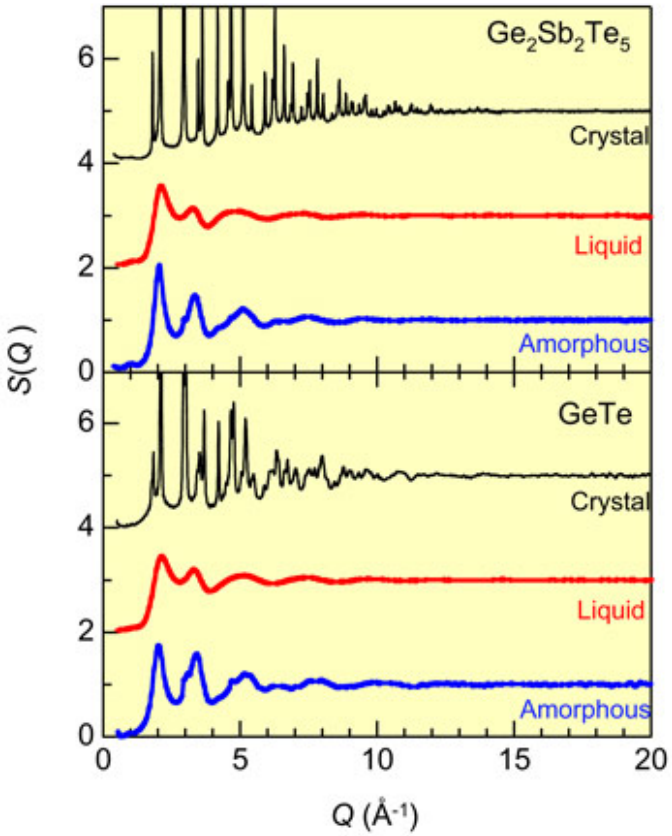
Observables

Structure factors



"RMC Analyses Solve High-Speed Phase-Change Mechanism"

Matsunaga, Kojima, Yamada, Kohara, Takata (2006)



Harmonic solids

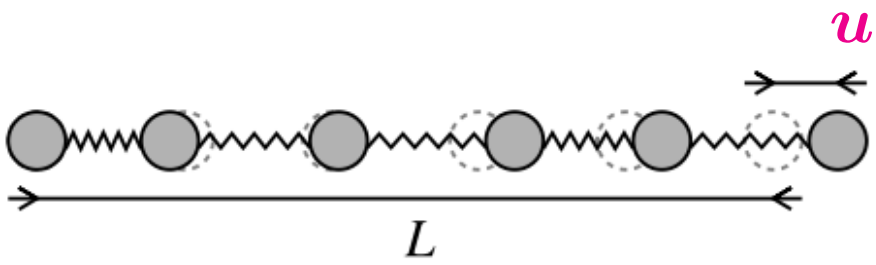
Peierls calculation

Consider a crystal made of atoms connected to their nearest-neighbours (nn) by Hooke springs.

Call $\phi_{\boldsymbol{R}_i}$ the position of the atom that, at zero temperature, is located at a vertex of a regular lattice with position $\boldsymbol{R}_i$.

At finite temperature the atomic positions fluctuate, $\phi_{\boldsymbol{R}_i} = \boldsymbol{R}_i + \boldsymbol{u}_{\boldsymbol{R}_i}$, with $\boldsymbol{u}_{\boldsymbol{R}_i}$ the local displacement from $\boldsymbol{R}_i$.

Sketch



Dashed: perfect lattice positions Gray: actual positions.

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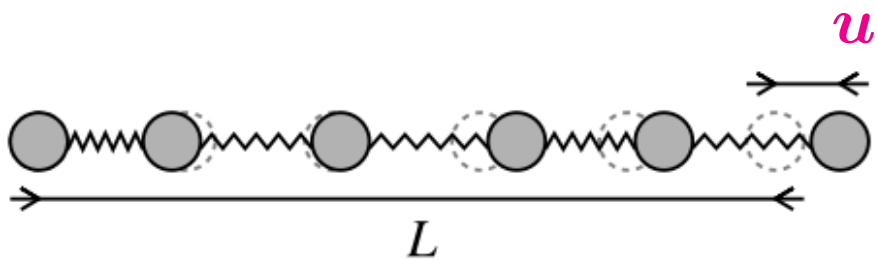

Does the long-range positional order survive at finite T ?

Harmonic solids

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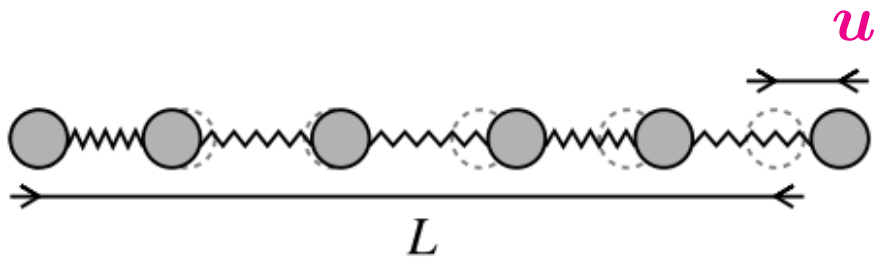
Sketch



In particular, do $2d$ crystals exist at finite T ?

Harmonic solids

Peierls calculation

Consider a crystal made of atoms connected to their nn by Hooke springs.

At finite temperature $\boldsymbol{\phi}_{\boldsymbol{R}_i} = \boldsymbol{R}_i + \boldsymbol{u}_{\boldsymbol{R}_i}$.

The potential energy is

$$U = \frac{K}{2} \sum_{\langle ij \rangle} (\boldsymbol{u}_{\boldsymbol{R}_i} - \boldsymbol{u}_{\boldsymbol{R}_j})^2 \approx \frac{K}{2} \int d^d r \, [\nabla \boldsymbol{u}(\boldsymbol{r})]^2$$

a quadratic Hamiltonian that can be diagonalised going to Fourier space

$$U \approx \frac{K}{2} \int \frac{d^d k}{(2\pi)^d} \, k^2 \, |\tilde{\boldsymbol{u}}(\boldsymbol{k})|^2$$

Harmonic solids

Peierls calculation

Look at the displacement field, $\boldsymbol{u}(\boldsymbol{r},t)$, in Fourier transform

$$\boldsymbol{u}(\boldsymbol{r}) = \int \frac{d^d\boldsymbol{k}}{(2\pi)^2}\, \tilde{u}(\boldsymbol{k})\, e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}$$

The Hamiltonian in the continuum limit

$$U = \frac{K}{2}\int d^d\boldsymbol{r}\, [\nabla \boldsymbol{u}(\boldsymbol{r})]^2 = \frac{K}{2}\int \frac{d^d\boldsymbol{k}}{(2\pi)^d}\, k^2\, |\tilde{\boldsymbol{u}}(\boldsymbol{k})|^2$$

is the one of a set of independent harmonic oscillators (phonons).

Assuming canonical equilibrium at inverse temperature β, for each $\boldsymbol{k}$

$$\langle |\tilde{u}(\boldsymbol{k})|^2 \rangle \propto \frac{k_B T}{K k^2}$$

The density of states of the phonons (how many of them there are with k between k and $k+dk$) is $\Omega(k) \propto k^{d-1}$

Harmonic solids

Peierls calculation

Let's go back to real space and compute the mean-square displacement

$$\Delta^2(\boldsymbol{r}) = \langle [\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{0})]^2 \rangle$$

Using the equipartition result $\langle |\tilde{u}(\boldsymbol{k})|^2 \rangle \propto k_B T/(K k^2)$,

$$\Delta^2(\boldsymbol{r}) \;=\; \frac{k_B T}{K} \int d^d \boldsymbol{k}\, \frac{1 - \cos \boldsymbol{k}\cdot\boldsymbol{r}}{k^2} \;\approx\; \frac{k_B T}{K} \int_{1/r}^{1/a} dk\; k^{d-1}\, \frac{1}{k^2}$$

and

$$\Delta^2(\boldsymbol{r}) \equiv \langle (\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{0}))^2 \rangle \simeq \frac{k_B T}{K} \begin{cases} r & d = 1 \\ \boxed{\ln r} & d = 2 \\ \text{cst} & d \geq 3 \end{cases}$$

Quasi long-range order in $d = 2$

Mermin-Wagner theorem

Consequences

A continuous symmetry cannot be spontaneously broken in $2d$.

(The Hamiltonian $\frac{K}{2}\int d^d r\ [\nabla \boldsymbol{u}(\boldsymbol{r})]^2$ is invariant under global rotations of $\boldsymbol{u}$)

Corollary: a crystal with long-range order cannot exist at $T>0$ in $d=2$.

Reason: in low d fluctuations are more effective and inhibit order.

