Active dumbbells

Leticia F. Cugliandolo

Université Pierre et Marie Curie
Sorbonne Universités
Institut Universitaire de France

leticia@lpthe.jussieu.fr
www.lpthe.jussieu.fr/~leticia

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, 2013-2017)

Amherst, USA, 2017

Problem & questions

From single to many-body

- How does an atypical force, the active force, alter the dynamics of an object (with a given form and mass distribution) immersed in a thermal bath, i.e. subject to friction $\longrightarrow$ dissipation and thermal fluctuations $\longrightarrow$ noise.
- Collective effects of an ensemble of such objects in interaction.
  - Dynamic phase transitions ? $3d$ *vs.* $2d$?
  - Active solid, liquid, gas phases ?
  - Collective dynamics ?

Some reviews : **Fletcher & Geissler 09, Vicsek 10, Menon 10, Ramaswamy 10, Romanczuk et al 12, Cates 12, Marchetti et al. 13, de Magistris & Marenduzzo 15**

Plan

1. Active Brownian dumbbells

2. Two-dimensional equilibrium phases

   Passive limit: Beyond the BKT-Halperin-Nelson-Young scenario

3. Two-dimensional collective behaviour of active systems

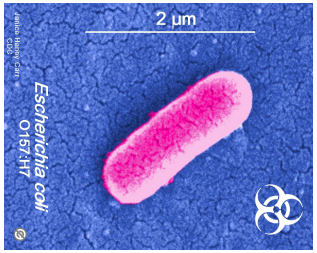
   No mobility induced phase transition (MIP)

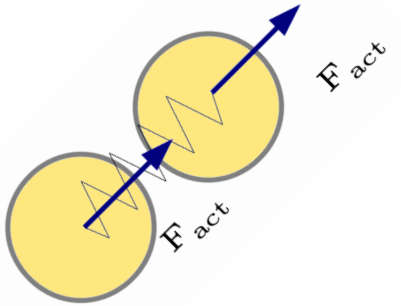
Particles with shape

e.g., a diatomic molecule or a dumbbell : bacteria

Two spherical atoms with diameter $\sigma_{\rm d}$ and mass $m_{\rm d}$

Persistent force





Massless spring modelled by a finite extensible non-linear elastic (fene) force between the atoms $\mathbf{F}_{\rm fene} = -\dfrac{k(\boldsymbol{r}_i - \boldsymbol{r}_j)}{1 - r_{ij}^2/r_0^2}$

Additional repulsive contribution (WCA truncated Lennard-Jones potential) to avoid atomic/colloidal overlapping

Langevin dynamics

a passive dumbbell made of a colloid i and a colloid j

$$
\begin{aligned}
m_{\rm d}\ddot{\boldsymbol{r}}_i(t) &= -\gamma\dot{\boldsymbol{r}}_i(t) + \mathbf{F}_{\rm pot_i}(\boldsymbol{r}_i,\boldsymbol{r}_j) + \boldsymbol{\eta}_i(t) \\
m_{\rm d}\ddot{\boldsymbol{r}}_j(t) &= -\gamma\dot{\boldsymbol{r}}_j(t) + \mathbf{F}_{\rm pot_j}(\boldsymbol{r}_i,\boldsymbol{r}_j) + \boldsymbol{\eta}_j(t)
\end{aligned}
$$

with $\mathbf{F}_{\rm pot} = \mathbf{F}_{\rm wca} + \mathbf{F}_{\rm fene}$, and

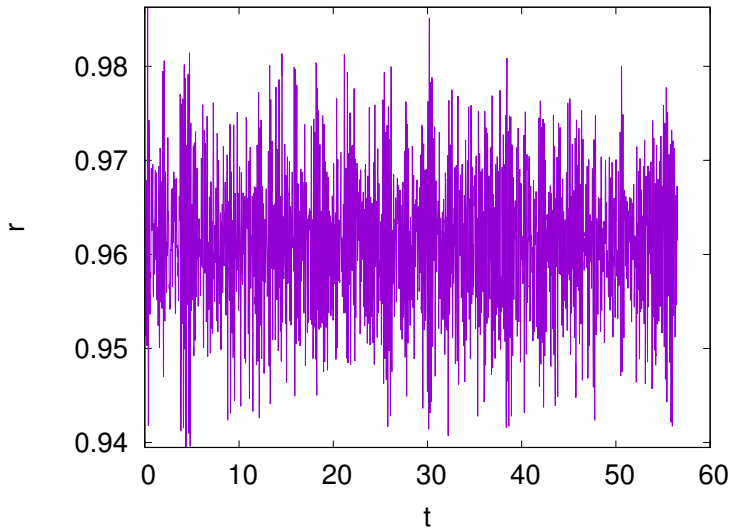
$\boldsymbol{\eta}_{i,j}$ independent thermal noises acting on the two beads, both with Gaussian statistics, zero average $\langle \eta_i^a(t)\rangle = 0$ at all times t, and δ-correlations $\langle \eta_i^a(t)\eta_j^b(t')\rangle = 2\,\gamma k_B T\,\delta_{ij}\delta_{ab}\,\delta(t-t')$. Friction coefficient γ

i, j bead labels, $a, b = 1, \ldots, d$ coordinate labels

Single passive dumbbell

Elongation of the molecule

Almost rigid molecule for the parameters chosen (note the vertical scale)



$$r(t) \simeq \sigma_{\mathrm{d}} = 1$$

Vibrations frozen

Langevin dynamics

a dumbbell under an active force

$$
\begin{aligned}
m_{\mathrm{d}}\ddot{\boldsymbol{r}}_i(t) &= -\gamma\dot{\boldsymbol{r}}_i(t) + \mathbf{F}_{\mathrm{pot}_i}(\boldsymbol{r}_i, \boldsymbol{r}_j) + \mathbf{F}_{\mathrm{act}} + \boldsymbol{\eta}_i(t) \\
m_{\mathrm{d}}\ddot{\boldsymbol{r}}_j(t) &= -\gamma\dot{\boldsymbol{r}}_j(t) + \mathbf{F}_{\mathrm{pot}_j}(\boldsymbol{r}_i, \boldsymbol{r}_j) + \mathbf{F}_{\mathrm{act}} + \boldsymbol{\eta}_j(t)
\end{aligned}
$$

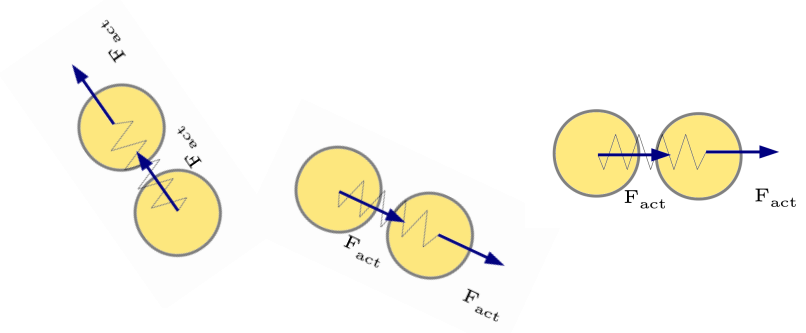
with $\mathbf{F}_{\mathrm{pot}} = \mathbf{F}_{\mathrm{wca}} + \mathbf{F}_{\mathrm{fene}}$

$\boldsymbol{\eta}_{i,j}$ independent thermal white noises acting on the two beads, and

The active force

$$\mathbf{F}_{\mathrm{act}} = F_{\mathrm{act}}\hat{\mathbf{n}}$$

along the main molecular axis

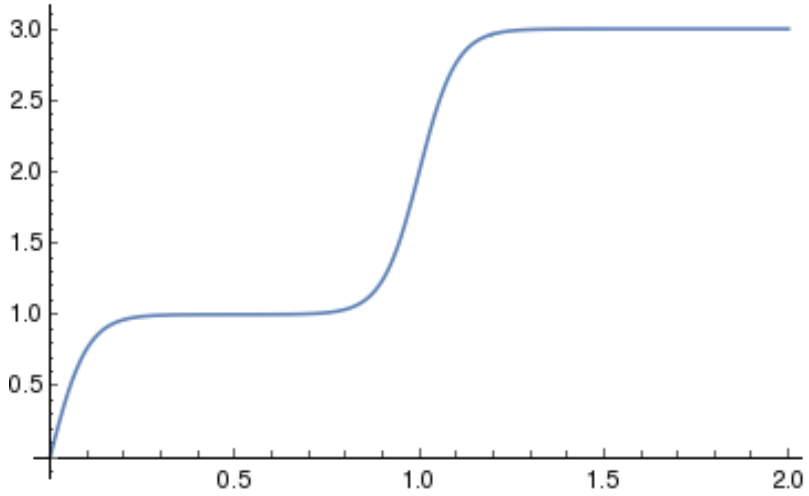


Single active dumbbell

Sketch of position mean-square displacement : new scales

Ballistic t_I Diffusive | $t^* = t_a/\mathrm{Pe}^2$ Ballistic $t_a = D_R^{-1} = \gamma\sigma_\mathrm{d}/(2k_BT)$ Diffusive

$$\Delta^2(t) = \langle[\mathbf{r}(t) - \mathbf{r}(0)]^2\rangle/t$$



t_I t^* t_a t

No $\mathrm{Pe} = \sigma_\mathrm{d}F_\mathrm{act}/(k_BT)$ effect on the angular motion of an isolated dumbbell

Problem & questions

From single to many-body

- How does an atypical force, the active force, alter the dynamics of a particle (with a given form and mass distribution) immersed in a thermal bath, i.e. subject to friction $\longrightarrow$ dissipation and

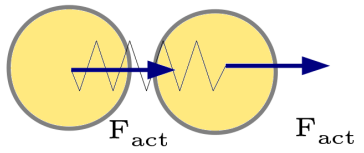
  thermal fluctuations $\longrightarrow$ noise

  Mean-square displacements

- Collective effects of an ensemble of such objects in interaction.
  - Dynamic phase transitions ? $3d$ *vs.* $2d$?
  - Active solid, liquid, gas phases ?
  - Collective dynamics ?

Interacting active dumbbells

Many-body interacting system



Two spherical atoms with diameter σ_{d} and mass m_{d}

Massless spring modelled by a finite extensible non-linear elastic (fene) force between the beads i and j in the same dumbbell, $\mathbf{F}_{\mathrm{fene}} = -\dfrac{k(\boldsymbol{r}_i - \boldsymbol{r}_j)}{1 - r_{ij}^2/r_0^2}$, with an additional repulsive contribution (WCA) to avoid colloidal overlapping.

Polar active force along the main molecular axis $\boxed{\mathbf{F}_{\mathrm{act}} = F_{\mathrm{act}}\,\hat{\mathbf{n}}}$

Purely repulsive WCA interaction between colloids in different molecules.

Langevin modelling of the interaction with the embedding fluid:

isotropic viscous forces, $-\gamma\dot{\boldsymbol{r}}_i$, and independent noises, $\boldsymbol{\eta}_i$, on the beads.

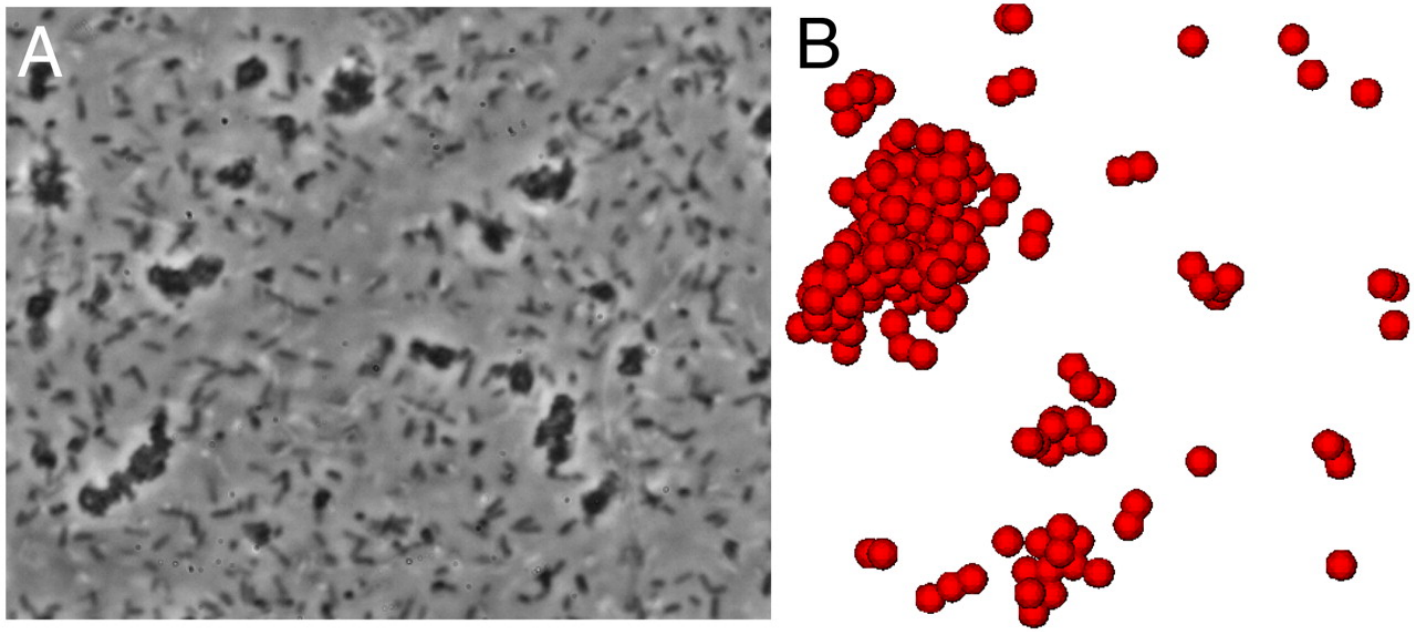
Active dumbbells

Collective effects at intermediate ϕ

$\phi = 0.4$, Pe = 40, $T = 0.05$

Bacteria colony

Phase segregation



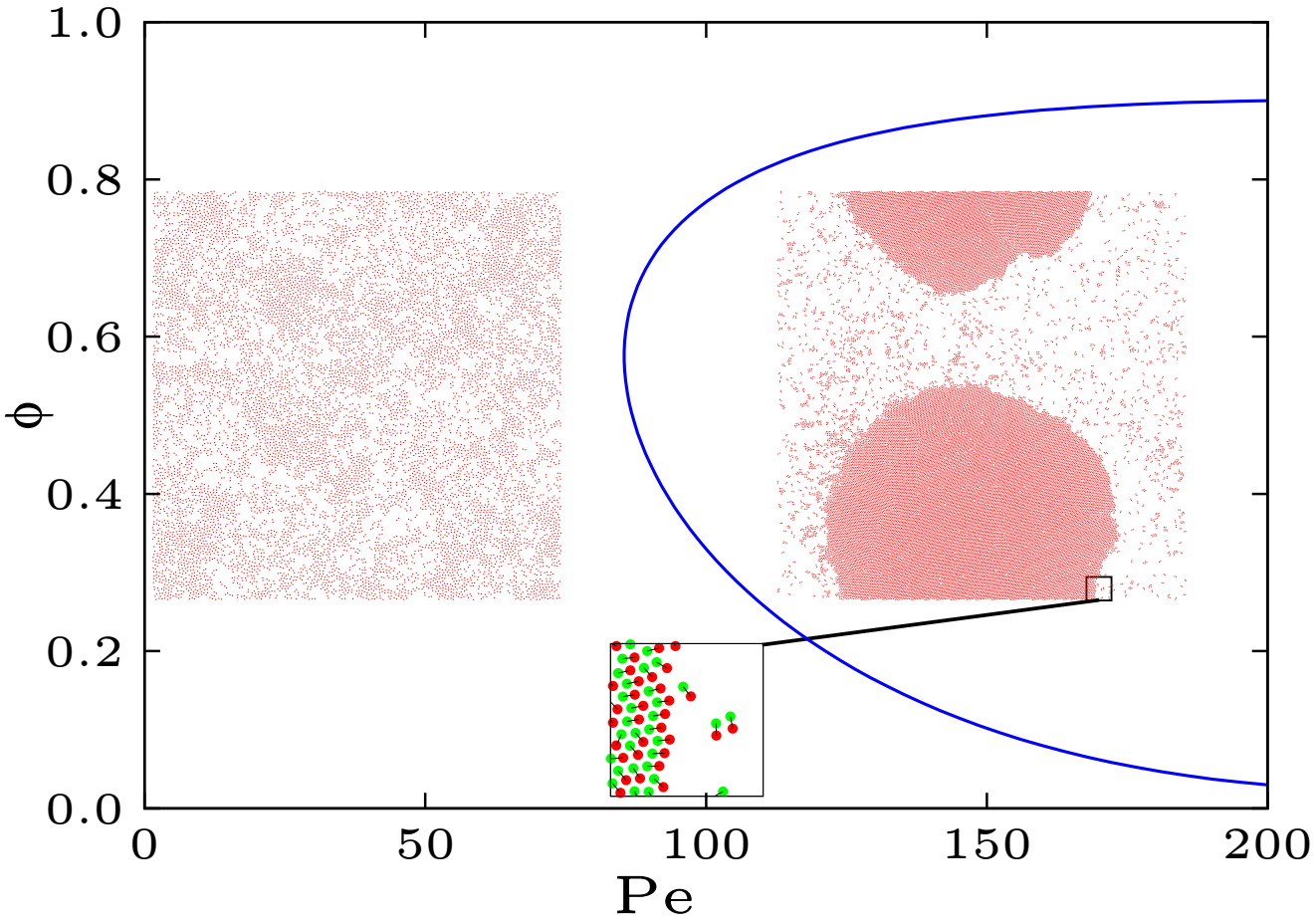
A. Bright-field microscopy image of a motile bacteria-polymer mixture

B. Snapshot of simulation of active dumbbells with parameters chosen to be similar to the experiments shown in A.

Schwarz-Linek et al 12

Active dumbbells in $2d$

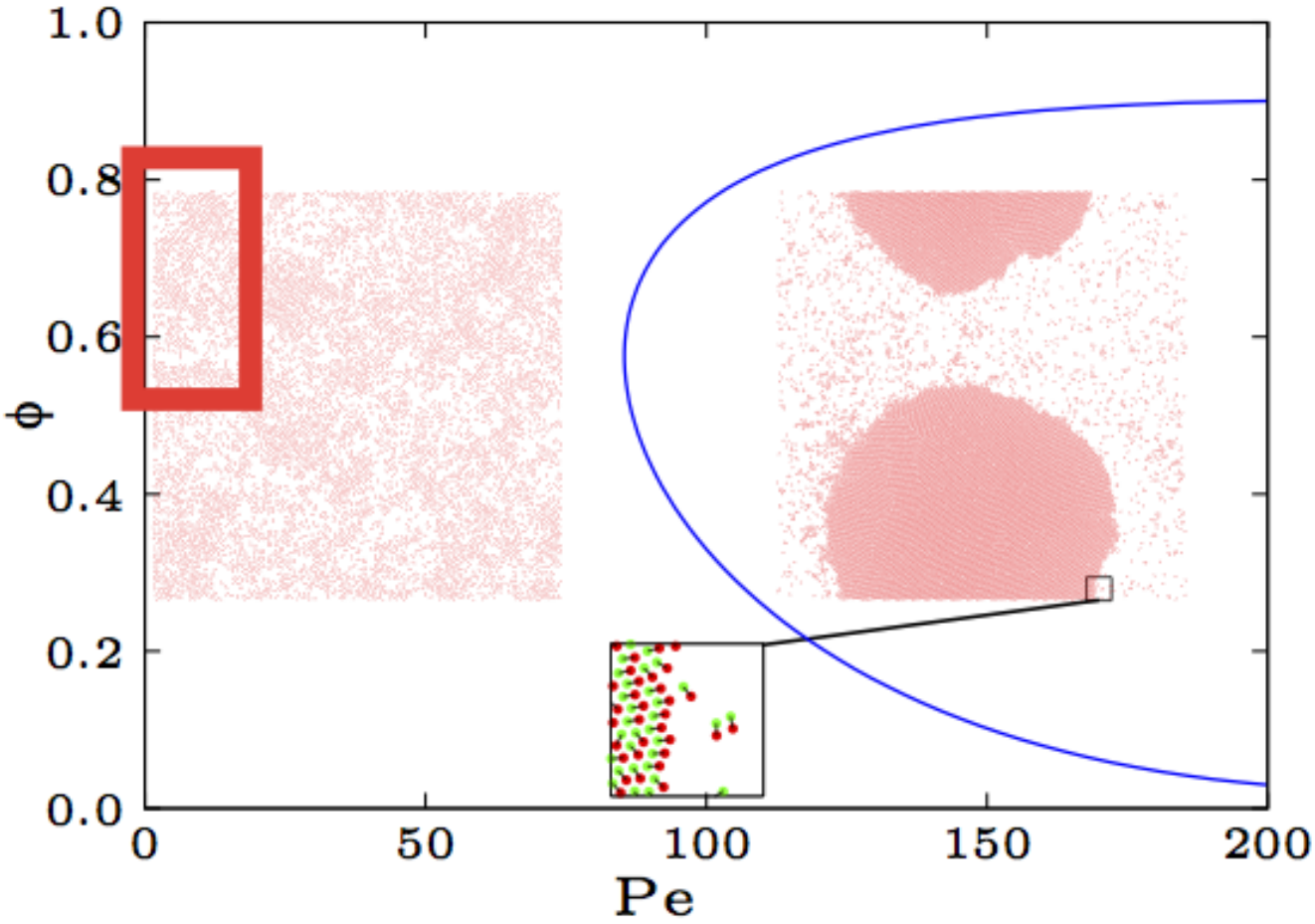
OLD phase diagram - motility induced phase transition



Mechanism for aggregation: note the head-tail alignment in the cluster.

