Dottorato di Ricerca Fisica (XXXII ciclo)

Phase transition and topological defects in a system of self-propelled disks

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Università degli Studi di Bari "Aldo Moro", INFN - Sezione di Bari

Tutor: Prof. Giuseppe Gonnella

Summary

- **Melting in two dimensional systems**:
  the original problem and the KTHN theory

- **Self-propelled disks**: persistent brownian motion & MIPS
- **Self-propelled dumbbells**

- **Results**: phase diagram, structure, dynamics, defects

Summary

- **Melting in two dimensional systems**: the original problem and the KTHN theory

equilibrium

- **Self-propelled disks**: persistent brownian motion & MIPS
- **Self-propelled dumbbells**
- **Results**: phase diagram, structure, dynamics, defects

out of equilibrium

Melting in 2D

Does an equilibrium ordered phase exist for 2d systems with short-range interactions?

Phase Transition in Elastic Disks*

B. J. Alder and T. E. Wainwright
University of California, Lawrence Radiation Laboratory, Livermore, California
(Received October 30, 1961)

The study of a two-dimensional system consisting of 870 hard-disk particles in the phase-transition region has shown that the isotherm has a van der Waals-like loop. The density change across the transition is about 4% and the corresponding entropy change is small.

Crystalline Order in Two Dimensions*

N. D. Mermin†
Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York
(Received 1 July 1968)

If N classical particles in two dimensions interacting through a pair potential $\Phi(\vec{r})$ are in equilibrium in a parallelogram box, it is proved that every $\vec{k}\neq 0$ Fourier component of the density must vanish in the thermodynamic limit, provided that $\Phi(\vec{r}) - \lambda r^2 |\nabla^2\Phi(\vec{r})|$ is integrable at $r=\infty$ and positive and nonintegrable at $r=0$, both for $\lambda=0$ and for some positive λ. This result excludes conventional crystalline long-range order in two dimensions for power-law potentials of the Lennard-Jones type, but is inconclusive for hard-core potentials. The corresponding analysis for the quantum case is outlined. Similar results hold in one dimension.

Phase transitions in 2d short-range interacting particles: Kosterlitz-Thouless-Halperin-Nelson

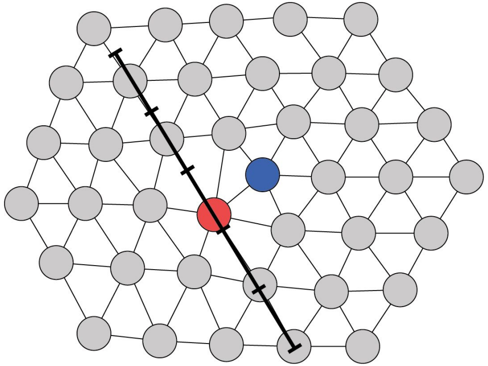
Phase transitions in 2d short-range interacting particles: Kosterlitz-Thouless-Halperin-Nelson

LIQUID ? **SOLID**

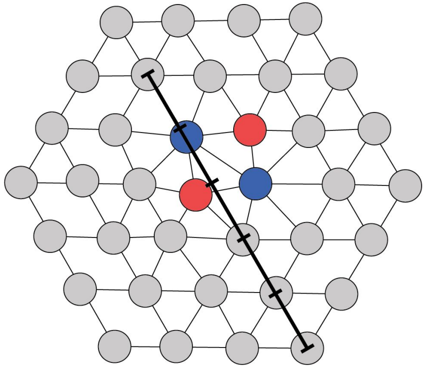
ϕ

Translational order

short-ranged



quasi-long-ranged



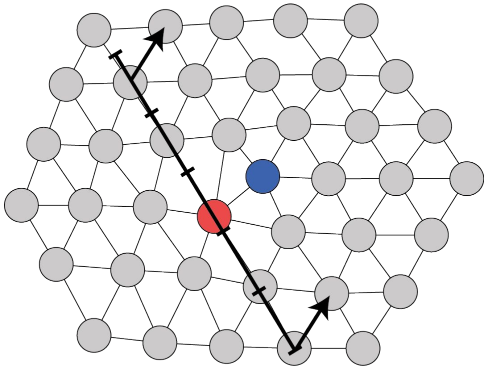
Phase transitions in 2d short-range interacting particles: Kosterlitz-Thouless-Halperin-Nelson

