Phase diagrams (& effect temperatures) of 2d active matter

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Work in collaboration with

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

G. Gonnella, **P. Digregorio**, G.-L. Laghezza, A. Lamura, A. Mossa, **I. Petrelli** (Bari, Italia, 2013-2019) & **A. Suma** (Trieste, Italia & Philadelphia, USA, 2014-2019)

D. Levis & I. Pagonabarraga (Barcelona, España & Lausanne, Suisse, 2017-2019)

Viña del Mar, Chile, 2019

Aim

Better understanding of dense (monodisperse) $2d$ active matter

Aim

Why $2d$?

Experimental realisations but...

in reality,

because $2d$ is interesting from a

fundamental viewpoint

Plan

1. Equilibrium phases: solidification/melting

   Special in two-dimensions

2. Self-propelled Brownian dumbbells & disks for active matter

3. Collective behaviour of dumbbells & disks in $2d$

   Passive case

   Active solid, hexatic, liquid, co-existence & Motility Induced Phase Separation (MIPS)

   Topological defects

   Effective temperatures

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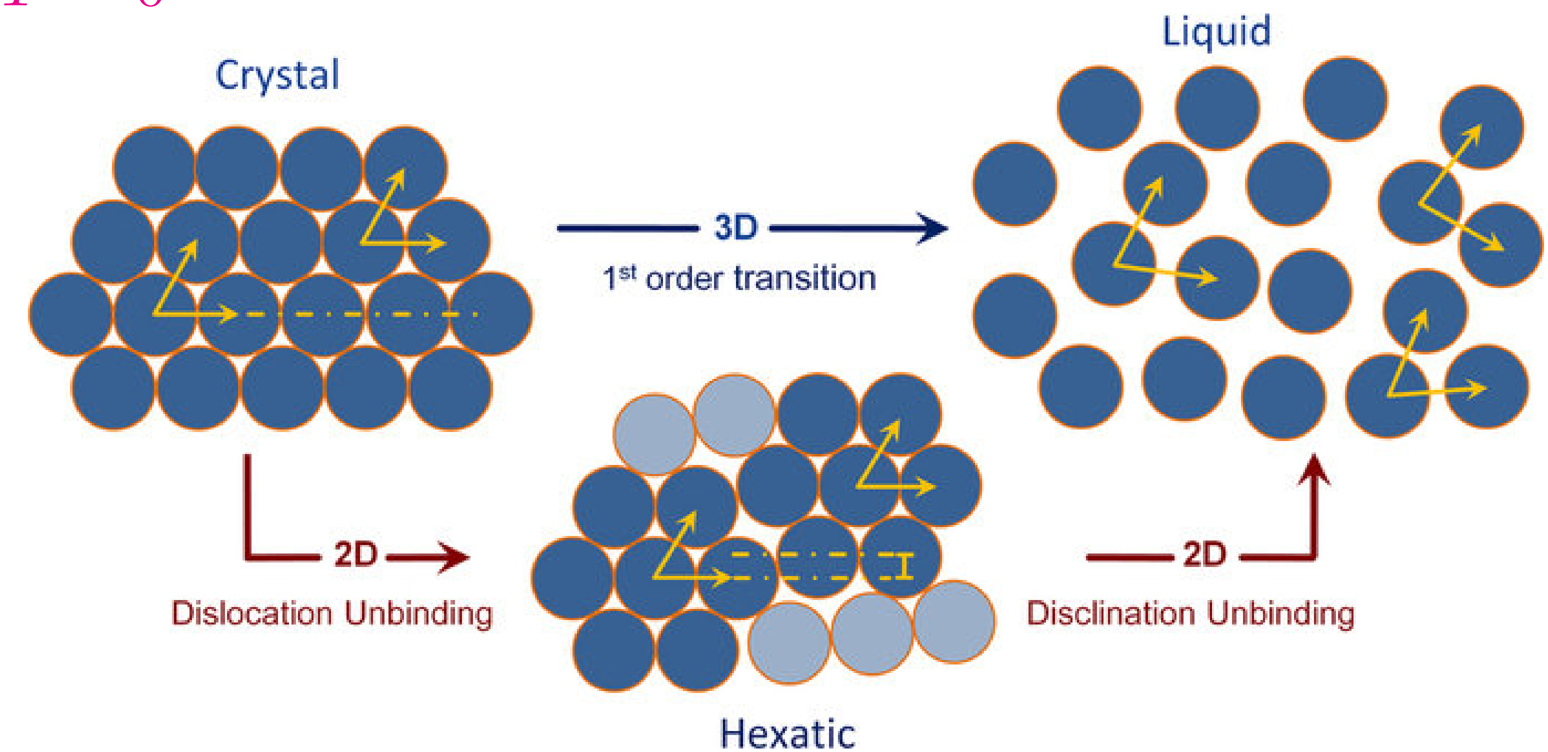
Freezing/Melting

Different routes in $3d$ and $2d$: mechanisms ?

$T = 0$



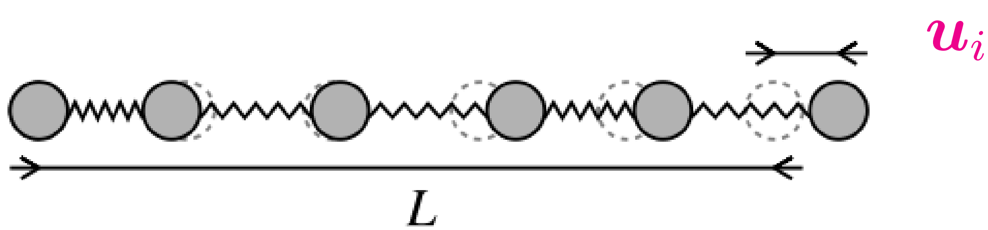
Orientation order preserved also lost

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

Harmonic solids

Peierls: no finite T long-range translational order in $2d$

Consider a crystal made of atoms connected to their nearest-neighbours by Hooke springs. At finite T the atomic positions, $\boldsymbol{\phi}_i$, fluctuate, $\boldsymbol{\phi}_i = \boldsymbol{R}_i + \boldsymbol{u}_i$, with $\boldsymbol{u}_i$ the local displacement from a regular lattice site i



Dashed: perfect lattice positions $\boldsymbol{R}_i$ Gray: actual positions $\boldsymbol{\phi}_i$

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

not in $d = 2$ since the mean-square displacement grows with distance

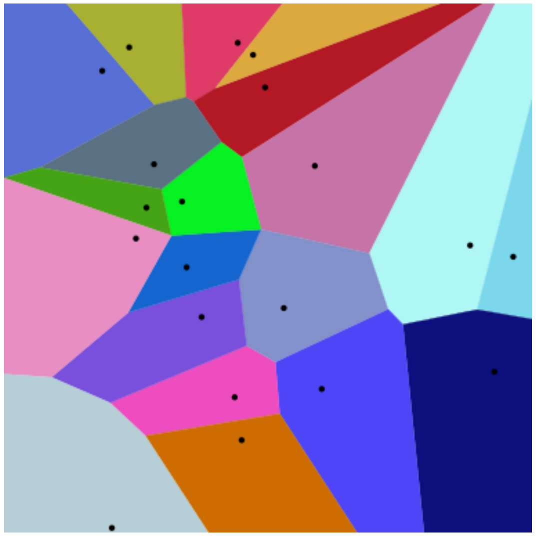
$$\Delta^2(\boldsymbol{r}) \equiv \langle (\boldsymbol{u}(\boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{0}))^2 \rangle \simeq \frac{k_B T}{K} \ln r$$

Other kind of order ?