Active dumbbells in $2d$

OLD phase diagram - to be revised



Focus on the homogeneous phase. Start from the analysis of the passive limit

Plan

1. Active matter

2. Active Brownian dumbbells

3. Two-dimensional equilibrium phases

   Passive limit: Beyond the BKT-Halperin-Nelson-Young scenario

4. Two-dimensional collective behaviour of active systems

   No mobility induced phase transition (MIP)

$2d$ 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

Plan

1. Active matter

2. Active Brownian dumbbells

3. Two-dimensional equilibrium phases

   Passive limit: Beyond the BKT-Halperin-Nelson-Young scenario

4. Two-dimensional collective behaviour of active systems

   No mobility induced phase transition (MIP)

Results & questions

- Brand new Bernard & Krauth two step transition scenario

Liquid	(1st order)	Hexatic	(BKTHNY)	Solid

confirmed for hard and soft passive disks

- Passive molecules ?
- Active disks and molecules ?
- Mobility induced phase transition for purely repulsive interactions *vs.*

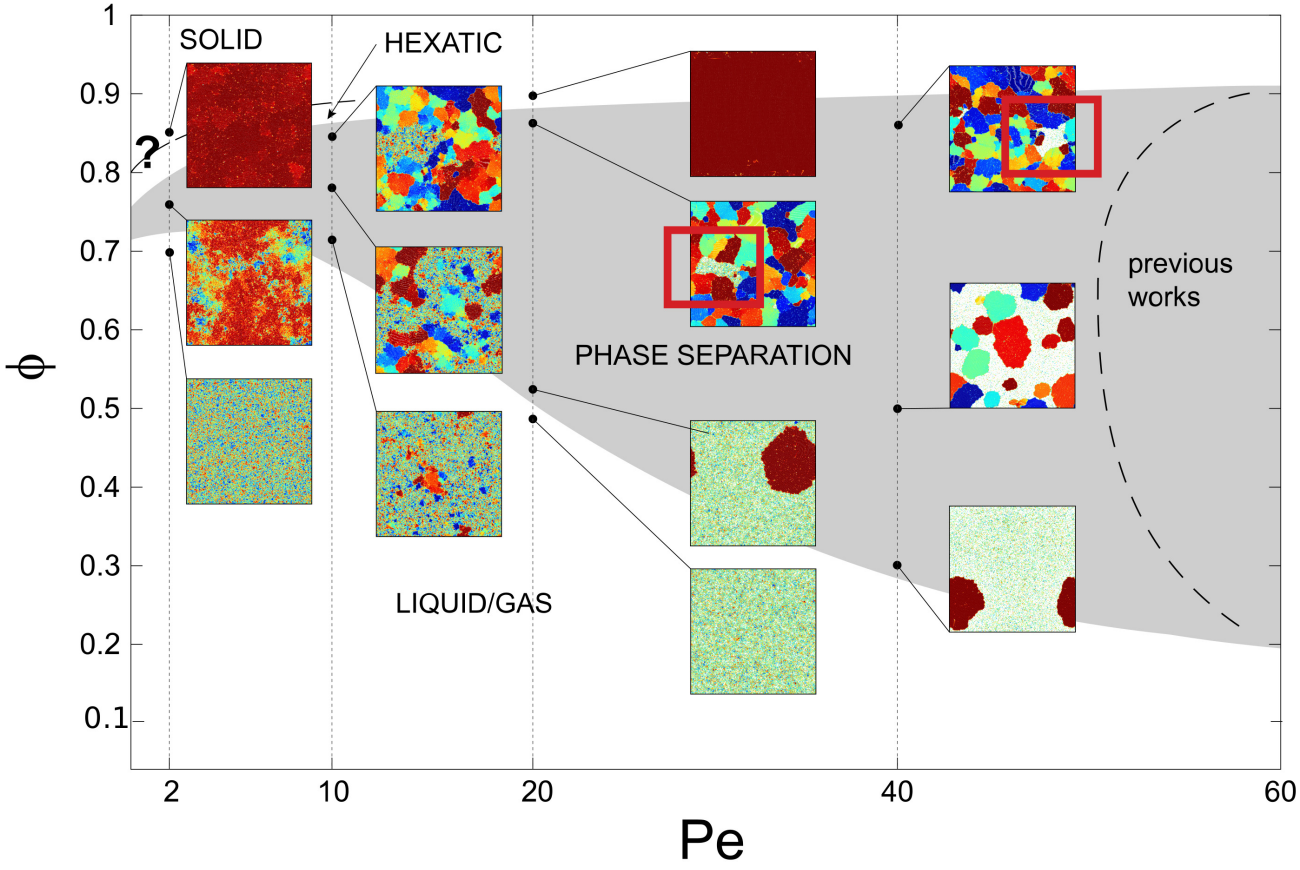
an extension of the Bernard & Krauth passive system scenario

to the active dumbbell problem

LFC, di Gregorio, Gonnella & Suma 16

Phase diagram

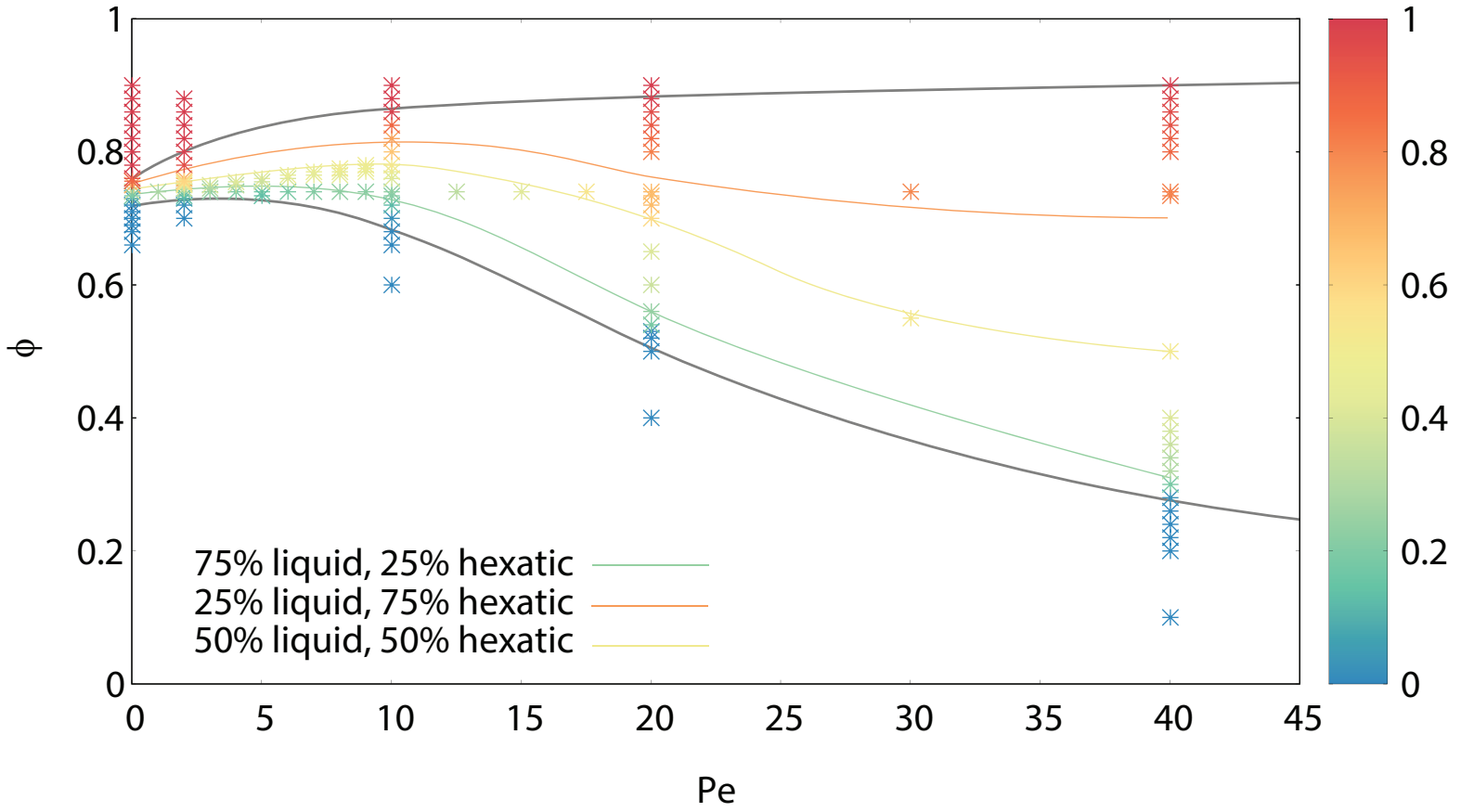
Active dumbbells



$T = 0.05$

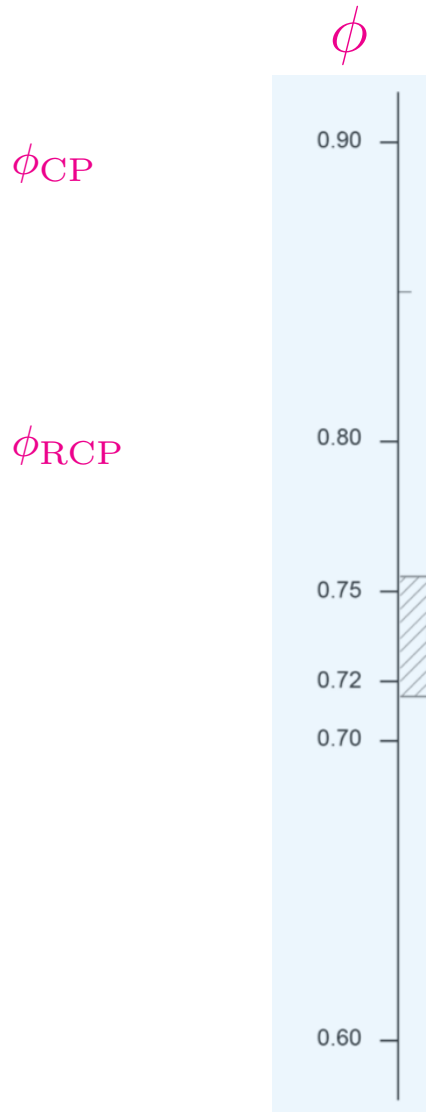
Coexistence region

& lines of constant proportion



Passive dumbbell system

Phase diagram (low T, as a function of packing fraction)



solid

hexatic

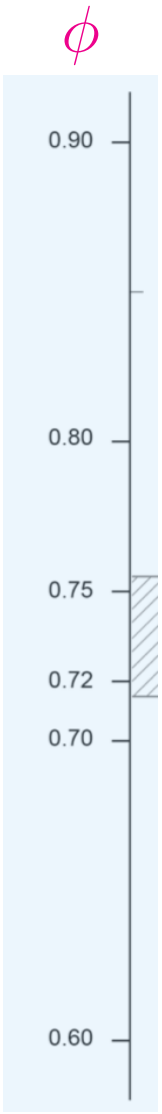
co-existence

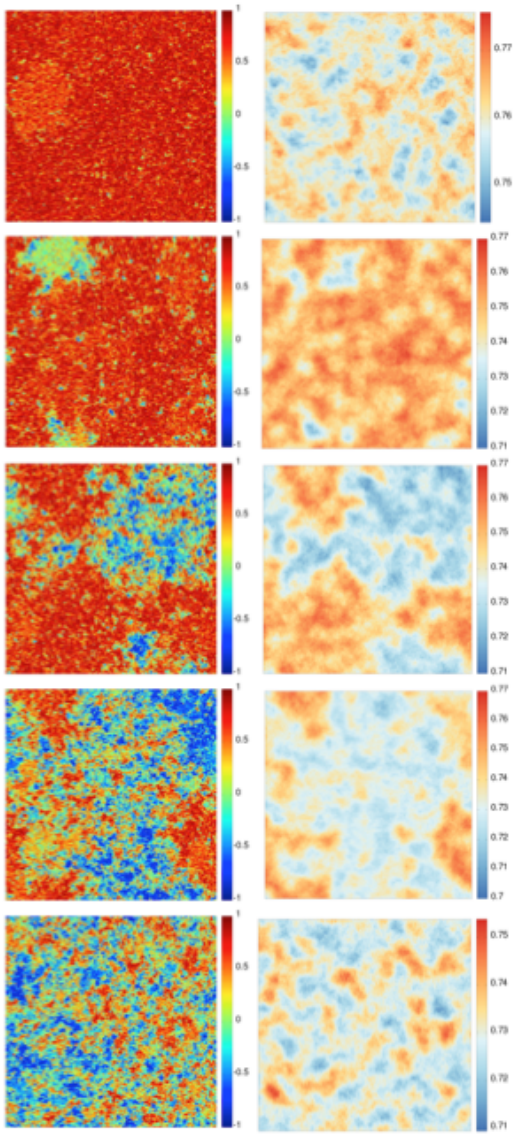
Really ?

liquid

Passive dumbbell system

Phase diagram





Local maps of

1st column

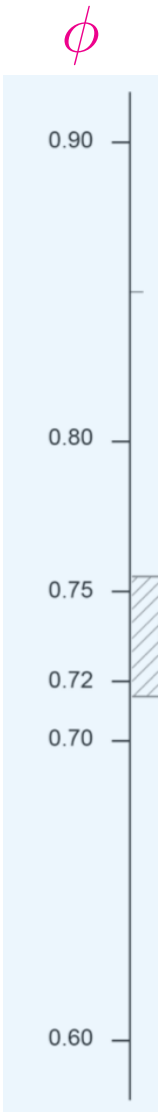
Local hexatic $|\psi_{6i}|$

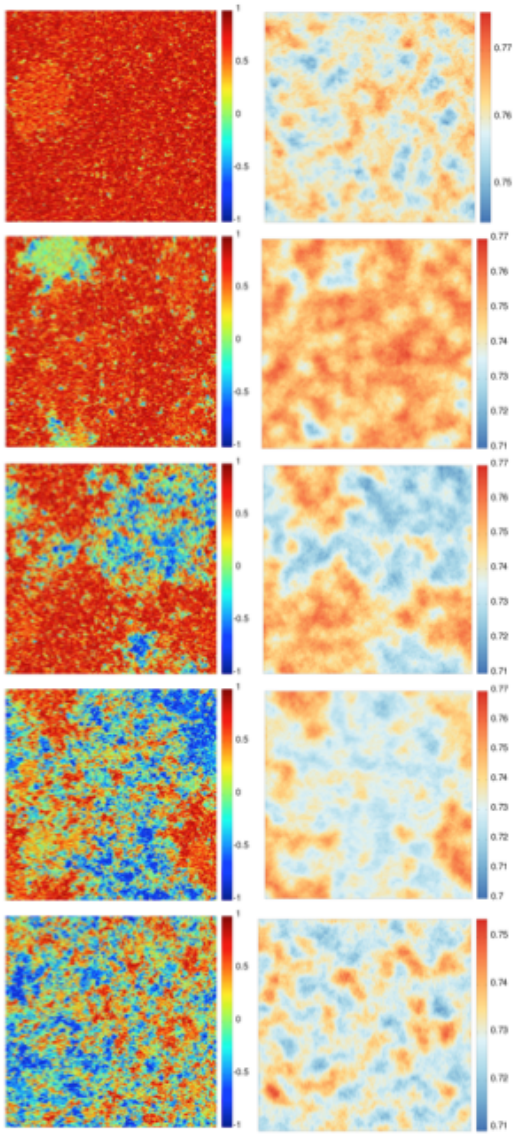
2nd column

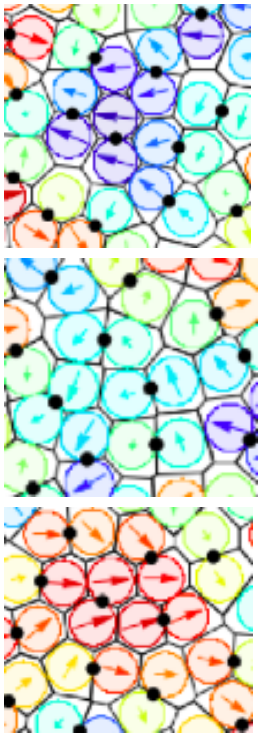
Local density ϕ_i

Passive dumbbell system

Phase diagram







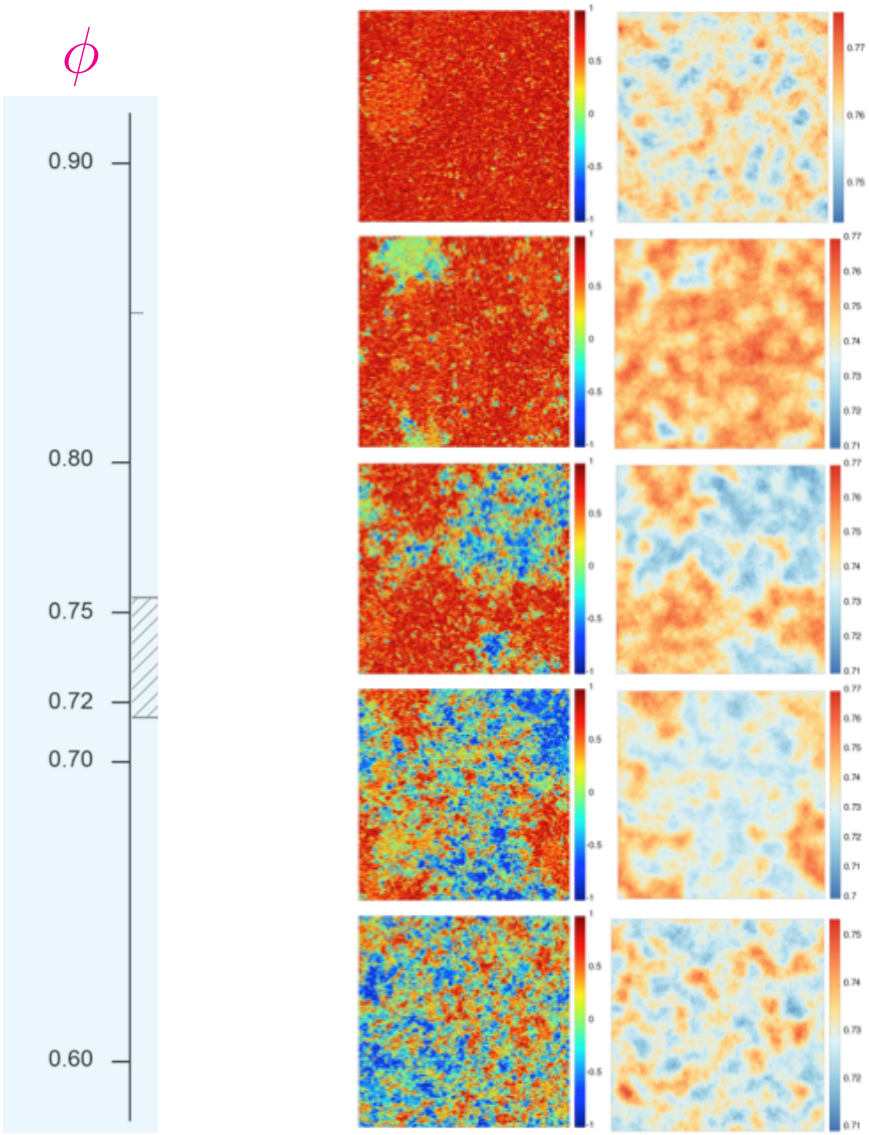
Same color =

same orientation

Then $|\psi_{6i}|$

Passive dumbbell system

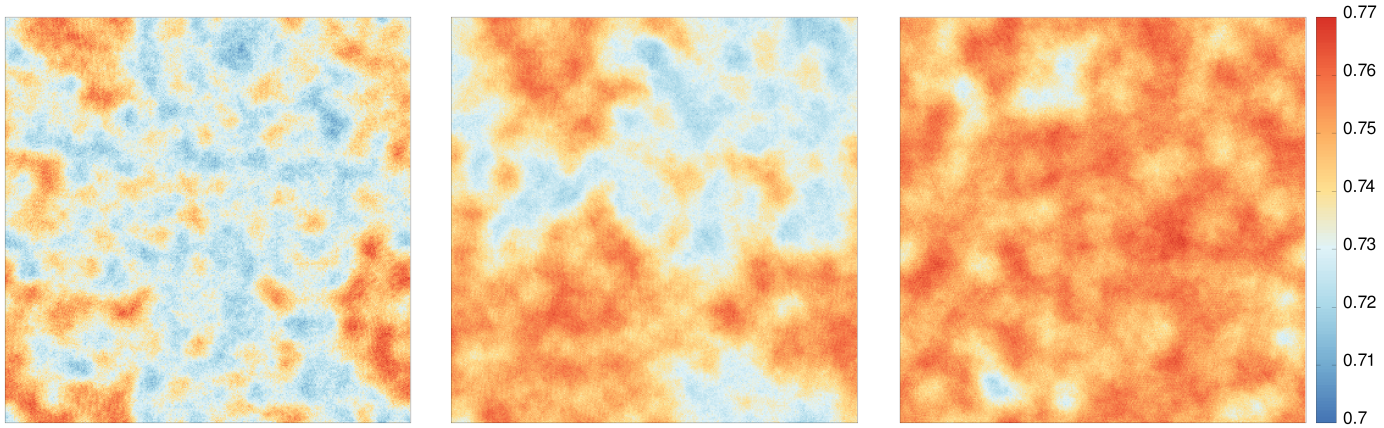
Phase diagram



Spatial correlation between regions of high density and regions of large absolute value of the local hexatic order parameter

Passive dumbbell system

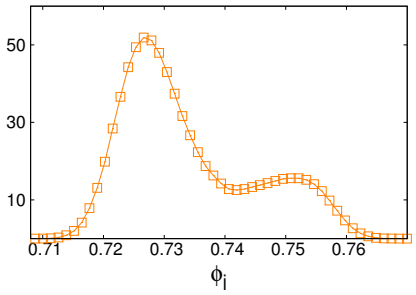
Local density & local hexatic parameter

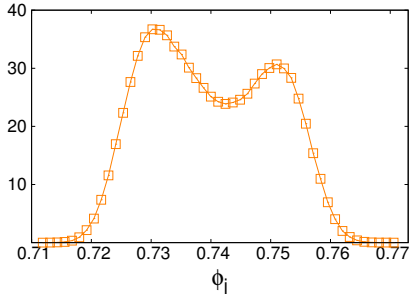


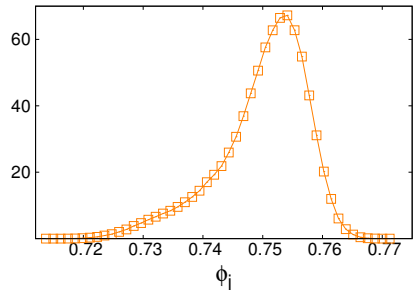
$\phi = 0.734$ (co-existence)

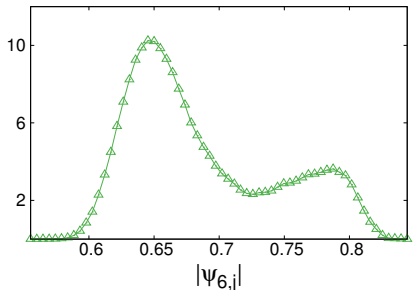
$\phi = 0.74$ (co-existence)

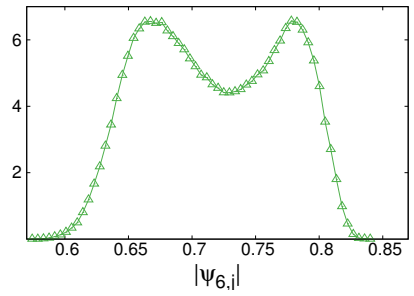
$\phi = 0.75$ (upper limit of co-existence)

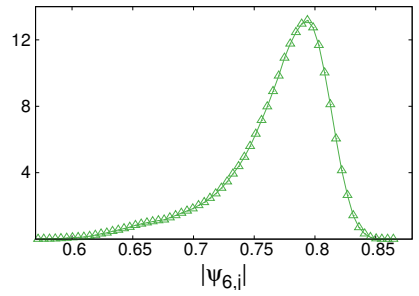






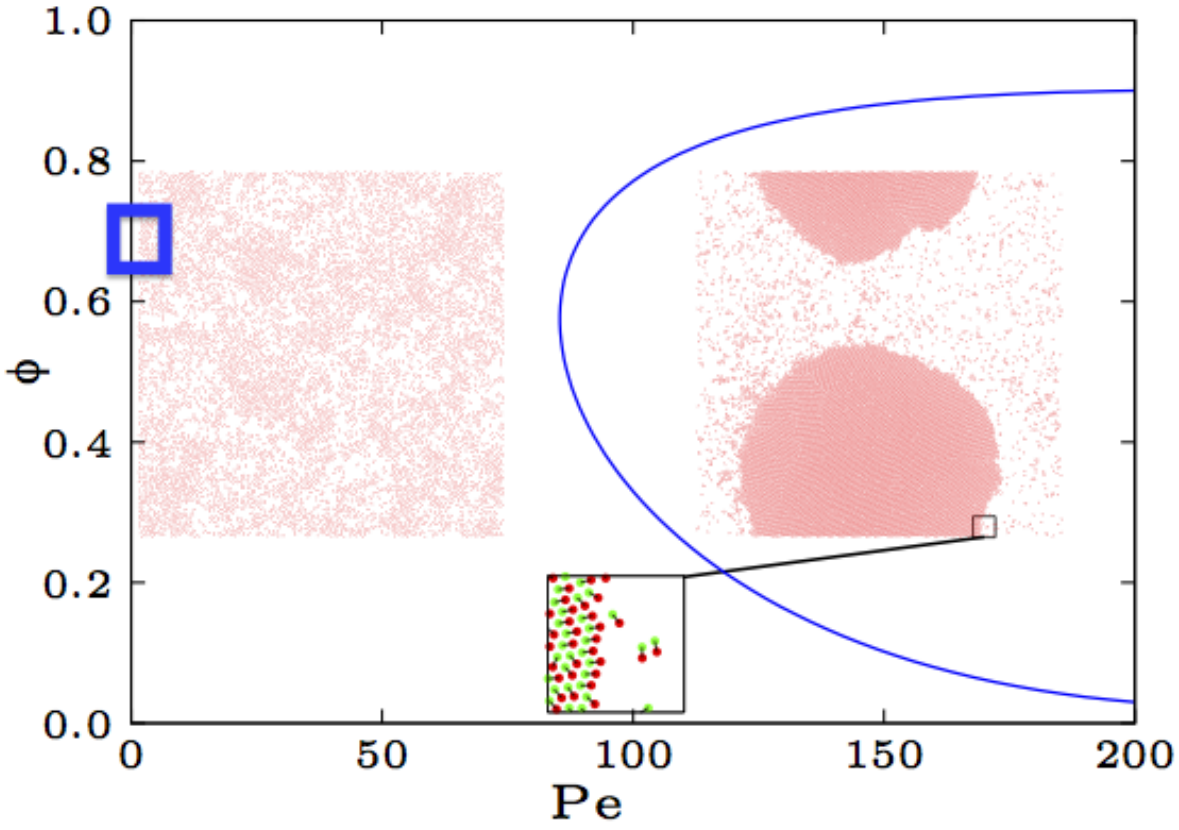






Active dumbbell system

OLD phase diagram & new result



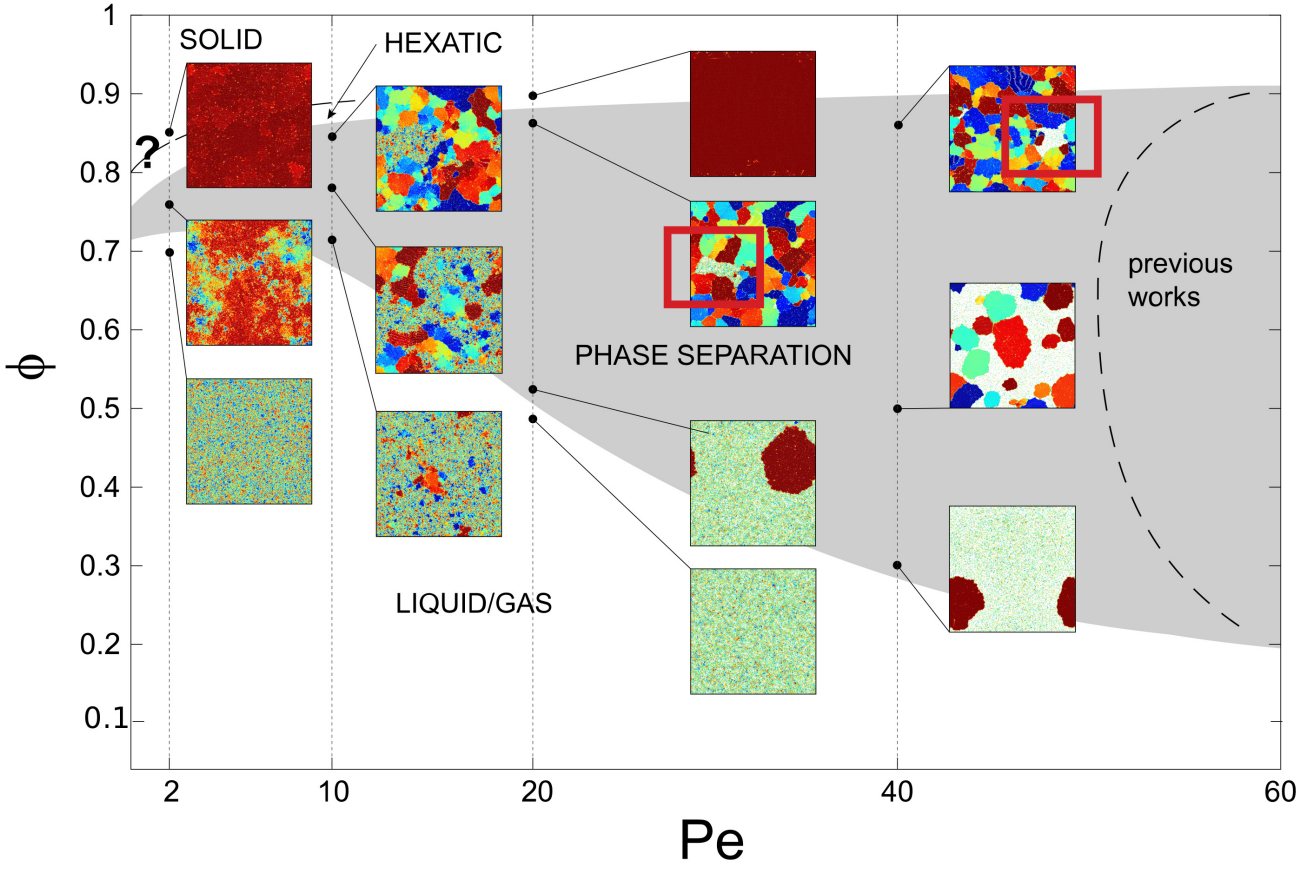
Connection between the two extremes !