LIQUID ? **SOLID**

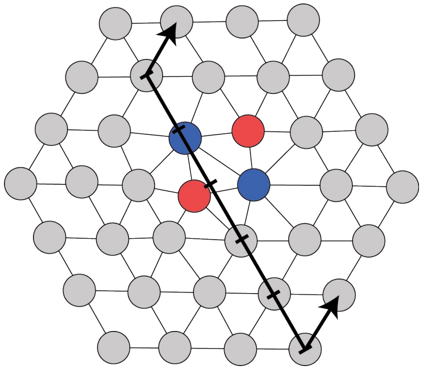
$\longrightarrow \phi$

Translational order

short-ranged

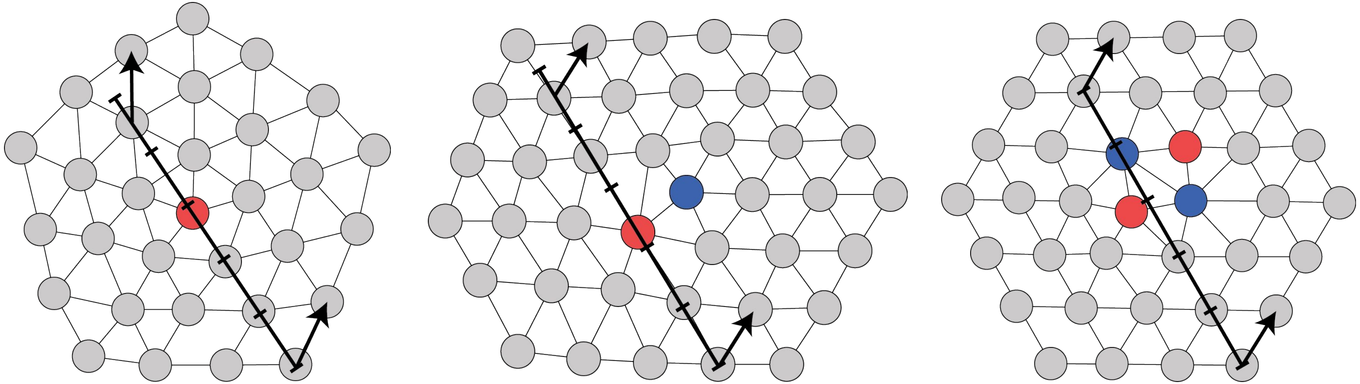


quasi-long-ranged



Phase transitions in 2d short-range interacting particles: Kosterlitz-Thouless-Halperin-Nelson

	LIQUID	**HEXATIC**	**SOLID** $\rightarrow \phi$
Bond-orientational order	short-ranged	quasi-long-ranged	long-ranged
Translational order	short-ranged	short-ranged	quasi-long-ranged

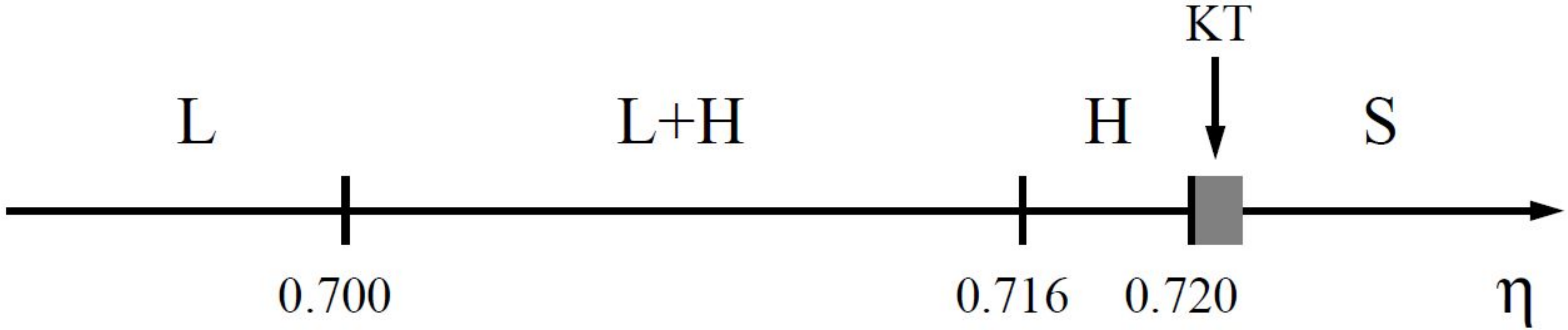


Melting scenario for hard disks. Recent results

Bernard P., Krauth W. F., Phys. Rev. Lett., 107 155704, (2015)
Dullens P.A., *et al.*, Phys. Rev. Lett., 118 158001 (2017)

Melting scenario for hard disks. Recent results

- First order phase transition between liquid and hexatic
- KTHN transition between hexatic and solid



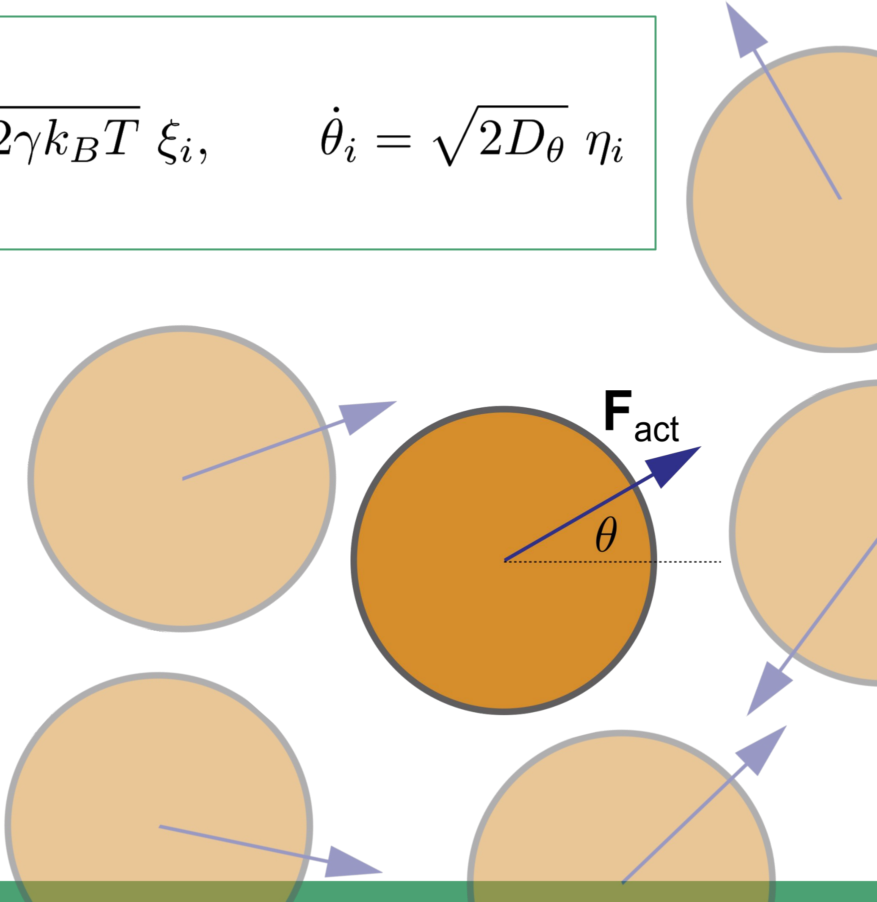
Bernard P., Krauth W. F., Phys. Rev. Lett., 107 155704, (2015)
Dullens P.A., *et al.*, Phys. Rev. Lett., 118 158001 (2017)

