
(Active) Matter in Two Dimensions

Melting & Phase Separation

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Work in collaboration with

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A. Tiribocchi (Roma), **L. Carenza** (Bari & Istanbul), **A. Suma** (Trieste, Philadelphia &
Bari), **D. Levis & I. Pagonabarraga** (Barcelona & Lausanne)

J^{20th}
stat
2004-2024

Bombay, India, 2025

Active Matter

Definition - Biological inspiration

Active matter is composed of large numbers of active "agents", which consume energy and thus move or exert mechanical forces

Due to the energy consumption, these systems are intrinsically out of thermal equilibrium

Homogeneous energy injection (not from the borders, *cfr.* shear)

Coupling to the environment (bath) allows for dissipation

Active Brownian Particles

(Overdamped) Langevin equations

Active force f_{act} along $\mathbf{n}_i = (\cos \theta_i, \sin \theta_i)$

$$\gamma \dot{\mathbf{r}}_i = f_{\text{act}} \mathbf{n}_i - \nabla_i \sum_{j(\neq i)} U_{\text{Mie}}(r_{ij}) + \boldsymbol{\xi}_i \quad \dot{\theta}_i = \eta_i ,$$

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

U_{Mie} **short-range strongly repulsive** Mie potential

$\boldsymbol{\xi}_i$ and η_i Gaussian white noises with $\langle \xi_i^a(t) \rangle = \langle \eta_i(t) \rangle = 0$,

$\langle \xi_i^a(t) \xi_j^b(t') \rangle = 2\gamma k_B T \delta_{ij}^{ab} \delta(t - t')$ with $k_B T = 0.05$, and $\langle \eta_i(t) \eta_j(t') \rangle = 2D_\theta \delta_{ij} \delta(t - t')$

Persistence time $\tau_p = D_\theta^{-1} = \gamma \sigma^2 / (3k_B T)$. Units of length σ and energy ε .

Péclet number $\text{Pe} = f_{\text{act}} \sigma / (k_B T)$ measures the activity and

$\phi = \pi \sigma^2 N / (4S)$ the packing friction

Active Matter

Global goal

To understand the **collective** behaviour of **active matter**

from the **statistical physics** viewpoint

with the help of extensive **numerical simulations**

and **theoretical arguments/analytic calculations**

Statistical Physics approach

2d Active Matter

Why two dimensions ?

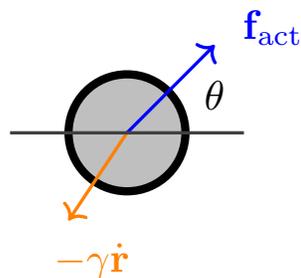
It is **experimentally** 'easier' than three dimensions

It is computationally lighter to **simulate** $2d$ systems than $3d$ ones

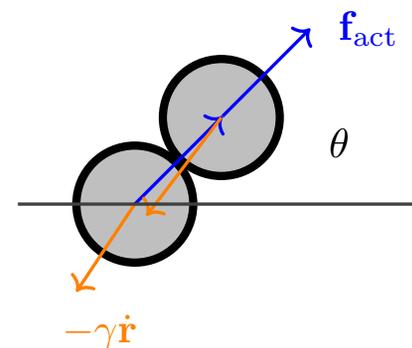
It is already **very rich** and **often realistic**

Focus here on two kinds of active constituents

Disks



Rigid Dumbbells



Active Brownian Matter

Questions – à la Statistical Physics – on bidimensional systems

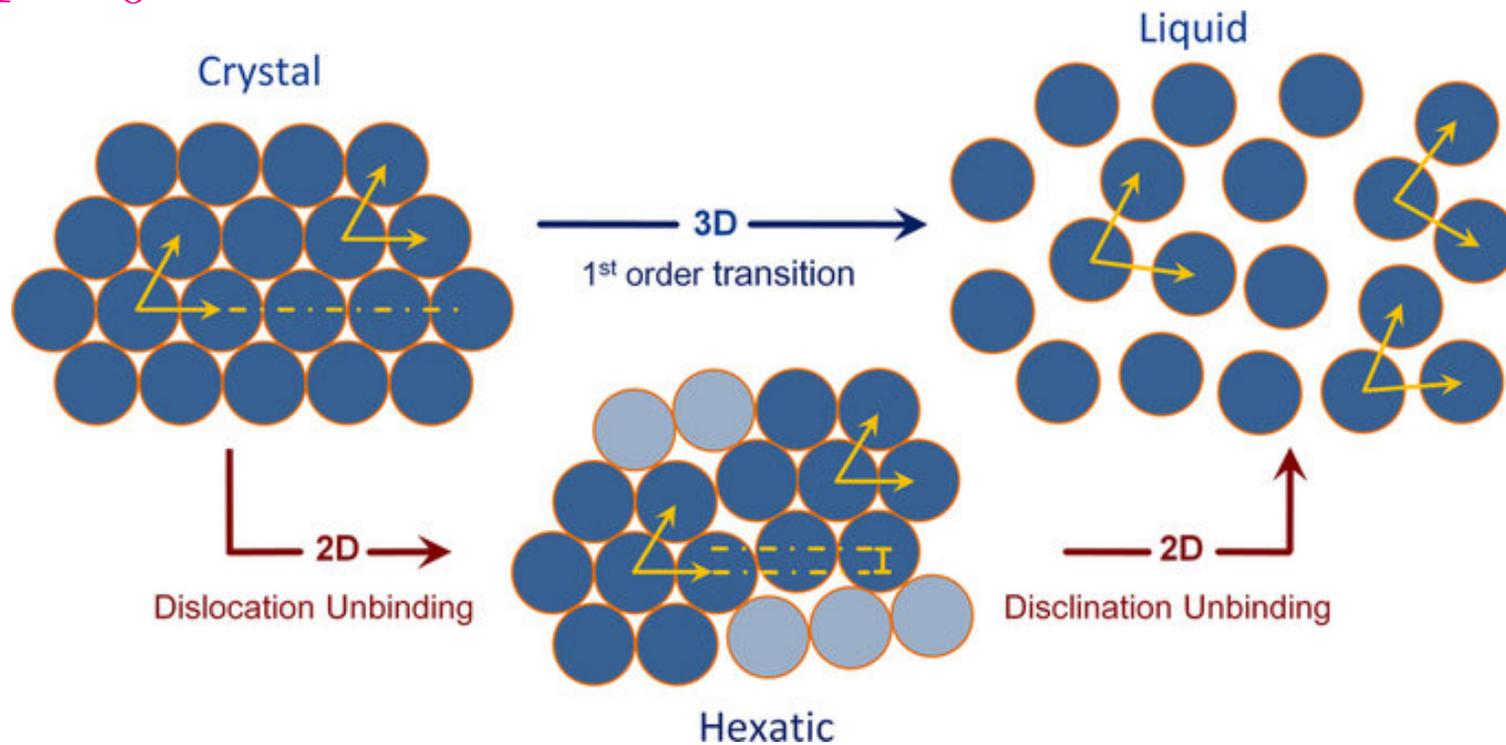
- Activity (Pe) - packing fraction (ϕ) phase diagram.
- Order of, and mechanisms for, the phase transitions.
 - Correlations, fluctuations.
 - Topological defects.

- Motility Induced Phase Separation.
 - Internal structure of the dense phase.
 - Mechanisms for growth of the dense phase.
 - Influence of particle shape, *e.g.* disks vs. dumbbells.

Freezing/Melting

Different routes in $3d$ and $2d$

$T = 0$



Orientation order preserved

also lost

Correlations & defects

Hexatic

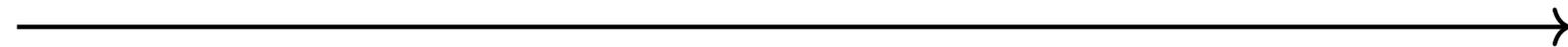
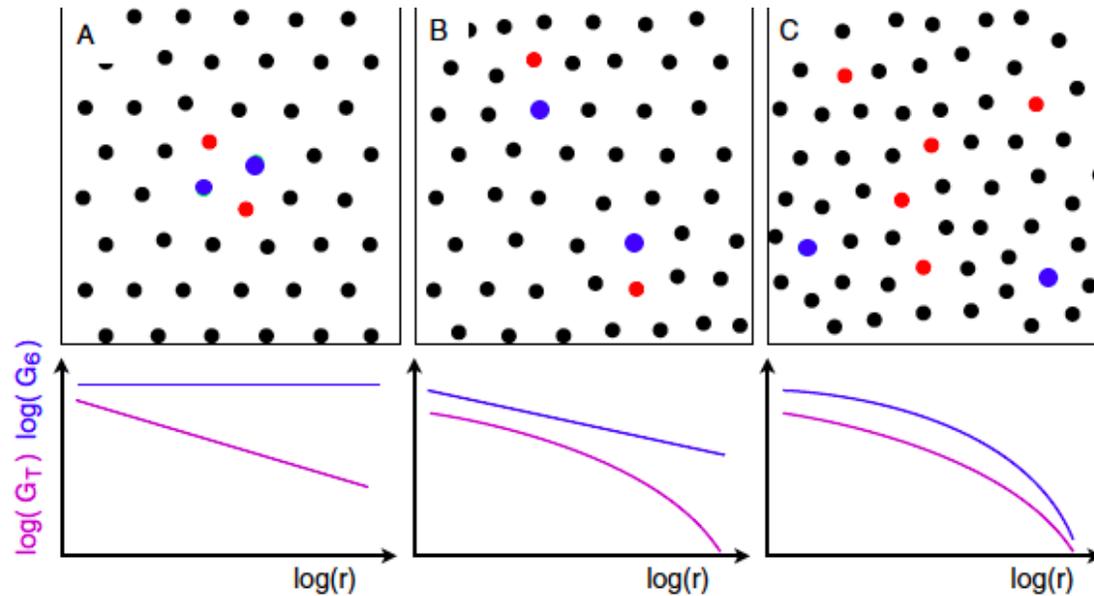
Positional