Dynamics

$|\psi_{6i}|$ **at** $\phi = 0.74$ **and Pe = 10 (co-existence)**

Phase diagram

Conclusions



$T = 0.05$

Discussion

Some things to do

- Confirm this picture for active hard and soft disks.
- Understand how to define a meaningful pressure.
- Investigate the dynamics taking into account the heterogeneity of the co-existence region.
  - Revisit the tracer motion under inhomogeneous conditions.
  - Revisit the effective temperature measurements.

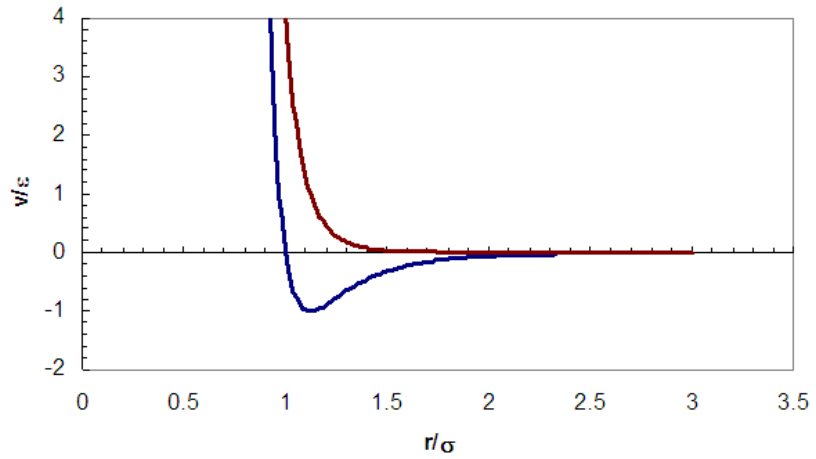
Interaction potential

Lennard-Jones vs WCA

$\mathbf{F}_{\rm pot} = \mathbf{F}_{\rm wca} + \mathbf{F}_{\rm fene}$, $V = V_{\rm wca} + V_{\rm fene}$ and hard repulsive $V_{\rm wca}$

$$V_{\rm wca}(\boldsymbol{r}_i, \boldsymbol{r}_j) = \begin{cases} V_{LJ}(r_{ij}) - V_{LJ}(r_c) & r < r_c \\ 0 & r > r_c \end{cases}$$

$$V_{LJ}(r_{ij}) = 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{2n} - \left(\frac{\sigma}{r_{ij}} \right)^{n} \right] \qquad r_c = 2^{1/n} \sigma = \sigma_{\rm d}$$



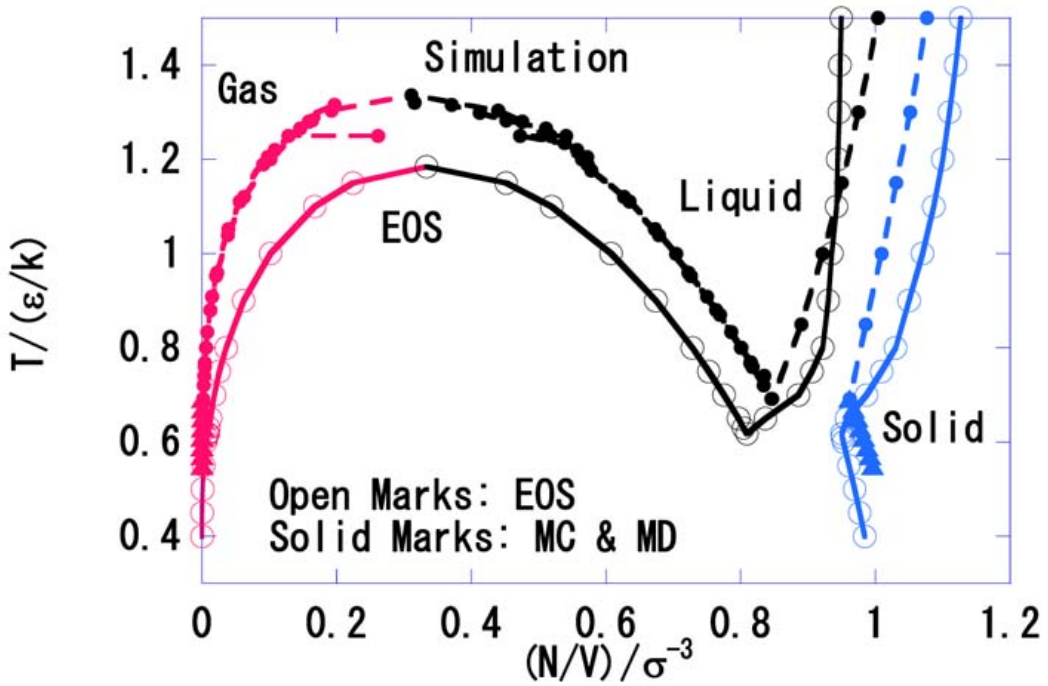
LJ potential has repulsive and attractive branches

WCA is purely repulsive

ϵ and $\sigma_{\rm d}$ are the energy and length scales

Passive molecular systems

Solid, liquid and gas equilibrium phases



Typical (simple) density-temperature (ϕ, T) phase diagram

Lennard-Jones model system for Argon (more later)

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

Freezing transition

Solid $\mapsto$ Liquid: Different routes in $3d$ and $2d$

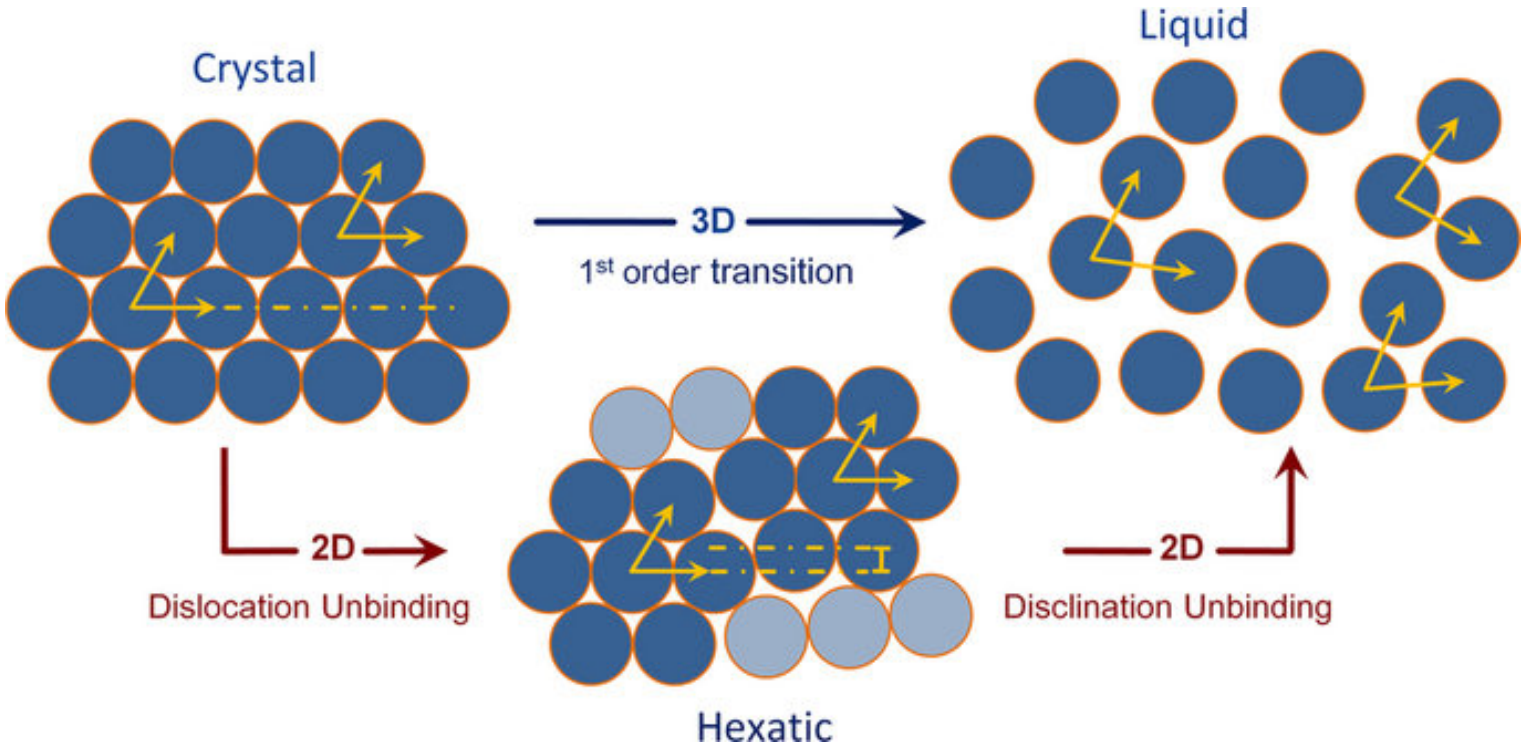


Image from **Pal, Kamal & Raghunathan, Sc. Rep. 6, 32313 (2016)**

Crystals *vs.* solids

$3d$ *vs.* $2d$

- A crystal is a system with *long-range positional order*.

  It has a periodic structure and its 'particles' are located close to the nodes of a lattice.

  The position fluctuations are bounded.

- A solid is a material with *non-vanishing shear modulus*.

- $2d$ solids exist and have a weaker ordering than $3d$ crystals.

  - They are *oriented crystals* with *quasi-long-range positional order*.
  - Critical phase with algebraic relaxation of position correlations.
  - Phase transition *à la* Kosterlitz-Thouless (Nobel Prize 2016).

Equilibrium phases of $2d$ matter

Historical development

- Peierls (1934) & Mermin-Wagner (1966-68) results.

  No positional long-range order in $2d$ at finite T

$$\Delta^2(\boldsymbol{r}) = \langle [\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{0})]^2 \rangle \simeq k_B T \ln r \quad \text{in} \quad d = 2$$

- Berenzinskii-Kosterlitz-Thouless-Halperin-Nelson-Young scenario

  Dislocations and disclinations

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

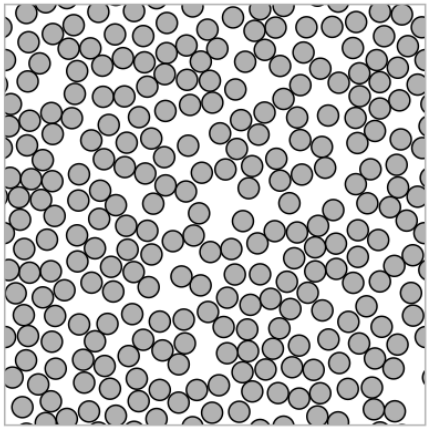
  Numerical simulations

- Brand new Bernard & Krauth two step transition scenario

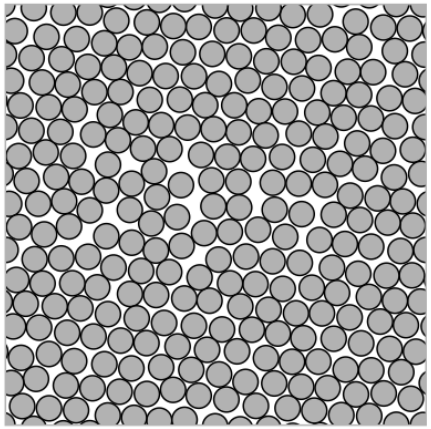
  Liquid to hexatic BKT transition preempted by a 1st order transition

Freezing

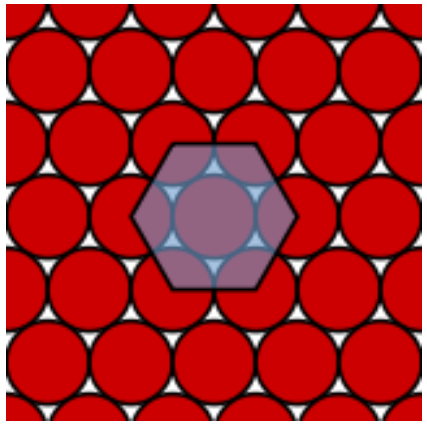
Disks in two dimensions



Low density liquid



Which phase ?



Crystalline triangular lattice

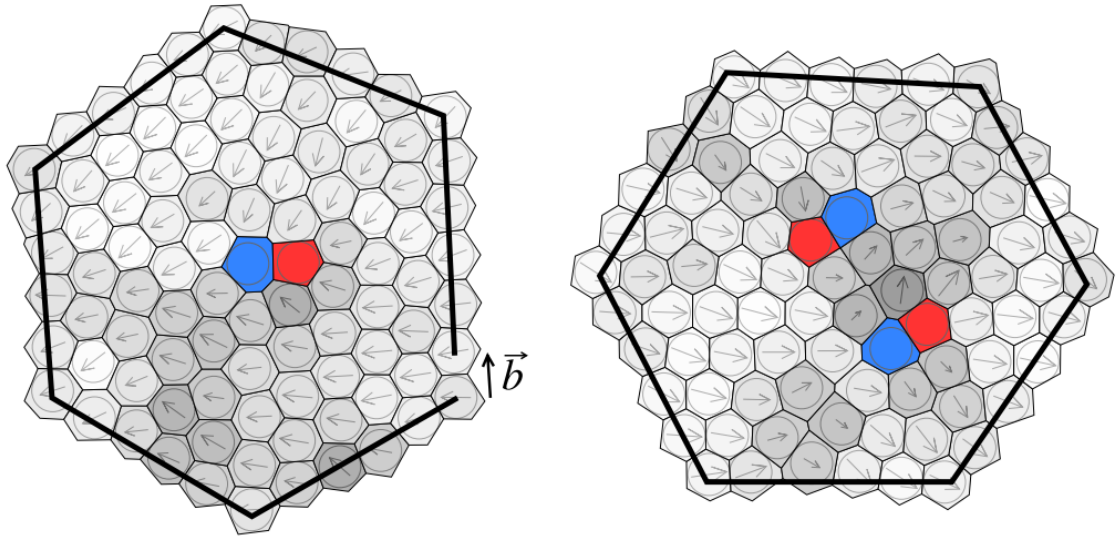
Note that in the crystal each disk has six neighbours

$\phi_{\mathrm{RCP}} \approx 0.82$ (random close packing) $\phi_{\mathrm{CP}} \approx 0.91$ (close packing)

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

Positional order

Disks, Voronoi cells & dislocations



A free dislocation (7-5)

A bound pair of dislocations (twice 7-5)

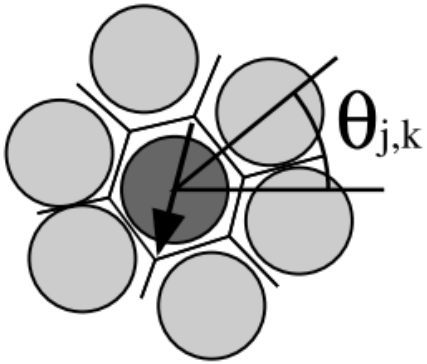
In the crystal the centers of the disks form a triangular lattice (six neighbours)

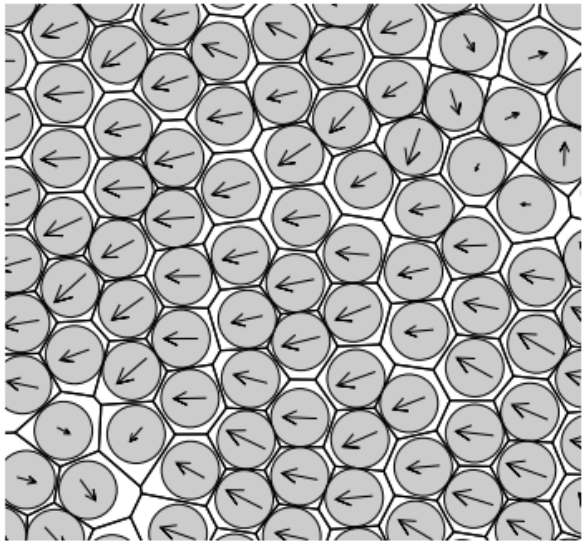
The **blue** disks have seven neighbours and the **red** ones have five.

On the left image: the effect of the defect spreads over the full system.

Orientational order

Hexatic order





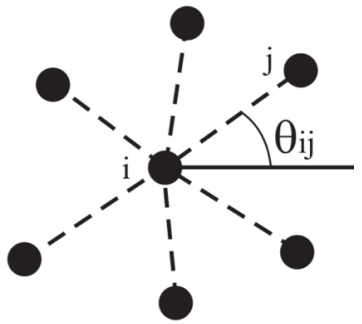
Associating arrows (directions) to disks

Orientational order

Hexatic order parameter

The local hexatic variable

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



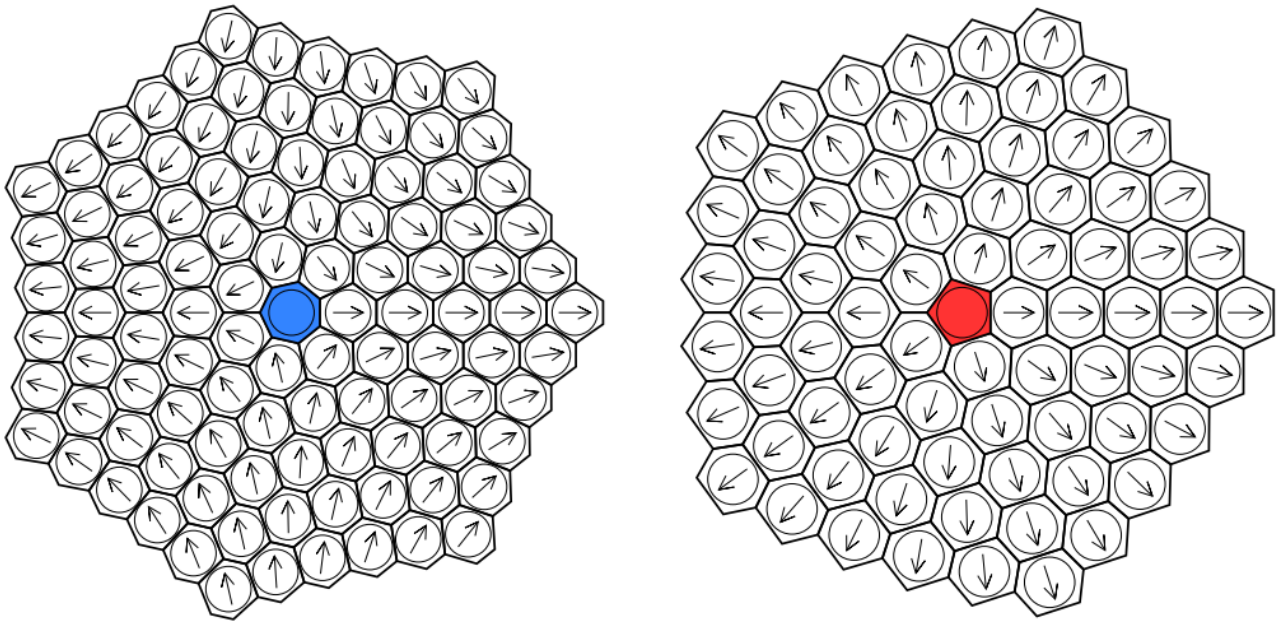
with $N^i_{\rm nn}$ the number of nearest (Voronoi) neighbours of bead i and θ_{ij} the angle between the segment that connects i with its neighbour j and the x axis.

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

Orientational order

Disks, arrows and disclinations



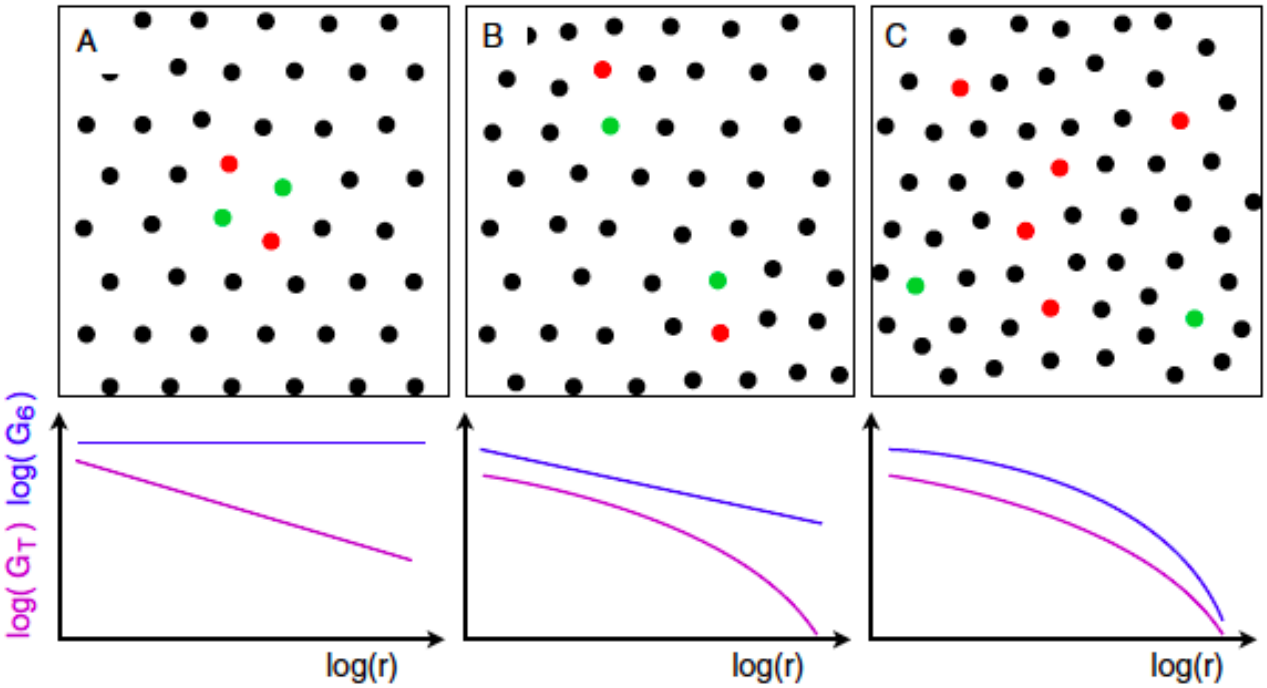
The orientation winds by $\pm 2\pi$ around the **blue** (seven) and **red** (five) defects.