Self-propelled particles

Self-propelled (active) brownian disks

$$\mathbf{n}_i = (\cos\theta_i(t), \sin\theta_i(t))$$
$$\gamma\dot{\mathbf{r}}_i = F_{act}\mathbf{n}_i - \nabla_i \sum_{j(\neq i)} U(r_{ij}) + \sqrt{2\gamma k_B T}\ \xi_i, \qquad \dot{\theta}_i = \sqrt{2D_\theta}\ \eta_i$$

- $U(r) = \begin{cases} U_{LJ}(r) - U_{LJ}(r_{min}) & \text{if } r < r_{min} \\ 0 \quad \text{if } r \geqslant r_{min} \end{cases}$
- $\langle \xi_i^\alpha(t) \rangle = 0, \quad \langle \xi_i^\alpha(t)\ \xi_j^\beta(t') \rangle = \delta_{ij}\delta^{\alpha\beta}\delta(t-t')$
- $\langle \eta_i(t) \rangle = 0, \quad \langle \eta_i(t)\ \eta_j(t') \rangle = \delta_{ij}\delta(t-t')$
- $D_\theta = 3k_B T/\gamma\sigma_d^2$



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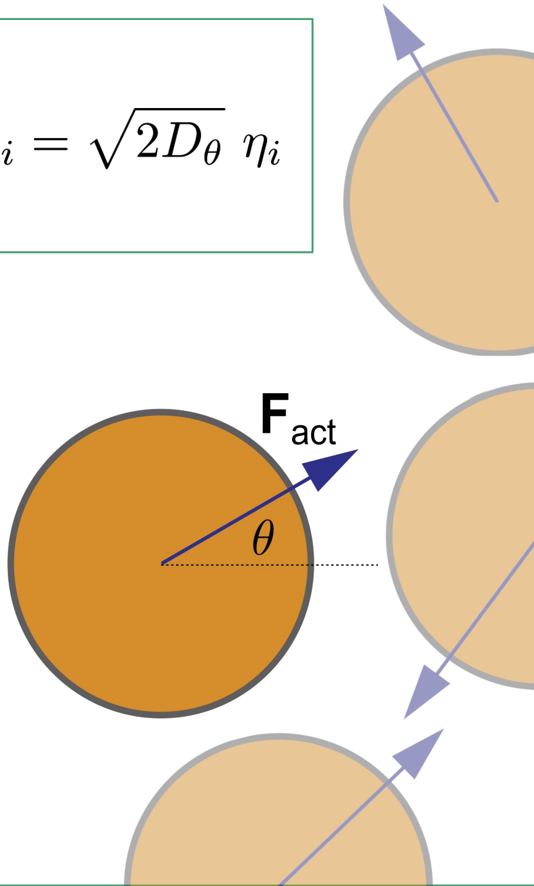
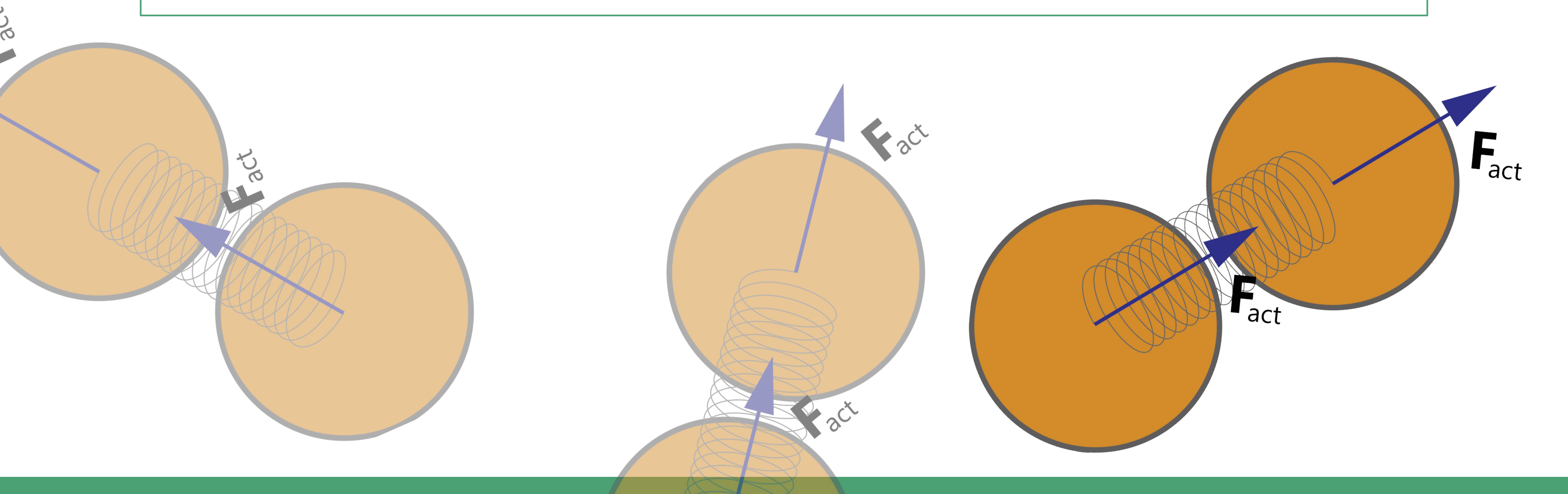
- $U(r) = \begin{cases} U_{LJ}(r) - U_{LJ}(r_{min}) & \text{if } r < r_{min} \\ 0 & \text{if } r \geqslant r_{min} \end{cases}$
- Surface fraction: $\phi = N\dfrac{\pi\sigma_d^2}{4S}$
- Péclet number: $\mathrm{Pe} = \dfrac{Lv_{act}}{D} = \dfrac{\sigma_d F_{act}}{k_B T}$