Quasi long-range positional order with algebraically decaying correlations is possible, $C(r)\simeq r^{-\eta}$.

Note the similarity with the $2d$ XY model of magnetism, $\boldsymbol{s}_i=(\cos\theta_i,\sin\theta_i)$

$$-\frac{H}{J}=\sum_{\langle ij\rangle}\boldsymbol{s}_i\cdot\boldsymbol{s}_j=\sum_{\langle ij\rangle}\cos\theta_{ij}\simeq\sum_{\langle ij\rangle}(1-\frac{\theta_{ij}^2}{2})\approx-\frac{1}{2}\int d^2r\ [\boldsymbol{\nabla}\theta(\boldsymbol{r})]^2$$

Berezinskii-Kosterlitz-Thouless

The $2d$ XY model

At very high temperature one expects disorder.

At very low temperature the harmonic approximation is exact and there is quasi long-range order.

There must be a transition in between.

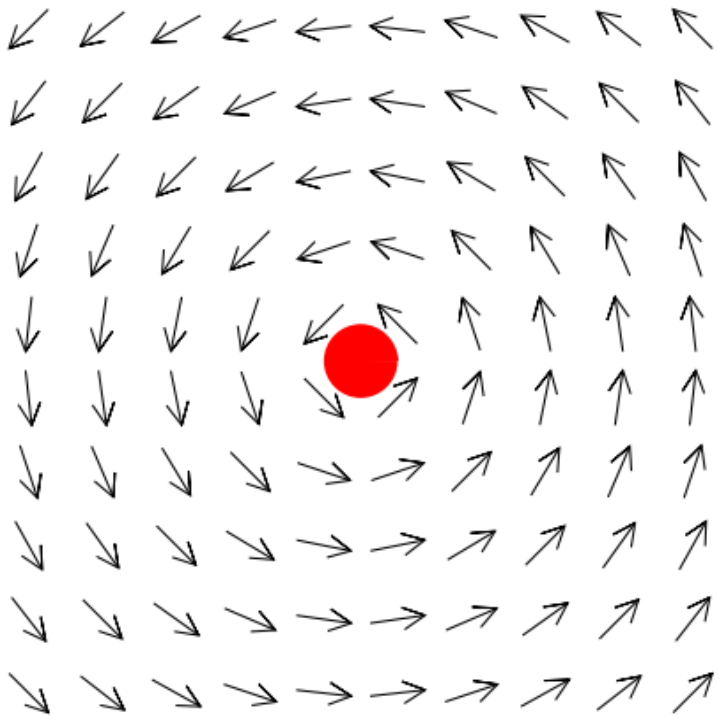
Assumption: the transition is continuous and it is determined by the unbinding of vortices (topological defects).

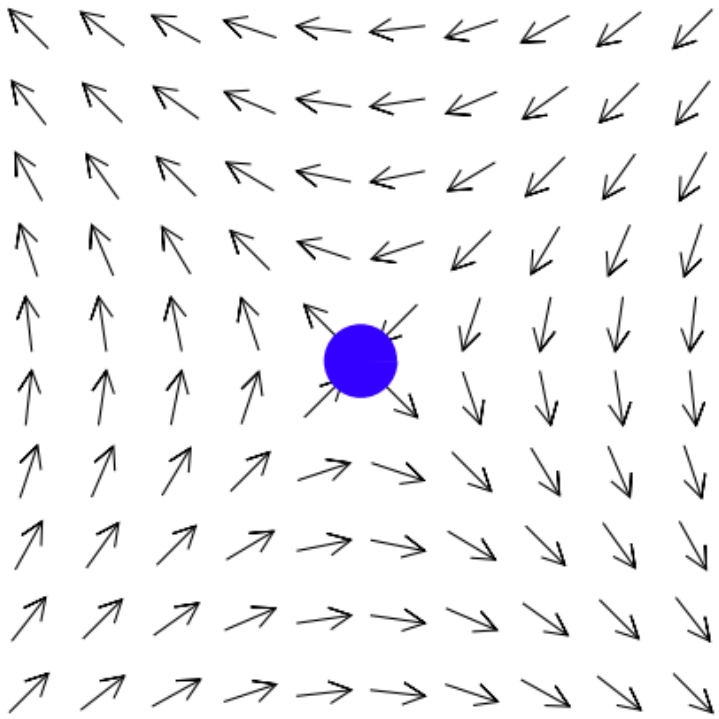
Proved with RG, assuming a continuous phase transition.

The correlation length diverges exponentially $\xi_{\rm eq} \simeq e^{a/|T-T_{\rm BKT}|^{-\nu}}$ at $T_{\rm BKT}$ and it remains infinite in the phase with quasi long-range order.

2d XY model

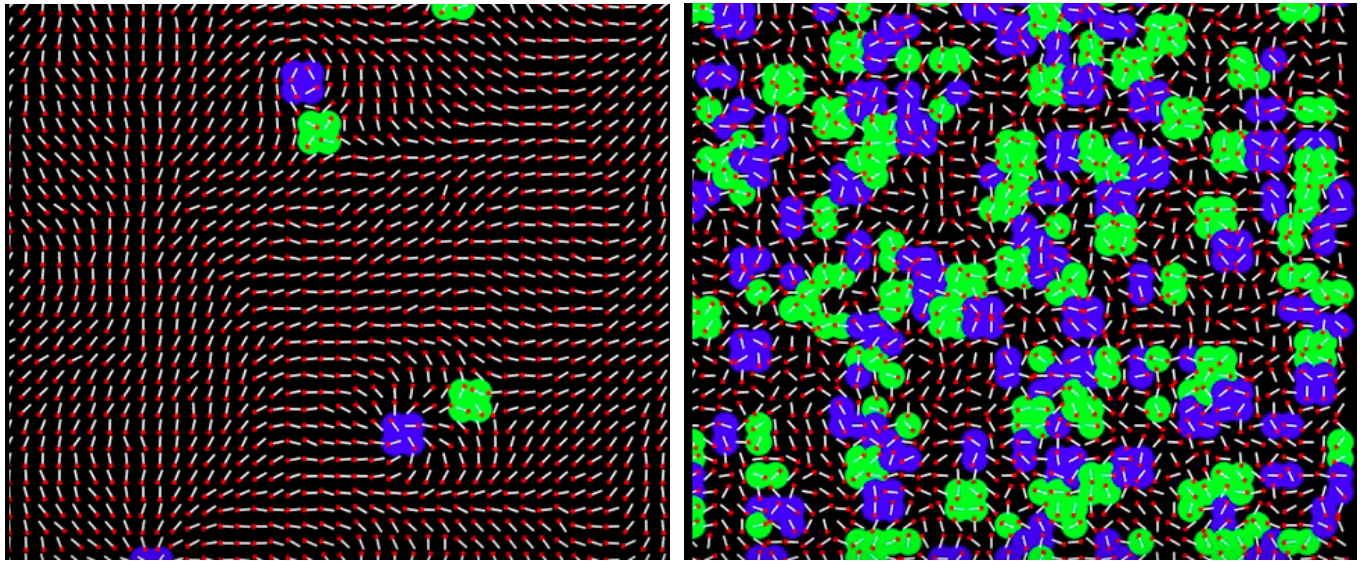
Vortices





2d XY model

BKT transition



$T < T_{\mathrm{BKT}}$

A few paired vortices

$T > T_{\mathrm{BKT}}$

Vortices are all over and unbound

A small portion of a much larger system with periodic boundary conditions is shown.

Images copied from **S. Burton's site**

BKT-Halperin-Nelson-Young

The $2d$ particle systems

At very high temperature one expects disorder.

At very low temperature the harmonic approximation is exact and there is quasi long-range order.

There must be a transition in between.

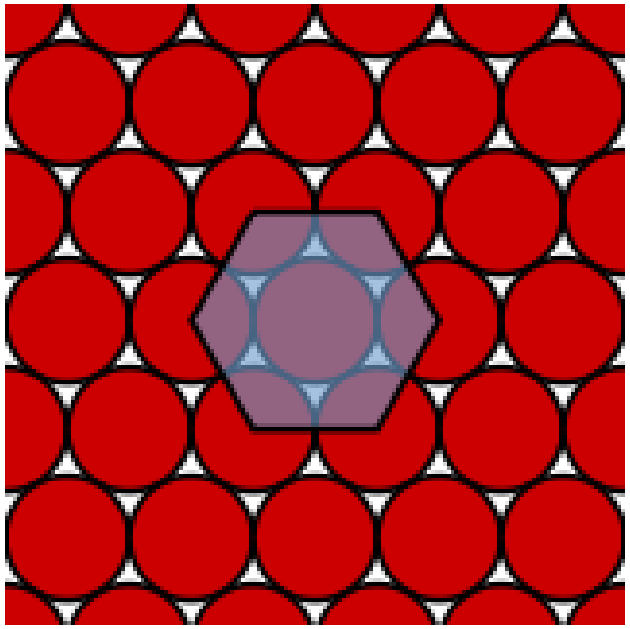
Assumption: the transition is continuous and it is determined by the unbinding of dislocations in the solid (topological defects).