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

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

Correlation functions

Sketches (green seven & red five neighbours)



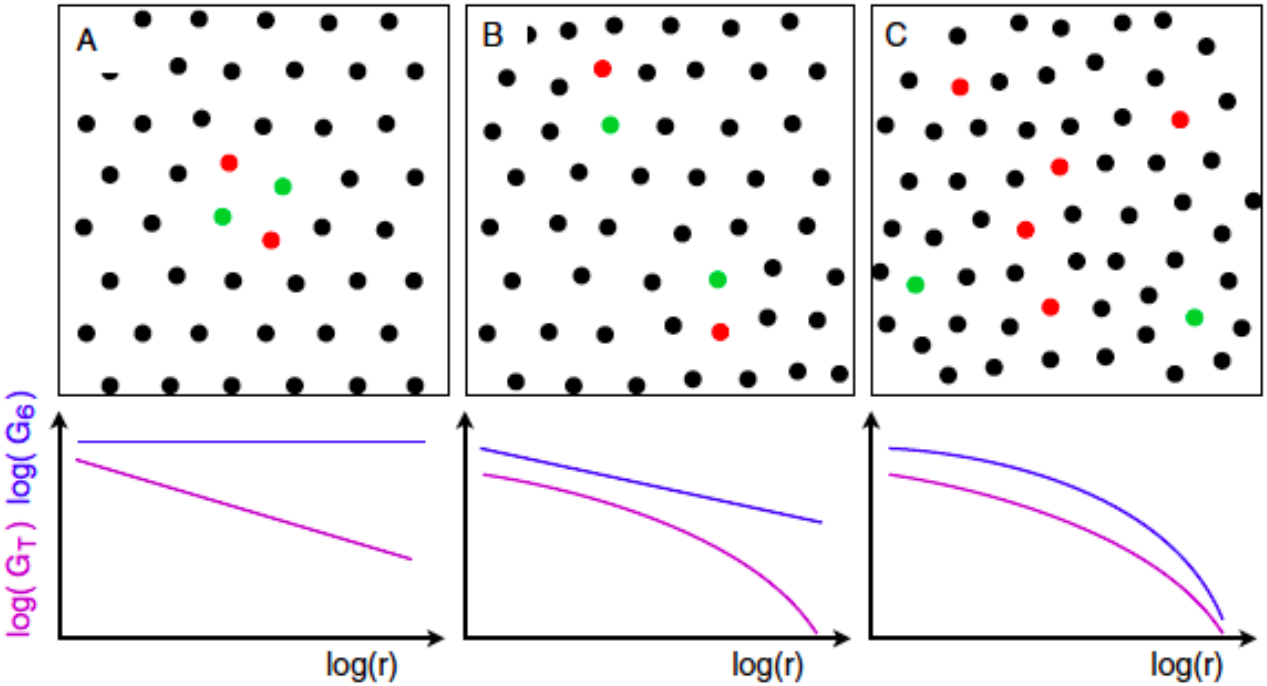
Solid Hexatic Liquid

Dislocations & disclinations bound Dislocations free Disclinations free

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

Correlation functions

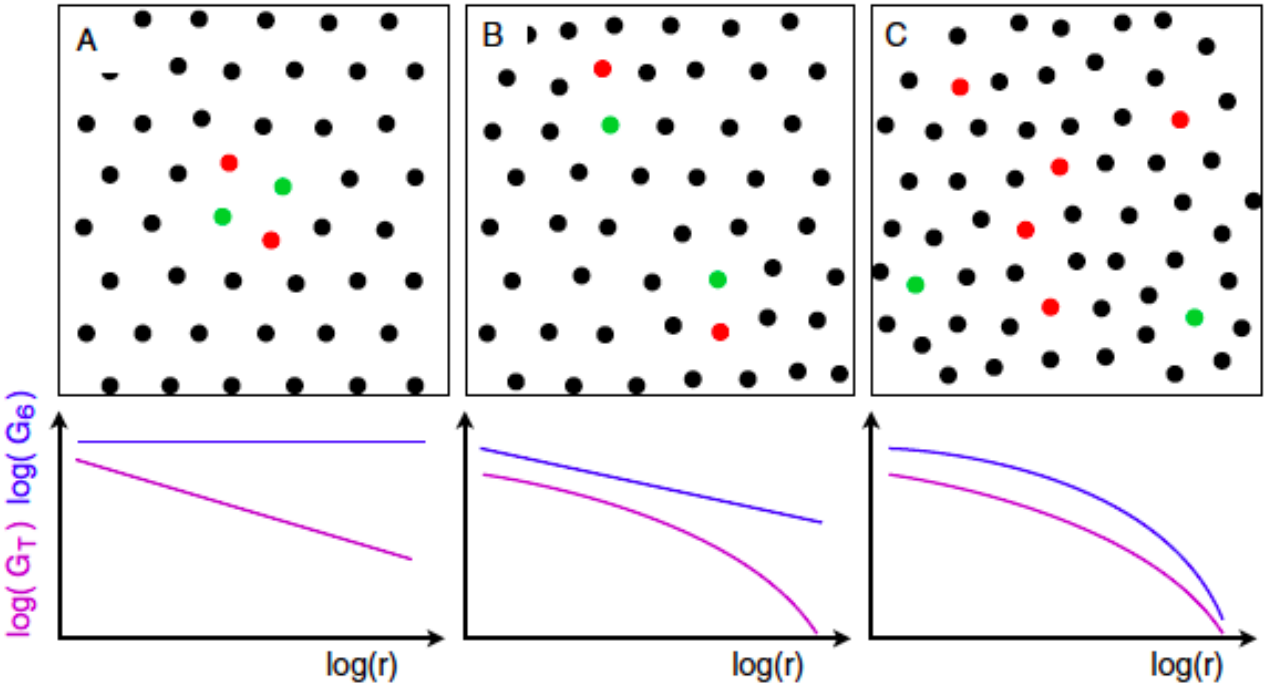
Positional



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

Correlation functions

Hexatic



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

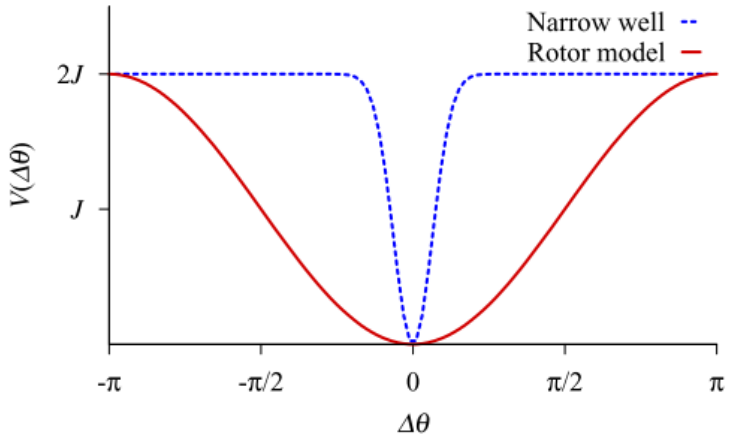
Berezinskii-Kosterlitz-Thouless

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:

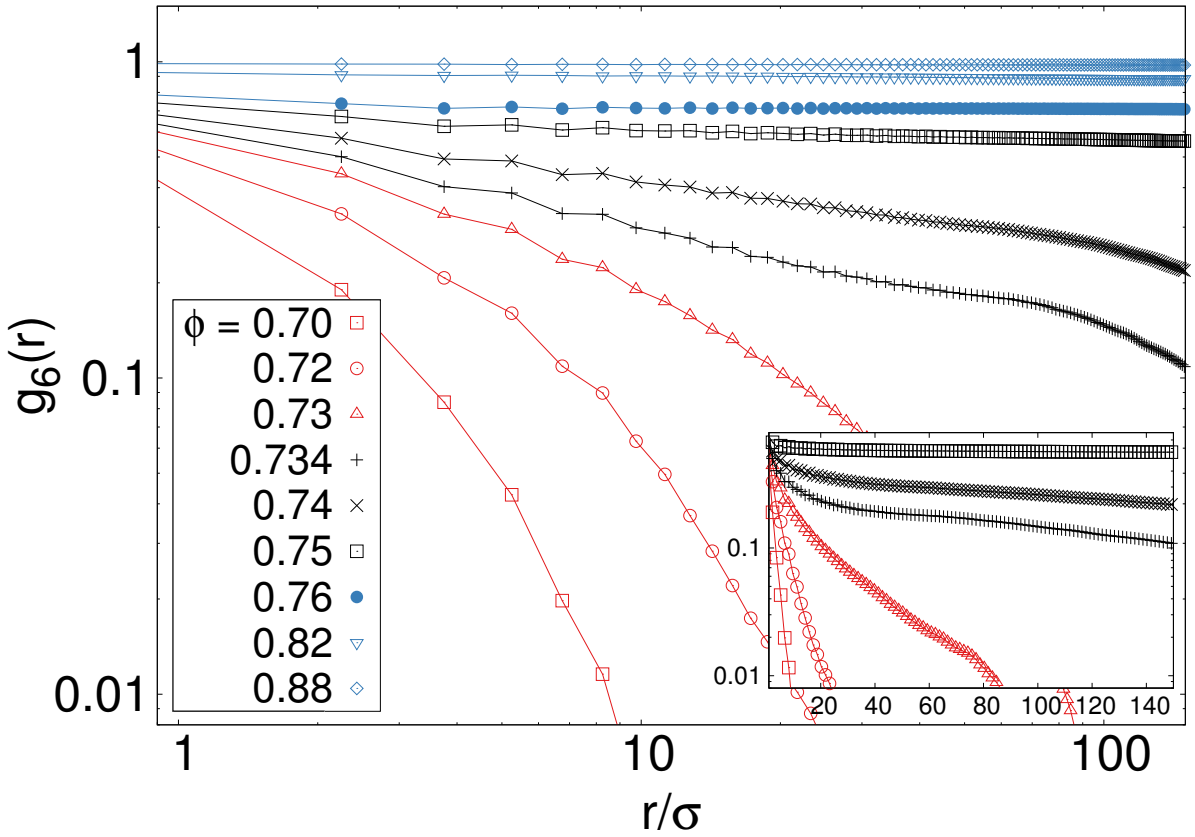


"First order phase transition in an XY model with nn interactions"