Self-propelled dumbbells

$$m\ddot{\mathbf{r}}_i = -\gamma\dot{\mathbf{r}}_i - \frac{\partial U_{FENE}}{\partial r_{i,i+1}}\hat{\mathbf{r}}_{i,i+1} - \sum_{j\neq i}^{2N}\frac{\partial U_{WCA}}{\partial r_{ij}}\ \hat{\mathbf{r}}_{ij} + F_{act}\hat{\mathbf{n}}_i + \sqrt{2D_0}\ \eta_i\ ,$$

$$m\ddot{\mathbf{r}}_{i+1} = -\gamma\dot{\mathbf{r}}_{i+1} + \frac{\partial U_{FENE}}{\partial r_{i,i+1}}\ \hat{\mathbf{r}}_{i,i+1} - \sum_{j\neq i+1}^{2N}\frac{\partial U_{WCA}}{\partial r_{i+1,j}}\ \hat{\mathbf{r}}_{i+1,j} + F_{act}\hat{\mathbf{n}}_{i+1} + \sqrt{2D_0}\ \eta_{i+1}$$



Persistent random walk

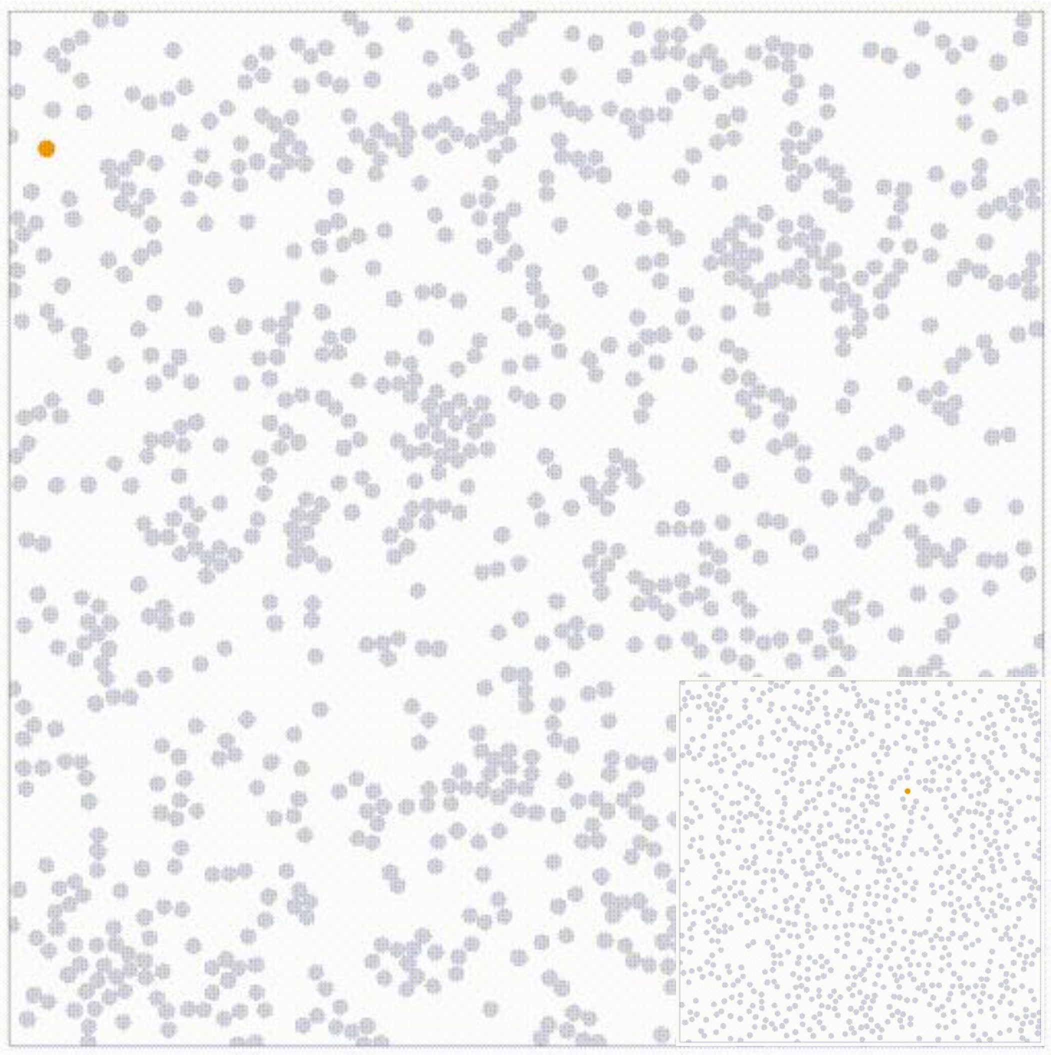
$$\gamma \dot{\mathbf{r}}(t) = F_{\mathrm{act}} \mathbf{n}(t) + \sqrt{2\gamma k_B T}\ \xi(t)$$
$$\theta(t) = \sqrt{2D_\theta}\ \eta(t)$$