Neighbours from 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

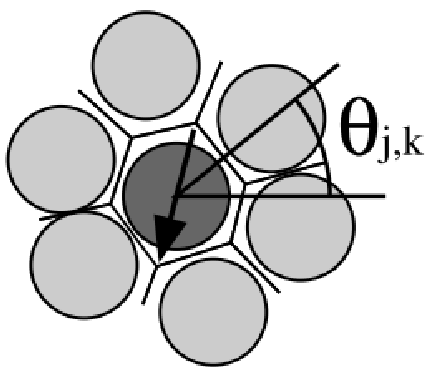
The region has five neighbouring cells from which it is separated by an edge

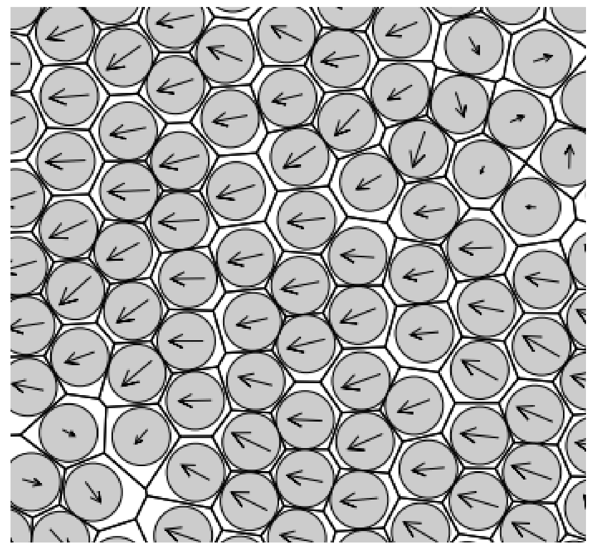
The grey zone has six neighbouring cells

Orientational order

Hexatic order parameter

The local (six) order parameter $\psi_{6_i} = \frac{1}{N^i_{\rm nn}} \sum_{k=1}^{N^i_{\rm nn}} e^{6{\rm i}\theta_{ik}}$ (vector)





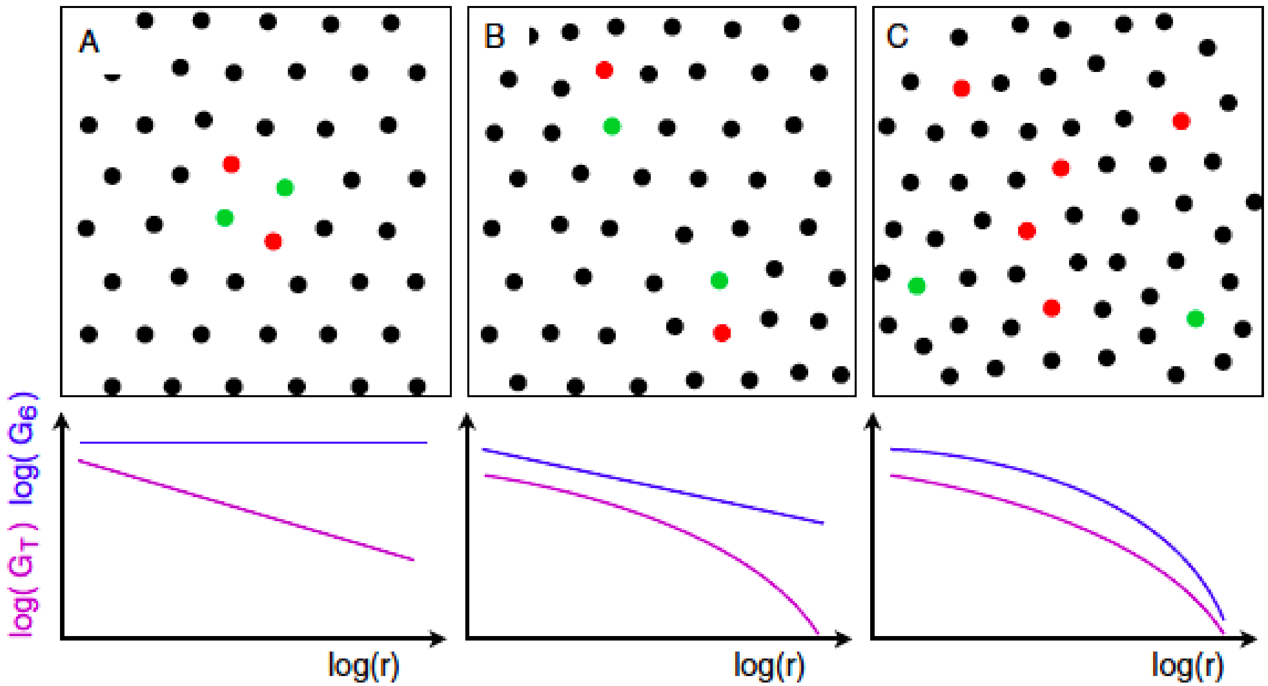
(For beads placed on the vertices of a triangular lattice, each bead i has six nearest-neighbours, $k = 1, \ldots, N^i_{\rm nn} = 6$, the angles are $\theta_{ik} = \frac{2\pi k}{6}$ + c and $\psi_{6_i} = 1$)

associates arrows (directions) to disks

and measures **orientational order**

Correlations & defects

Hexatic **Positional** ● **7 neighb** ● **5 neighb**



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

Phases & transitions

BKT-HNY *vs.* a new scenario by Bernard & Krauth (2011)

	BKT-HNY	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 for hard enough particles

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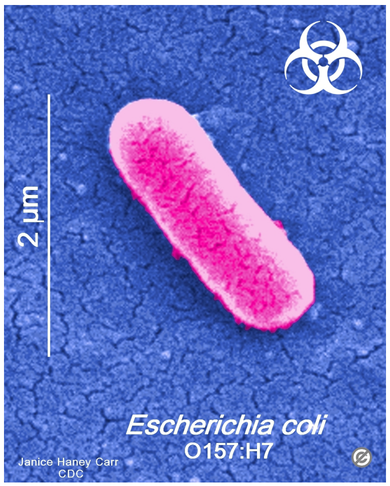
Single active dumbbell

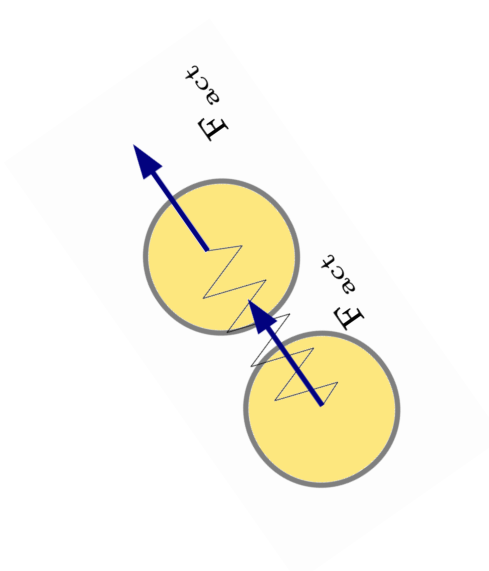
Diatomic molecule - toy model for bacteria



Escherichia coli

Picture borrowed

from the internet

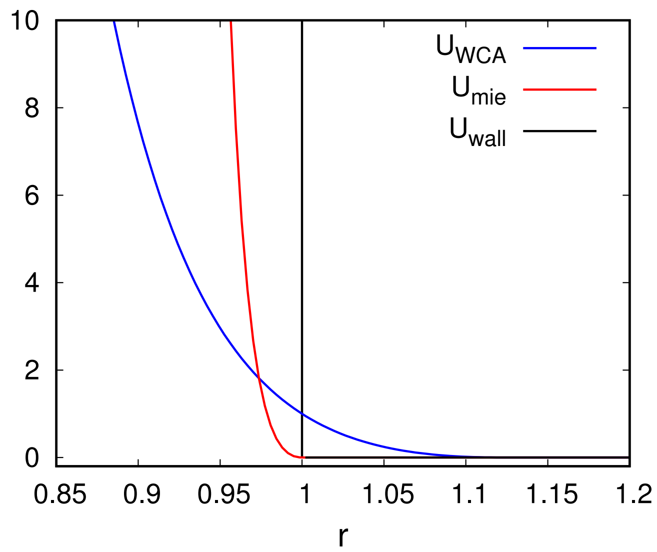


A rigid dumbbell

Interacting active dumbbells

Dissipation, noise, repulsive potential, propulsion

$$m_{\mathrm{d}}\ddot{\boldsymbol{r}}_i(t) = -\gamma\dot{\boldsymbol{r}}_i(t) + \mathbf{F}_{\mathrm{mie}_i}(t) + \mathbf{F}_{\mathrm{act}_i}(t) + \boldsymbol{\eta}_i(t)$$
$$m_{\mathrm{d}}\ddot{\boldsymbol{r}}_{i+1}(t) = -\gamma\dot{\boldsymbol{r}}_{i+1}(t) + \mathbf{F}_{\mathrm{mie}_{i+1}}(t) + \mathbf{F}_{\mathrm{act}_{i+1}}(t) + \boldsymbol{\eta}_{i+1}(t)$$