Proved with RG that assumes a continuous phase transition.

The correlation length diverges exponentially $\xi_{\rm eq} \simeq e^{a/|T-T_{\rm c}|^{-\nu}}$ at T_c and it remains infinite in the phase with quasi long-range order.

Close packing of disks

Triangular lattice for identical disks: the perfect crystal



The centres of the disks form a triangular lattice.

By joining these centres in the form shown in the figure one forms an hexagon.

The connectivity of the triangular lattice is six.

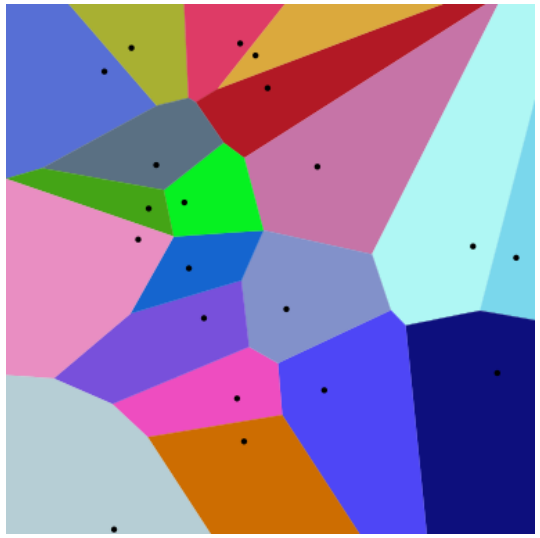
Defects will be associated to centres with less or more neighbours.

Observables

Voronoi tessellation

A Voronoi diagram is induced by a set of points, called sites, that in our case are the centres of the disks.

The plane is subdivided into faces that correspond to the regions where one site is closest.



Focus on the central light-green face

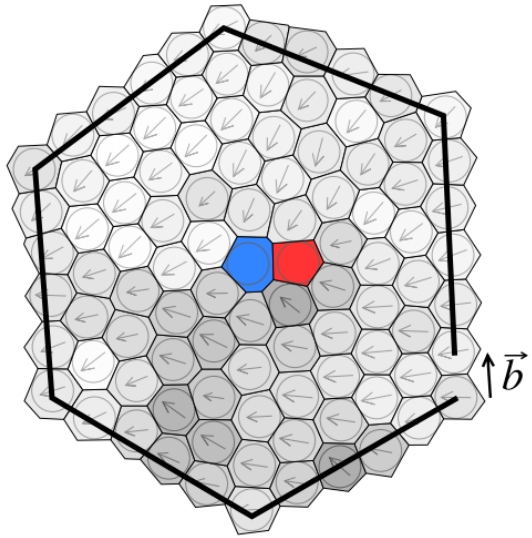
All points within this region are closer to the dot within it than to any other dot on the plane

The region has five neighbouring cells from which it is separated by an edge

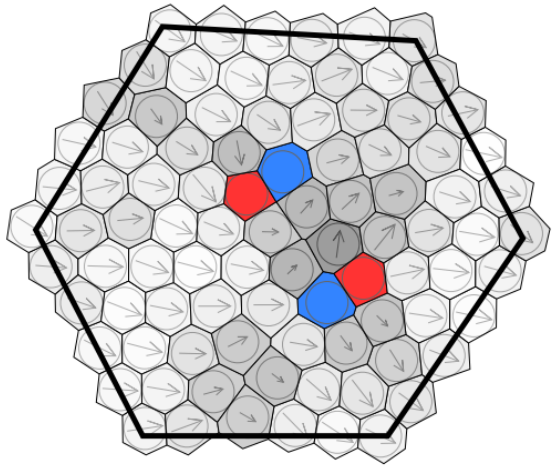
The grey zone has six neighbouring cells

Close packing of disks

Disks, Voronoi cells & dislocations



A free dislocation



A bound pair of dislocations

In the crystal the centers of the disks form a triangular lattice

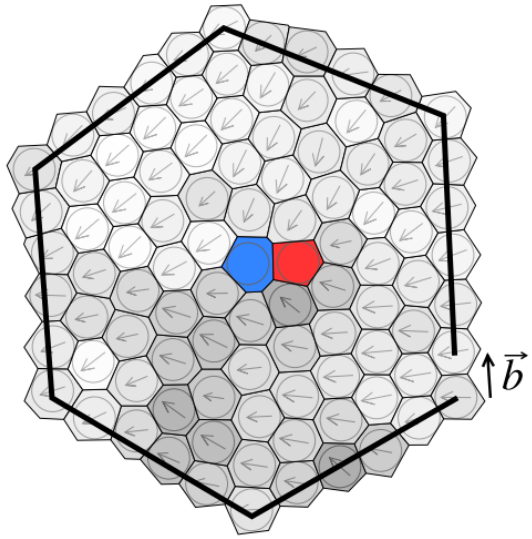
The **blue** disks have seven neighbours and the **red** ones have five.

On the left image : the external path fails to close and form a perfect hexagon.

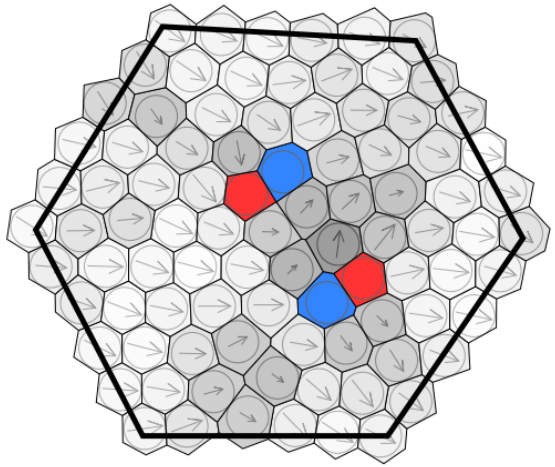
The effect of the defect spreads over the full system.

Close packing of disks

Disks, Voronoi cells & dislocations



A free dislocation



A bound pair of dislocations

In the crystal the centers of the disks form a triangular lattice

The **blue** disks have seven neighbours and the **red** ones have five.

On the right image : the external path closes and forms a perfect hexagon. The effects of the defects are confined.

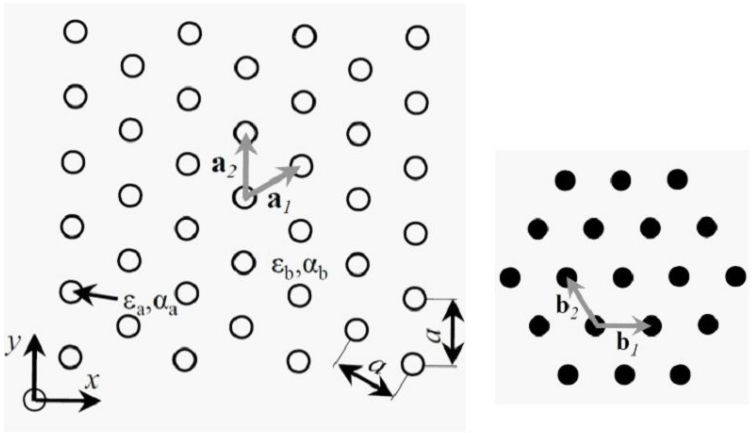
Observables

Structure factor

$\boldsymbol{r}_i$ and $\boldsymbol{r}_j$ are the positions of the beads i and j and $\boldsymbol{q}$ is the wave-vector :

$$S(\boldsymbol{q}) = \frac{1}{N} \sum_{ij} e^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)}$$

Visualisation : two dimensional representation in the (q_x, q_y) plane.