- Ballistic short-time

$$v_0 = \frac{F_{\mathrm{act}}}{\gamma}$$

- Diffusive long-time

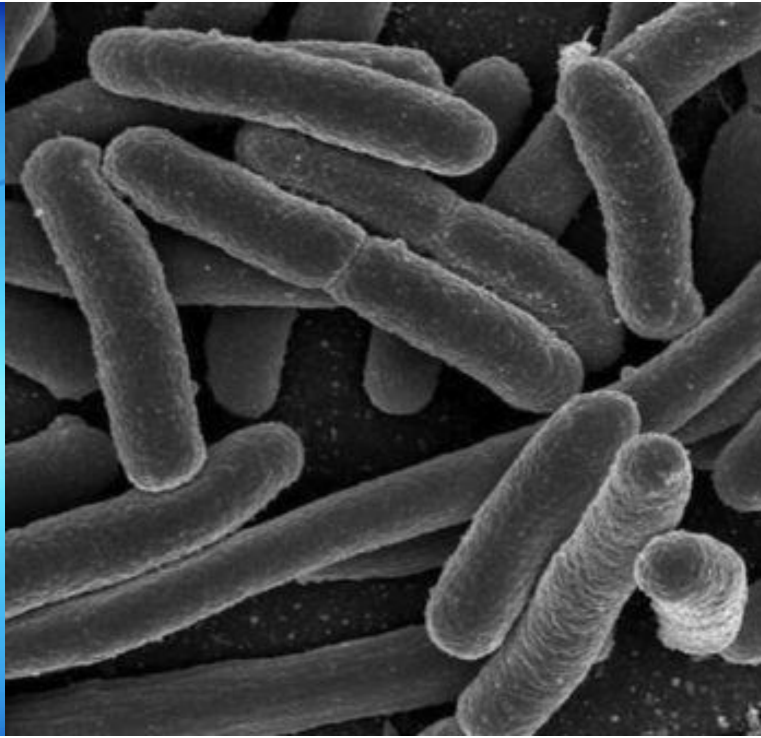
$$D = D_0 + \frac{v_0^2}{2D_\theta}$$



Active systems

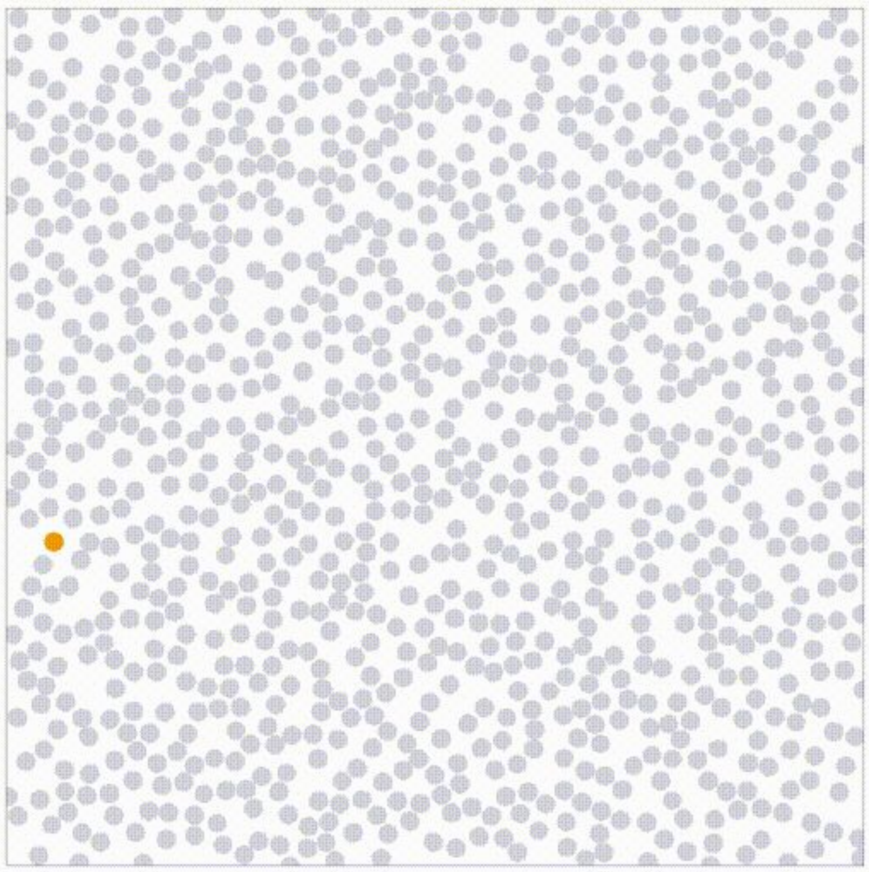
Birds flocking

Fish schools



Bacteria

Motility-induced phase separation (MIPS)



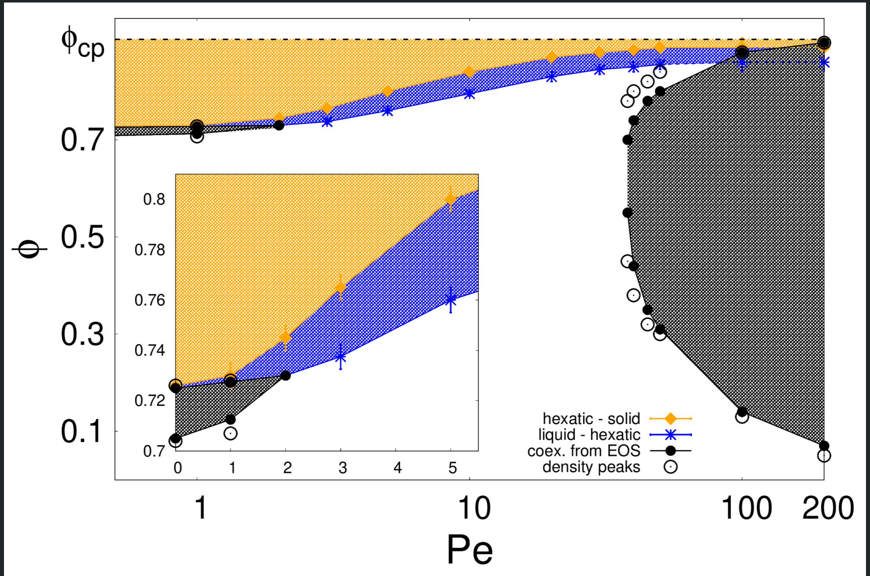
Review of the results

Review of the results

- **Phase diagram of active disks**
- Dynamical scaling for MIPS

- Phase diagram of active dumbbells
- Structural behavior and dynamics of the clusters in MIPS