Mie potential

from truncated Lennard-Jones

with $n = 32$

very hard

Active dumbbell

Control parameters

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

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

Energy scales:

Active work $2\sigma_\mathrm{d}\, F_\mathrm{act}$

thermal energy k_BT

Péclet number Pe = $\frac{2F_\mathrm{act}\sigma_\mathrm{d}}{k_BT}$

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 Re = $\frac{m_\mathrm{d}F_\mathrm{act}}{\sigma_\mathrm{d}\gamma^2}$

Pe $\in [0, 200]$ Re $< 10^{-2}$ $N = 512^2 \simeq 2.6 \times 10^5$

Stiff molecule limit: vibrations frozen.

Interest in the ϕ, F_act and k_BT dependencies, $k_BT = 0.05$ fixed.

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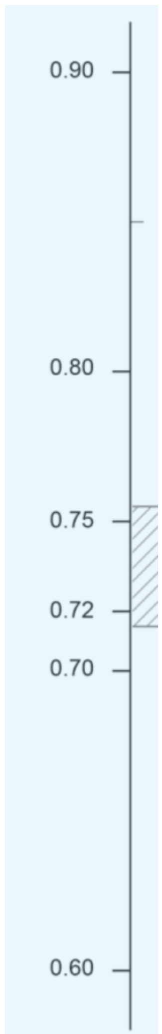
Passive dumbbells

Phase diagram

ϕ



ϕ_{CP}

ϕ_{RCP}

solid

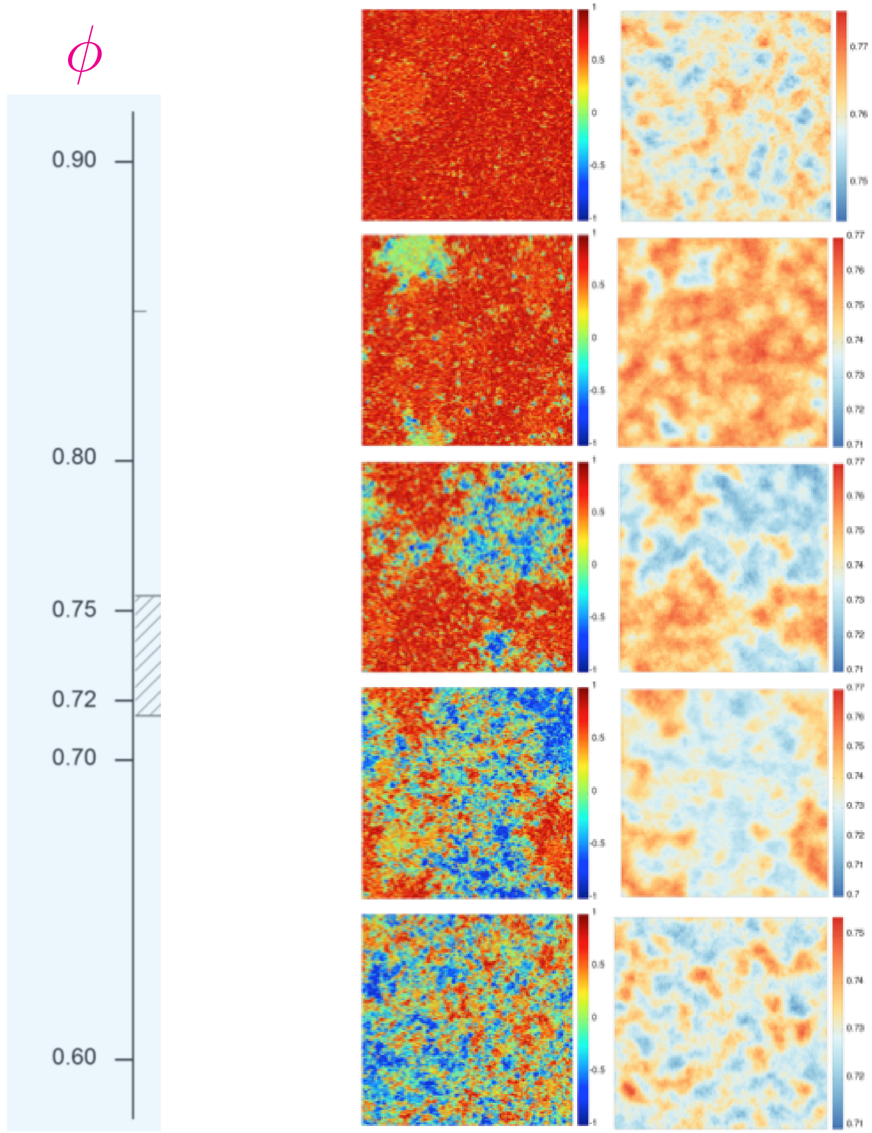
hexatic

co-existence Really ?