● 7 neighb ● 5 neighb

Solid

Hexatic

Liquid



T $1/\phi$

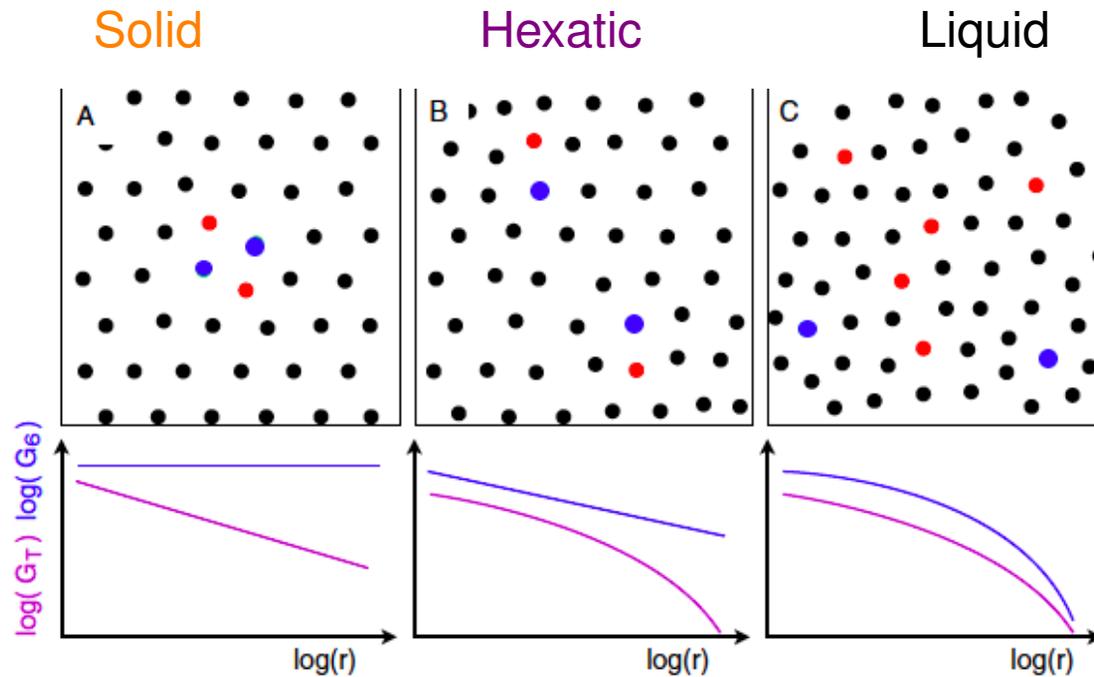
$$\text{long } r: G_6(r) = \begin{cases} \text{cst} & \text{solid} & \text{long range order} \\ r^{-\eta_6} & \text{hexatic} & \text{quasi long range order} \\ e^{-r/\xi_6} & \text{liquid} & \text{disorder} \end{cases}$$

Correlation functions

Hexatic

Positional

● 7 neighb ● 5 neighb

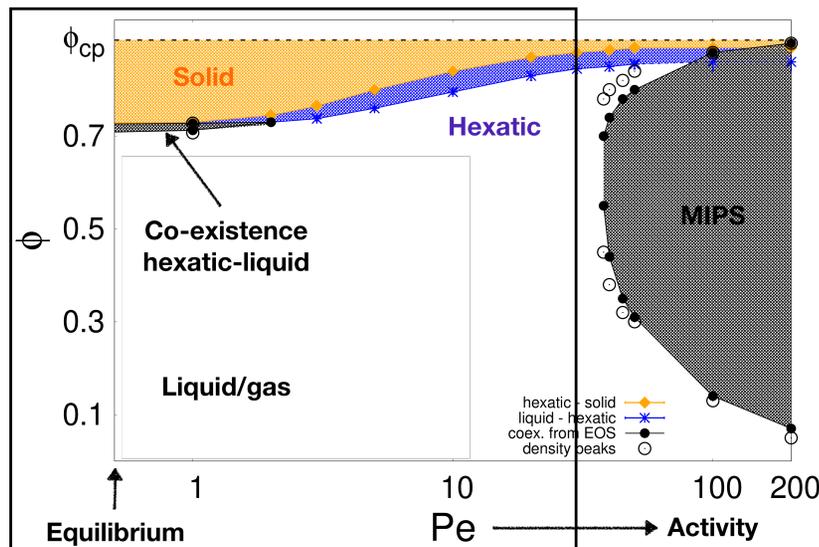


$T \quad 1/\phi$

$$\text{long } r: \quad G_{q_0}(r) = \begin{cases} r^{-\eta} & \text{solid} & \text{quasi long range order} \\ e^{-r/\xi_h} & \text{hexatic} & \text{disorder} \\ e^{-r/\xi_l} & \text{liquid} & \text{disorder} \end{cases}$$

Active Brownian disks

Phase diagram with **solid**, **hexatic**, **liquid**, co-existence and MIPS



Different from BKT-HNY picture

1st order **hexatic-liquid** close to $Pe = 0$

KT-HNY **solid-hexatic** dislocation unbinding
disclination unbinding in liquid

percolation of defect clusters in liquid

Pressure $P(\phi, Pe)$ (EOS), correlations $C_{q_0}(r)$, $g_6(r)$, and distributions of ϕ_i , $|\psi_{6i}|$
defect identification & counting

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

Klamser, Kapfer & Krauth, Nature Comm. 9, 5045 (2018)

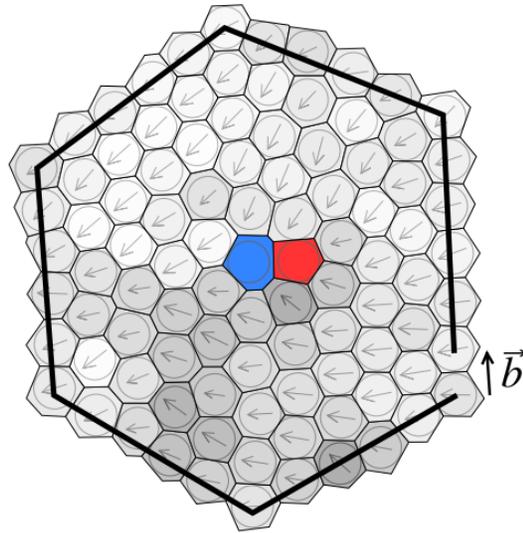
What drives the phase transitions ?

We highlighted the particles with **5** & **7** neighbours

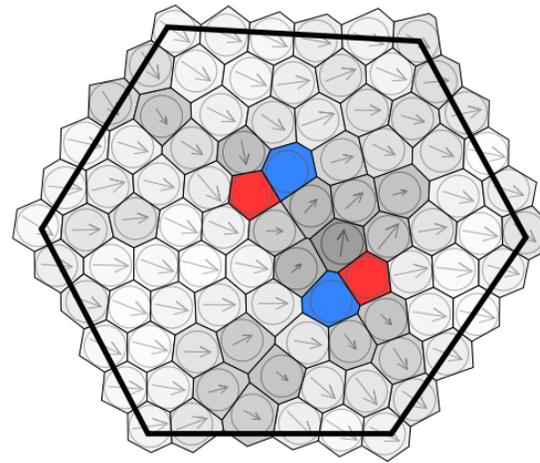
Defects

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

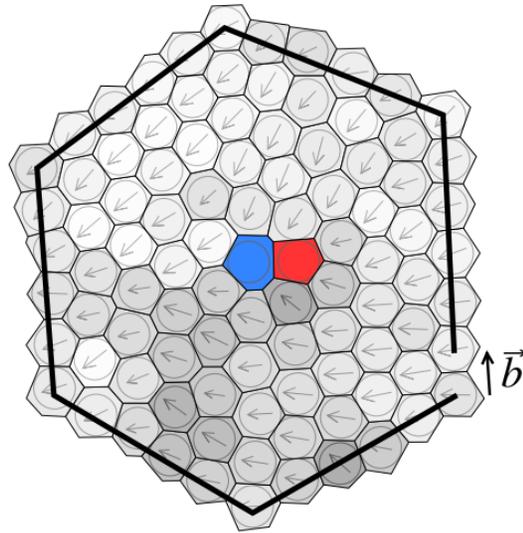
The **blue** disks have seven neighbours and the **red** ones have five.

On the right image: the external path closes and forms a perfect hexagon.

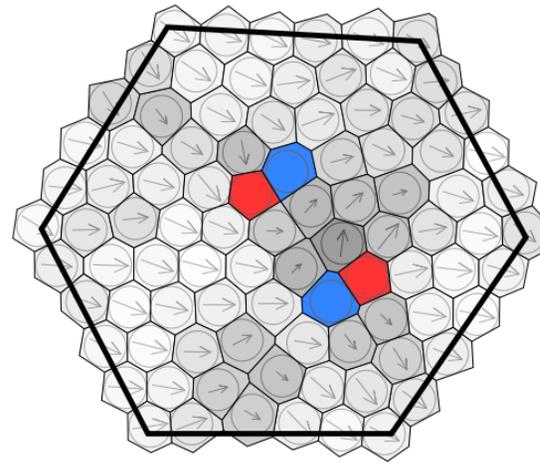
The effects of the defects are confined. This is the **solid** phase.

Close packing of disks

Disks, Voronoi cells & dislocations



A free dislocation



A bound pair of dislocations

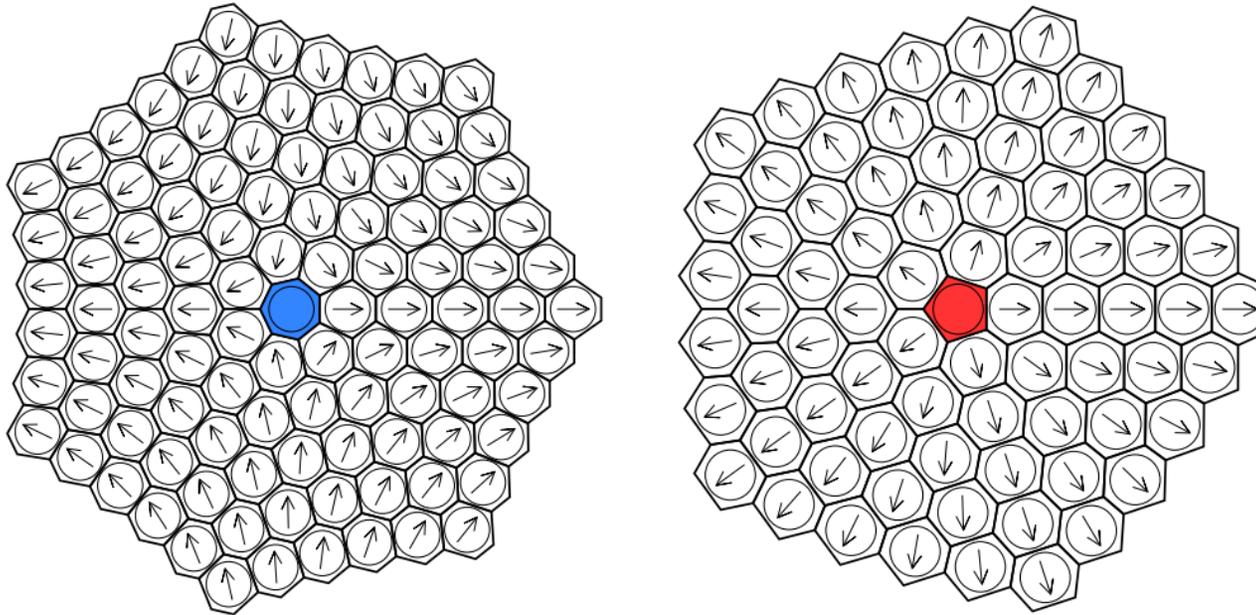
In the crystal the centres of the disks form a triangular lattice

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

On the left image: the external path fails to close, no perfect hexagon. The effect of the defects spreads & kills translation order: **hexatic** phase.