- Topological defects for active disks



DP, Levis D., Suma A., Cugliandolo L.F., Gonnella G., Pagonabarraga I., Phys. Rev. Lett., 121 098003 (2018)

Review of the results

- Phase diagram of active disks
- **Dynamical scaling for MIPS**

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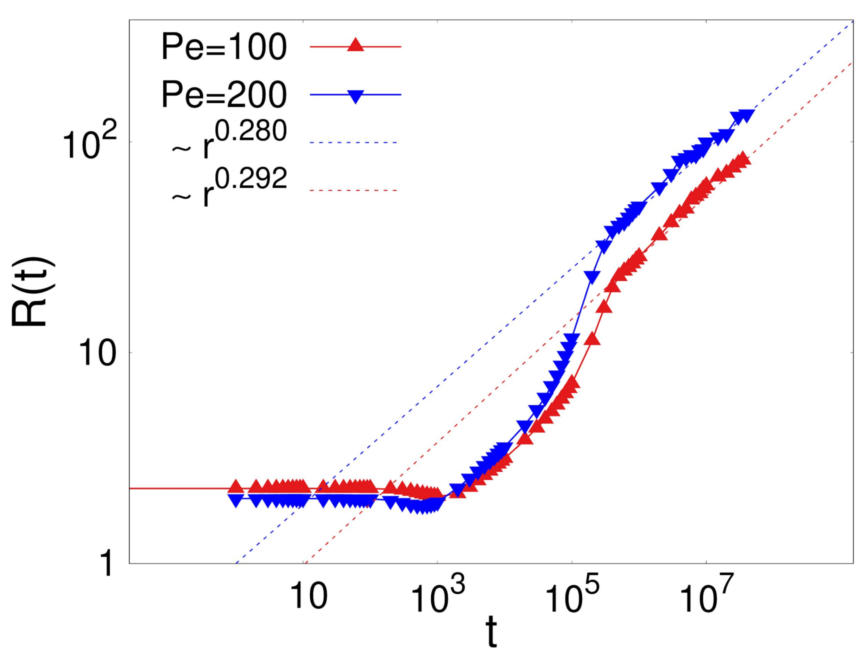


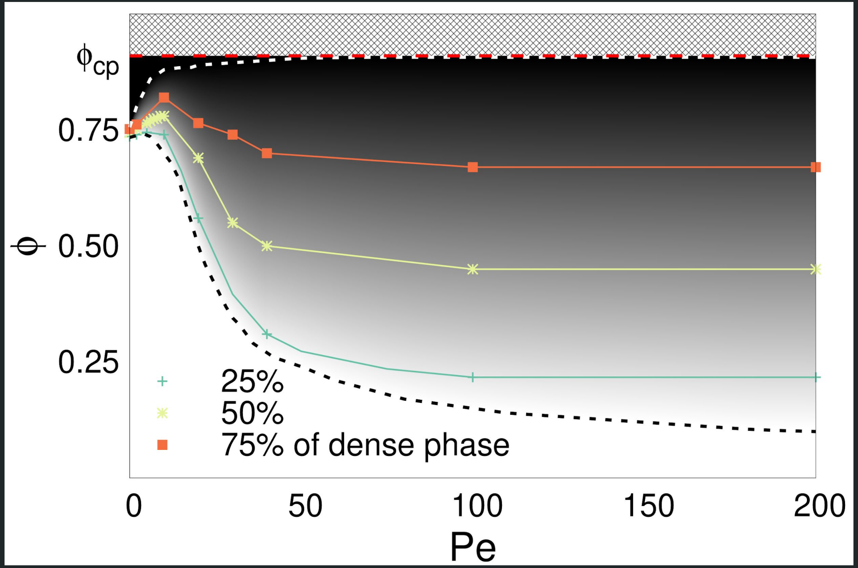
Ongoing work

Review of the results

- Phase diagram of active disks
- Dynamical scaling for MIPS

- **Phase diagram of active dumbbells**
- Structural behavior and dynamics of the clusters in MIPS

- Topological defects for active disks



Cugliandolo L.F., DP, Gonnella G., Suma A., Phys. Rev. Lett., 1119268002 (2017)

Review of the results

- Phase diagram of active disks
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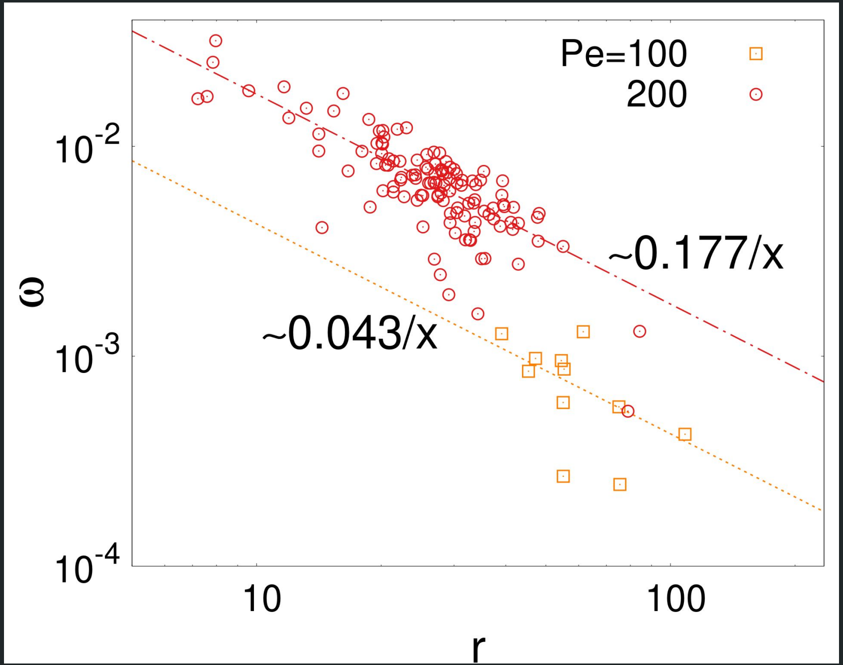
- **Structure and dynamics of the clusters in MIPS**