liquid

Passive dumbbells

Phase diagram



Images for ϕ

in the striped region

1st column

Local hexatic ψ_{6i}

projected onto the direction

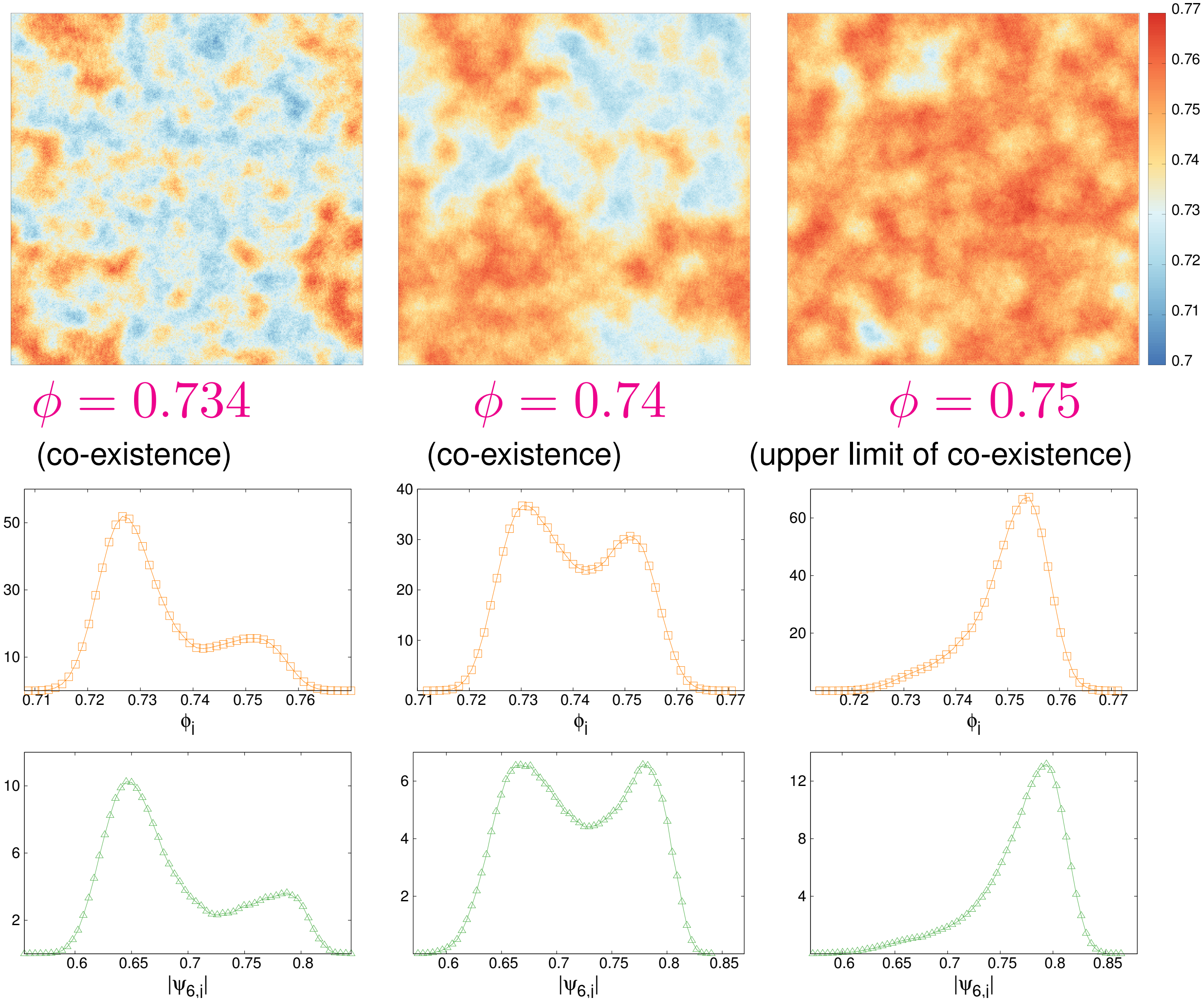
of the average

2nd column

Local density ϕ_i

Passive dumbbells

Local density & local hexatic parameter



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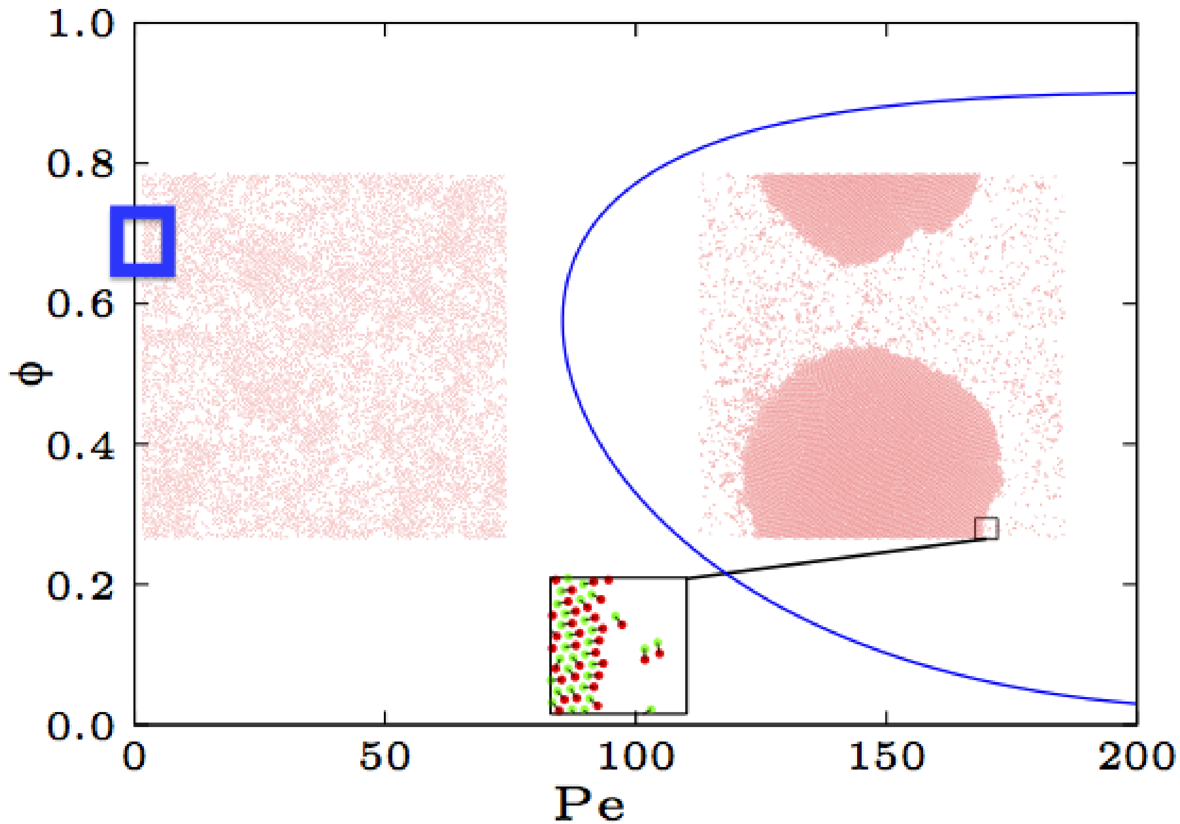
Active dumbbells

OLD phase diagram & new Pe = 0 result

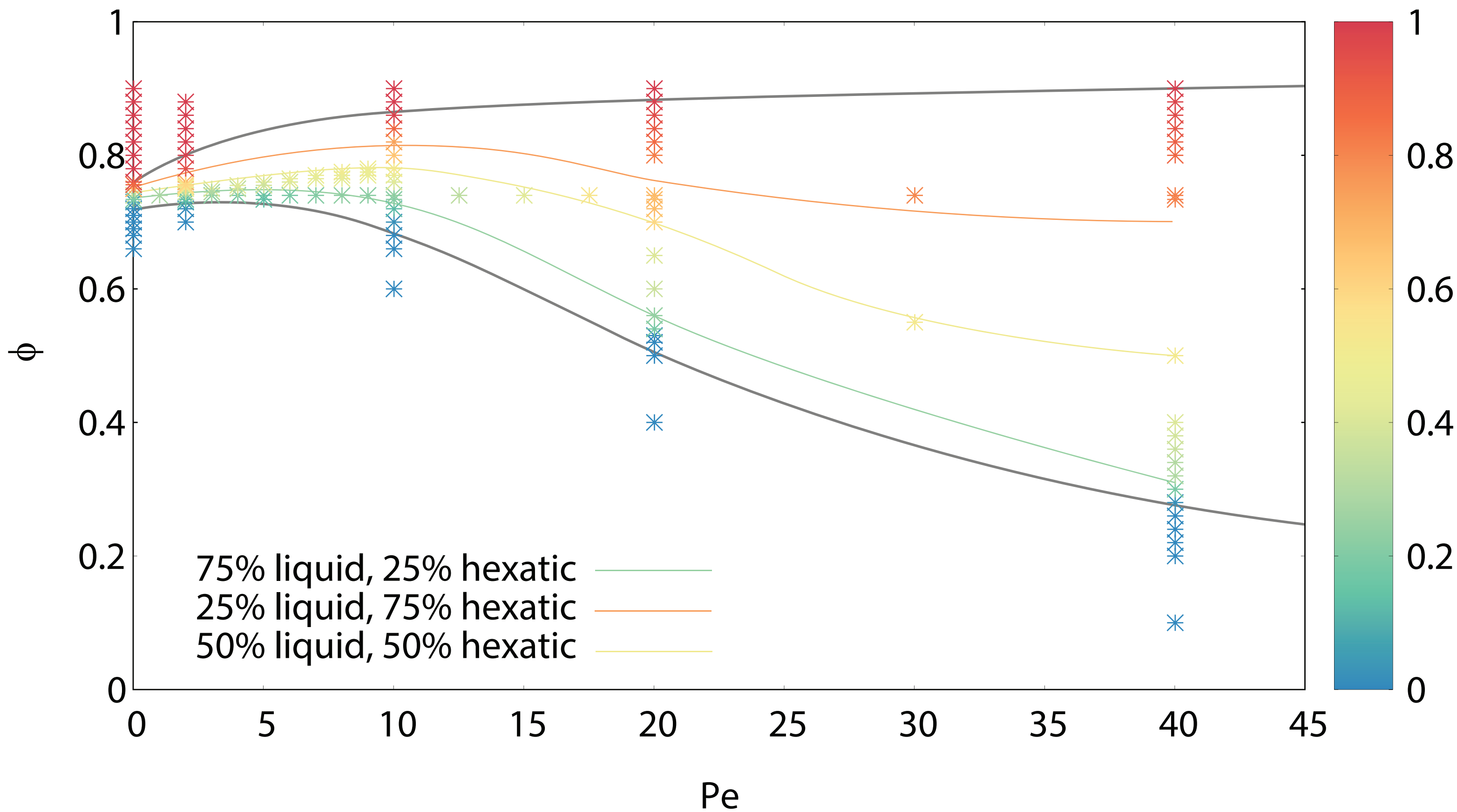


Connection between co-existence at Pe = 0 and MIPS at high Pe ?