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

Passive dumbbell system

Hexatic correlation function



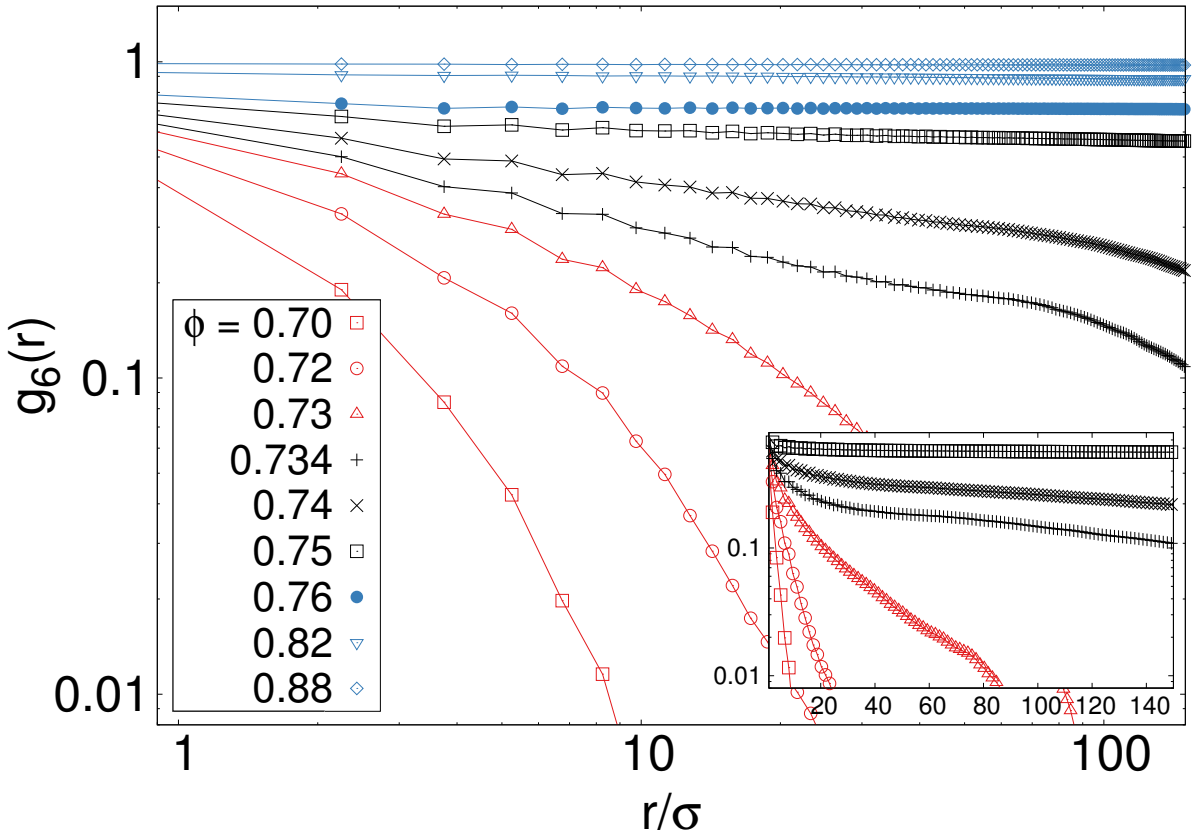
Solid

Hexatic

Liquid

Passive dumbbell system

Hexatic correlation function



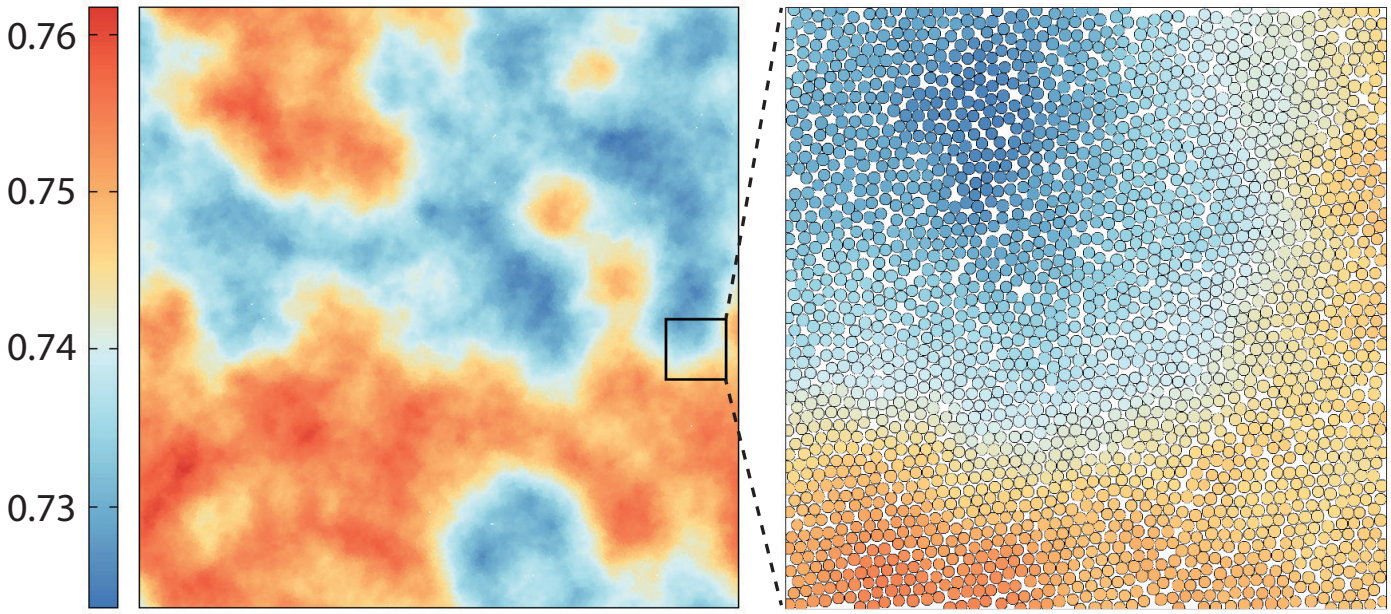
Saturation

Algebraic

Exponential

Passive dumbbell system

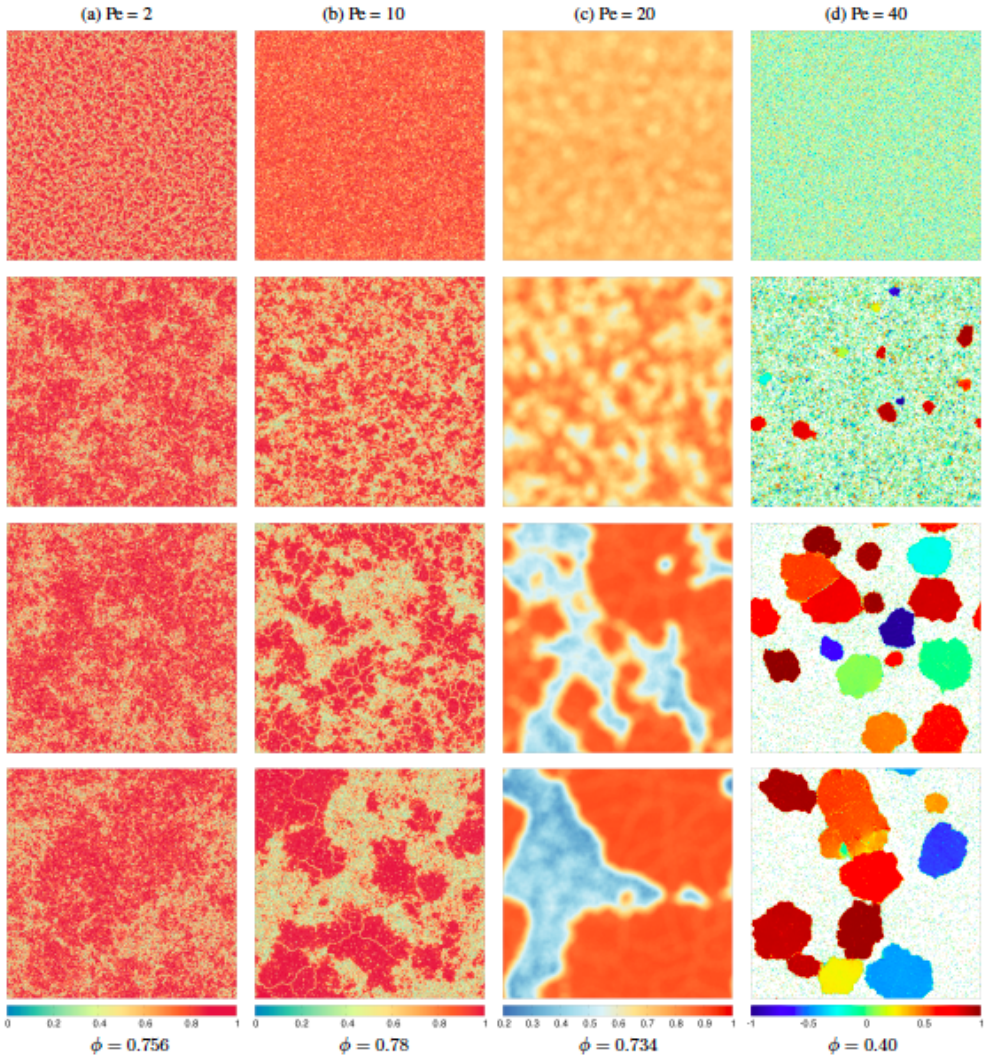
Local density colour map



Co-existence between dense and loose regions

Active coarsening

at lower limit of coexistence



$|\psi_{6i}|$ $|\psi_{6i}|$ ϕ_i ψ_{6i}

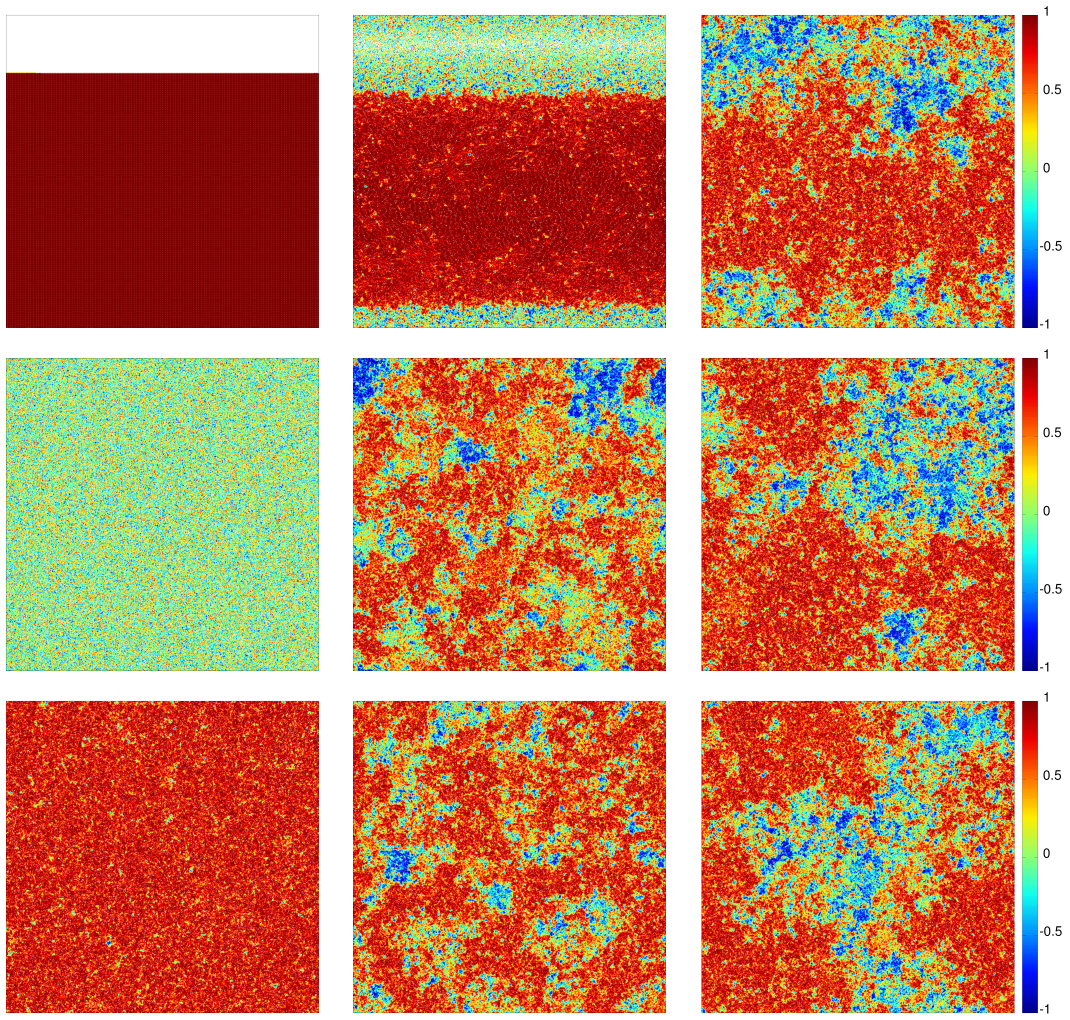
Passive dumbbell system

Co-existence region : independence of the initial conditions

crystal

random

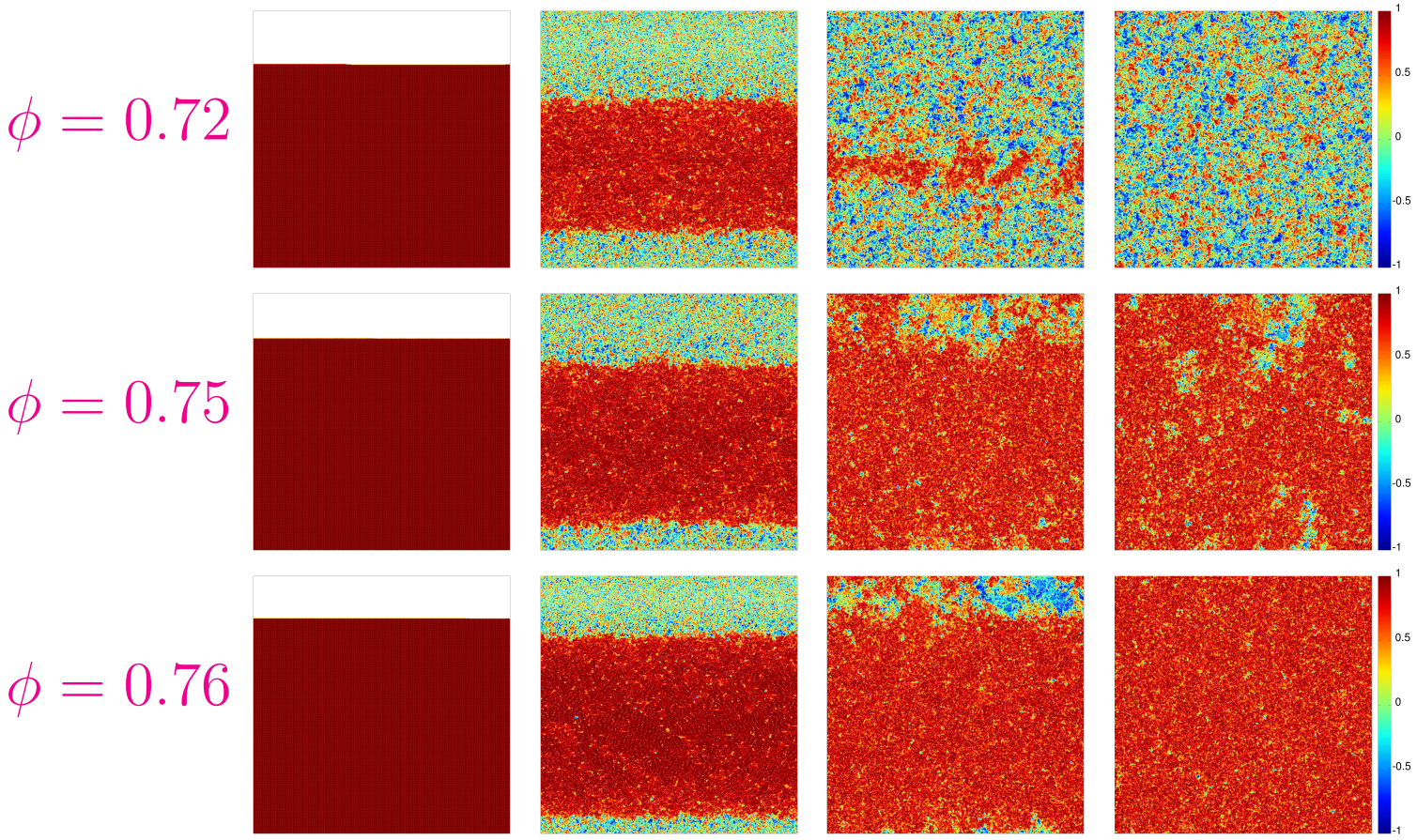
hexatic



$t = 0$ t_1 t_2

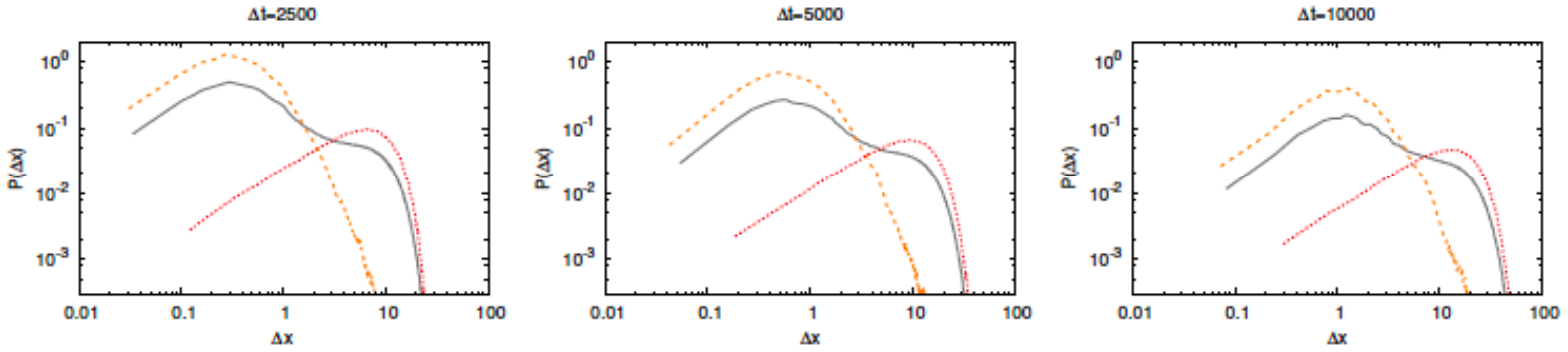
Passive dumbbell system

Dynamics: Below, in and above the co-existence region



Discussion

Two populations in co-existence region



Pe = $10, \phi = 0.78$ at $t = 2500,\ 5000,\ 10000$

The averaged hexatic modulus is computed for each particle on a radius of 10 σ_{d} around the particle itself, and a particle is considered to be inside a cluster only if this value is greater than 0.75. Only such particles were taken into account in the red peak on the right.

In black : all dumbbells

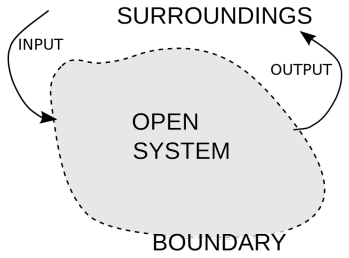
Open systems

Aim

Our interest is to describe the statics and dynamics of a classical (or quantum) system coupled to a classical (or quantum) environment.

The Hamiltonian of the ensemble is

$$H = H_{syst} + H_{env} + H_{int}$$



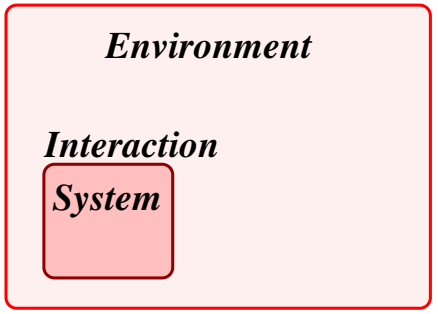
The dynamics of all variables are given by Newton (or Heisenberg) rules, depending on the variables being classical (or quantum).

The total energy is conserved, $E = \text{ct}$ but each contribution is not, in particular, $E_{syst} \neq \text{ct}$, and we'll take $e_0 \ll E_{syst} \ll E_{env}$.

Dynamics in equilibrium

Conditions

Take an open system coupled to an environment



Necessary :

— The bath should be in equilibrium

same origin of noise and friction.

— Deterministic force :

conservative forces only, $\vec{F} = -\vec{\nabla} V$.

— Either the initial condition is taken from the equilibrium pdf, or the latter should be reached after an equilibration time t_{eq} :

$$P_{eq}(v, x) \propto e^{-\beta(\frac{mv^2}{2}+V)}$$

Microscopic scales

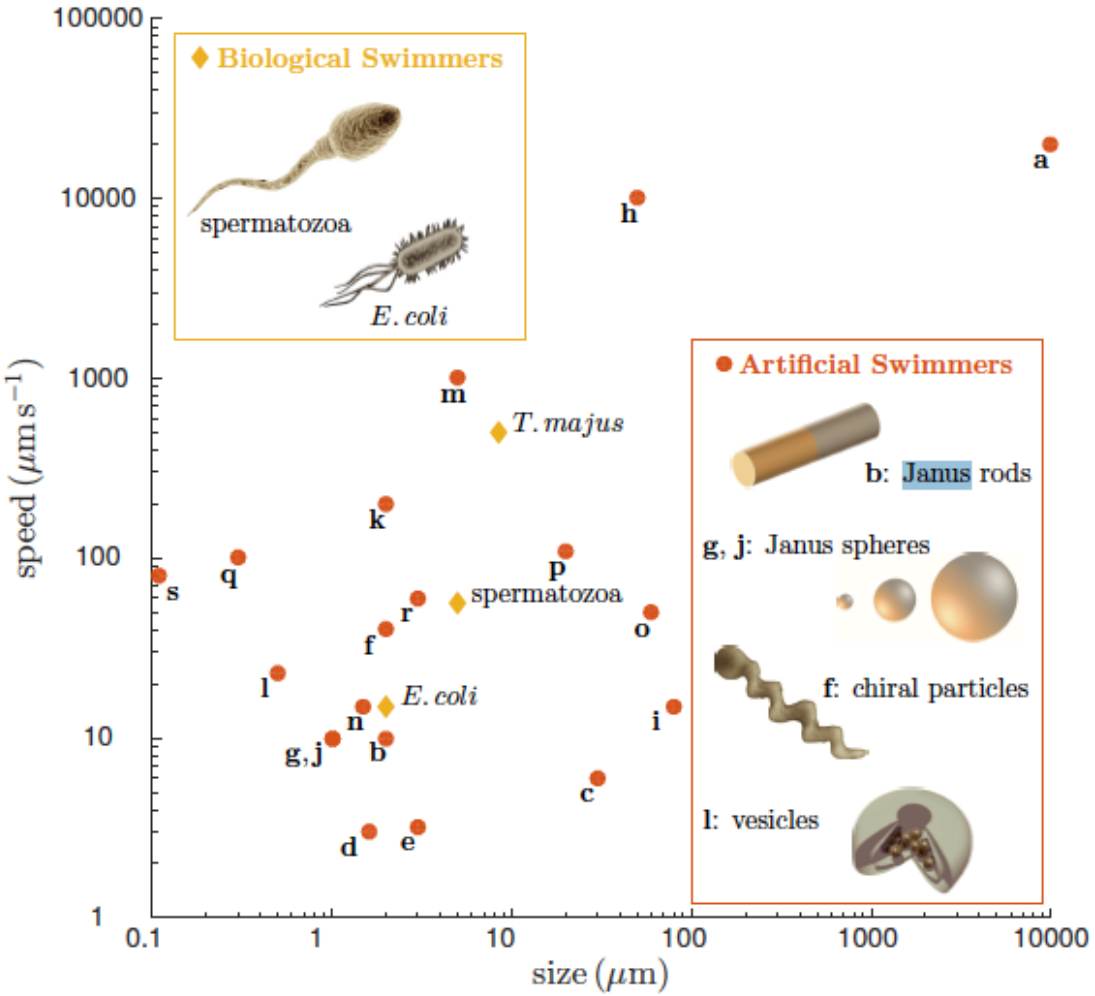


Image taken from **Bechinger et al, Rev. Mod. Phys. 88, 045006 (2016)**

Models & Methods

From very detailed to approximate

	Biological	Statistical physics	Non-linear dynamics
Microscopic		Brownian/Run&Tumble	Cellular automata
Collective		Phases & transitions	Bifurcations
Experiments		Soft-condensed matter	
Numerical		MD, MC, Lattice Boltzmann	Integration
Analytical		Liquid/Glass theory	Hydrodyn/Mechanics

Vicsek model

Minimal (cellular automata) model for flocking

Flocking due to any kind of self-propulsion and alignment with neighbours.

The position and velocity of an agent are $\boldsymbol{r}_i$ and $\boldsymbol{v}_i = v_0 \hat{\boldsymbol{v}}_i$ with $v_0 = \text{cst}$.

Each microscopic update is such that the individual's direction is updated according to the mean $\overline{\ldots}$ over its neighbours

$$\hat{\boldsymbol{v}}_i(t+\delta t) = \overline{\hat{\boldsymbol{v}}_j(t)}_{|\boldsymbol{r}_i - \boldsymbol{r}_j|<r} + \boldsymbol{\eta}_i(t)$$

plus some noise $\boldsymbol{\eta}_i$ (normalisation is imposed after each step) and moves at constant speed v_0 in the new direction

$$\boldsymbol{r}_i(t+\delta t) = \boldsymbol{r}_i(t) + v_0 \hat{\boldsymbol{v}}_i(t+\delta t)\, \delta t$$

"Novel Type of Phase Transition in a System of Self-Driven Particles",

Vicsek, Czirók, Ben-Jacob, Cohen, Shochet, Phys. Rev. Lett. 75 1226 (1995)

Vicsek model

Minimal (cellular automata) model for flocking

Flocking due to any kind of self-propulsion and alignment with neighbours.

The particles are self-propelled due to v_0

The total number of particles is conserved (no birth/death).

The velocity direction plays a similar role to the one of the spin in the Heisenberg (or XY) ferromagnetic models (more later)

As the particles move in the direction of their velocity, the "connectivity matrix" is not constant, but evolves (if the interaction range is finite).

There is no momentum conservation and Galilean invariance is broken.

Spontaneous symmetry breaking of polar order, $\boldsymbol{p}(t) = \frac{1}{N} \sum_{i=1}^{N} \hat{\boldsymbol{v}}_i(t) \neq 0$

At $v_0 = 0$ the model is the Heisenberg one. However, this is a singular limit.

Vicsek model

Minimal (cellular automata) model for flocking

Flocking due to any kind of self-propulsion and alignment with neighbours.

The global behaviour is controlled by the density ϕ, the noise amplitude $k_B T$ and the particles' modulus of the velocity v_0.

Dynamic phase diagram $(k_B T, \phi)$ (v_0 fixed) from

the polar order parameter $\boldsymbol{p}(t) = \frac{1}{N} \sum_{i=1}^{N} \hat{\boldsymbol{v}}_i(t)$

- Homogenous collective motion (high density, weak noise)
- Ordered bands (intermediate)
- Disordered (low density, strong noise)

"Novel Type of Phase Transition in a System of Self-Driven Particles",
Vicsek, Czirók, Ben-Jacob, Cohen, Shochet, Phys. Rev. Lett. 75 1226 (1995)

Ginelli, arXiv:1511.01451 in Microswimmers Summer School, Jülich

Models

Continuum model

The mean center-of-mass velocity $\langle \boldsymbol{v} \rangle$ is the order parameter.

The development of $\langle \boldsymbol{v} \rangle \neq \boldsymbol{0}$ for the flock as a whole requires spontaneous breaking of the continuous rotational symmetry.

Out of equilibrium feature possible also in low dimensions.

Breakdown of linearized hydrodynamics imply large fluctuations in dimensions smaller than four.

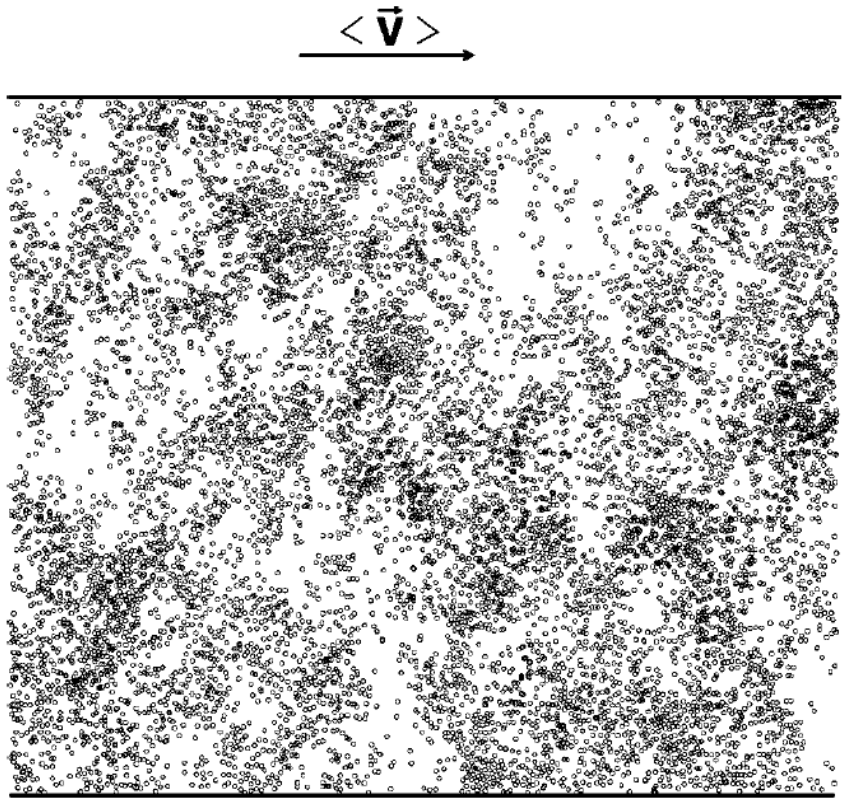
Argument: Improved transport suppresses the very fluctuations that give rise to it, leading to long-range order in $d = 2$.

"Flocks, herds, and schools : A quantitative theory of flocking",

Toner & Tu, Phys. Rev. E 58, 4828 (1998)

Models

Continuum model : giant density fluctuations



"Long-Range Order in a $2d$ Dynamical XY Model : How Birds Fly Together"

"Flocks, herds, and schools : A quantitative theory of flocking",

J. Toner & Y. Tu, Phys. Rev. Lett. 75, 4326 (1995), Phys. Rev. E 58, 4828 (1998)

Models

Continuum model

$$\partial_t \boldsymbol{v} + \underbrace{\lambda_1(\boldsymbol{\nabla}\cdot\boldsymbol{v})\boldsymbol{v} + \lambda_2(\boldsymbol{v}\cdot\boldsymbol{\nabla})\boldsymbol{v} + \lambda_3\boldsymbol{\nabla}v^2}_{\text{Navier-Stokes w/no Galilean invariance}} =$$

$$\underbrace{\alpha_1\boldsymbol{v} - \alpha_2 v^2\boldsymbol{v}}_{\text{“Potential force” imposing } v^2=\alpha_1/\alpha_2} \qquad \underbrace{-\boldsymbol{\nabla}P}_{\text{“Pressure variation”}}$$

$$\underbrace{+D_B\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{v}) + D_T\nabla^2\boldsymbol{v} + D_2(\boldsymbol{v}\cdot\boldsymbol{\nabla})^2\boldsymbol{v}}_{\text{Dissipative terms}} \underbrace{+\boldsymbol{\eta}}_{\text{Noise}}$$

$$P = \sum_{n=1}^{\infty}\sigma_n(\rho-\rho_0)^n$$

Pressure tending to impose $\rho-\rho_0$ small

$$\partial_t\rho + \boldsymbol{\nabla}\cdot(\boldsymbol{v}\rho) = 0$$

Toner & Tu, Phys. Rev. E 58, 4828 (1998)

$\alpha_1 < 0$ ($\alpha_1 > 0$) in the homogenous (flocking) phase

“Hydrodynamic eqs. for self-propelled part.: microscopic derivation & stability analysis”

Bertin, Droz and Grégoire, J. Phys. A 42, 445001 (2009)

Models

Run & tumble particles

This mechanism can be described as a repeating sequence of two actions:

(i) a period of nearly constant-velocity translation (run) followed by

(ii) a seemingly erratic rotation (tumble).

Observed by **Berg & Brown, Nature (1972)**

Simulation

from **M. Kardar**'s webpage

Run with $v = 20\,\mu m/s$; tumble with rate $\alpha = 1/s$ and duration $\tau = 0.1\,s$

Diffusion constants

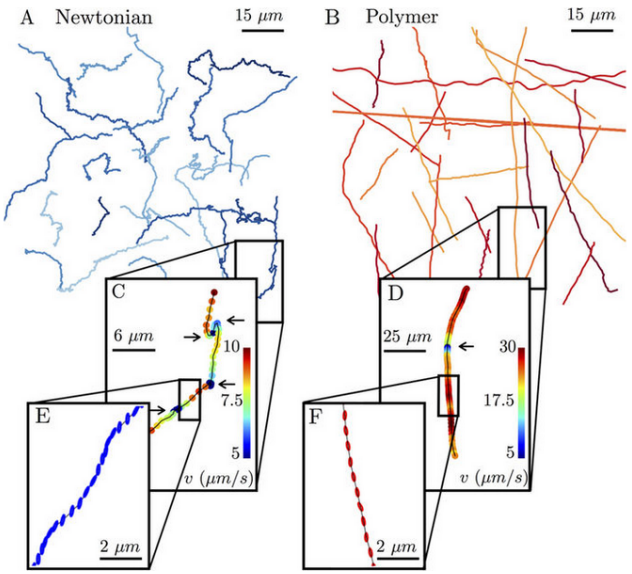
$$D_{RT} = \frac{v^2}{d\alpha(1+\alpha\tau)} \simeq 100\,\mu m^2/s$$

$$D_{BM} = \frac{k_B T}{6\pi\eta R} \simeq 0.2\,\mu m^2/s$$

Models

Run & tumble particles

Some trajectories depending on the environment



Trajectories of E. coli cells in (A) buffer and (B) polymeric solution

"Running and tumbling with E. coli in polymeric solutions",

Patteson, Gopinath, Goulian and Arratia, Scient. Rep. 5, 15761 (2015)

Models

Fluctuating hydrodynamic theories in low density limits

Local density scalar field $\rho(\boldsymbol{r},t) = \sum_{i=1}^{N} \delta(\boldsymbol{r} - \boldsymbol{r}_i(t))$

Local polar vector field $\boldsymbol{p}(\boldsymbol{r},t) = \frac{1}{\rho(\boldsymbol{r},t)} \sum_{i=1}^{N} \hat{\boldsymbol{v}}_i(t) \delta(\boldsymbol{r} - \boldsymbol{r}_i(t))$

$$\begin{aligned} \partial_t \rho + v_0 \boldsymbol{\nabla} \cdot (\rho \boldsymbol{p}) &= -\boldsymbol{\nabla} \cdot \left(-\frac{1}{\gamma_\rho} \boldsymbol{\nabla} \frac{\delta F}{\delta \rho} + \boldsymbol{\eta}_\rho \right) \\ \partial_t \boldsymbol{p} + \lambda_1 (\boldsymbol{p} \cdot \boldsymbol{\nabla}) \boldsymbol{p} &= -\frac{1}{\gamma_{\boldsymbol{p}}} \frac{\delta F}{\delta \boldsymbol{p}} + \boldsymbol{\eta}_{\boldsymbol{p}} \end{aligned}$$

with wise proposals for the "free-energy" F and noises $\boldsymbol{\eta}_\rho$ and $\boldsymbol{\eta}_{\boldsymbol{p}}$.