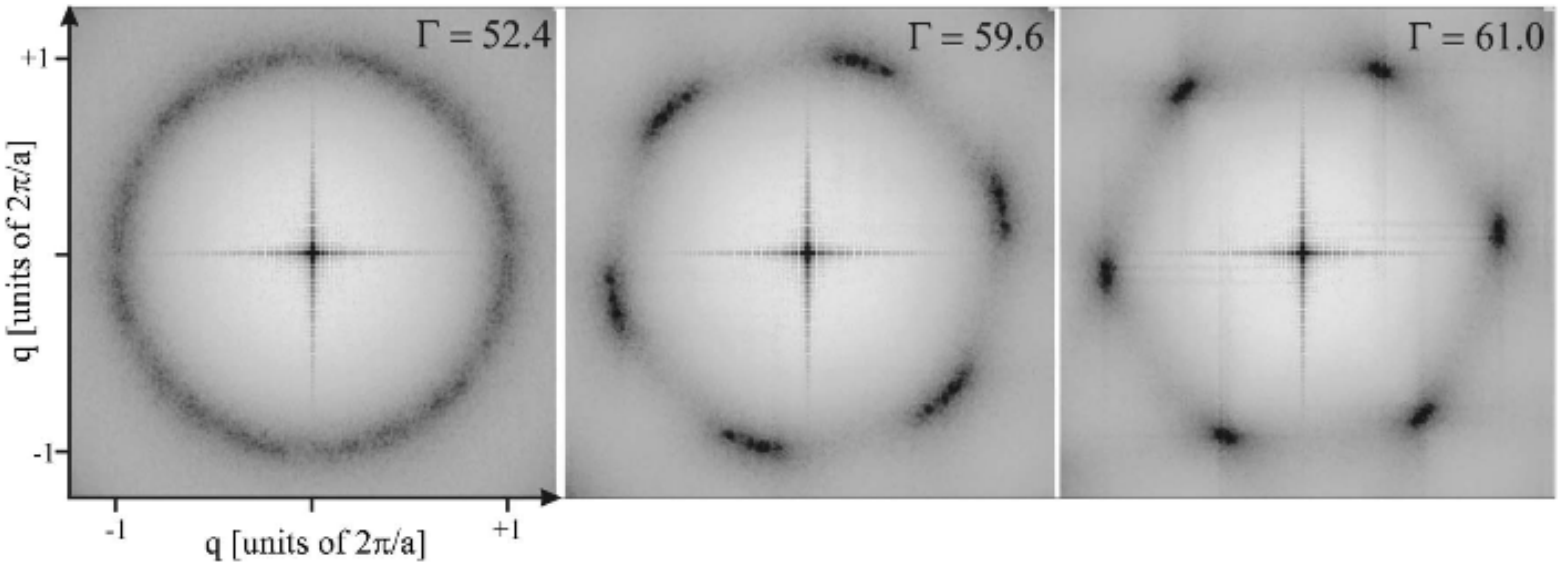


Triangular lattice in real space

Hexagonal lattice in reciprocal space

$2d$ Freezing

Structure factor in $2d$ colloidal suspensions



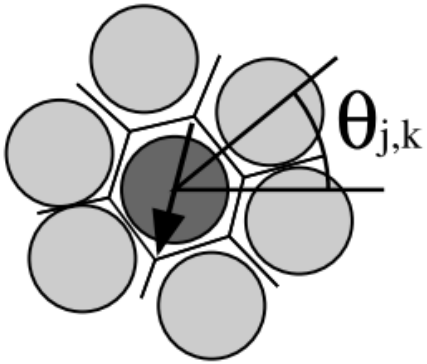
Liquid (later) Solid

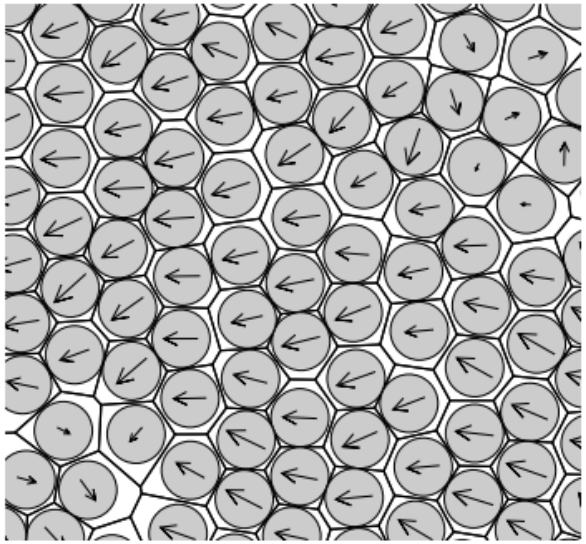
Γ is the inverse temperature

Figure from **Keim et al. Maret and von Grünberg, Phys. Rev. E 75, 031402 (2007)**

Observables

Hexatic (orientational) order





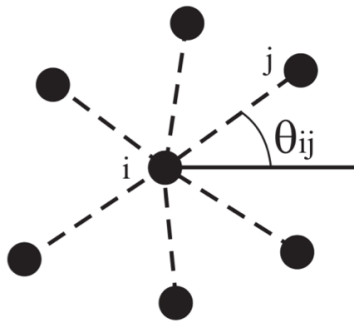
Associating arrows (directions) to disks

Observables

Hexatic order

The local hexatic variable

$$\psi_{6i} = \frac{1}{N^i_{\rm nn}} \sum_{j=1}^{N^i_{\rm nn}} e^{6{\rm i}\theta_{ij}}$$



with $N^i_{\rm nn}$ the number of nearest (Voronoi) neighbours of bead i and θ_{ij} the angle between the segment that connects i with its neighbour j and the x axis.

For beads placed on the vertices of a triangular lattice, each bead has six nearest-neighbours, $j = 1, \ldots, 6$, the angles are $\theta_{ij} = 2\pi j/6$ and $\psi_{6i} = 1$ for all i.

measures orientational order

Observables

Hexatic order

The local hexatic fluctuating order

$$\psi_{6i} = \frac{1}{N^i_{\rm nn}} \sum_{j=1}^{N^i_{\rm nn}} e^{6{\rm i}\theta_{ij}}$$

We also look at the average of the modulus and modulus of the average

$$2N\,\psi_6 = \left| \sum_{i=1}^{N} \psi_{6i} \right| \qquad\qquad 2N\,\Gamma_6 = \sum_{i=1}^{N} |\psi_{6i}|$$

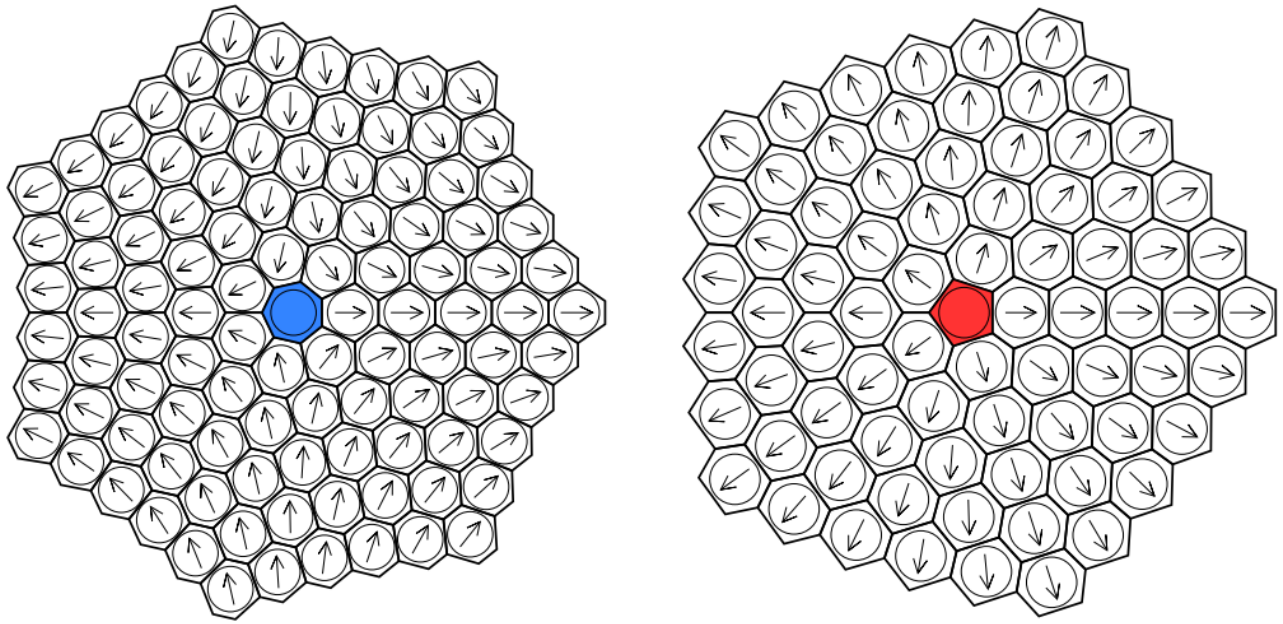
and the correlation functions

$$g_6(r) = \frac{\sum_{ij} [\langle \psi^*_{6i} \psi_{6j} \rangle] \Big|_{r_{ij}=r}}{[\langle |\psi_{6i}|^2 \rangle]}$$