MIPS: motility induced phase separation (a dense bubble in a dilute background

Phase diagram

Active dumbbells



LFC, Digregorio, Gonnella & Suma, PRL 119, 268002 (2017) $T = 0.05$

Petrelli, Digregorio, LFC, Gonnella & Suma, EPJE (2018)

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Active disks

Overdamped Brownian particles (the standard model)

Active force $\mathbf{F}_{\rm act}$ along $\mathbf{n}_i = (\cos\theta_i(t), \sin\theta_i(t))$

$$\gamma \dot{\mathbf{r}}_i = F_{\rm act}\mathbf{n}_i - \boldsymbol{\nabla}_i \sum_{j(\neq i)} U_{\rm Mie}(r_{ij}) + \boldsymbol{\xi}_i \ , \qquad \dot{\theta}_i = \eta_i \ ,$$

$\mathbf{r}_i$ position of the centre of ith part & $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ inter-part distance,

short-ranged repulsive Mie potential,

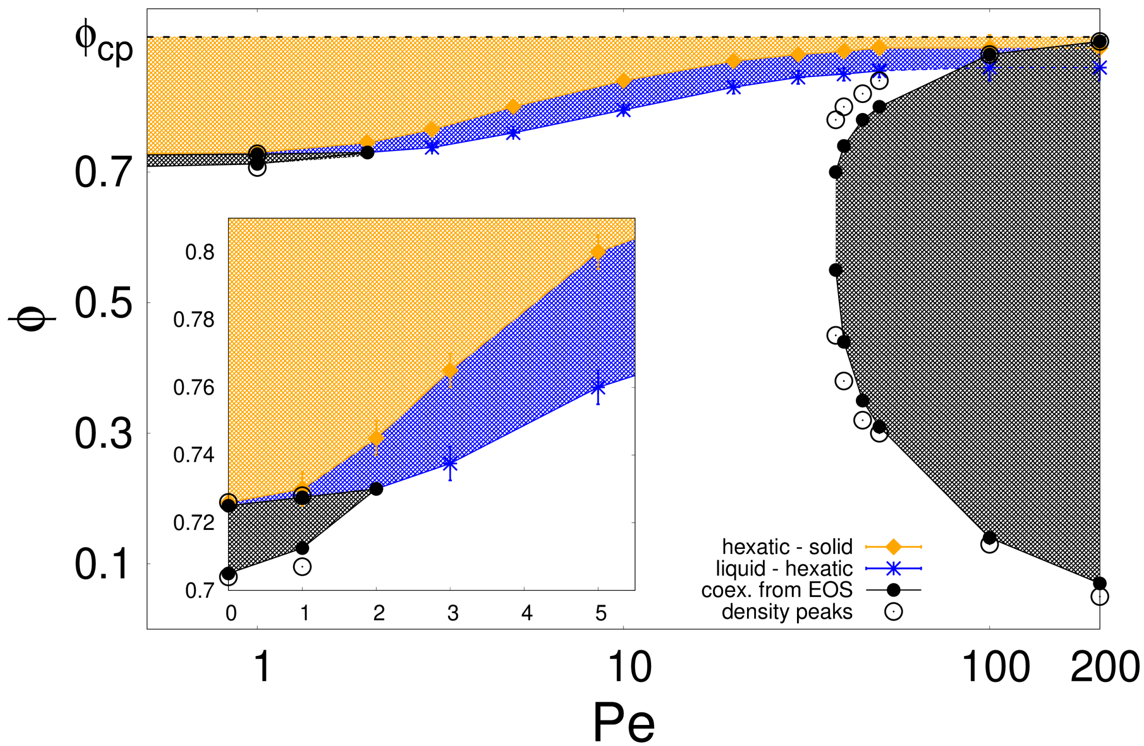
$\boldsymbol{\xi}$ and η zero-mean Gaussian noises with
$\langle \xi_i^a(t)\, \xi_j^b(t')\rangle = 2\gamma k_B T \delta_{ij}^{ab}\delta(t-t')$ and $\langle \eta_i(t)\, \eta_j(t')\rangle = 2D_\theta \delta_{ij}\delta(t-t')$.

The units of length, time and energy are given by σ_d, $\tau = D_\theta^{-1}$ and ε

$D_\theta = 3k_BT/(\gamma\sigma_d^2)$, packing fraction $\phi = \pi\sigma_d^2 N/(4S)$, Péclet number Pe = $F_{\rm act}\sigma_d/(k_BT)$. Parameters $\gamma = 10$, $k_BT = 0.05$ and $\tau_p \simeq 60$

Active disks

Phase diagram

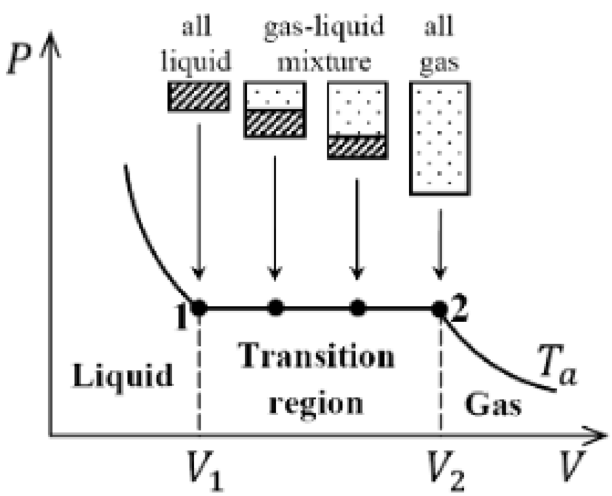


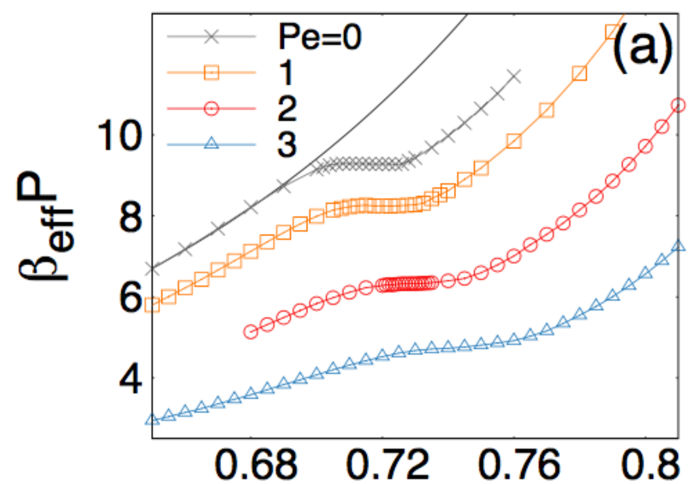
Digregorio, Levis, Suma, LFC, Gonnella & Pagonabarraga, PRL 121, 098003 (2018)