Close packing of disks

Unbinding of disclinations



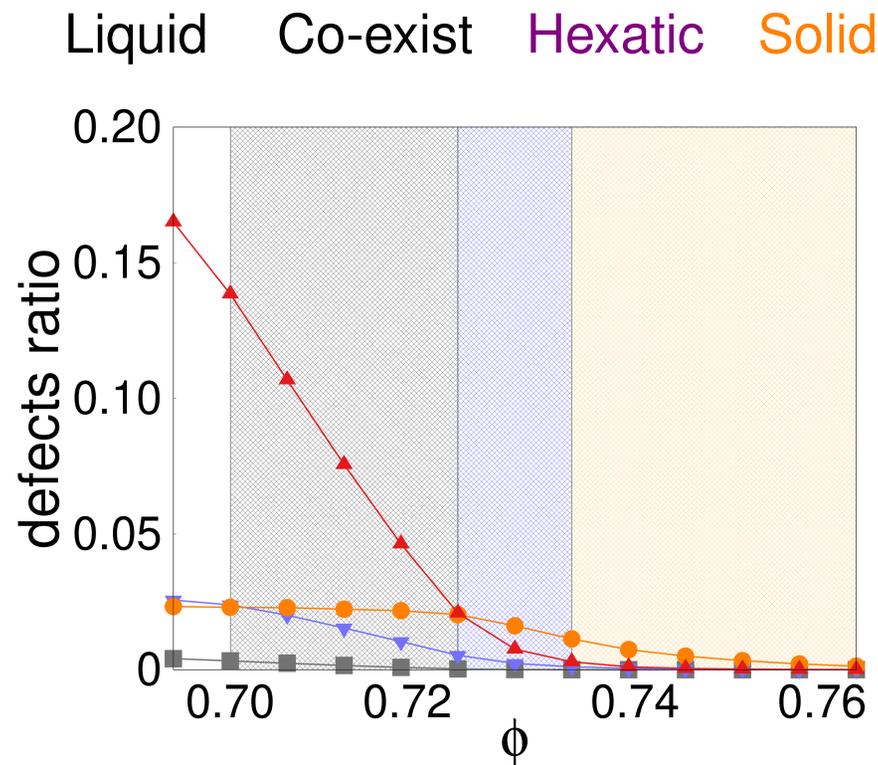
The orientation winds by $\pm 2\pi$ around the **blue** (seven) and **red** (five) defects. Very similar to the vortices in the $2d$ XY magnetic model.

Halperin, Nelson & Young scenario: the unbinding of disclinations drives a second BKT-like transition to the **liquid**.

What happens with the defects ?

Proliferation of clusters

Within the co-existence region & all along the hextic-liquid transition



Clusters ▲ of defects proliferate within the co-existence region

Vacancies ● remain approximately constant within the co-existence region

Topological defects

Summary of results

- **Solid - hexatic** à la BKT HNY even quantitatively (ν value) and independently of the activity (Pe) *Universality ? **
- **Hexatic - liquid** very few disclinations and not even free *Breakdown of the BKT-HNY picture for all Pe (even zero)*
- Close to, but in the liquid, **percolation** of *clusters of defects* with properties of uncorrelated critical percolation (d_f, τ)
- In **MIPS**, network of defects on top of the interfaces between hexatically ordered regions, interrupted by the *gas bubbles in cavitation*

Digregorio, D Levis, LF Cugliandolo, G Gonnella, I Pagonabarraga, *Soft Matter* 18, 566 (2022)

* Shi, Cheng & Chaté, *Phys. Rev. Lett.* 131, 108301 (2023)

Active Brownian Matter

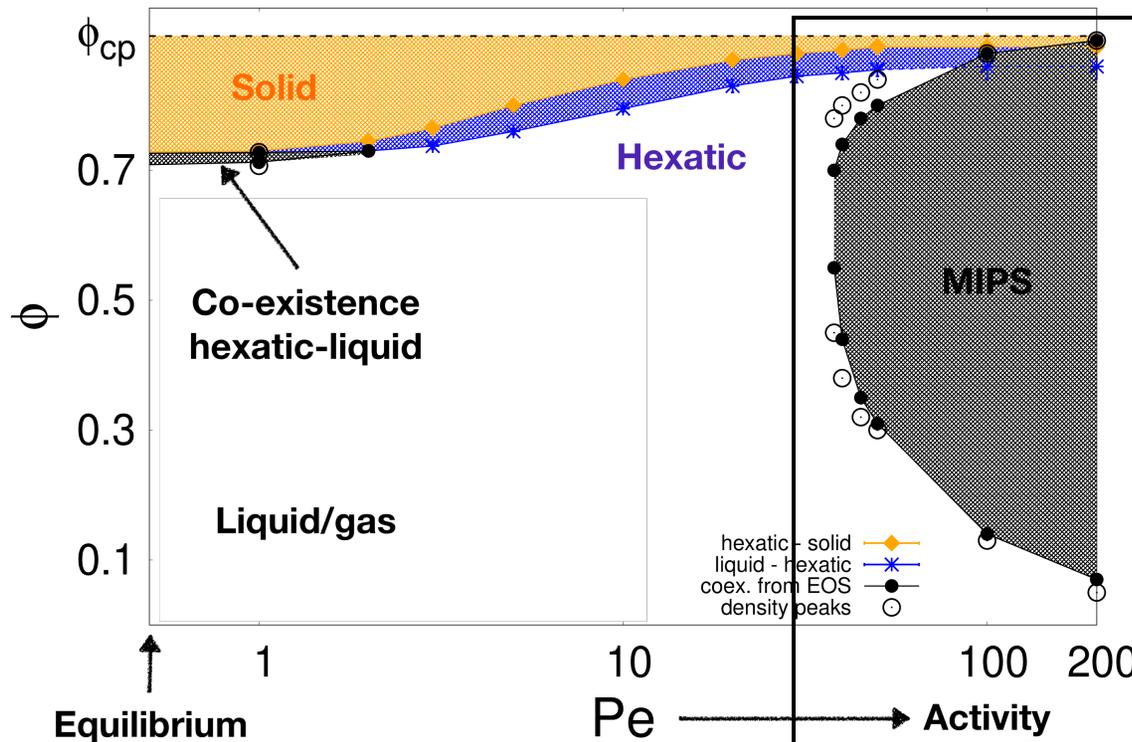
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Active Brownian disks

Phase diagram with **solid**, **hexatic**, **liquid**, co-existence and MIPS



**Motility induced
phase separation (MIPS)
gas & dense**

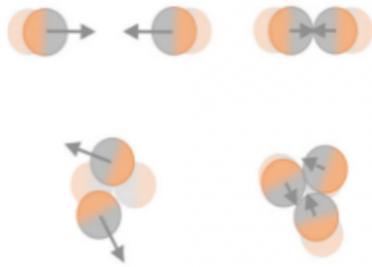
Cates & Tailleur
Ann. Rev. CM 6, 219 (2015)
Farage, Krinninger & Brader
PRE 91, 042310 (2015)

Pressure $P(\phi, Pe)$ (EOS), correlations $G_T(r)$, $G_6(r)$, and distributions of ϕ_i , $|\psi_{6i}|$

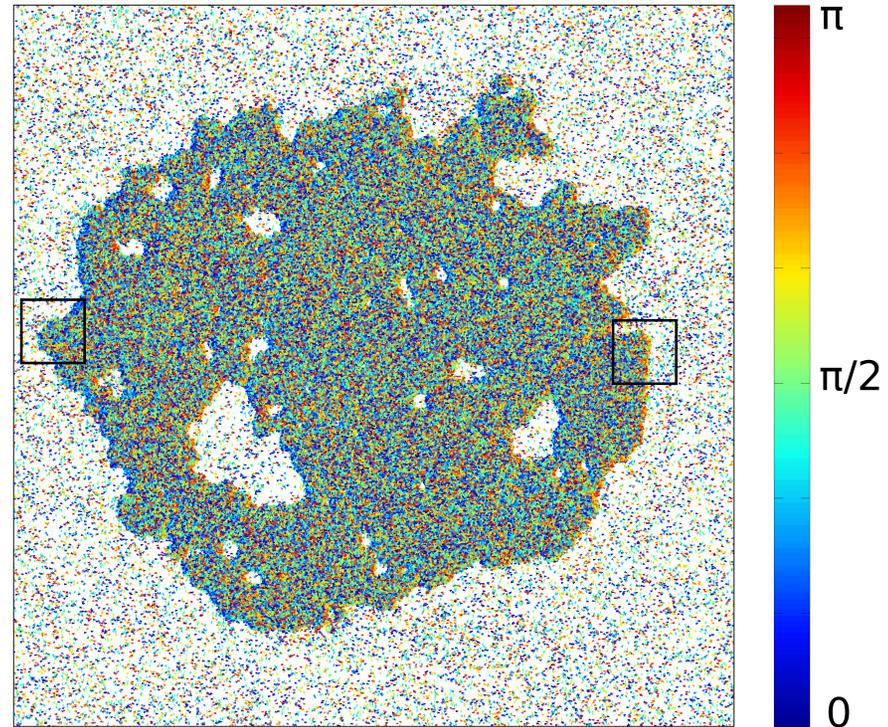
Digregorio, Levis, Suma, LFC, Gonnella & Pagonabarraga, PRL 121, 098003 (2018)

MIPS - ABP

The basic mechanism



Particles collide heads-on
and cluster even in the
absence of attractive forces



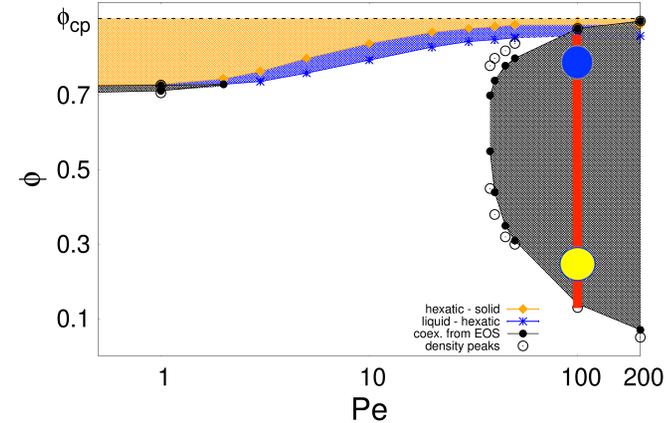
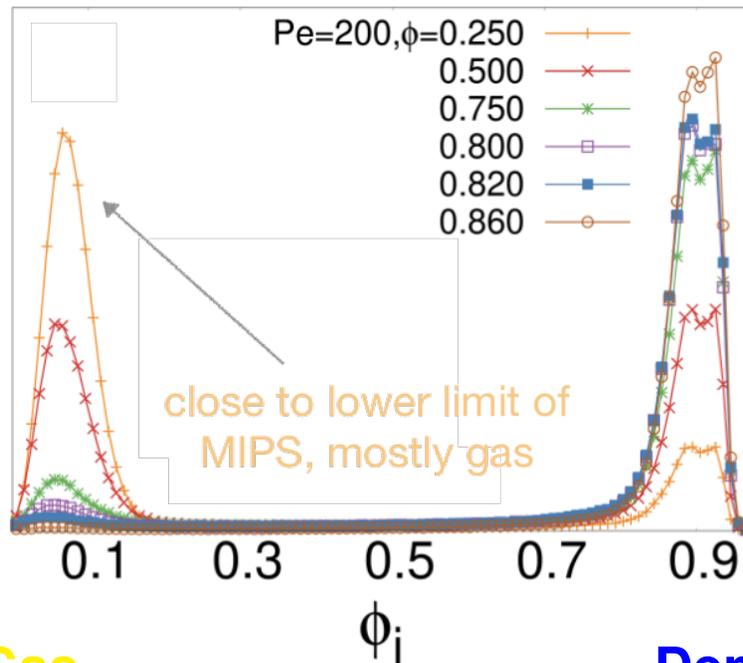
→ blue 0