- Topological defects for active disks



Petrelli I., DP, Cugliandolo L.F., Gonnella G., Suma A., Eur. Phys. J. E (2018) 41: 128

Review of the results

- Phase diagram of active disks
- Dynamical scaling for MIPS

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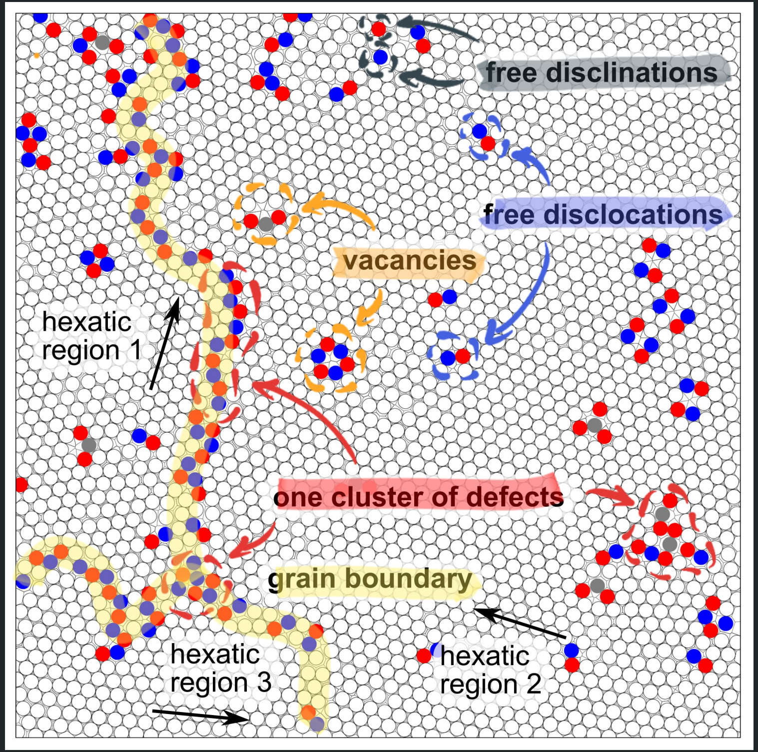
- Structural behavior and dynamics of the clusters in MIPS

- **Topological defects for active disks**



Ongoing work

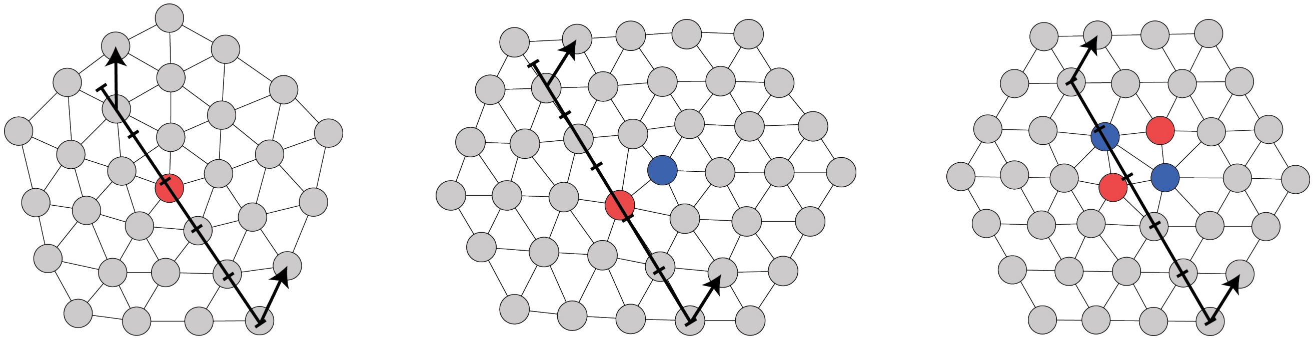
Topological defects

MD simulations: **512^2 particles** on a rectangular box with $L_x/L_y=2/\sqrt{3}$
~**10^3 runs lasting 96 hours on (parallel) 48 cpus**
on Marconi-CINECA and Marenostrum-BSC (Barcelona)

Halperin-Nelson phase transition (passive)

	LIQUID	HEXATIC	SOLID
Bond-orientational order	short-ranged	quasi-long-ranged	long-ranged
Translational order	short-ranged	short-ranged	quasi-long-ranged