$T = 0.05$

Active disks

Equation of state (eos) : pressure



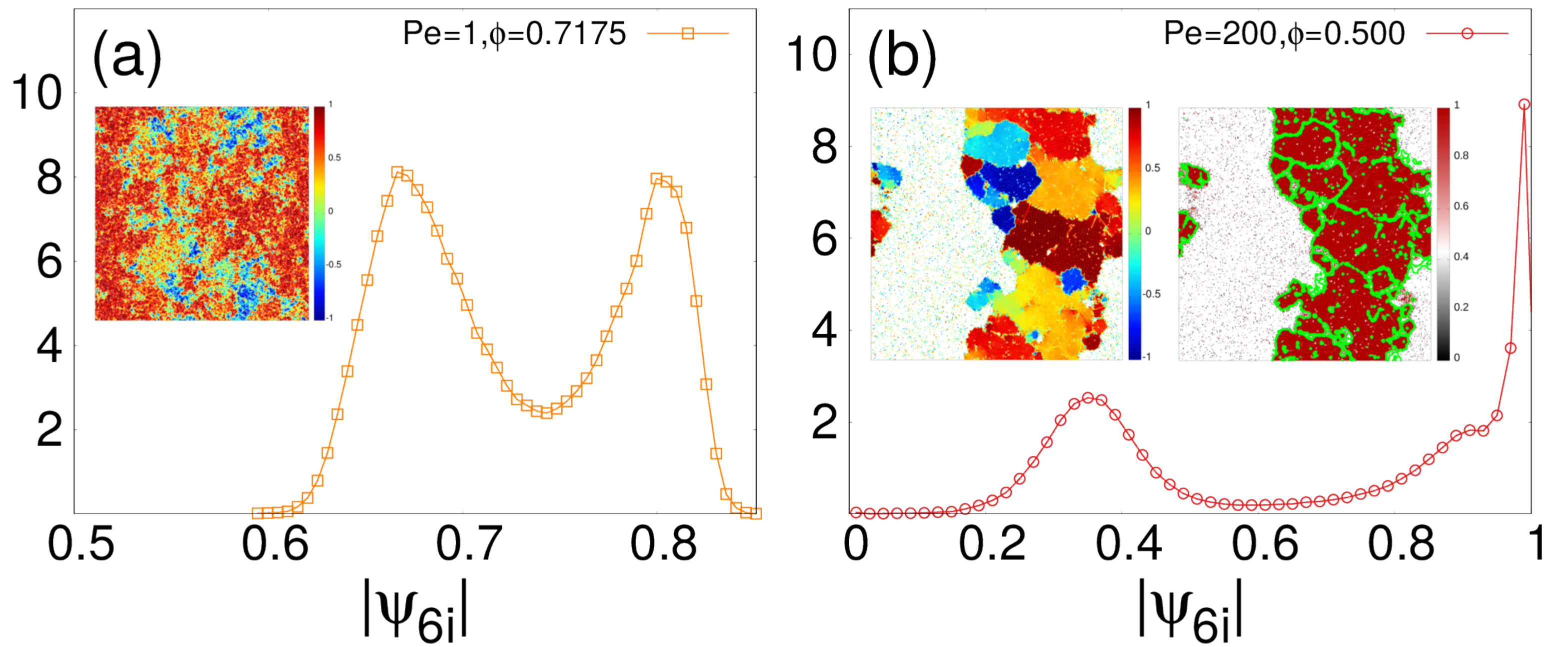


$$\Delta P = P - P_{\rm gas} = \frac{F_{\rm act}}{2V}\sum_i \langle \mathbf{n}_i \cdot \mathbf{r}_i \rangle - \frac{1}{4V}\sum_{i,j}\langle \boldsymbol{\nabla}_i U(r_{ij}) \cdot (\mathbf{r}_i - \mathbf{r}_j)\rangle$$

Active disks

Modulus of the local hexatic order parameter

Pe = 1 Pe = 200



Co-existence in passive limit and in MIPS

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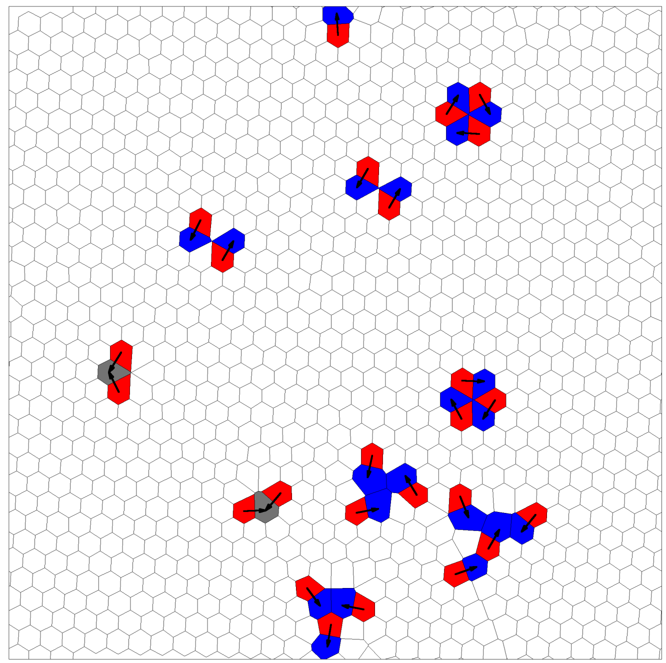
   Topological defects (work in progress)

   Effective temperatures

Active disks

Topological defects (Voronoi cells with $\neq 6$ neighbours)



Dislocations, pairs of dislocations, vacancies, disclinations, grain boundaries

The classification in **Pertsinidis & Ling, PRL 87, 098303 (2001)**

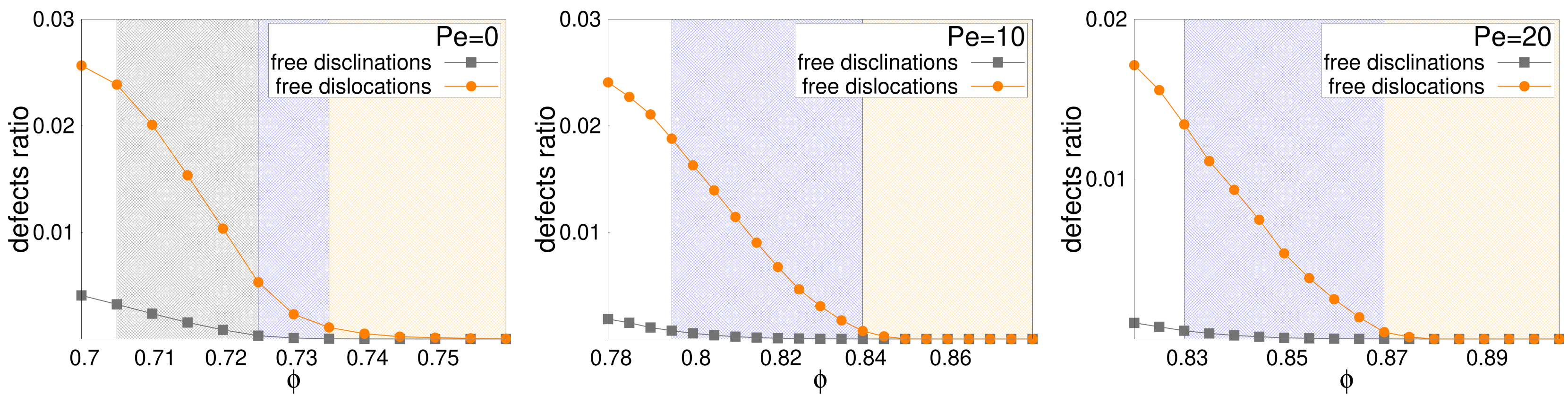
Digregorio, Levis, Suma, LFC, Gonnella & Pagonabarraga, in preparation

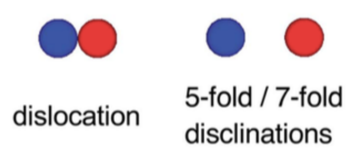
Active disks

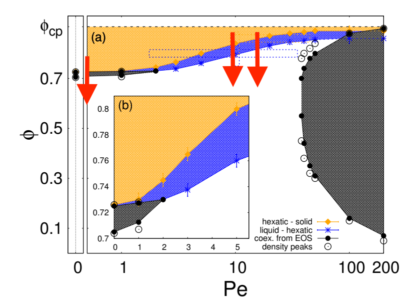
Solid-hexatic transition & the emergence of the liquid