← red π

The colours indicate the direction \mathbf{n}_i along which the particles are pushed by the active force f_{act}

MIPS - ABP

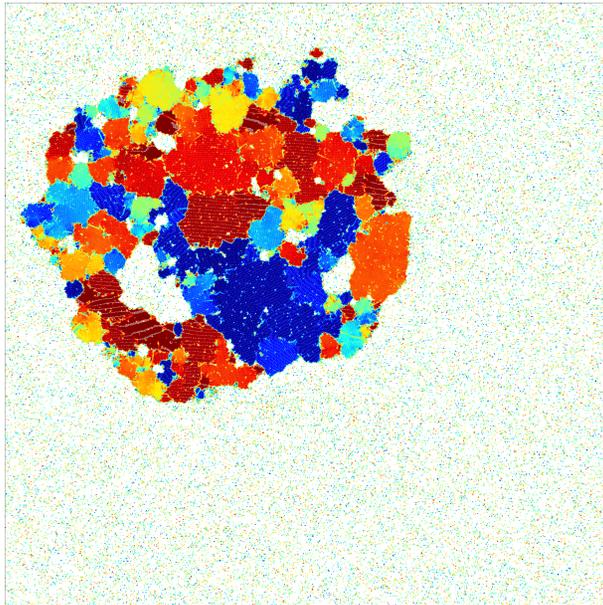
Identification via the local density distributions - dense & gas



The position of the peaks does not change while changing the global packing fraction ϕ but their relative height does. Transfer of mass from **gas** to **dense** component as ϕ increases

The Dense Phase - ABP

Hexatic patches, defects & bubbles in the stationary limit



Dense/dilute separation¹

For low packing fraction ϕ
a single round droplet

Growth² of clusters³ with a mosaic
of hexatic orders³ with
gas bubbles^{2,4,5} & defects⁶

¹ Cates & Tailleur, Annu. Rev. Cond. Matt. Phys. 6, 219 (2015)

² Caporusso, Digregorio, Levis, LFC & Gonnella, PRL 125, 178004 (2020)

³ Caporusso, LFC, Digregorio, Gonnella, Levis & Suma, PRL 131, 068201 (2023)

⁴ Tjhung, Nardini & Cates, PRX 8, 031080 (2018)

⁵ Shi, Fausti, Chaté, Nardini & Solon, PRL 125, 168001 (2020)

⁶ Digregorio, Levis, LFC, Gonnella & Pagonabarraga, Soft Matter 18, 566 (2022)

Active Brownian Matter

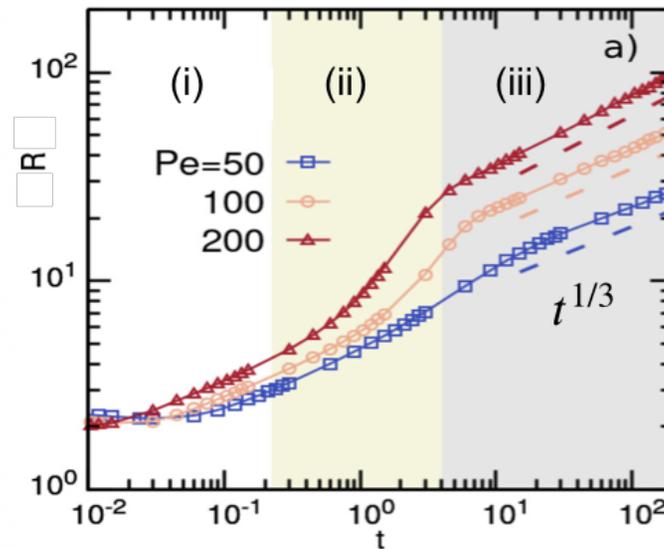
Table with results

	Disks	Dumbbells
Non-Eq Steady-State (NESS)	$R \sim aL$ $R_H \sim R_H^* \ll L$ $P(R_B) \sim R_B^{-\tau} e^{-\frac{R_B}{R_B^*}}$	
Approach to NESS	Next	

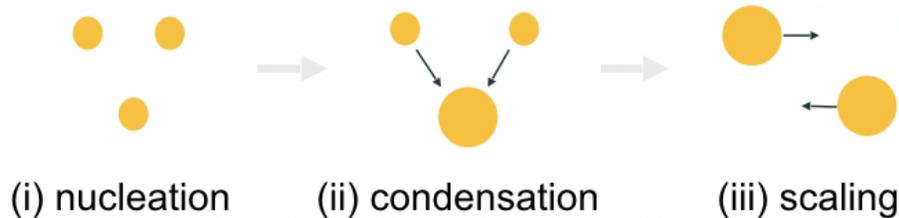
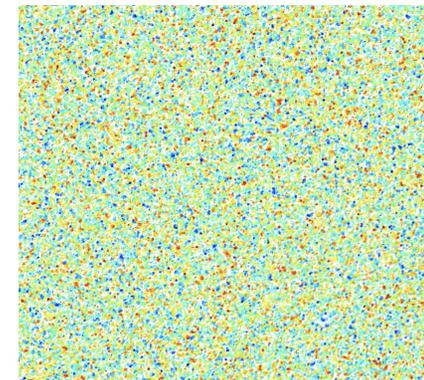
The Growth Law

Growing length of the dense component and regimes

Different Pe



Movie



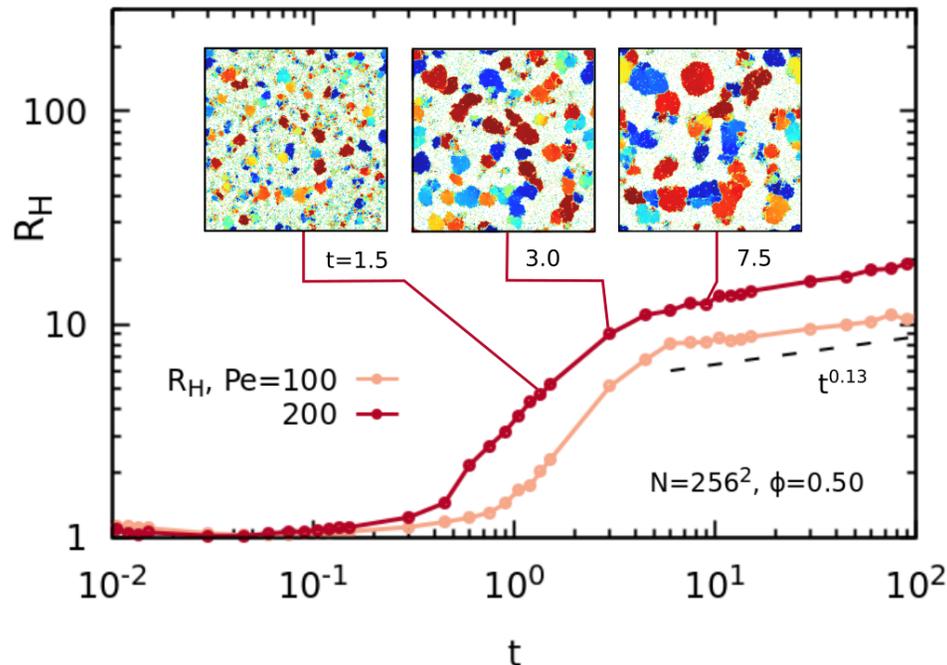
$$R(t) \sim t^{1/3} \text{ for all } Pe$$

Lifshitz-Slyozov-Wagner

In scaling regime $t^{1/3}$ like in passive scalar phase separation.

Local Hexatic Order - ABP

Growing length of the orientational order – regimes

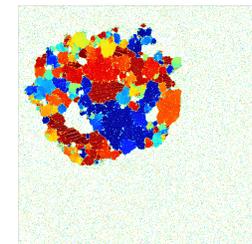
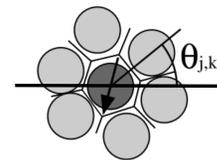


Full hexatically ordered small clusters

Larger clusters with several orientational order within

Local hexatic order parameter

$$\psi_{6j} = \frac{1}{nn_j} \sum_{k=1}^{nn_j} e^{i6\theta_{jk}}$$



$R_H \sim t^{0.13}$ in the scaling regime and $R_H \rightarrow R_H^* \ll L$

Similar to pattern formation, e.g.

Vega, Harrison, Angelescu, Trawick, Huse, Chaikin & Register, PRE 71, 061803 (2005)

Active Brownian Matter

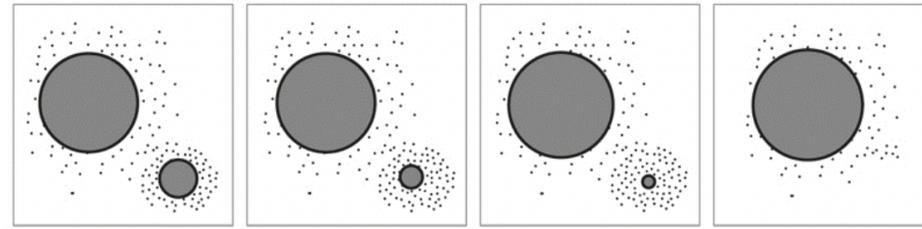
Table with results

	Disks	Dumbbells
Non-eq Steady-State	$R \sim aL$ $R_H \sim R_H^* \ll L$ $P(R_B) \sim R_B^{-\tau} e^{-\frac{R_B}{R_B^*}}$	
Approach to NESS	$R \sim t^{1/3} \rightarrow aL$ $R_H \sim t^{0.13} \rightarrow R_H^*$	