Note that the normalisation is site independent

Close packing of disks

Disclinations



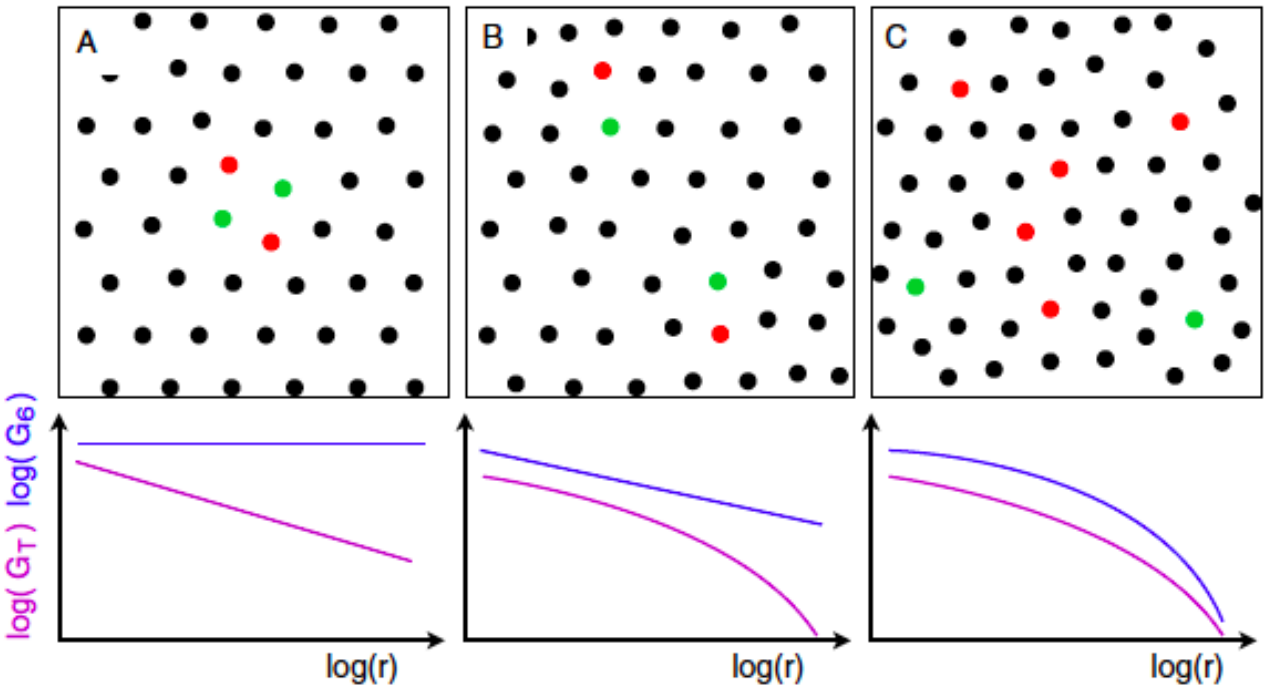
The orientation winds by $\pm 2\pi$ around the **blue** (seven) and **red** (five) defects.

Very similar to the vortices in the $2d$ XY magnetic model.

BKTNHY scenario : the unbinding of vortices drives another BKT-like transition.

Correlation functions

Sketches

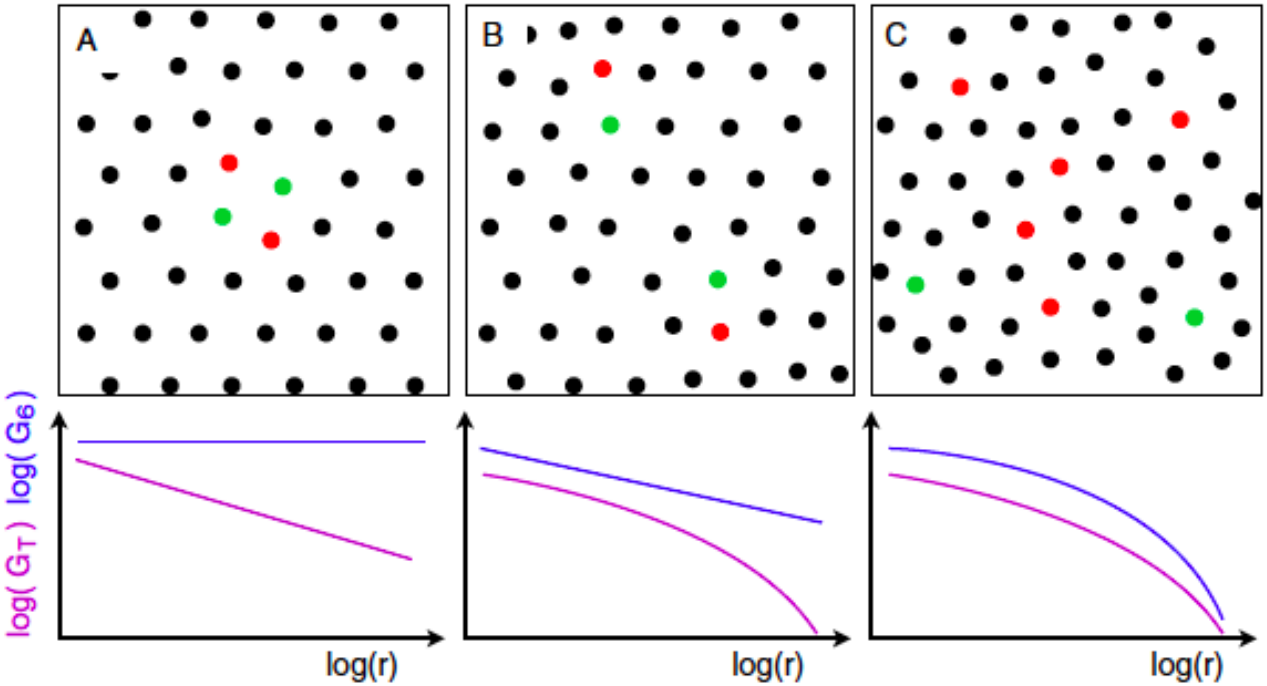


Solid Hexatic Liquid

Figure from **Gasser, J. Phys. : Cond. Matt. 21, 203101 (2009)**

Correlation functions

Hexatic



long r: $G_6(r) = \begin{cases} \text{ct} & \text{solid} & \text{long range order} \\ r^{-\eta_6} & \text{hexatic} & \text{short range order} \\ e^{-r/\xi_6} & \text{isotropic} & \text{disorder} \end{cases}$