1st order
w/co-existence

à la KTHNY
free dislocations at solid-hex
free disclinations in the liquid

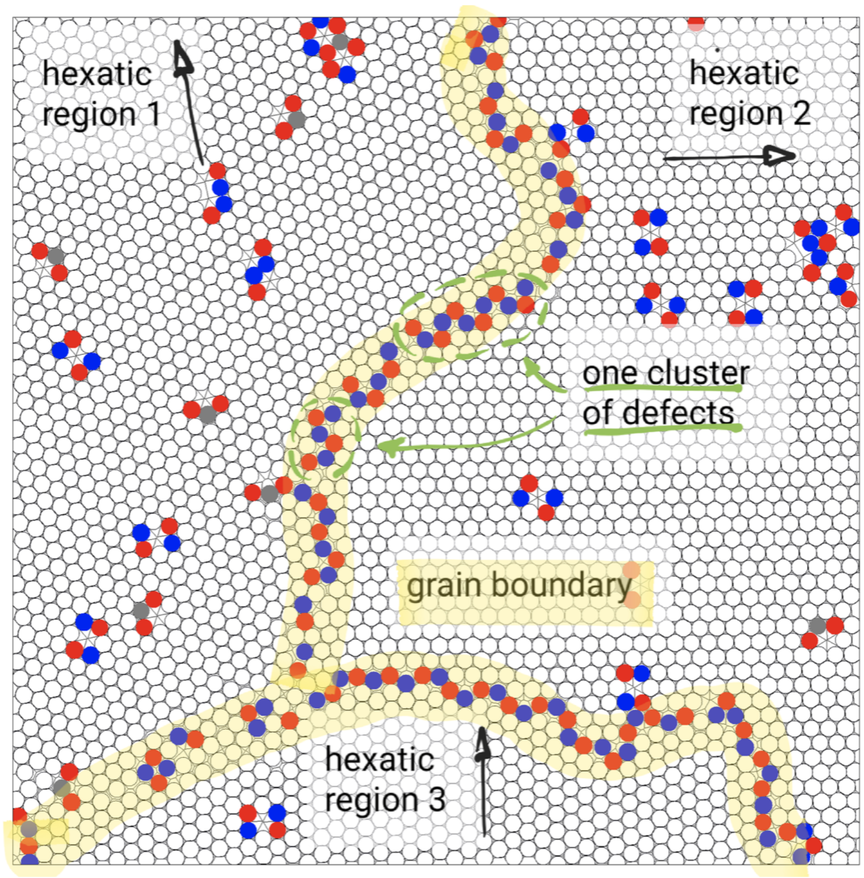






Active disks

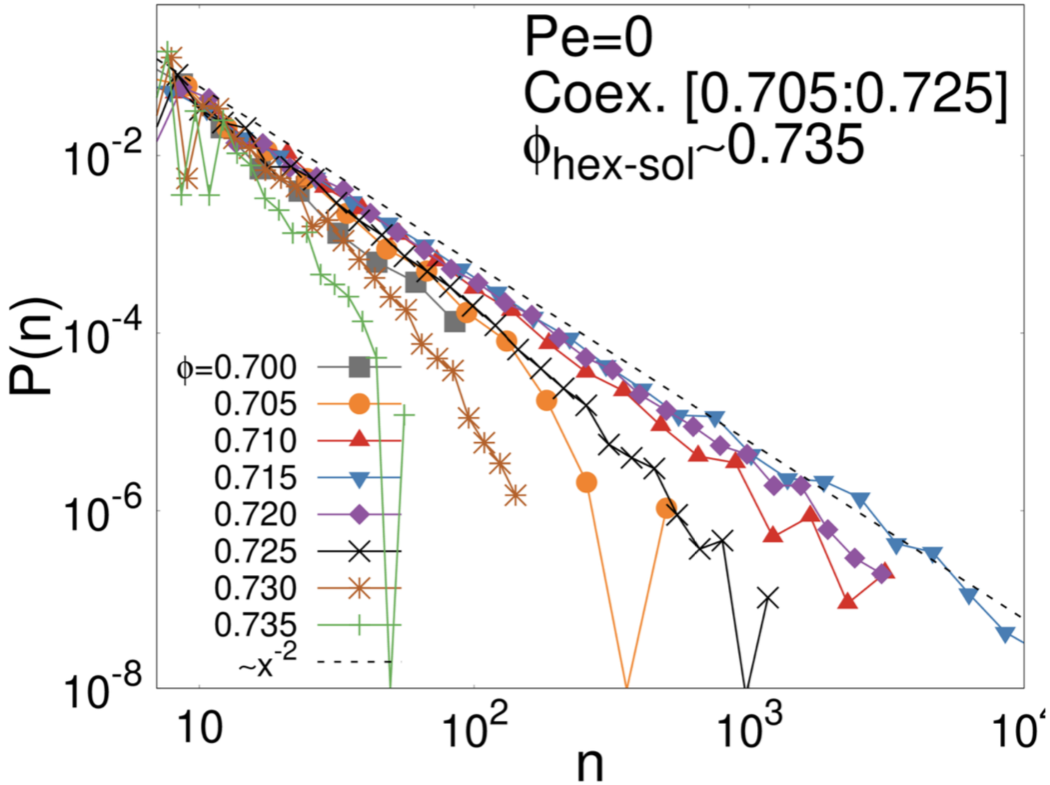
Lines of defects in dense region



Percolation of grain boundaries ?

Active disks

Algebraic distribution of defect cluster sizes



$\phi = 0.715$

within the coexistence region

$\simeq$ percolation of grain boundaries

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Fluctuation-dissipation

Linear relation between χ and Δ^2 in equilibrium

$$P(\zeta, t_w) \to P_{\rm eq}(\zeta)$$

- The dynamics are stationary

$$\Delta^2_{AB}(t,t_w) = \langle [A(t) - B(t_w)]^2\rangle = [C_{AA}(0) + C_{BB}(0) - 2C_{AB}(t-t_w)]$$

$$\to \Delta^2_{AB}(t-t_w)$$

- The fluctuation-dissipation theorem between spontaneous (Δ^2_{AB}) and induced (R_{AB}) fluctuations

$$R_{AB}(t-t_w) = \frac{1}{2k_BT}\frac{\partial \Delta^2_{AB}(t-t_w)}{\partial t}\,\theta(t-t_w)$$

holds and implies

$$\chi_{AB}(t-t_w) \equiv \int_{t_w}^{t} dt'\, R_{AB}(t,t') = \frac{1}{2k_BT}[\Delta^2_{AB}(t-t_w) - \Delta^2_{AB}(0)]$$

Fluctuation-dissipation

Linear relation between χ and Δ^2 out of equilibrium ?