"Hydrodynamics of soft active matter"

Marchetti, Joanny, Ramaswamy, Liverpool, Prost, Rao, Simha

Rev. Mod. Phys. 85 (2013)

Langevin approach

Lennard-Jones potential

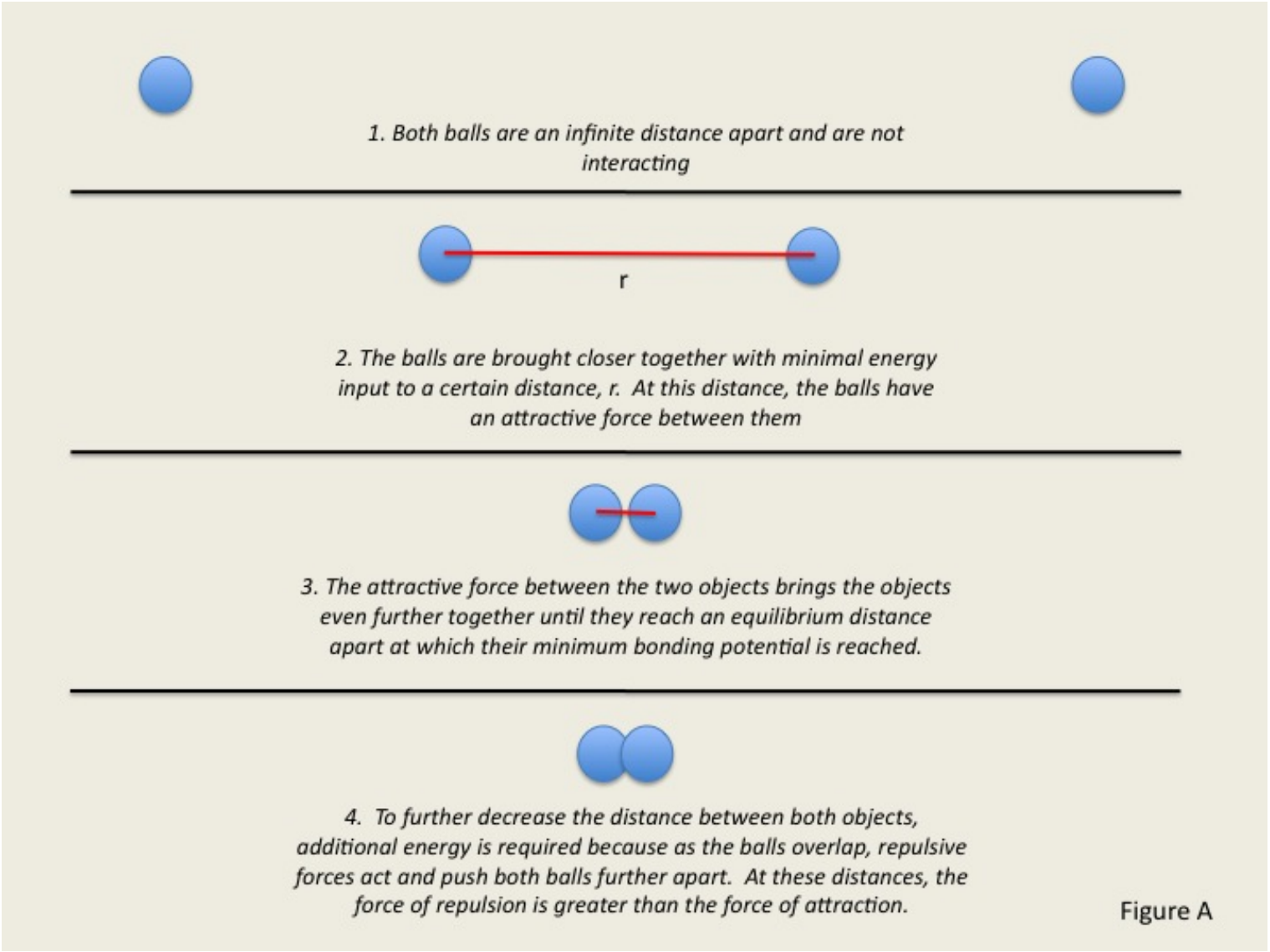


Figure A

Langevin approach

Lennard-Jones potential

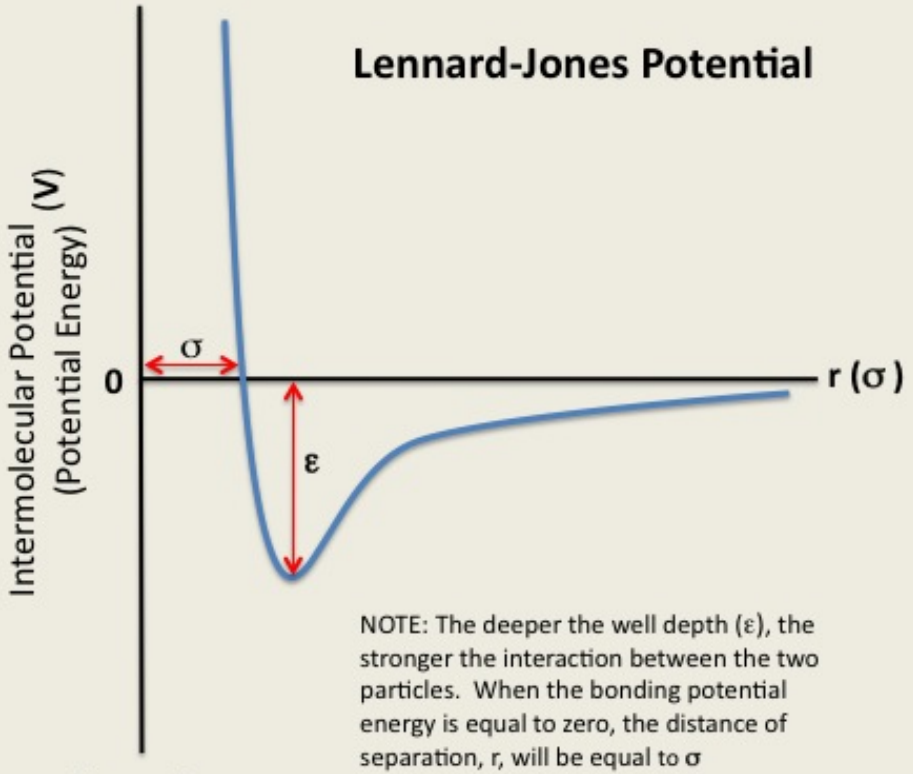


Figure B

Langevin approach

Lennard-Jones potential

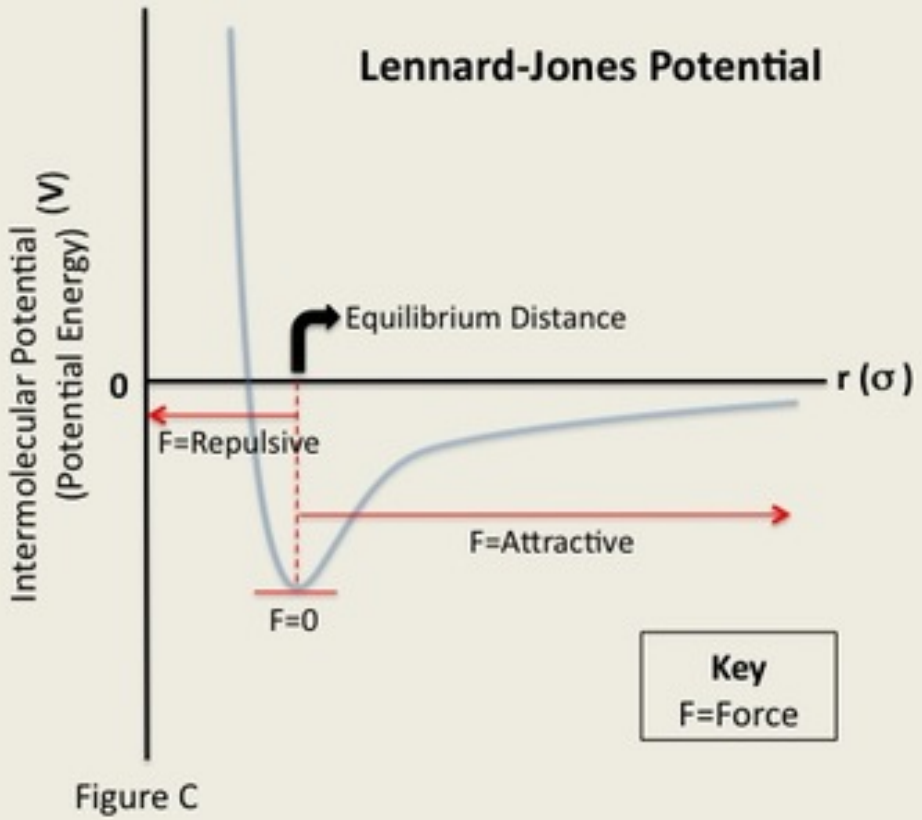
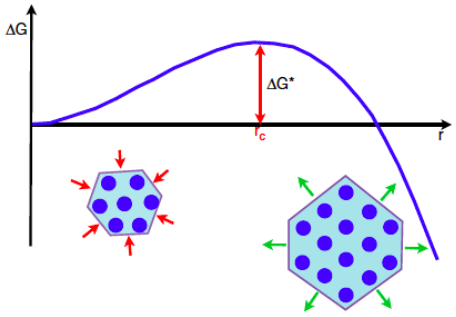


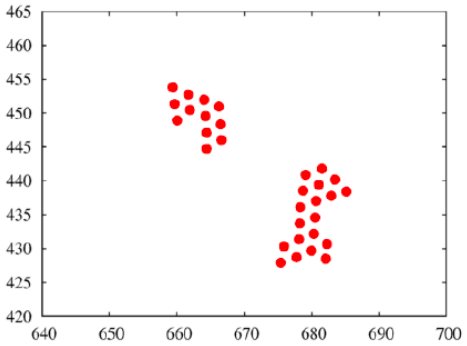
Figure C

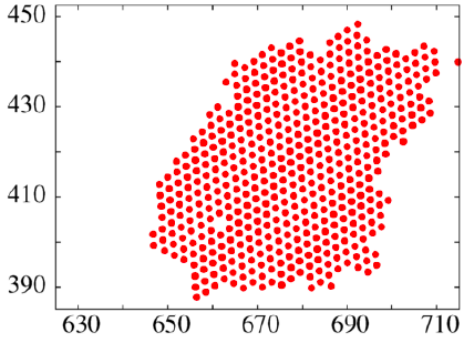
Figures : credit **Chemistry LibreTexts UC Davis**

Freezing

First order route: nucleation & growth







Nucleation barrier $\Delta F(R)$

Examples of two crystalline configurations

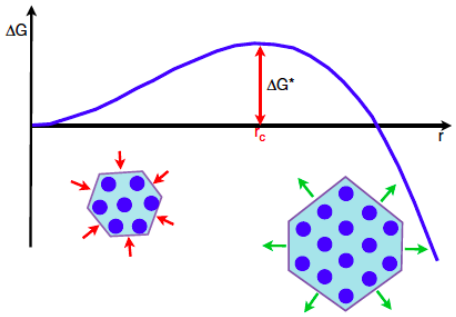
$$\Delta F(R) \equiv F_{\text{bubble}}(R) - F_{\text{no bubble}}(R) \approx -\delta f \, R^d + s \, R^{d-1}$$

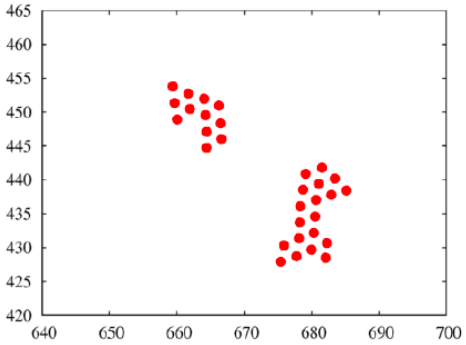
$$\Delta F(R_c) \approx \frac{s^d}{(\delta f)^{d-1}} \quad \text{and} \quad R_c \approx \frac{s}{\delta f} \quad \text{in} \quad d \geq 2$$

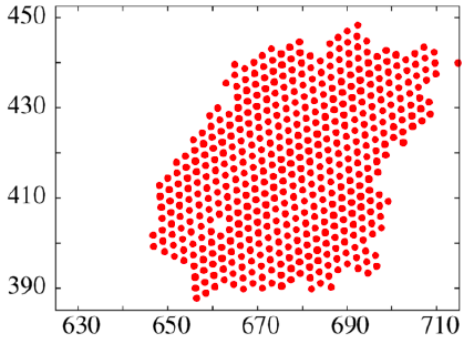
Left image from **Gasser, J. Phys. : Cond. Matt. 21, 203101 (2009)**

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)**

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.

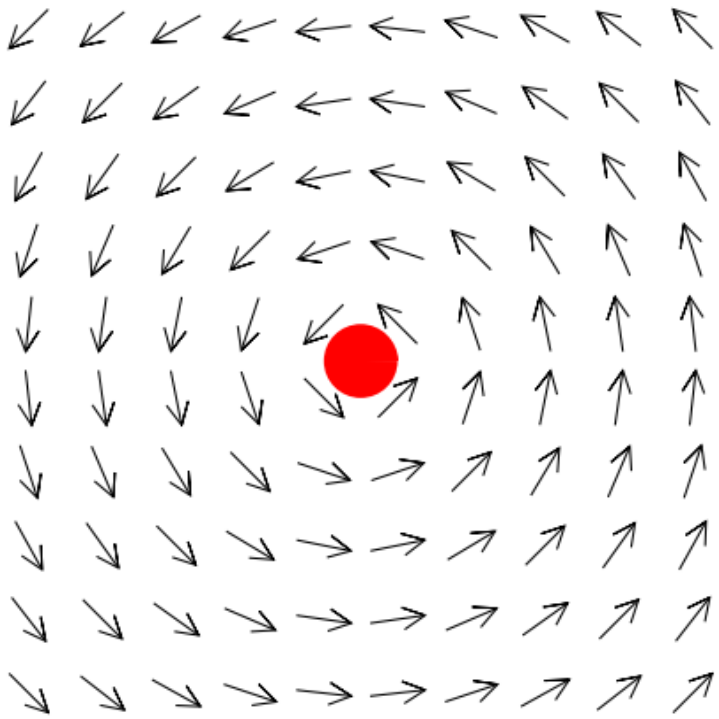
Assumption: the transition is continuous and it is determined by the unbinding of vortices (topological defects).

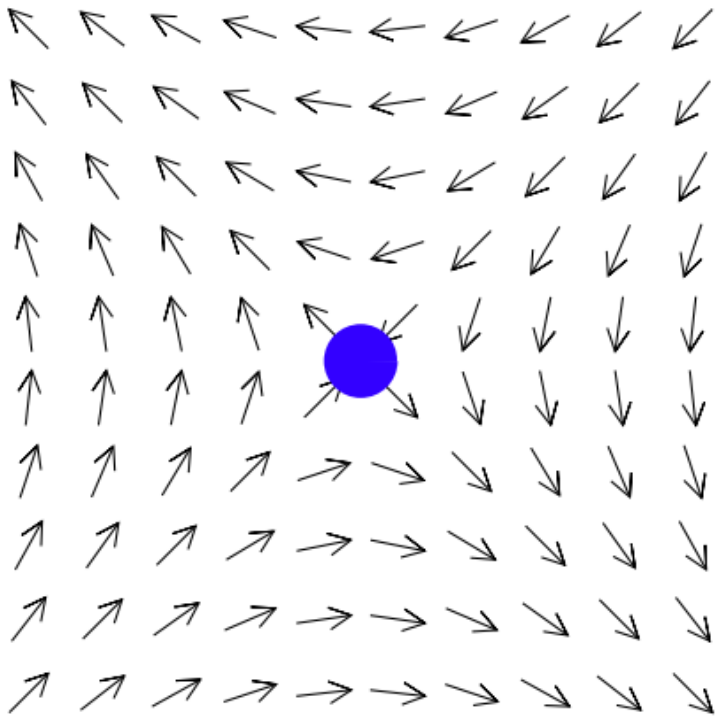
Proved with RG, assuming a continuous phase transition.

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

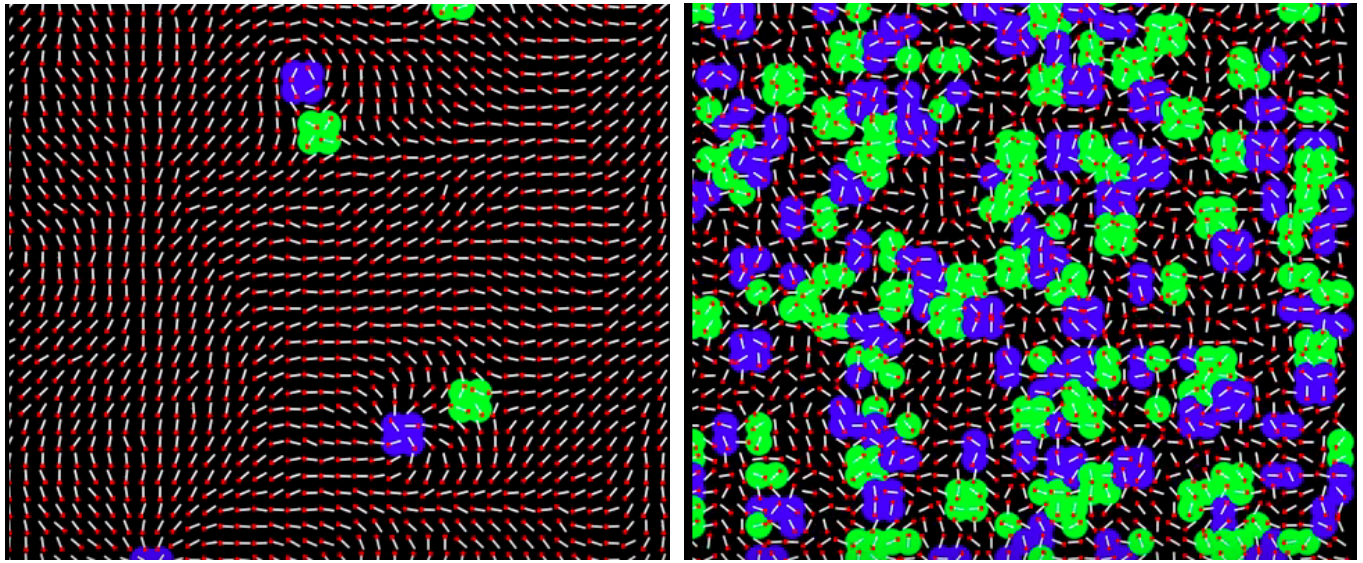
Vortices





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**

Equilibrium phases

Macroscopic properties

- A gas is an an air-like fluid substance which expands freely to fill any space available, irrespective of its quantity.
- A liquid is a substance that flows freely but is of constant volume, having a consistency like that of water or oil. It takes the shape of its container
- A solid is a material with non-vanishing shear modulus.
- A crystal is a system with long-range positional order.

  It has a periodic structure and its ‘particles’ are located close to the nodes of a lattice.

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, $\boldsymbol{s}_i=(\cos\theta_i,\sin\theta_i)$

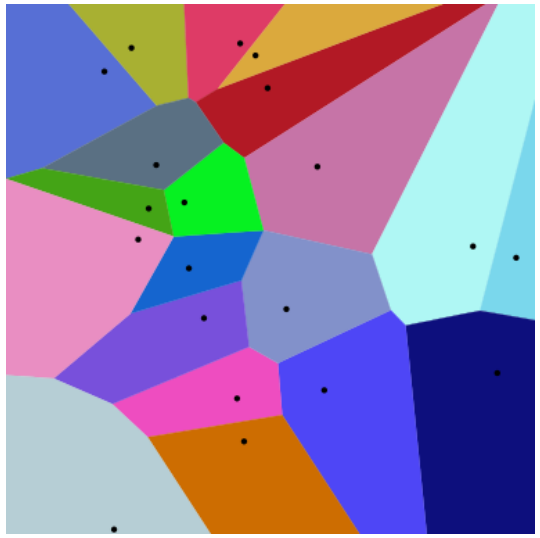
$$-\frac{H}{J}=\sum_{\langle ij\rangle}\boldsymbol{s}_i\cdot\boldsymbol{s}_j=\sum_{\langle ij\rangle}\cos\theta_{ij}\simeq\sum_{\langle ij\rangle}(1-\frac{\theta_{ij}^2}{2})\approx-\frac{1}{2}\int d^2r\ [\boldsymbol{\nabla}\theta(\boldsymbol{r})]^2$$

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

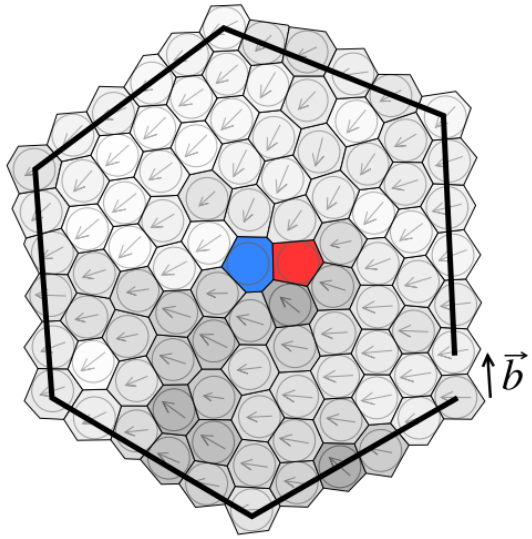
All points within this region are closer to the dot within it than to any other dot on the plane

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

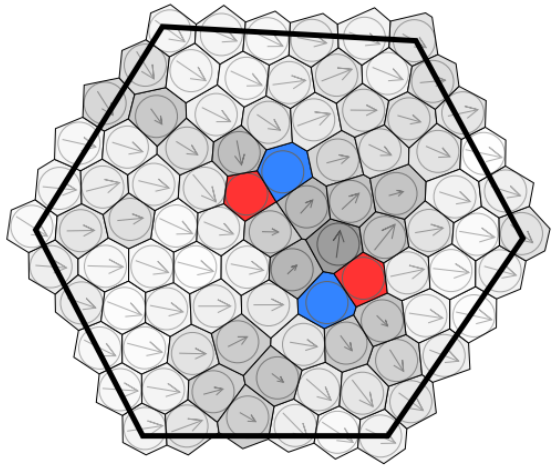
The grey zone has six neighbouring cells

Close packing of disks

Disks, Voronoi cells & dislocations



A free dislocation



A bound pair of dislocations

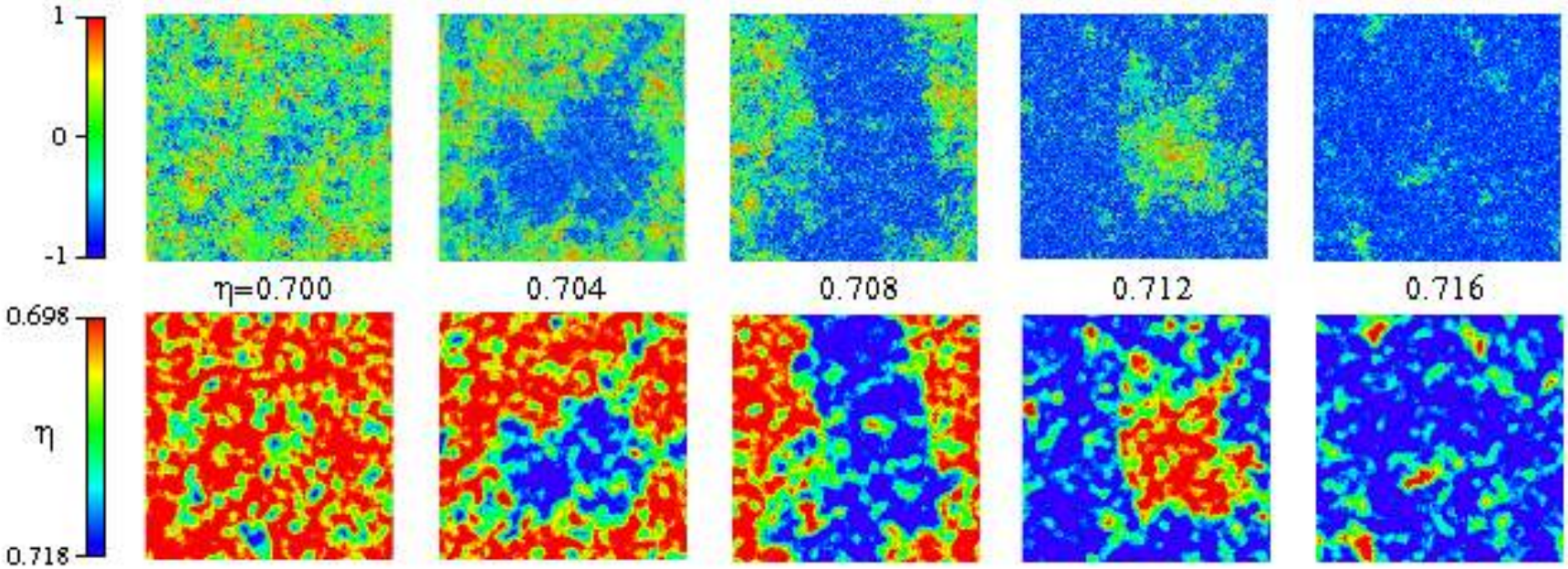
In the crystal the centers of the disks form a triangular lattice

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

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

Hard disks in two dimensions

Correlation between the local orientation and density

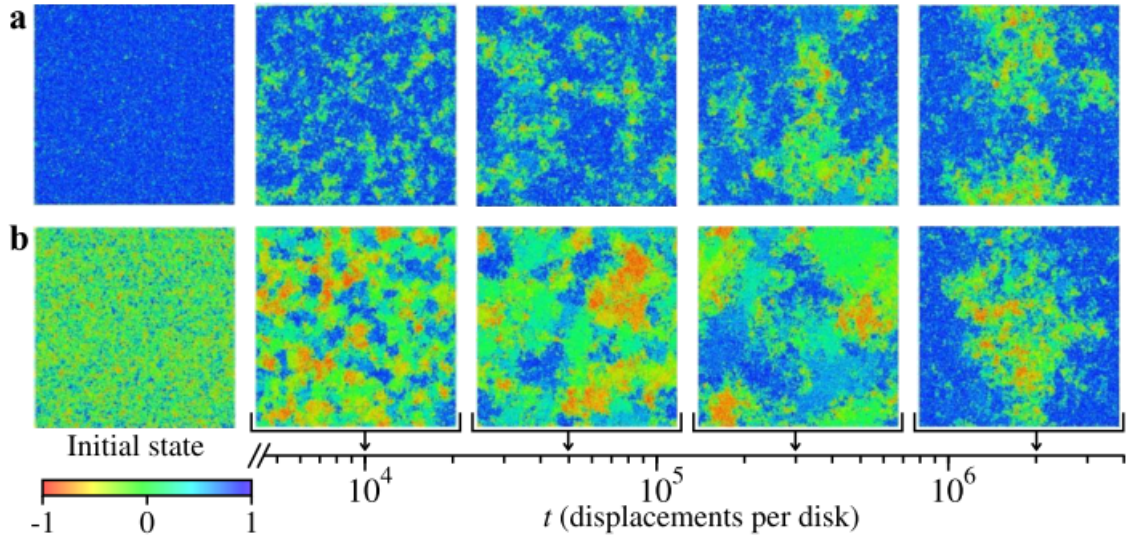


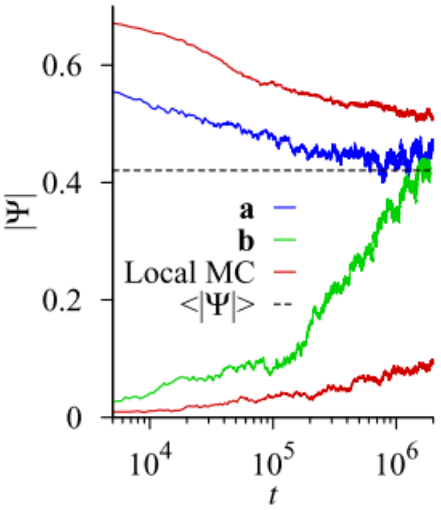
"Two-step melting in two dimensions : first-order liquid-hexatic transition"