Mechanism for $t^{1/3}$

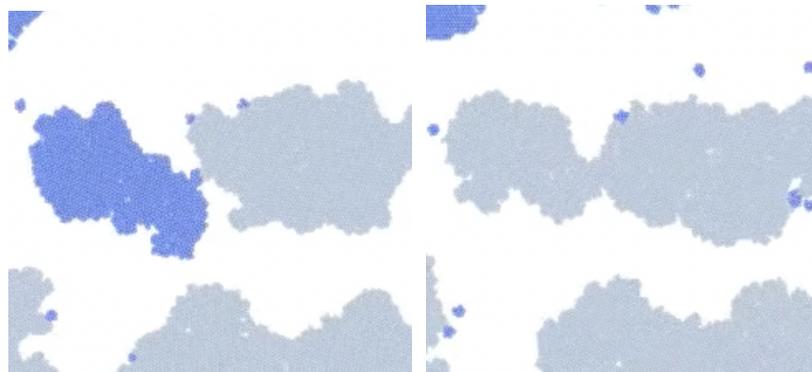
Two (non-exclusive) possibilities

1. Is it like the one of **passive attractive particles** ?



Ostwald ripening

2. Are there other **processes** at work in the active case ?

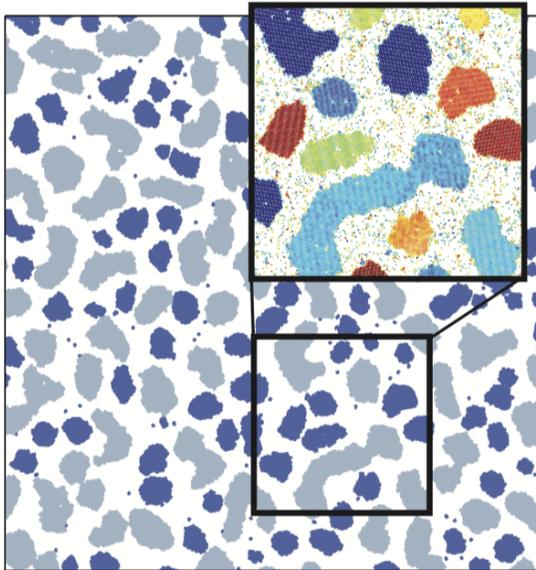


Cluster-cluster aggregation

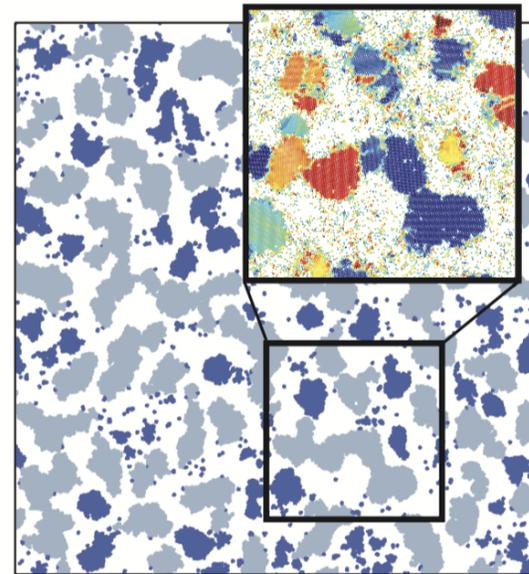
Dense Clusters - ABP

Instantaneous configurations (DBSCAN)

Passive - attractive



Active - repulsive



The Mie potential is not truncated in the passive case \Rightarrow attractive

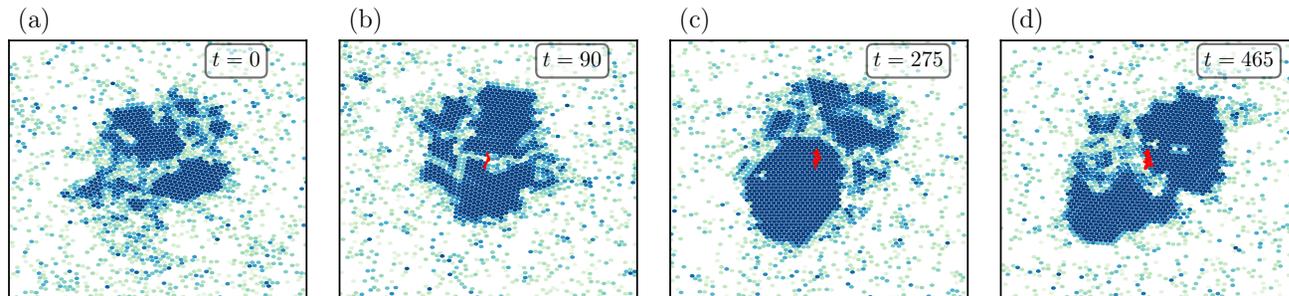
Parameters are such that $R(t)$ is the same in the two systems

Colors in the zoomed box indicate orientational order

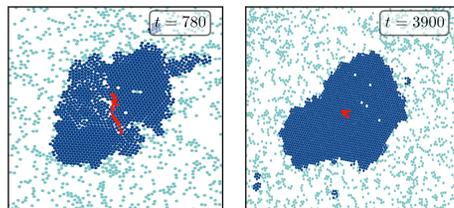
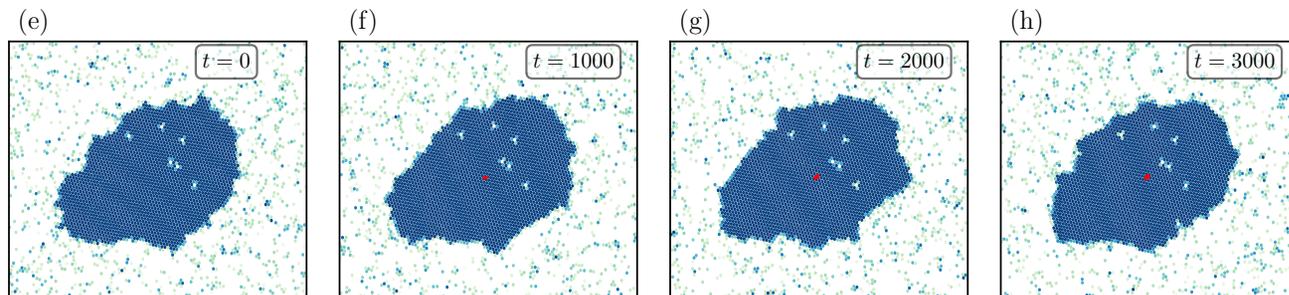
Clusters' Dynamics - ABP

Tracking of individual cluster motion - video

Active



Passive



In **red** the center of mass trajectory

Active is much faster than passive

Cluster-Cluster Aggregation

Smoluchowski argument

From $\overline{R}_g \sim t^{1/z}$ and using $D(M) \sim M^{-\alpha}$

Smoluchowski eq. $\Rightarrow z = d_f(1 + \alpha) - (d - d_w)$

Regular clusters $M_k < \overline{M}$

$$d_f = d = d_w = 2$$

$$\alpha = 0.5$$

$$z = 2(1 + 0.5) = 3$$

Fractal clusters $M_k > \overline{M}$

$$d_f = 1.45, d = 2 \text{ and } d_w \sim 2$$

$\alpha = 0.5$ in the bulk

$$z = 1.45(1 + 0.5) = 2.18 < 3$$

Reviews on the application of fractals to colloidal aggregation

R. Jullien, Croatia Chemica Acta 65, 215 (1992) P. Meakin, Physica Scripta 46, 295 (1992)

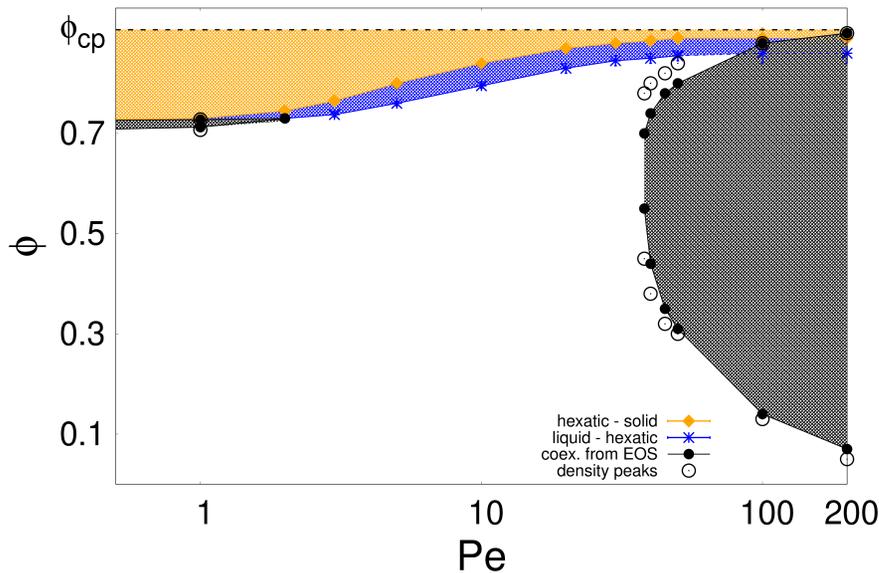
Active Brownian Matter

Table with results

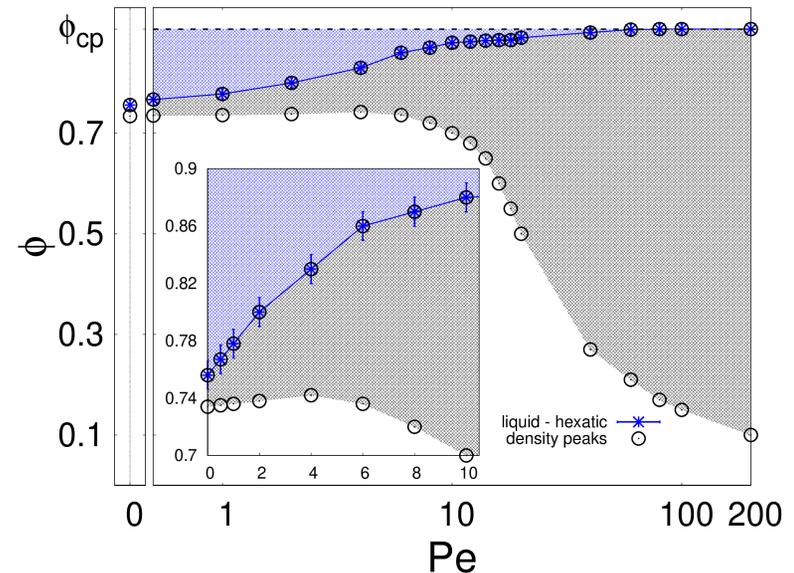
	Disks	Dumbbells
Non-eq Steady-State	$R \sim aL$ $R_H \sim R_H^* \ll L$ $P(R_B) \sim R_B^{-\tau} e^{-\frac{R_B}{R_B^*}}$	Next
Approach to NESS	$R \sim t^{1/3}$ $R_H \sim t^{0.13}$ Ostwald ripening & Cluster-cluster aggregation Thanks to $D(M) \sim M^{-1/2}$	Next