$2d$ colloidal suspensions

Hexatic correlation functions

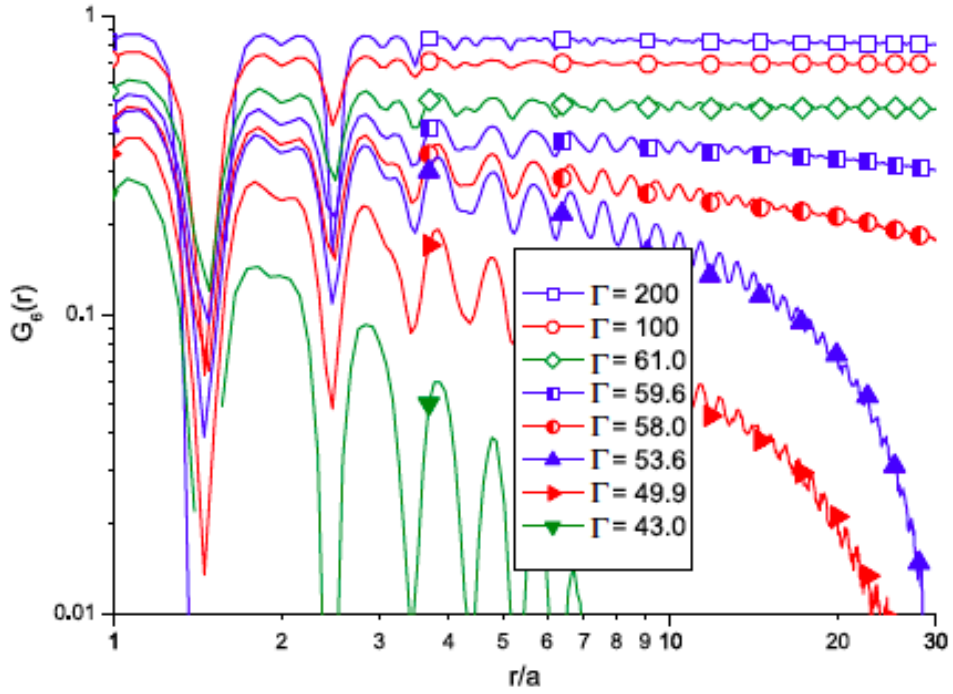
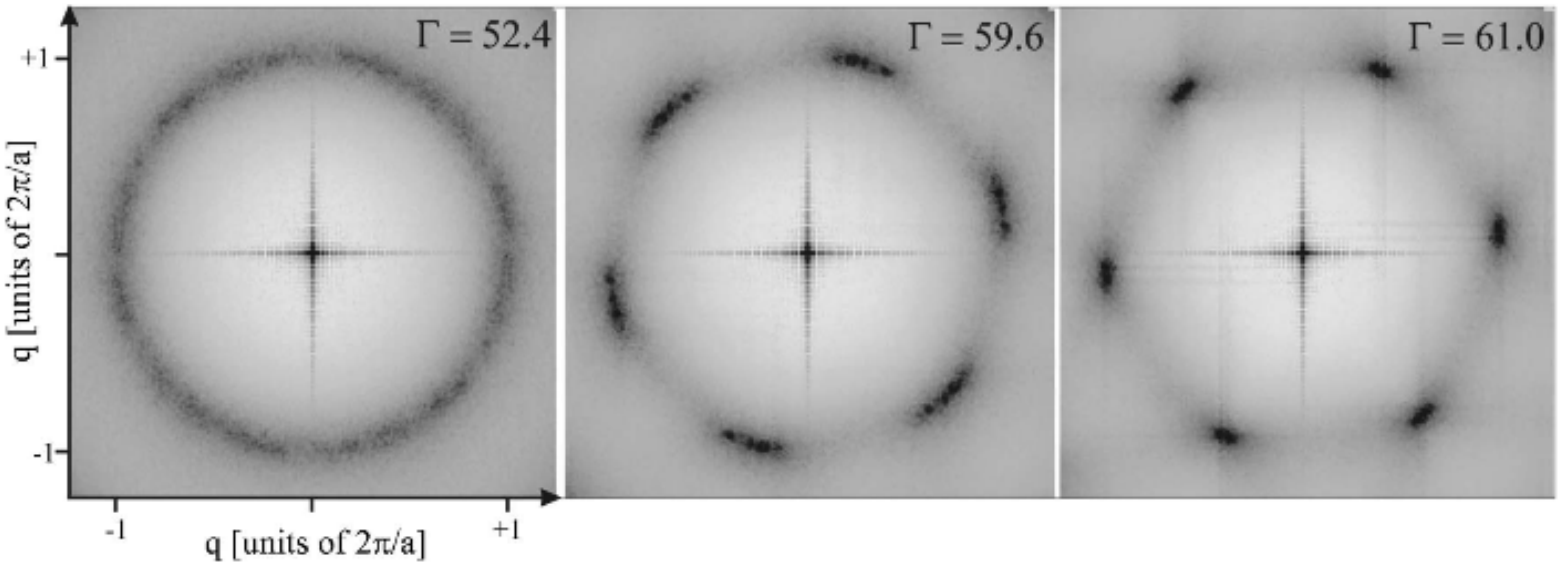


Figure from **Keim, Maret and von Grünberg, Phys. Rev. E 75, 031402 (2007)**

$2d$ Freezing

Structure factor in $2d$ colloidal suspensions



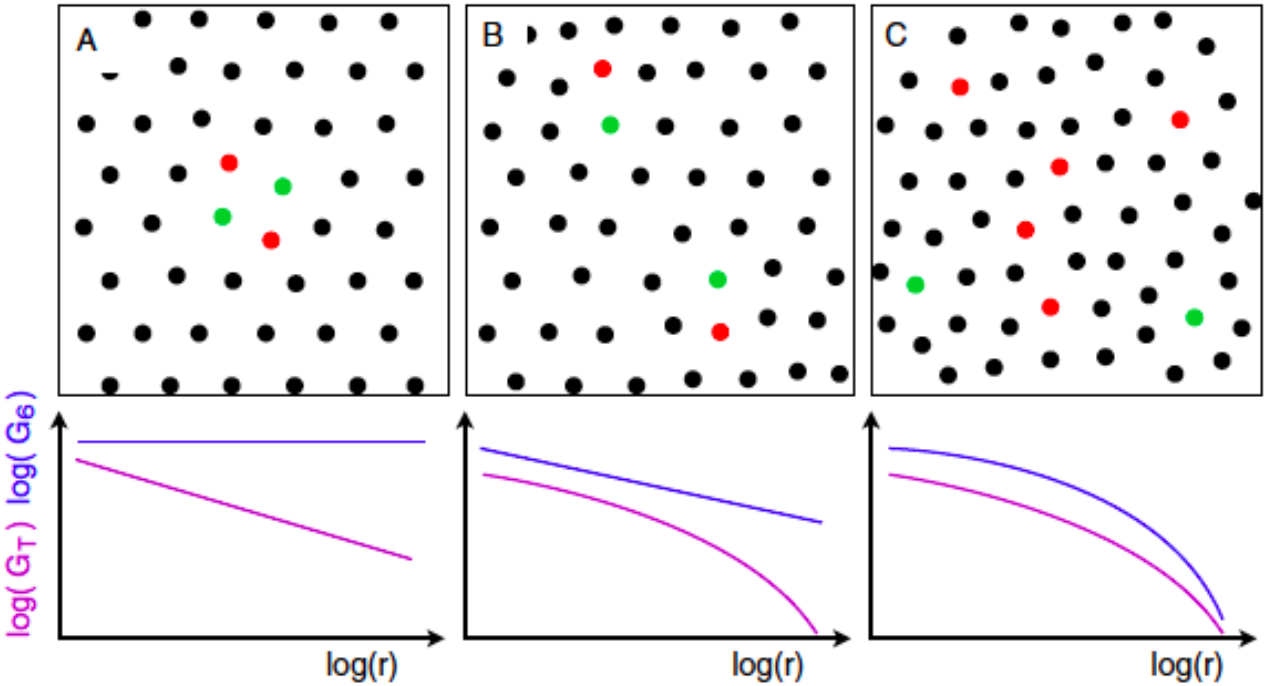
Liquid Hexatic Solid

Γ is the inverse temperature

Figure from **Keim et al. Maret and von Grünberg, Phys. Rev. E 75, 031402 (2007)**

Correlation functions

Positional



long r: $G_T(r) = \begin{cases} r^{-\eta} & \text{solid} \quad \text{quasi long range order} \\ e^{-r/\xi} & \text{hexatic} \quad \text{disorder} \\ e^{-r/\xi} & \text{isotropic} \quad \text{disorder} \end{cases}$

$2d$ Freezing

BKTHNY

	BKTHNY
Solid	QLR positional & LR orientational
transition	BKT (unbinding of dislocations)
Hexatic phase	SR positional & QLR orientational
transition	BKT (unbinding of disclinations)
Liquid	SR positional & orientational

In the (T, ϕ) phase diagram.

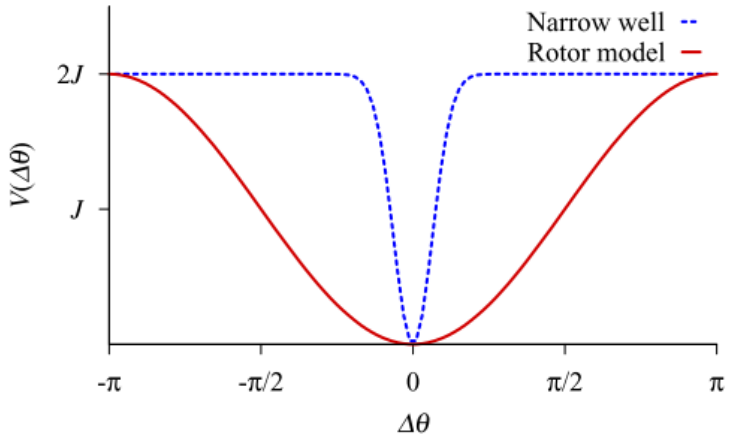
Berezinskii-Kosterlitz-Thouless

Lack of universality of the transition in XY models

The RG proof yields, actually, an upper limit for the stability of the quasi long-range ordered phase.

A first order phase transition at a lower T can preempt the BKT one.

It does for sufficiently steep potentials:



"First order phase transition in an XY model with nn interactions"

Domany, Schick & Swendsen, Phys, Rev. Lett. 52, 1535 (1984)

$2d$ Freezing

BKTHNY *vs.* a new scenario by Bernard & Krauth

	BKTHNY	BK
Solid	QLR pos & LR orient	QLR pos & LR orient
transition	BKT (unbinding of dislocations)	BKT
Hexatic phase	SR pos & QLR orient	SR pos & QLR orient
transition	BKT (unbinding of disclinations)	**1st order**
Liquid	SR pos & orient	SR pos & orient

Basically, the phases are the same, but the low-lying transition is different, allowing for coexistence of the liquid and hexatic phases.