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

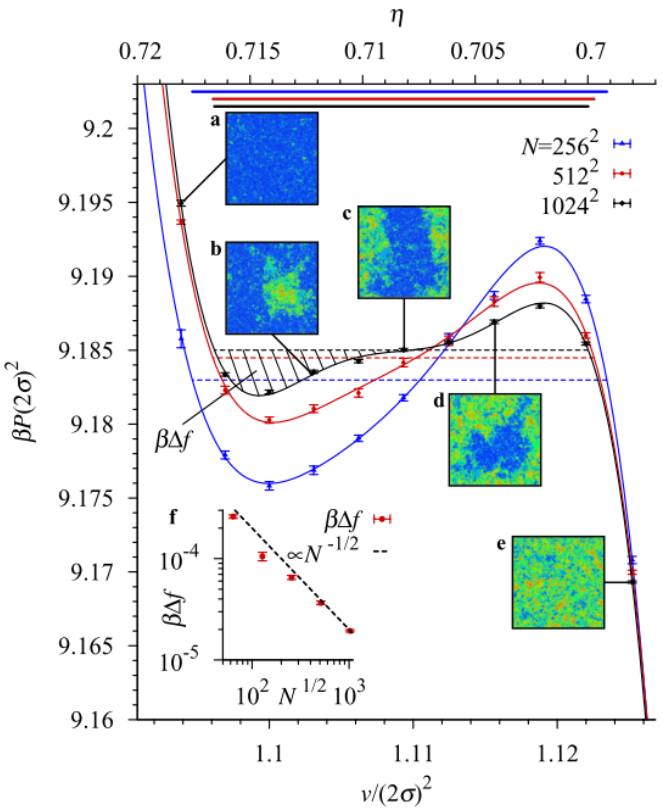
"Two-step melting in two dimensions : first-order liquid-hexatic transition"

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

Hard disks in two dimensions

Pressure loop and finite N dependence

Hexatic Liquid



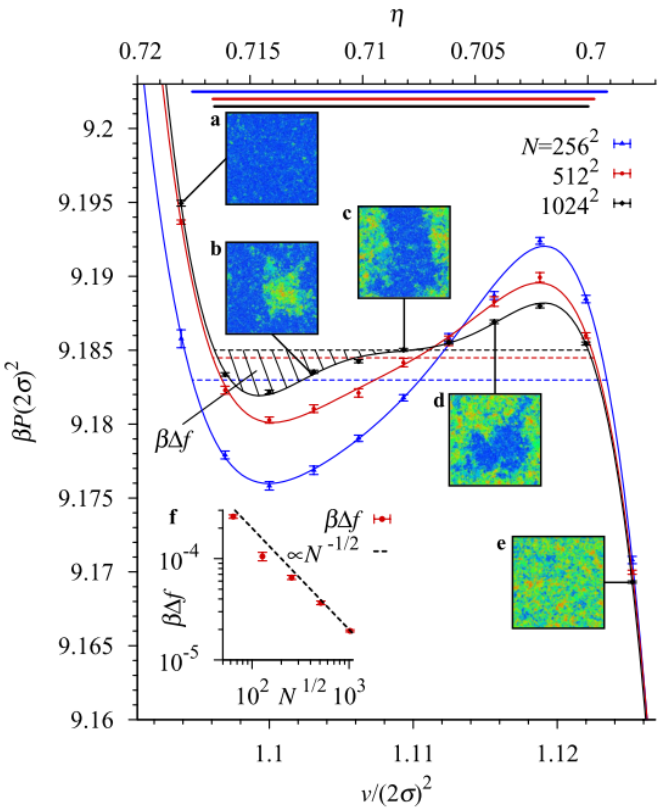
Similar to Van der Waals model for 1st order phase transitions

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 $\phi \simeq 0.708$

Observables

Local density

For each bead, i the first estimate of the local density ϕ_i^{Vor} is the ratio between its surface and the area A_i^{Vor} of its Voronoi region:

$$\phi_i^{\mathrm{Vor}} = \frac{\pi\sigma_{\mathrm{d}}^2}{4A_i^{\mathrm{Vor}}}$$

We next coarse-grain this value by averaging the single-bead densities ϕ_i^{Vor} over a disk $S_R^{(i)}$ with radius R

$$[[\phi_i]] \equiv \sum_{i \in S_R^{(i)}} \phi_i^{\mathrm{Vor}} / (\pi R^2)$$

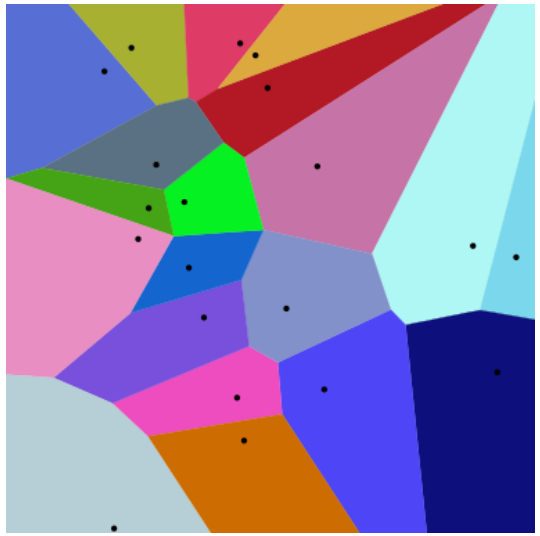
Visualisation: each bead is painted with the colour of its coarse-grained local density value, $[[\phi_i]]$, denser in red, looser in blue.

Observables

Voronoi tessellation

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

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

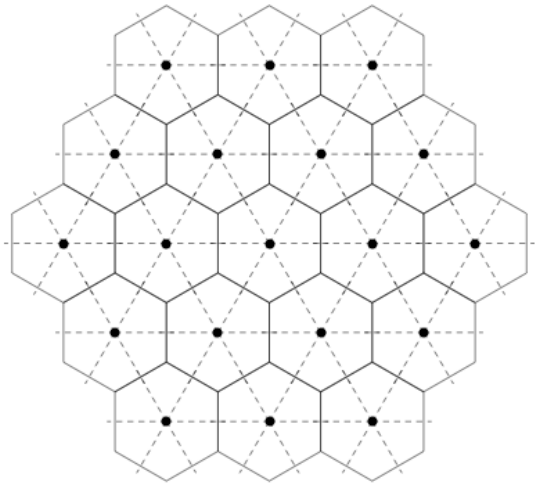
The grey zone has six neighbouring cells

Observables

Voronoi tessellation

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

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



With dashed lines, the triangular lattice

The vertices are the sites

Each site has six nearest neighbours

The angles of the edges of the triangular lattice are

$$\theta_{ij} = 2\pi j/6$$

The hexagonal lattice is the Voronoi tessellation

Observables

Local density

For each bead, i the first estimate of the local density ϕ_i^{Vor} is the ratio between its surface and the area A_i^{Vor} of its Voronoi region:

$$\phi_i^{\mathrm{Vor}} = \frac{\pi\sigma_{\mathrm{d}}^2}{4A_i^{\mathrm{Vor}}}$$

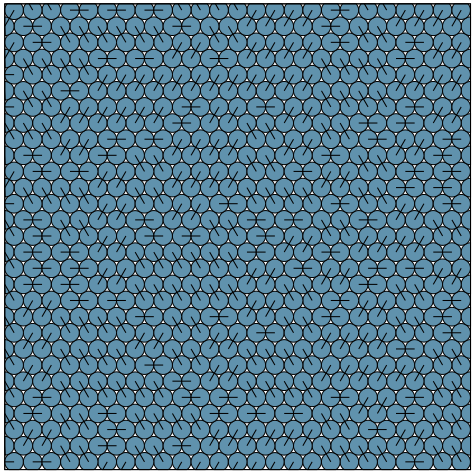
We next coarse-grain this value by averaging the single-bead densities ϕ_i^{Vor} over a disk $S_R^{(i)}$ with radius R

$$[[\phi_i]] \equiv \sum_{i \in S_R^{(i)}} \phi_i^{\mathrm{Vor}} / (\pi R^2)$$

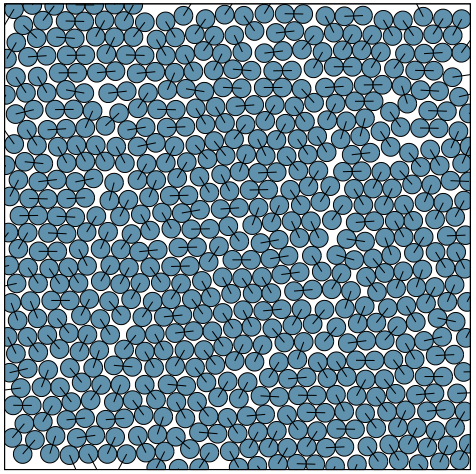
Visualisation: each bead is painted with the colour of its coarse-grained local density value, $[[\phi_i]]$, denser in red, looser in blue.

Initial conditions

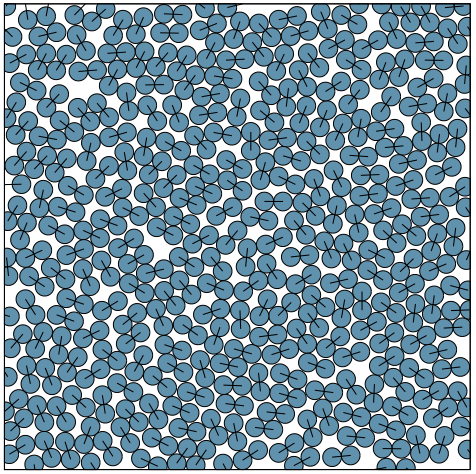
Three cases



Crystal



Hexatic order



Random

with the desired ϕ

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

Observables

Positional order

The density-density correlation function

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

is linked to the structure factor

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

by

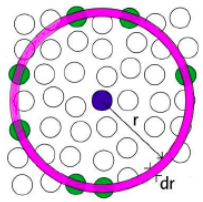
$$N\,S(\boldsymbol{q})\;=\;\int d^d\boldsymbol{r}_1\int d^d\boldsymbol{r}_2\,C(\boldsymbol{r}_1,\boldsymbol{r}_2)\,e^{-\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)}$$

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

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

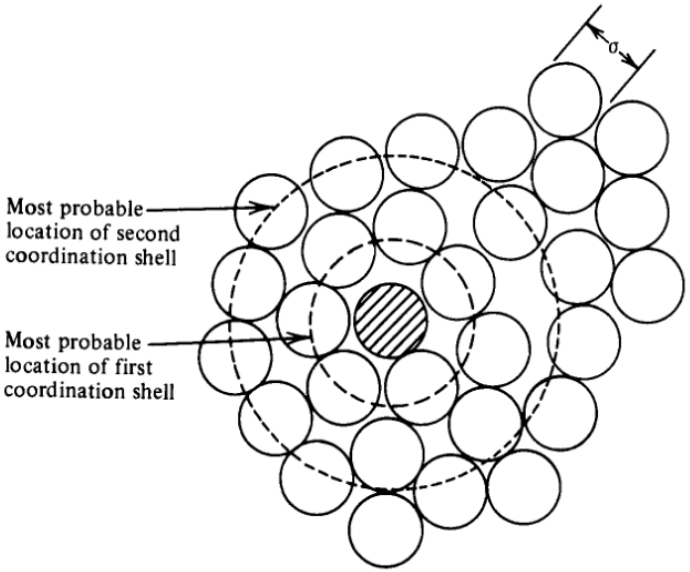
by

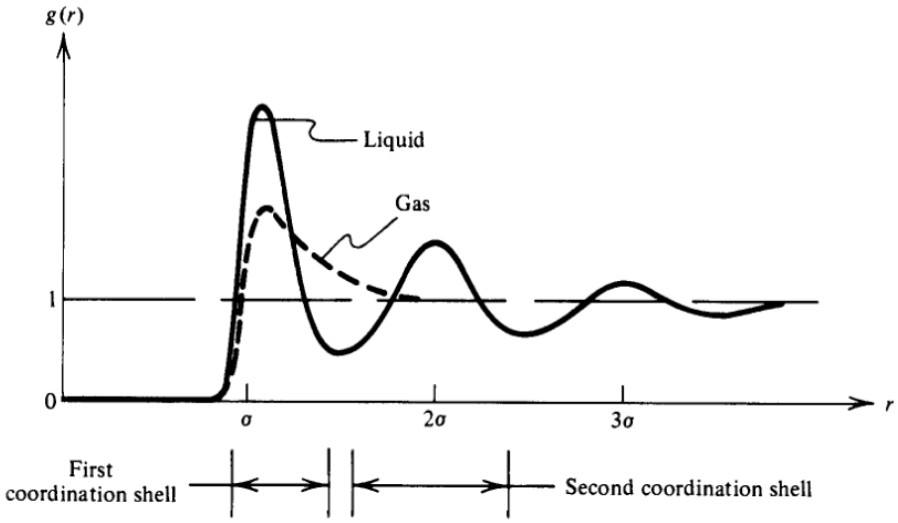
$$S(\boldsymbol{q}) = 1 + \frac{N}{V} \int d^d\boldsymbol{r}\; g(r)\, e^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}$$

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

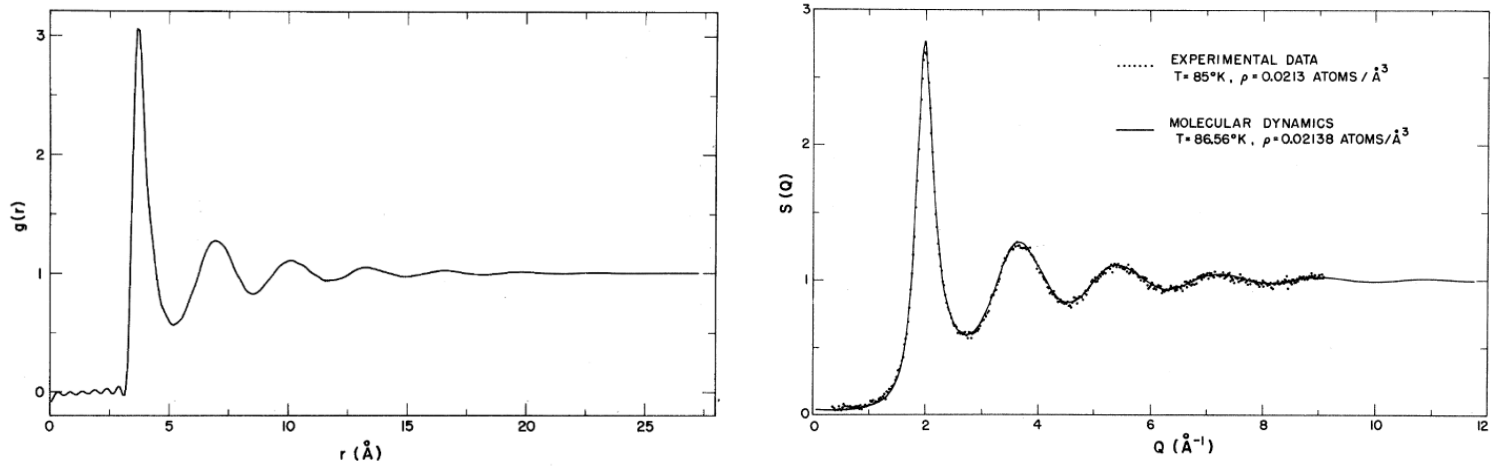




"Introduction to Modern Statistical Mechanics", **Chandler** (OUP)

Observables

Experiments & simulations of liquids



Inter-peak distance in $g(r)$ is $\Delta r \simeq \sigma \simeq 3\text{Å}$

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

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

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

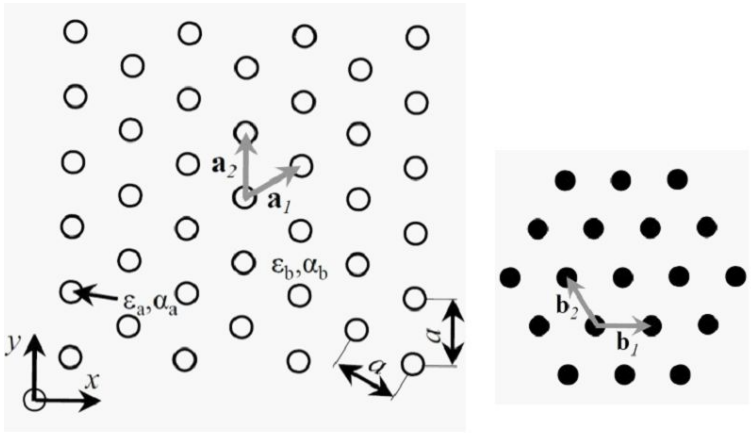
Observables

Structure factor for crystals

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

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

Visualisation : $2d$ representation in the (q_x, q_y) plane, Bragg peaks.



(a) (b)

Triangular lattice in real space — Hexagonal lattice in reciprocal space

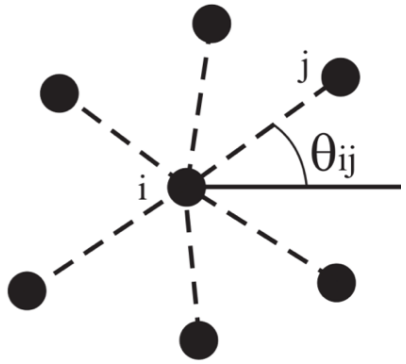
Voronoi cell — Brillouin zone

Observables

Hexatic order

The local hexatic fluctuating order

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



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

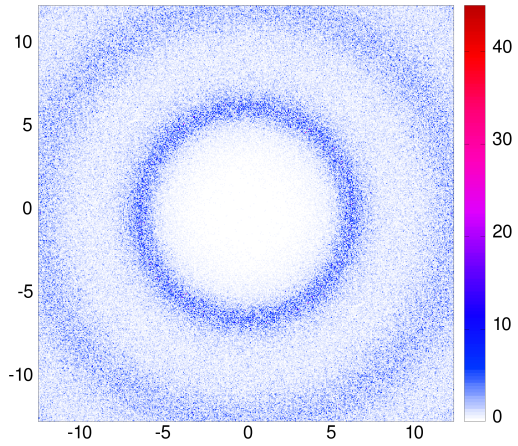
$$g_6(r) = \frac{\sum_{ij} [\langle \psi^*_{6i} \psi_{6j} \rangle] \Big|_{r_{ij}=r}}{[\langle |\psi_{6i}|^2 \rangle]}$$

Note that the normalisation is site independent

Passive system

Structure factor - very low and very high density

$\phi = 0.66$

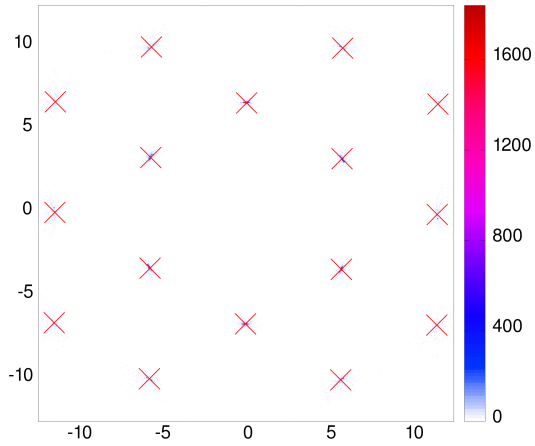


Liquid

Solid

Bragg peaks

$\phi = 0.76$



Primitive vectors

$$\boldsymbol{q}_1 = \frac{4\pi}{a\sqrt{3}}\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)$$

$$\boldsymbol{q}_2 = \frac{4\pi}{a\sqrt{3}}(0, 1)$$

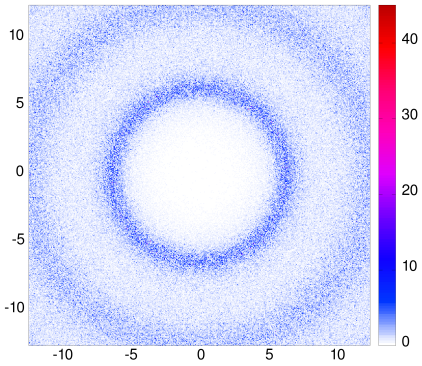
Unit of length

$$a = \left(\frac{\pi}{2\sqrt{3}\phi}\right)^{1/2} \sigma_{\mathrm{d}}$$

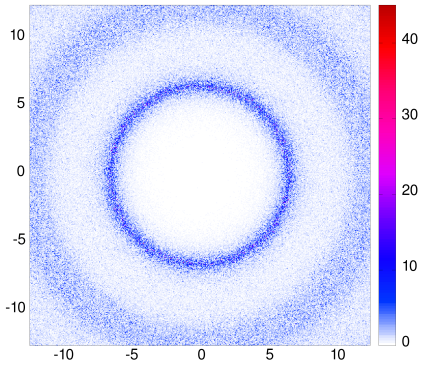
Passive system

Structure factor - progressive increase in density

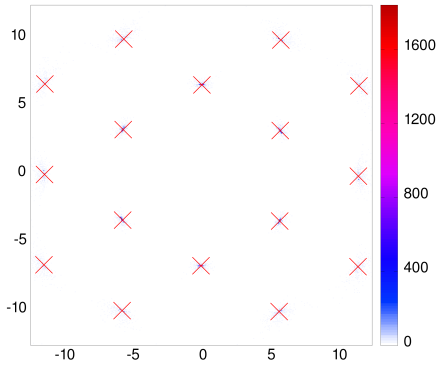
$\phi = 0.66$ (liquid)



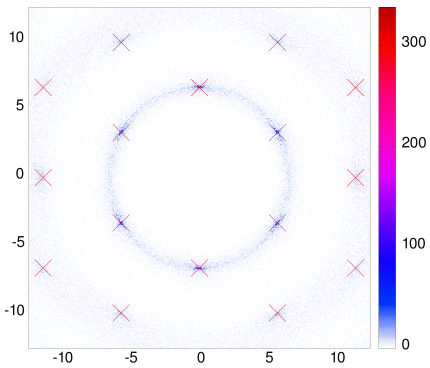
$\phi = 0.72$ (liquid)



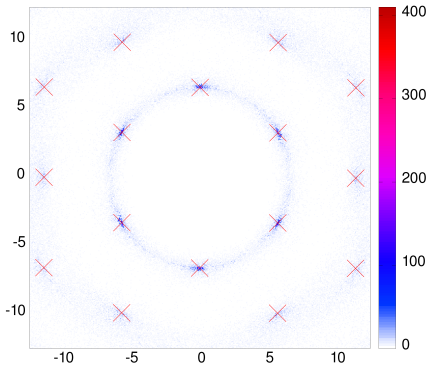
$\phi = 0.76$ (solid)



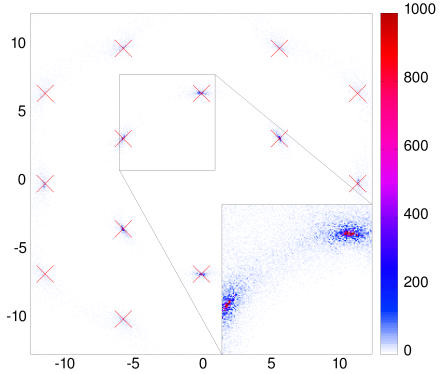
$\phi = 0.734$ (co-existence)



$\phi = 0.74$ (co-existence)