Phase Diagram - ABD

cfr. ABPs, plenty of interesting differences



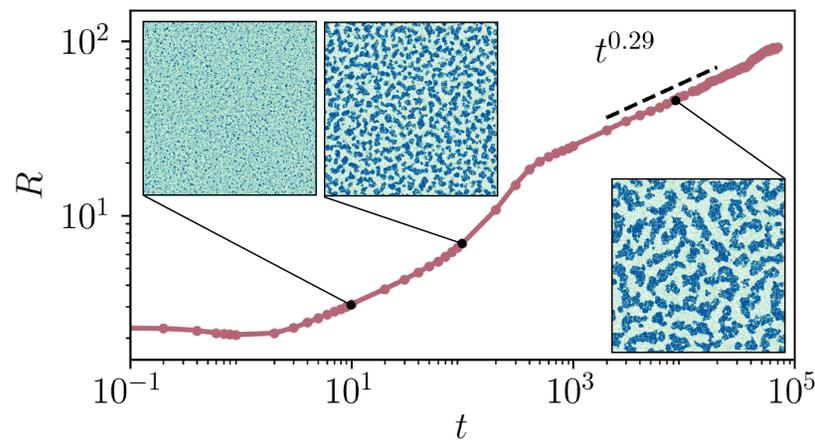
AB Particles



AB Dumbbells

Growth of the Dense Phase

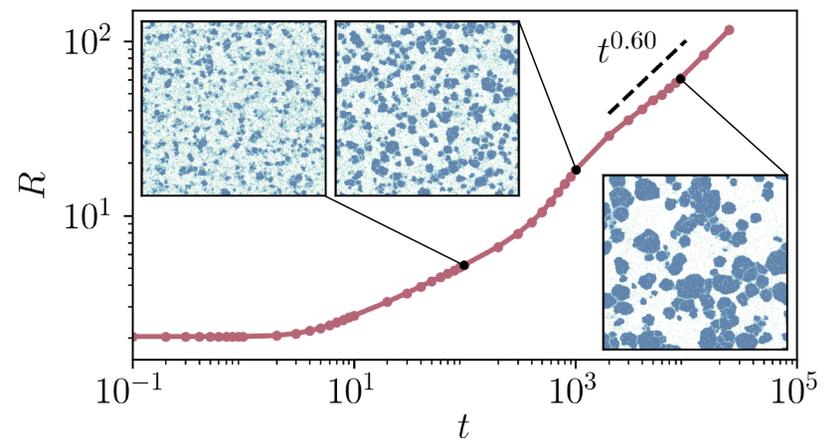
ABP vs ABD both at $Pe = 100$ and 50:50



AB Particles

slower

$$t^{0.3}$$

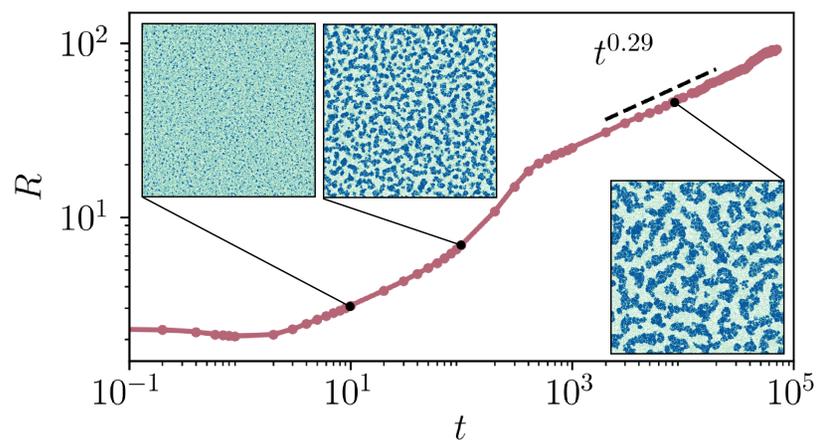
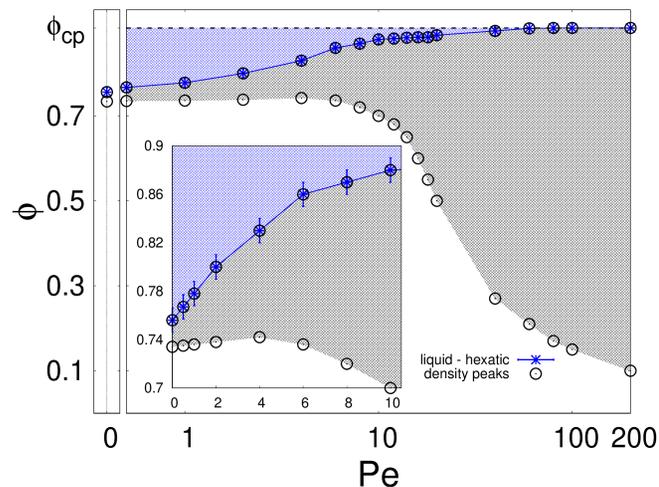
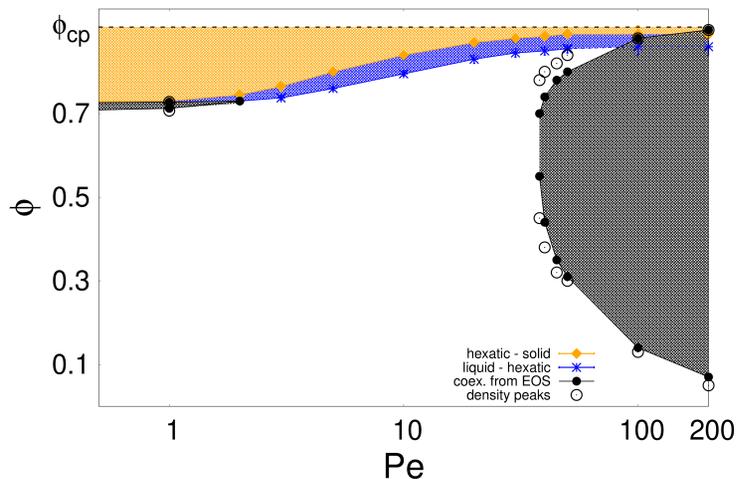


AB Dumbbells

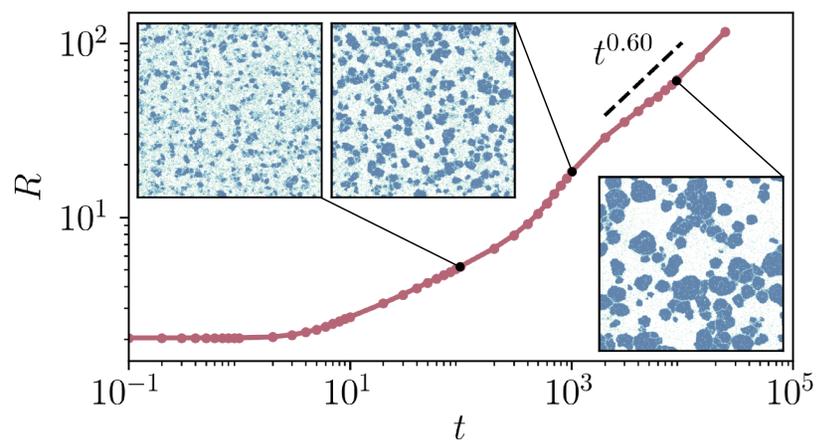
faster

$$t^{0.6}$$

ABPs vs ABDs



AB Disks
Cluster diffusion



AB Dumbbells
Cluster rotation

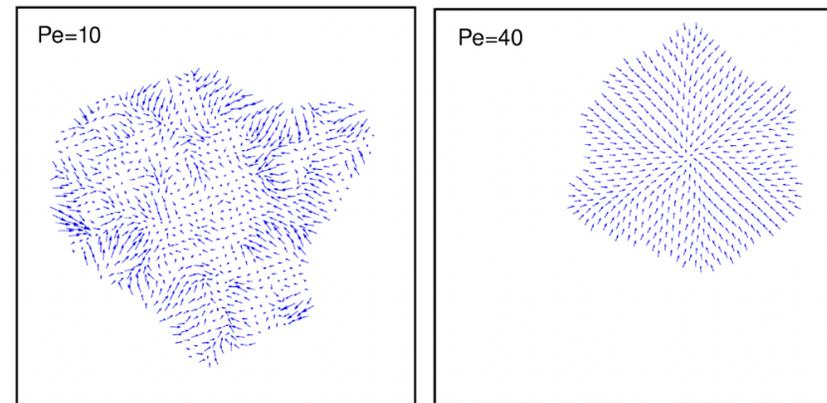
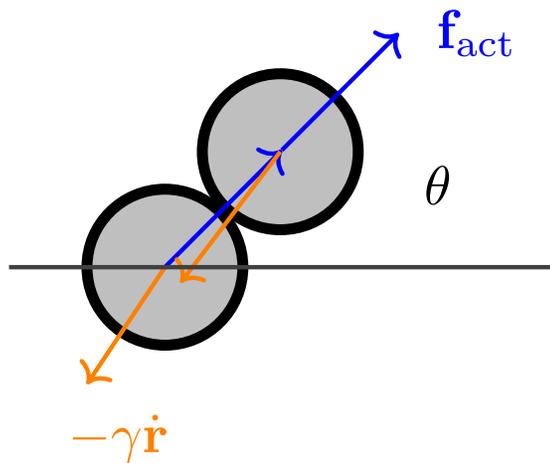
Active Brownian Matter

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Non-eq Steady-State	$R \sim L$ $R_H \sim R_H^* \ll L$ $P(R_B) \sim R_B^{-\tau} e^{-\frac{R_B}{R_B^*}}$	$R \sim L$ $R_H \sim L$ no bubbles
Approach to NESS	$R \sim t^{1/3} \rightarrow L$ $R_H \sim t^{0.13} \rightarrow R_H^*$ Ostwald ripening & Cluster-cluster aggregation	$R \sim t^{2/3} \rightarrow L$ $R_H \sim t^{0.3} \rightarrow L$ Rotation polarization

ABPs vs ABDs

What is special about dumbbells ?



Coarse-grained **polarization**

Vortex & aster patterns emerge

ABPs vs. ABDs

Field Theory - density ϕ coupled to polarity \mathbf{p}

$$F = \int d^d x \left\{ \frac{\alpha_\phi}{2\phi_{cr}} \phi^2 (\phi - \phi_0)^2 + k_\phi |\nabla \phi|^2 - \alpha_{\mathbf{p}} \frac{\phi - \phi_{cr}}{\phi_{cr}} |\mathbf{p}|^2 + \frac{\alpha_{\mathbf{p}}}{2} |\mathbf{p}|^4 + k_{\mathbf{p}} (\nabla \mathbf{p})^2 \right\}$$

$$\partial_t \phi + \boxed{\lambda \nabla \cdot (\mathbf{p} \phi)} = M \nabla^2 \mu_\phi$$

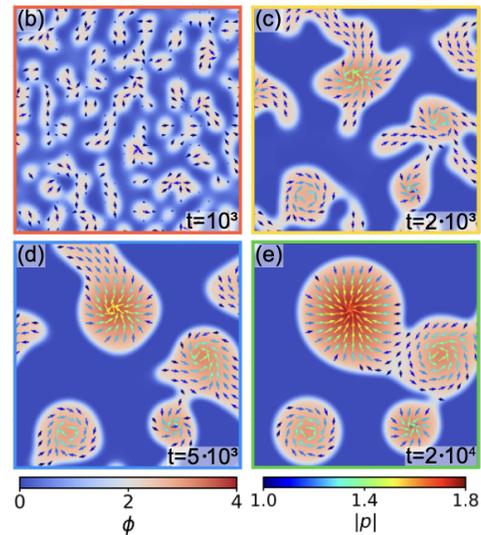
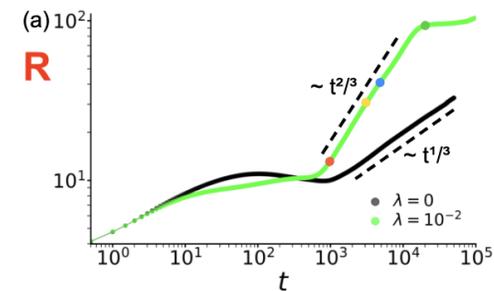
$$\partial_t \mathbf{p} = -\Gamma \mu_{\mathbf{p}}$$

$$R(t) \simeq t^{0.6} \quad \lambda = 10^{-2}$$

Advection accelerates growth

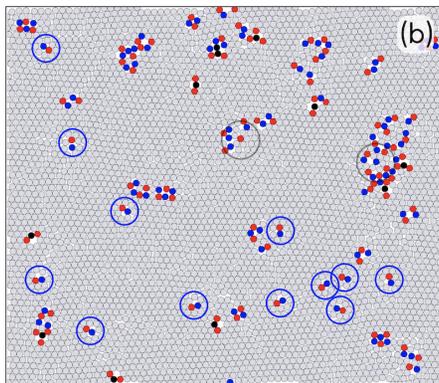
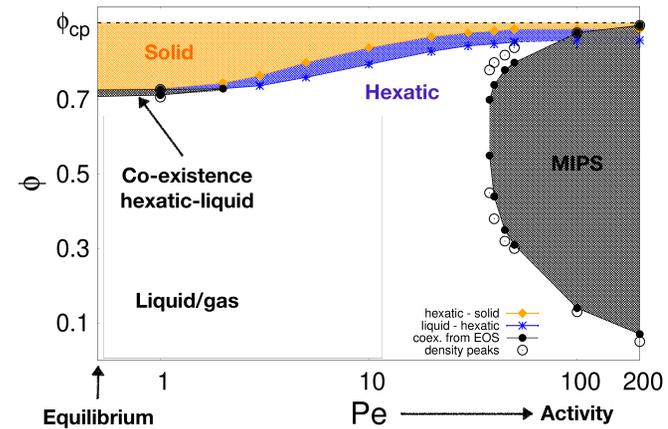
$$\mu_\phi = \frac{\delta F}{\delta \phi} \quad \mu_{\mathbf{p}} = \frac{\delta F}{\delta \mathbf{p}}$$