Hard disks in two dimensions

Orientation vector construction

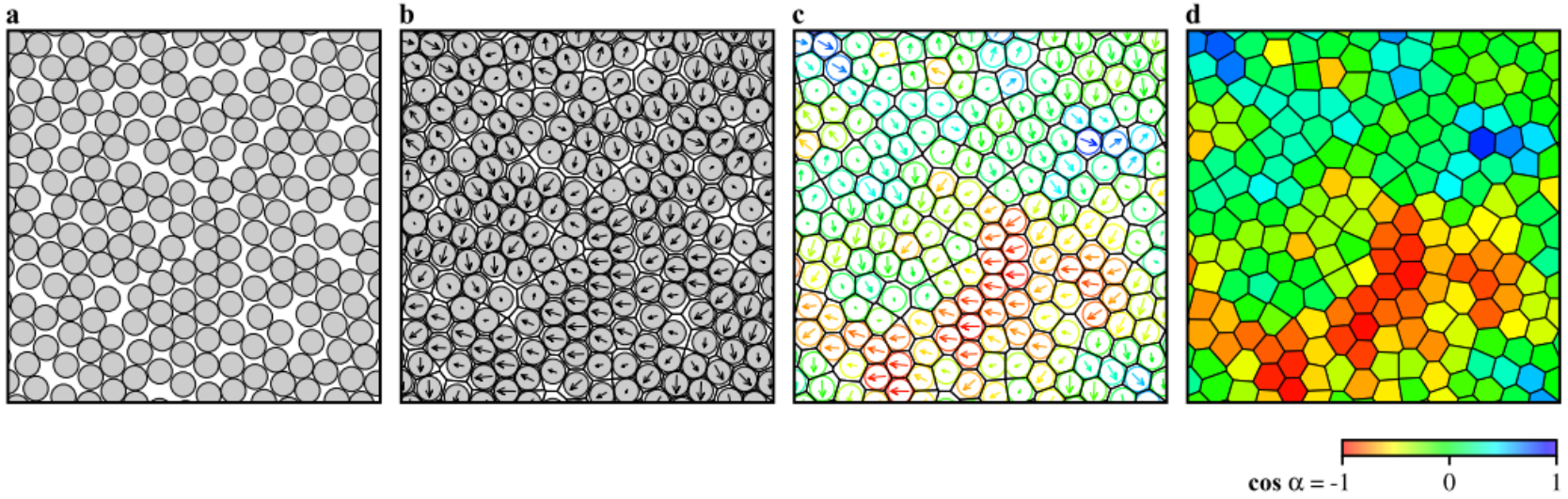


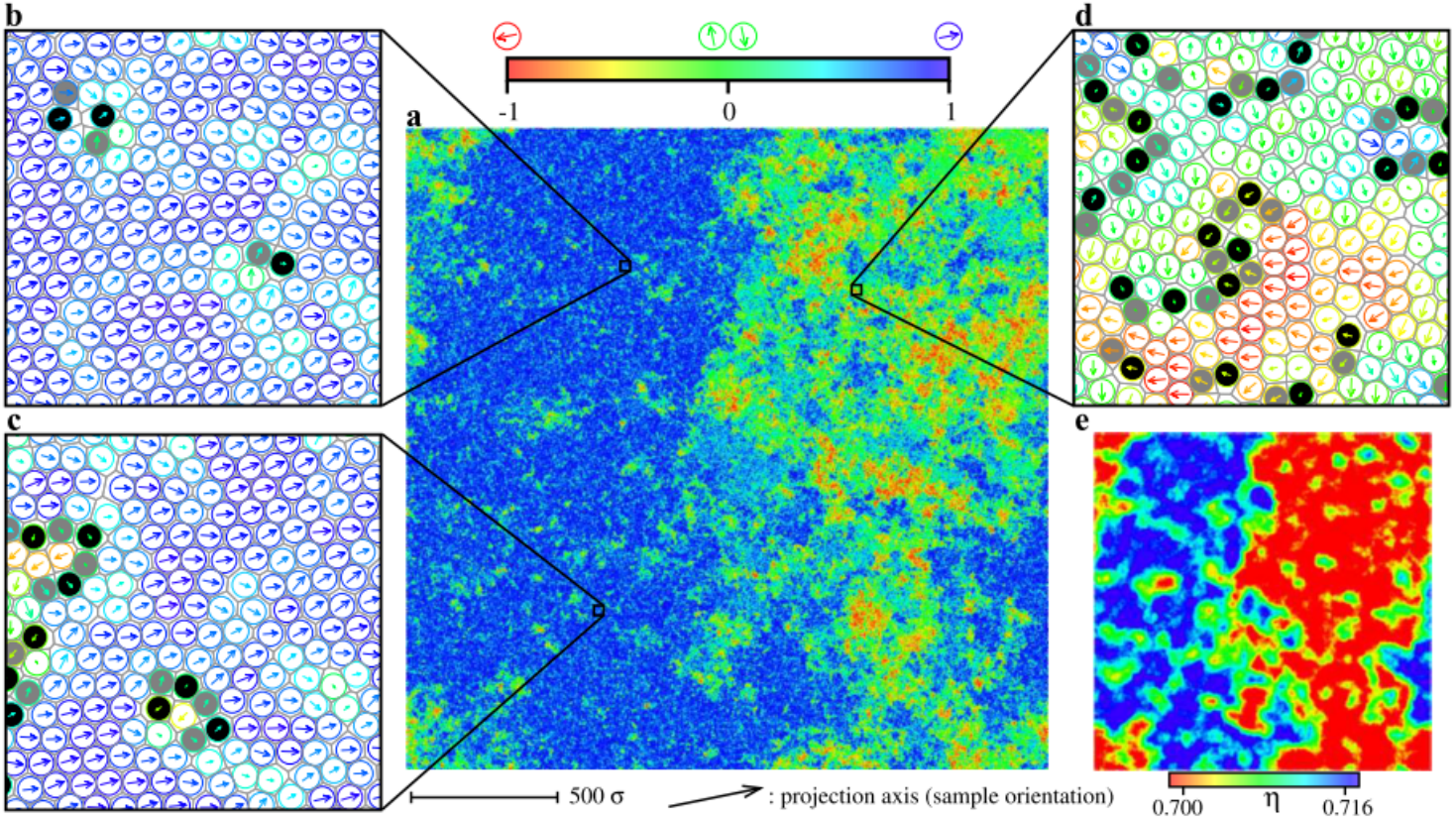
Figure 3.4: Close view of the construction for the visualization of the orientational field. **a**: Hard disks **b**: Voronoi construction, the arrows represent the local orientations. **c**: Coloration of the orientation depending on their projection toward a given axis. **d**: The Voronoi cells are colored. (Ref [6], cf. Section 7.3).

"Two-step melting in two dimensions : first-order liquid-hexatic transition"

Bernard & Krauth, Phys. Rev. Lett. 107, 155704 (2011)

Hard disks in two dimensions

Coexistence

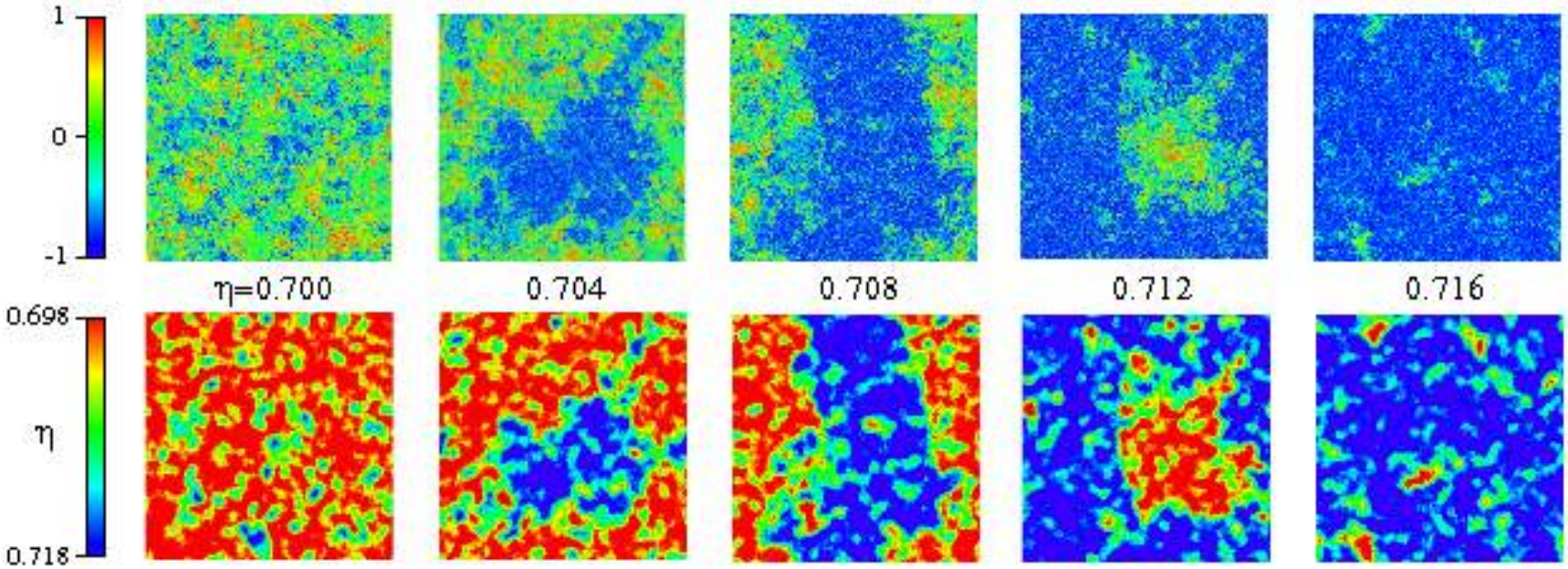


"Two-step melting in two dimensions : first-order liquid-hexatic transition"