$$\boxed{P(\zeta, t_w) \neq P_{\rm eq}(\zeta)}$$

- The dynamics are stationary

$$\Delta^2_{AB}(t,t_w) = \langle [A(t) - B(t_w)]^2 \rangle = [C_{AA}(0) + C_{BB}(0) - 2C_{AB}(t-t_w)]$$

$$\to \Delta^2_{AB}(t-t_w)$$

- The fluctuation-dissipation theorem between spontaneous (Δ^2_{AB}) and induced (R_{AB}) fluctuations

$$R_{AB}(t-t_w) \neq \frac{1}{2k_BT} \frac{\partial \Delta^2_{AB}(t-t_w)}{\partial t} \, \theta(t-t_w)$$

does not hold but one can propose

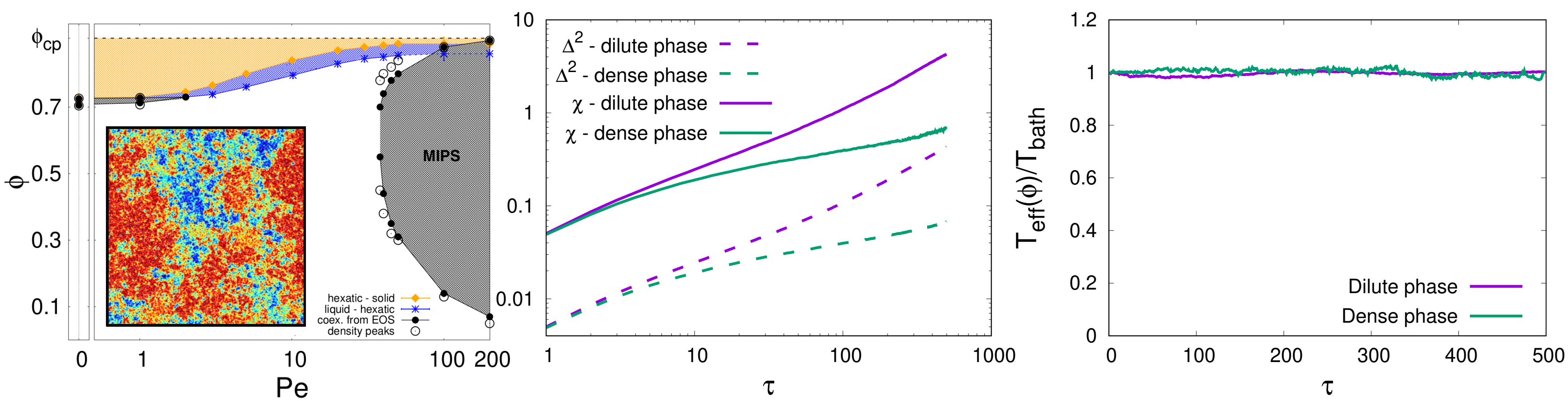
$$\boxed{\chi_{AB}(t-t_w) \equiv \int_{t_w}^{t} dt' \, R_{AB}(t,t') = \frac{[\Delta^2_{AB}(t-t_w) - \Delta^2_{AB}(0)]}{2k_BT_{\rm eff}(t-t_w)}}$$

Teff = T

Co-existence in equilibrium

Pe = 0 $\phi = 0.710$

Integrated linear response & mean-square displacement: their ratio (FDT) $\tau = t - t_w$



Method: linear response computed with Malliavin weights (no perturbation applied) as proposed by **G. Szamel** for active matter systems.

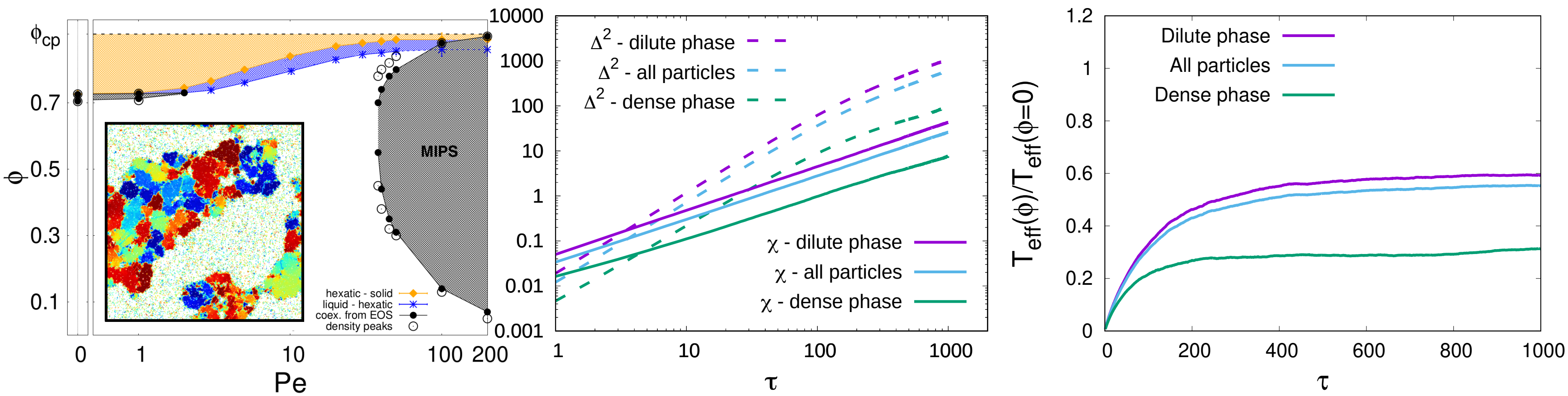
Petrelli, LFC, Gonnella & Suma, in preparation

Teff $\neq$ T

Co-existence in MIPS

Pe = 50 $\quad \phi = 0.5$

Integrated linear response & mean-square displacement: their ratio (FDR) $\tau = t - t_w$



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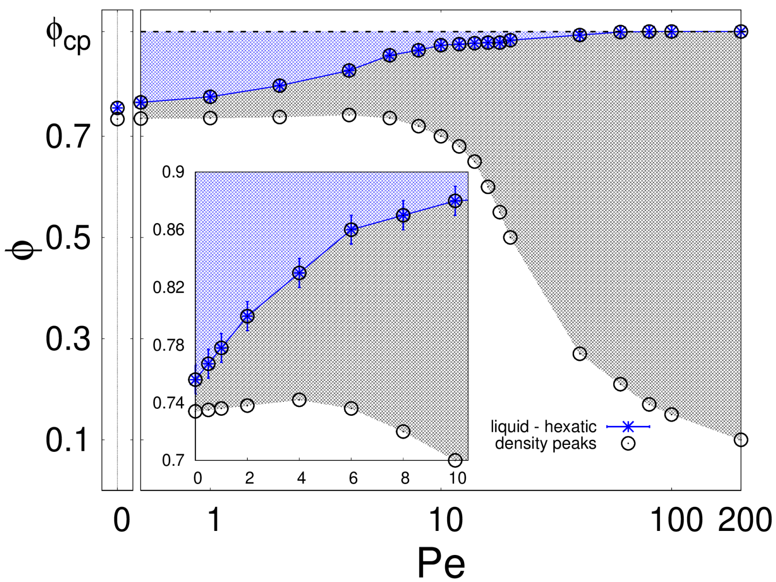
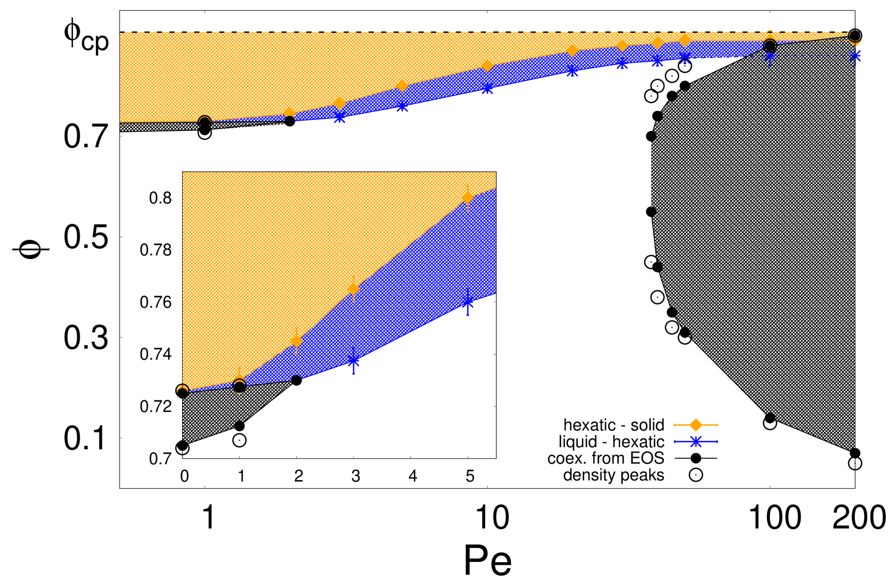
Petrelli, LFC, Gonnella & Suma, in preparation

Active Brownian systems

Conclusions : phase diagrams & plenty of interesting facts



Dumbbells



Disks

Thanks !