$\lambda = 0$ Model B



Results I

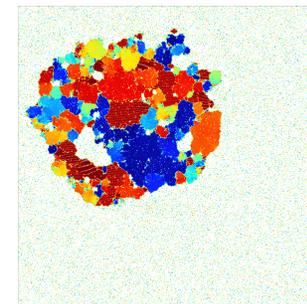
We established the full phase diagram of ABPs
solid, **hexatic**, **liquid** & MIPS



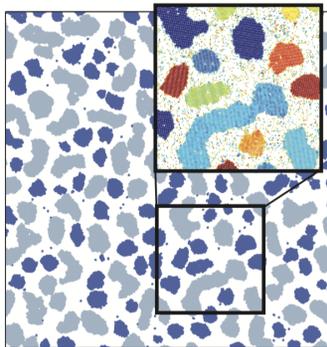
We clarified the role played by point-like
(**dislocations** & **disclinations**)
and **clustered** defects in
passive & active $2d$ models.

In MIPS

Micro vs. macro: hexatic patches & bubbles

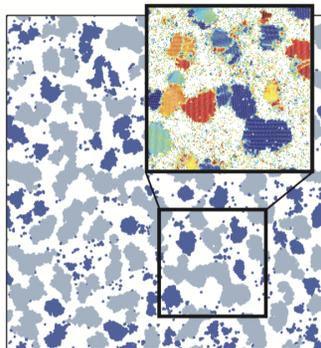


Results II



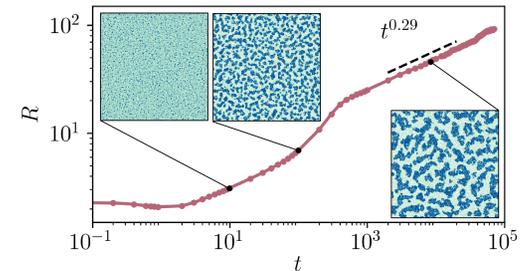
Difference between

Passive

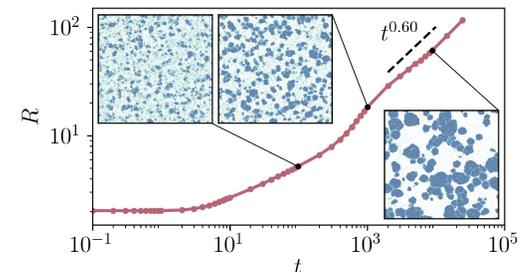


Active

growth



ABPs $R \sim t^{1/3}$



ABDs $R \sim t^{3/5}$

Ostwald ripening & cluster-cluster diffusive aggregation in ABP case
cluster-cluster aggregation almost not present in passive

Co-existence of regular and fractal clusters

Heterogeneous/homogenous orientational order in large ABP/ABD clusters

Extras

Cluster-cluster aggregation

Extended Smoluchowski argument

From $\bar{R}_g \sim t^{1/z}$ and using $D(M) \sim M^{-\alpha}$

Smoluchowski eq. $\Rightarrow z = d_f(1 + \alpha) - (d - d_w)$

Regular clusters $M < \bar{M}$ **Fractal** clusters $M > \bar{M}$

$$d_f = d = d_w = 2$$

$$\alpha = 0.5$$

$$z = 2(1 + 0.5) = 3$$

$$d_f = 1.45, d = 2 \text{ and } d_w \sim 2$$

if, instead, $\alpha = 1$

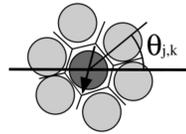
$$z = 1.45(1 + 1) \sim 3$$

Reviews on the application of fractals to colloidal aggregation

R. Jullien, Croatia Chemica Acta 65, 215 (1992) P. Meakin, Physica Scripta 46, 295 (1992)

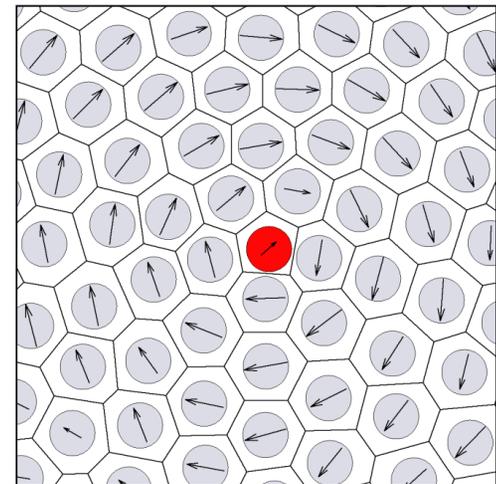
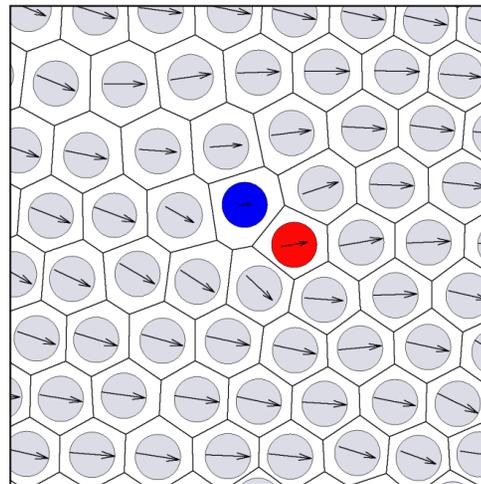
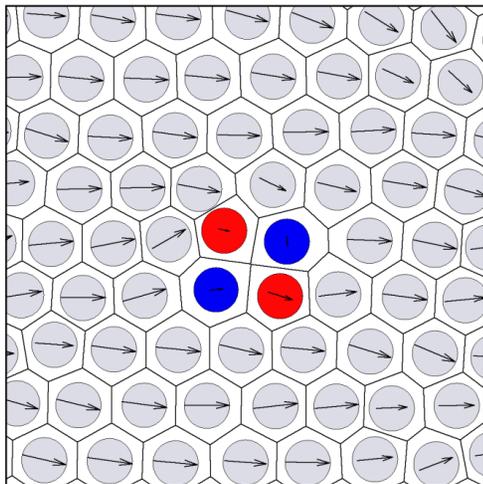
Freezing/Melting - arrows

Hexatic (orientational) order parameter $\psi_{6j} = \frac{1}{nn_j} \sum_{k=1}^{nn_j} e^{i6\theta_{jk}}$



ϕ ← **SOLID** **HEXATIC** **LIQUID**

LR orient.
QLR transl. QLR orient.
SR transl. SR orient.
SR transl.



arrows oriented (LR) less oriented (QLR) order lost (SRL)

● five neighbours

● seven neighbours

Voronoi tessellation

Phases & transitions

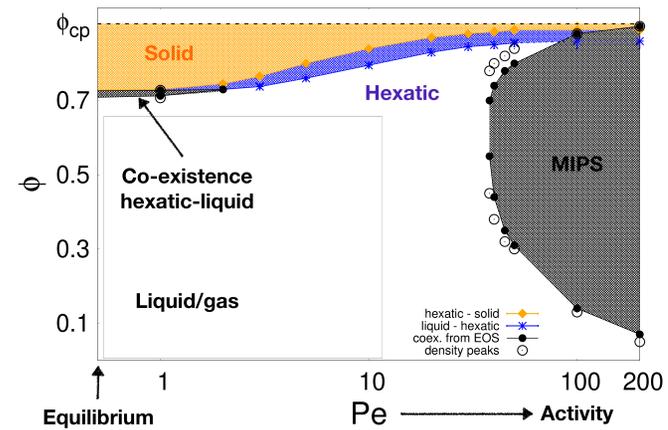
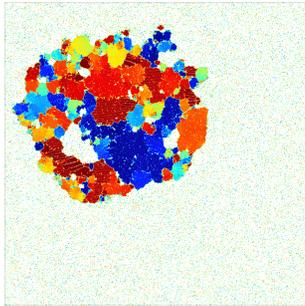
2d passive $Pe = 0$ systems: BKT-HNY vs. a new scenario

	BKT-HNY	BK
Solid	QLR pos & LR orient	QLR pos & LR orient
transition	BKT	BKT
Hexatic	SR pos & QLR orient	SR pos & QLR orient
transition	BKT	1st order
Liquid	SR pos & orient	SR pos & orient

Basically, the phases are the same, but the **hexatic-liquid** transition is different, allowing for **coexistence of the two phases** for **hard enough particles**

Event driven MC simulations. Bernard & Krauth PRL 107, 155704 (2011)

Results I on ABPs

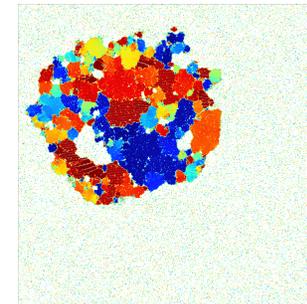


In MIPS

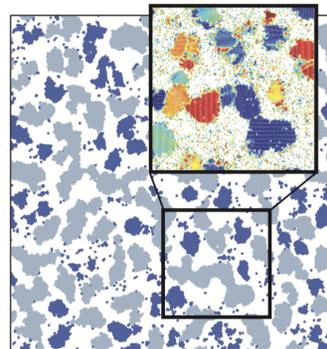
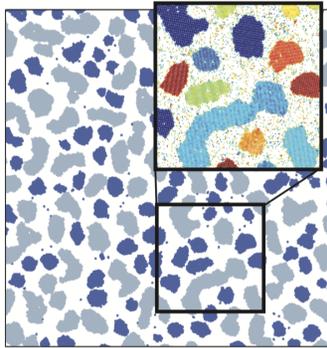
Ostwald ripening & Cluster-cluster aggregation

$$R(t) \sim t^{1/3}, R_H(t) \sim t^{0.13}$$

Micro vs. macro: hexatic patches & bubbles



Results II on ABPs



Difference between

Passive

Active

growth

Ostwald ripening & cluster-cluster diffusive aggregation in active case
cluster-cluster aggregation almost not present in passive