Bernard & Krauth, Phys. Rev. Lett. 107, 155704 (2011)

Hard disks in two dimensions

Correlation between the local orientation and density

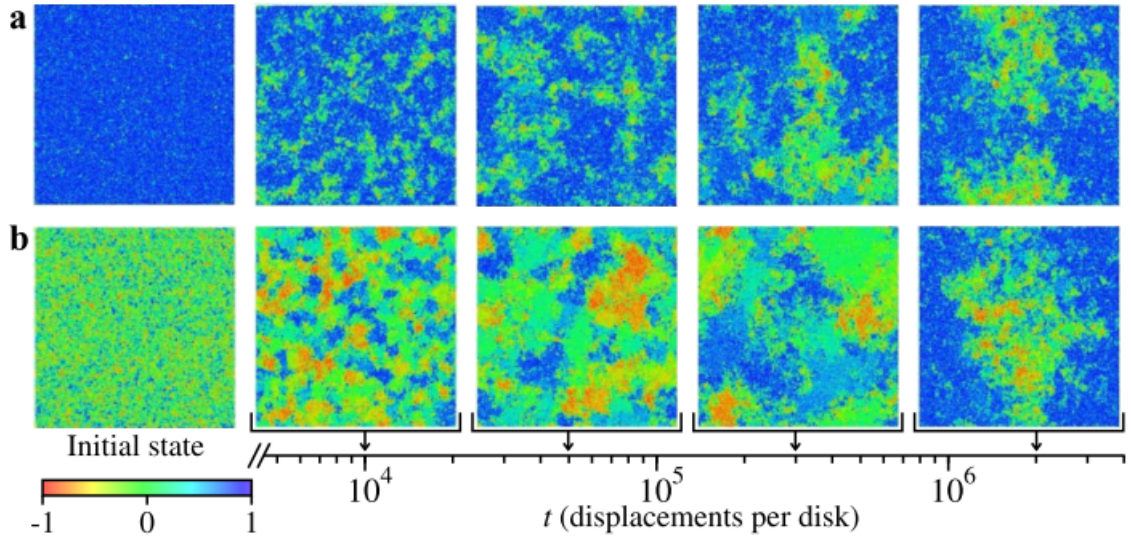


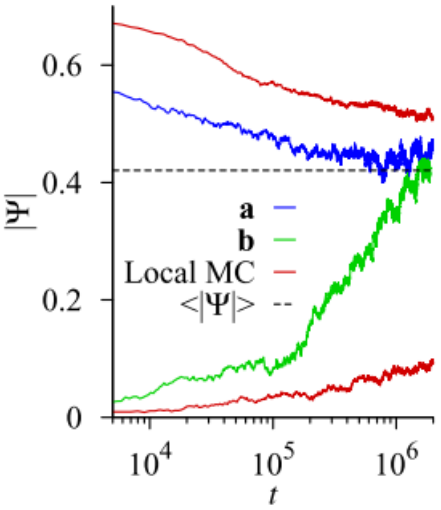
"Two-step melting in two dimensions : first-order liquid-hexatic transition"

Bernard & Krauth, Phys. Rev. Lett. 107, 155704 (2011)

Hard disks in two dimensions

Time evolution from different initial states in the co-existence region





Initial state solid in **a**, liquid in **b**.

Red lines obtained w/simple MC, other w/smart algorithm

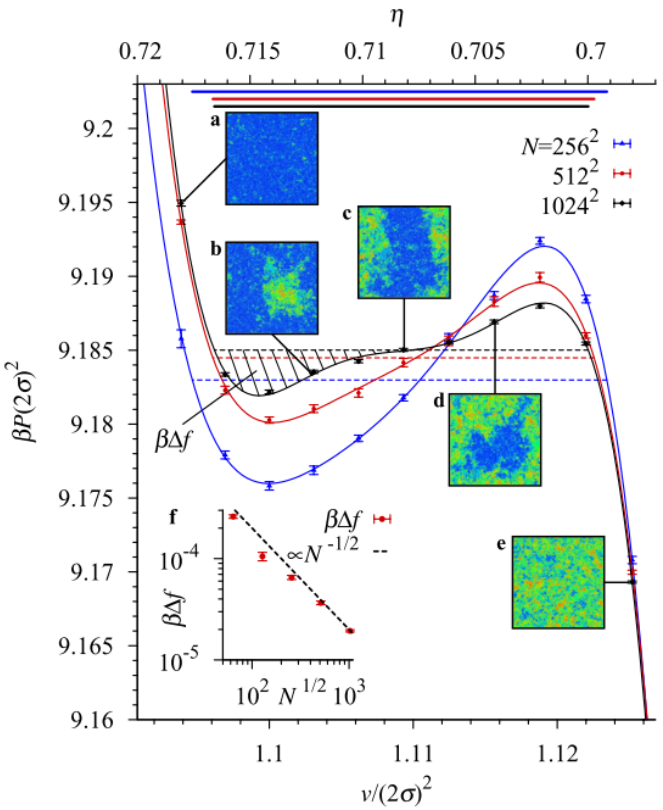
"Two-step melting in two dimensions : first-order liquid-hexatic transition"

Bernard & Krauth, Phys. Rev. Lett. 107, 155704 (2011)

Hard disks in two dimensions

Pressure loop and finite N dependence

Hexatic Liquid



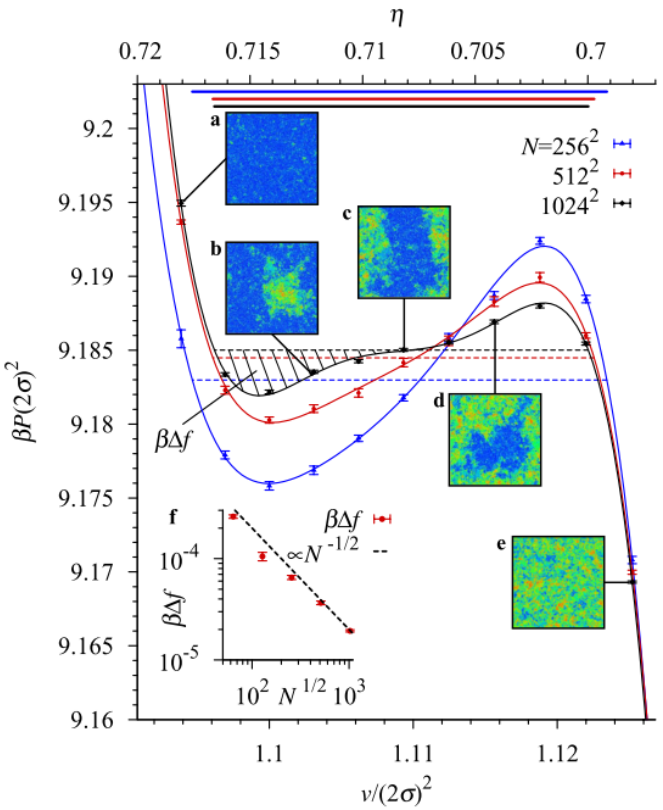
Similar to Van der Waals model for 1st order phase transitions

P cannot increase with V (stability): phase separation *via* Maxwell construction

Hard disks in two dimensions

Pressure loop and finite N dependence

Hexatic Liquid



A system with PBCs has a $\sim$ flat interface with surface energy scaling as $S \simeq L^{d-1} = \sqrt{N}$ and $f \simeq N^{-1/2}$. Verified in the inset for $\phi \simeq 0.708$

Summary

4th Lecture : equilibrium phases of $2d$ matter

- 2d passive systems made of hard or soft disks in interaction

	BKTHNY	BK
Solid	QLR pos & LR orient	QLR pos & LR orient
transition	BKT (unbinding of dislocations)	BKT
Hexatic phase	SR pos & QLR orient	SR pos & QLR orient
transition	BKT (unbinding of disclinations)	**1st order**
Liquid	SR pos & orient	SR pos & orient