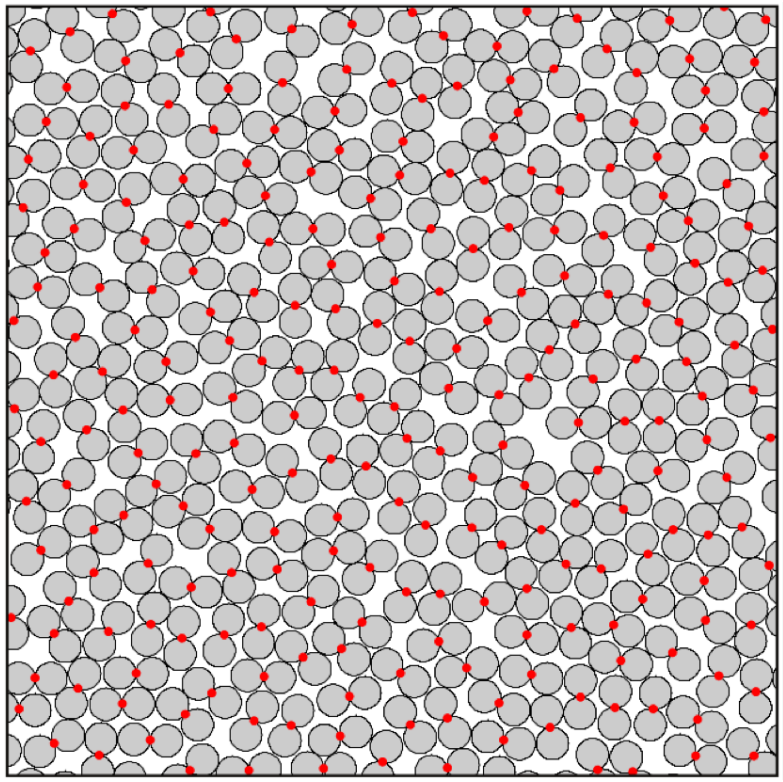


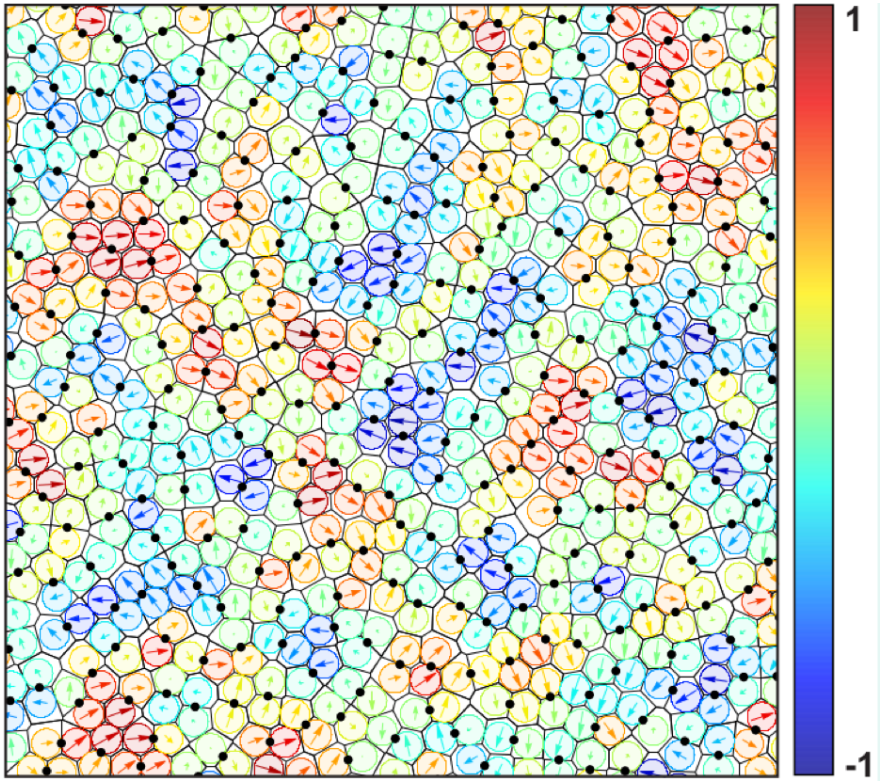
$\phi = 0.75$ (co-existence)



Passive system

Hexatic order parameter





Dumbells

Hexatic local vector

Plan

1. The result : new phase diagram
2. The interacting dumbbells model
3. Passive case
4. Active case
5. Discussion of

   Mobility induced phase transition for purely repulsive interactions

   vs.

   just an extension of the Bernard & Krauth passive system scenario

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

Single active dumbbell

Control parameters

Number of dumbbells $N = 1$ and box volume S in two dimensions:

packing fraction $\phi = \dfrac{\pi \sigma_{\mathrm{d}}^2}{2S}$

Transport rates:

Advective transport $Lv \mapsto \sigma_{\mathrm{d}} F_{\mathrm{act}}/\gamma$

diffusive transport $D \mapsto k_B T/(2\gamma)$

Péclet number $\mathrm{Pe} = \dfrac{2F_{\mathrm{act}}\sigma_{\mathrm{d}}}{k_B T}$

Active force $Lv \mapsto \sigma_{\mathrm{d}} F_{\mathrm{act}}/\gamma$

viscous force $\nu \mapsto \gamma \sigma_{\mathrm{d}}^2/m_{\mathrm{d}}$

Reynolds number $\mathrm{Re} = \dfrac{m_{\mathrm{d}} F_{\mathrm{act}}}{\sigma_{\mathrm{d}} \gamma^2}$

$\mathrm{Pe} \in [0, 40]$ $\mathrm{Re} < 10^{-2}$

We keep the parameters in the harmonic (fene) and WCA (repulsive) potential fixed. Stiff molecule limit: vibrations frozen.

Interest in the Pe (and later ϕ) dependencies.

Hard disks in two dimensions

Orientation vector construction

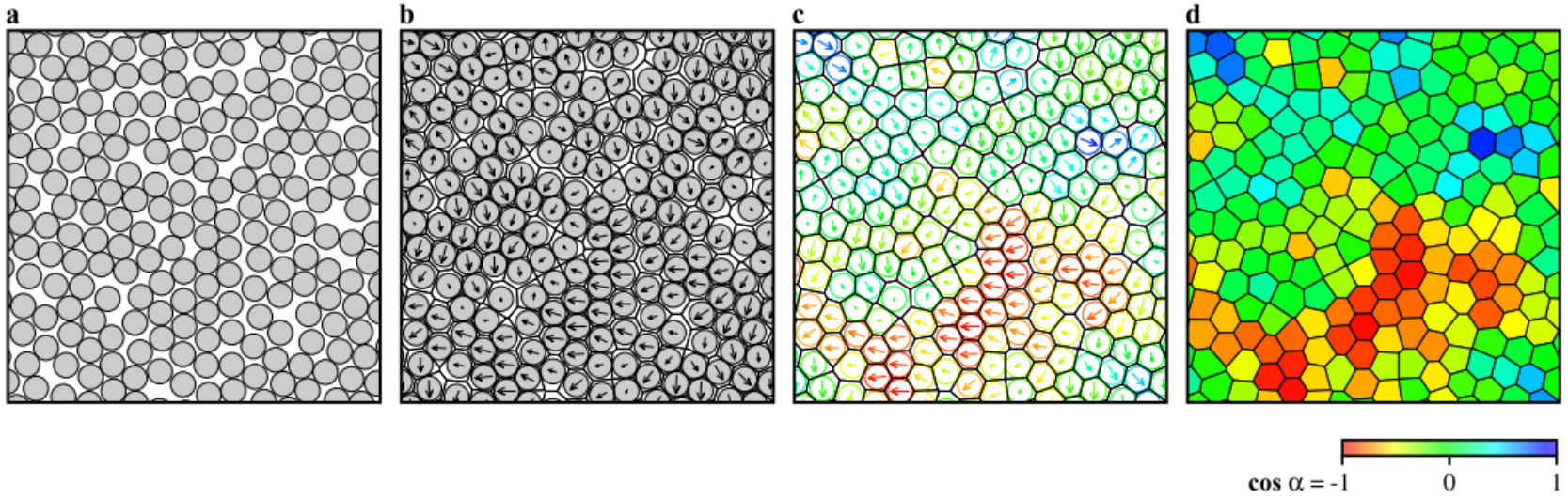


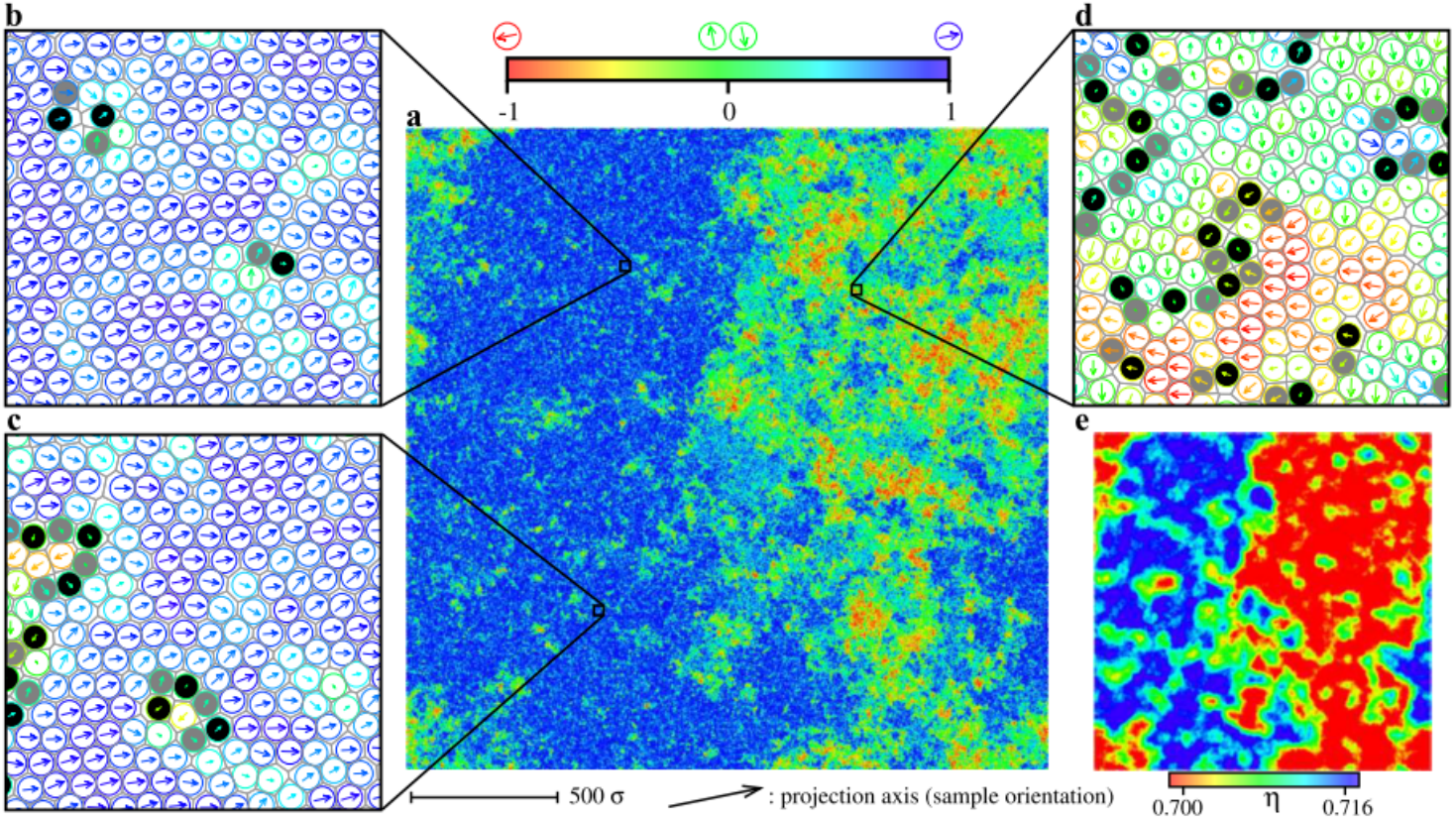
Figure 3.4: Close view of the construction for the visualization of the orientational field. **a**: Hard disks **b**: Voronoi construction, the arrows represent the local orientations. **c**: Coloration of the orientation depending on their projection toward a given axis. **d**: The Voronoi cells are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

Summary

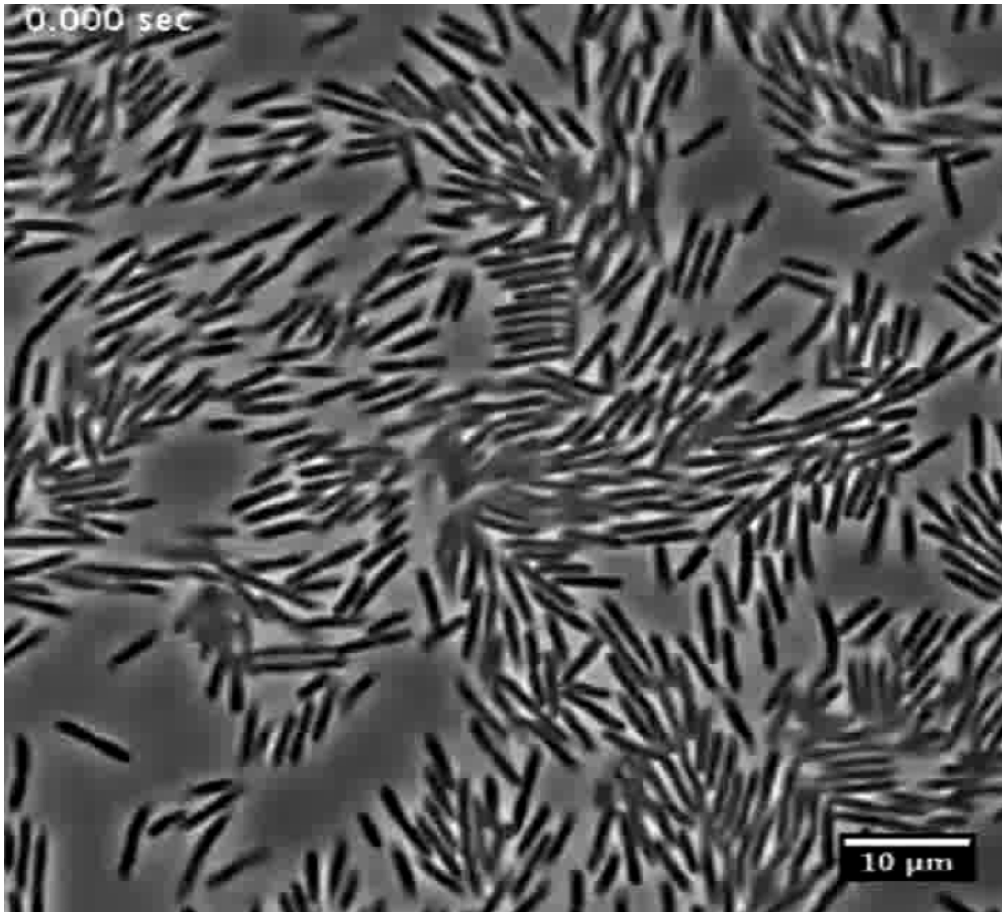
Equilibrium phases of $2d$ matter

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

	BKTHNY	BeKr
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

Active dumbbell system

Mechanism for segregation

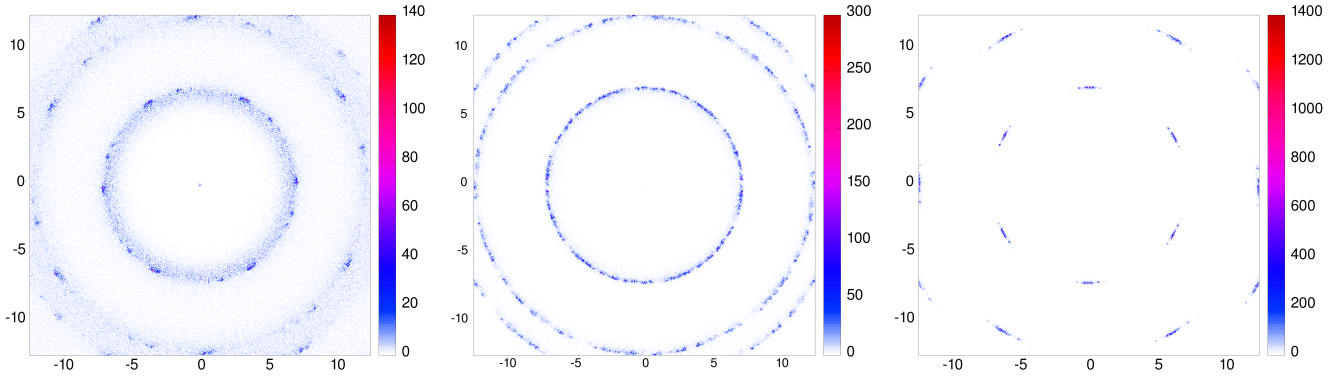


Active dumbbell system

Structure factor Pe = 10 & Pe = 40

$\phi = 0.734$ $\phi = 0.84$ $\phi = 0.88$

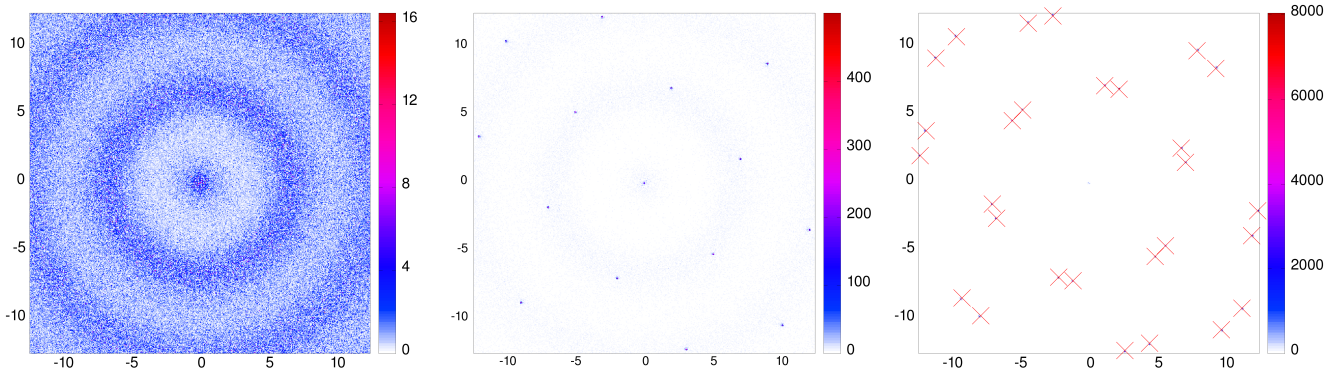
Pe = 10



(liquid) (upper limit of co-existence)

$\phi = 0.26$ $\phi = 0.28$ $\phi = 0.34$

Pe = 40



(liquid) (lower limit of co-existence

Harmonic solids

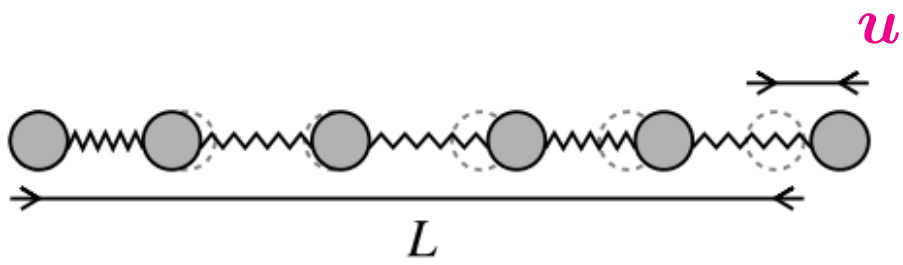
Peierls calculation

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

Call $\boldsymbol{\phi_{R_i}}$ the position of the ith atom that, at zero temperature, is located at a vertex $\boldsymbol{R_i}$ of a regular lattice, the equilibrium positions of the springs.

At finite temperature the atomic positions fluctuate, $\boldsymbol{\phi_{R_i} = R_i + u_{R_i}}$, with $\boldsymbol{u_{R_i}}$ the local displacement from $\boldsymbol{R_i}$.

$1d$ sketch



Does the long-range positional order survive at finite T in $2d$?

Harmonic solids

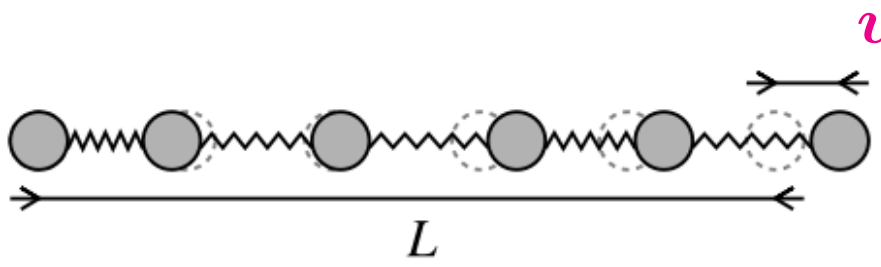
Peierls calculation

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

Call $\boldsymbol{\phi_{R_i}}$ the position of the ith atom that, at zero temperature, is located at a vertex $\boldsymbol{R_i}$ of a regular lattice, the equilibrium positions of the springs.

At finite temperature the atomic positions fluctuate, $\boldsymbol{\phi_{R_i} = R_i + u_{R_i}}$, with $\boldsymbol{u_{R_i}}$ the local displacement from $\boldsymbol{R_i}$.

$1d$ sketch



No ! $\Delta^2(\boldsymbol{r}) = \langle [\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{0})]^2 \rangle \simeq \frac{k_B T}{K} \ln r$ **in** $d = 2$

BKT-Halperin-Nelson-Young

The $2d$ particle systems

At very high temperature (low density) one expects disorder.

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

There must be a transition in between.

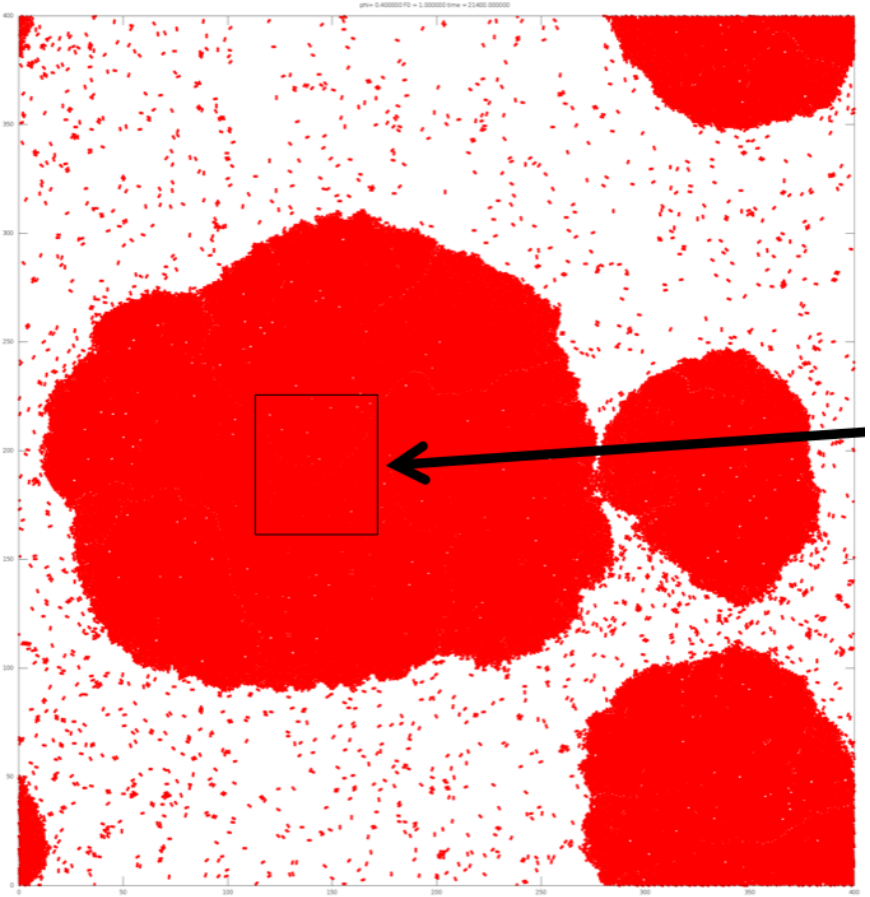
Assumption: the transition is continuous and it is determined by the unbinding of dislocations in the solid (topological defects).

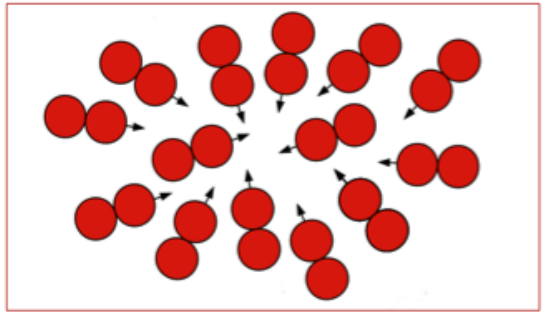
Proved with RG that assumes a continuous phase transition.

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.

Active dumbbell system

Active mechanism for segregation





Activity favours segregation