Co-existence of regular and fractal clusters in both cases

Heterogeneous orientational order in large active clusters only

Dense Clusters - ABP

Visual facts about the cluster dynamics

In both cases, **Ostwald ripening** features

- small clusters evaporate
- gas particles attach to large clusters

In the **active system**

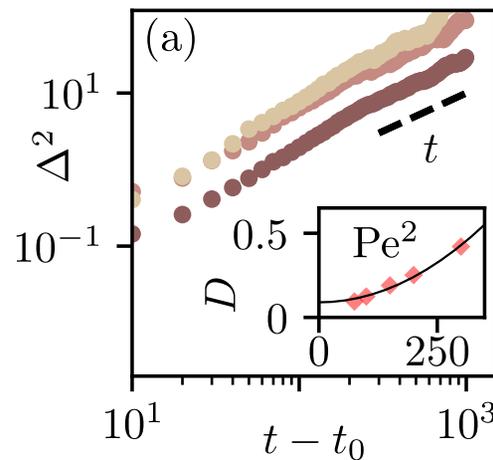
- clusters displace much more & sometimes aggregate
- they also break & recombine

like in **diffusion limited cluster-cluster aggregation**

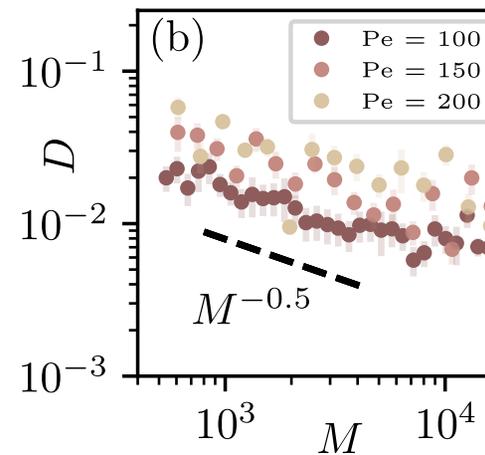
Clusters' Diffusion - ABP

Mean Square Displacement

Average over all clusters



Mass dependence



$$\Delta_k^2(t, t_0) = [\mathbf{r}_{\text{c.o.m.}}^{(k)}(t) - \mathbf{r}_{\text{c.o.m.}}^{(k)}(t_0)]^2 \sim 2d D(M_k, \text{Pe}) (t - t_0)$$

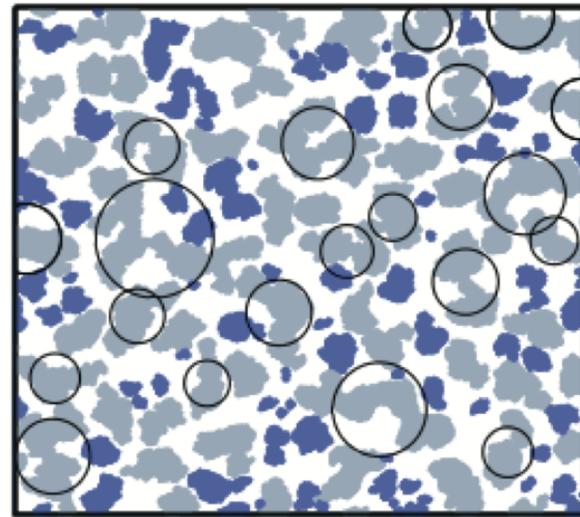
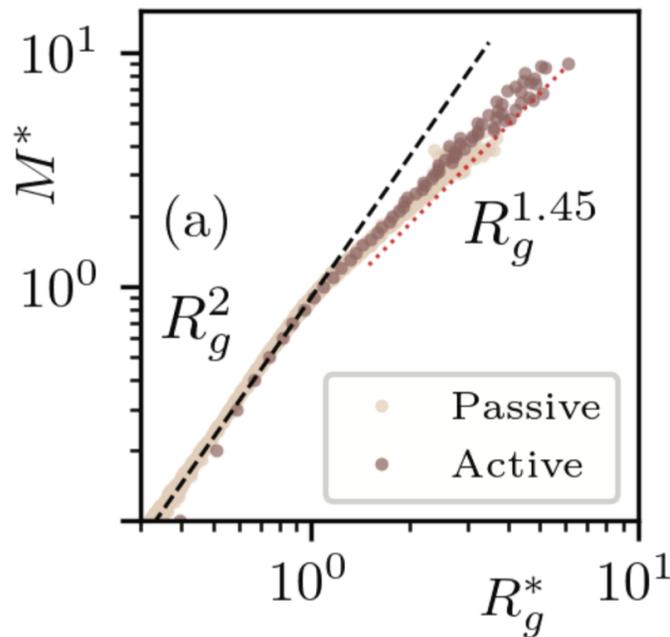
A sum of random forces yields $D \sim M^{-1}$

Passive tracer in a dilute active bath $D \sim R^{-1} \sim M^{-1/2}$ Solon & Horowitz (22)

Passive & very heavy isolated active clusters $D \sim M^{-1}$

Clusters' Geometry - ABP

Scatter plots: small regular – large fractal



Cluster mass $M_k^*(t) = \frac{M_k(t)}{\overline{M}(t)}$

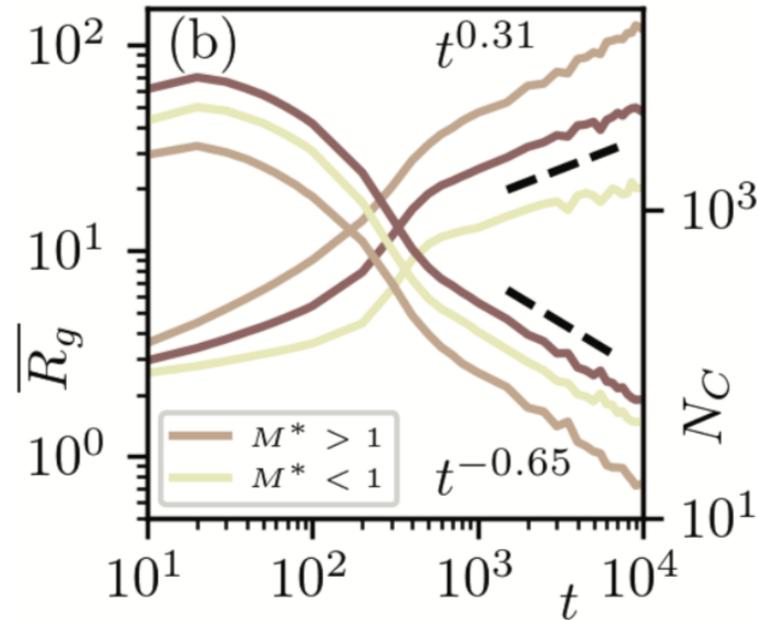
Gyration radius $R_{gk}^*(t) = \frac{R_{gk}(t)}{R_g(t)}$

Data sampled in the scaling regime $t = 10^3 - 10^5$ every 10^3 time steps

$\overline{O}(t) = \frac{1}{N_c(t)} \sum_{k=1}^{N_c(t)} O_k(t)$ and $N_c(t)$ the total number of clusters at time t

Regular vs Fractal Clusters

Radius of gyration and number of ABP clusters



regular $z \gtrsim 3$

More

Dominate

fractal $z < 3$

Less

average $z = 1/0.31 \sim 3$

All

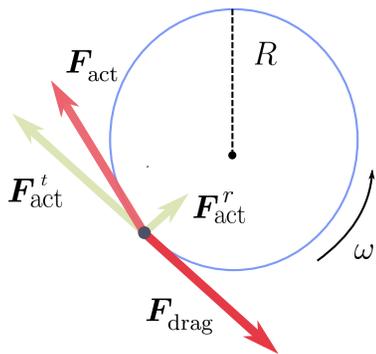
Model

Solid body motion

$$M\ddot{\mathbf{R}}_{\text{cm}} = \mathbf{F}_{\text{drag}} + \mathbf{F}_{\text{act}} \quad (\text{with } \mathbf{F}_{\text{act}} = \sum_{i \in \mathcal{C}} \mathbf{f}_{\text{act}i} \text{ and } \mathbf{F}_{\text{drag}} = -\gamma \frac{M}{m} \dot{\mathbf{R}}_{\text{cm}})$$

$$\dot{\mathbf{L}} = \mathbf{T}_{\text{drag}} + \mathbf{T}_{\text{act}} \quad \text{with}$$

$$\left. \begin{array}{l} \mathbf{L} \\ \mathbf{T}_{\text{drag}} \\ \mathbf{T}_{\text{act}} \end{array} \right\} = \sum_{i \in \mathcal{C}} (\mathbf{r}_i - \mathbf{R}_{\text{cm}}) \times \left\{ \begin{array}{l} m \frac{d}{dt} (\mathbf{r}_i - \mathbf{R}_{\text{cm}}) \\ -\gamma \frac{d}{dt} (\mathbf{r}_i - \mathbf{R}_{\text{cm}}) = -\frac{\gamma}{m} \mathbf{L} \\ \mathbf{f}_{\text{act}i} \end{array} \right.$$



Sketch of forces acting on

the c.o.m. of the cluster

ω angular velocity

How does $R = R_{\text{cm}}$ depend on M, R_g, f_{act} ?

Model

Circular motion

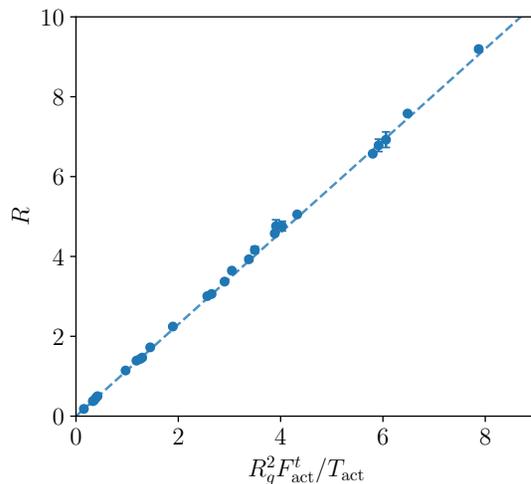
Overdamped approximation for angular momentum

$$\dot{\mathbf{L}} = \mathbf{T}_{\text{act}} + \mathbf{T}_{\text{drag}} \approx 0 \implies \mathbf{T}_{\text{act}} - \gamma/m \mathbf{L} \approx 0 \implies L \approx \frac{m}{\gamma} T_{\text{act}}$$

Using now $L = I\omega = MR_g^2 \omega$ in the last equation $\omega \approx \frac{m}{M} \frac{T_{\text{act}}}{\gamma R_g^2}$

On the other hand the balance of the tangential forces yields

$$F_{\text{act}}^t = F_{\text{drag}} = (M/m) \gamma \dot{R}_{\text{cm}} \approx (M/m) \gamma \omega R \implies R = \frac{m}{M} \frac{F_{\text{act}}^t}{\gamma} \frac{1}{\omega}$$



Putting these two equations together

← Test $R = R_g^2 \underbrace{\frac{F_{\text{act}}^t}{T_{\text{act}}}}_{\text{independent of } f_{\text{act}}}$

Is there a field-theory model for $R(t) \sim t^{0.6}$