ϕ



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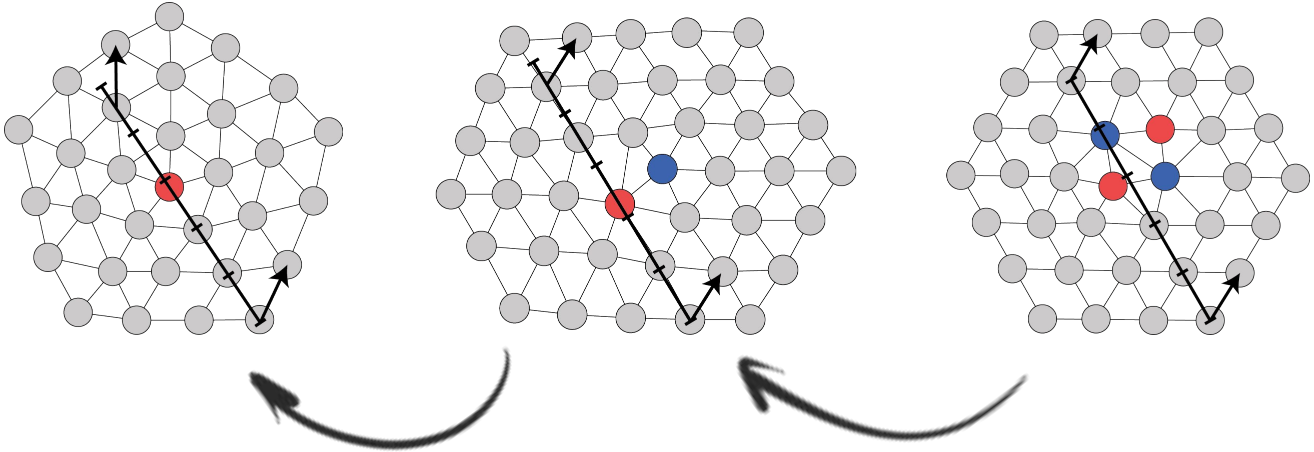
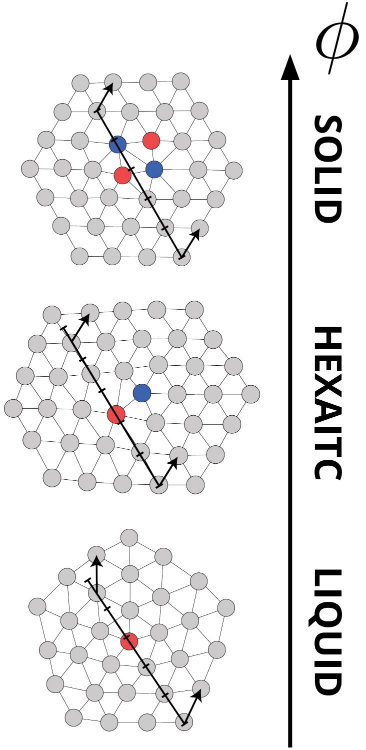


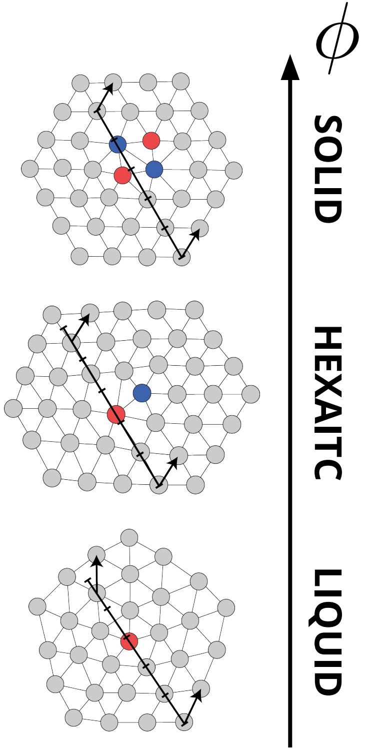
DISLOCATION UNBINDING

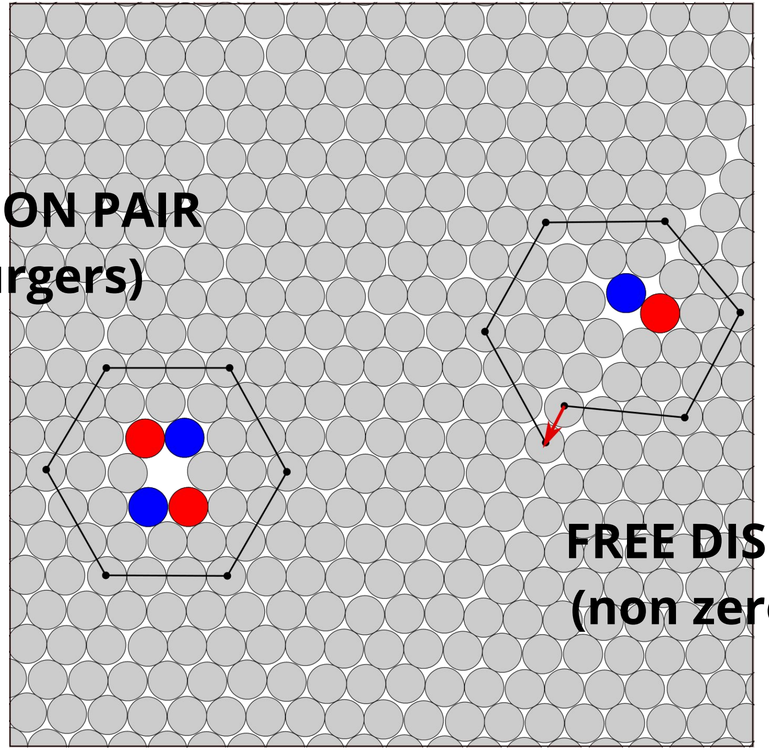
DISLOCATION-PAIRS UNBINDING

Equilibrium-like KTHN defects unbinding mechanism for the active system?



Equilibrium-like KTHN defects unbinding mechanism for the active system?





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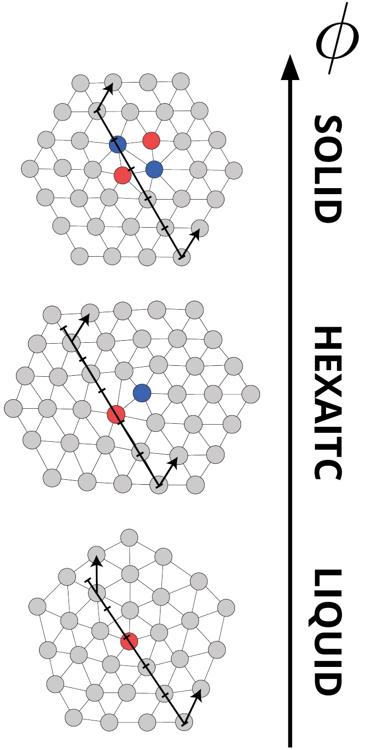
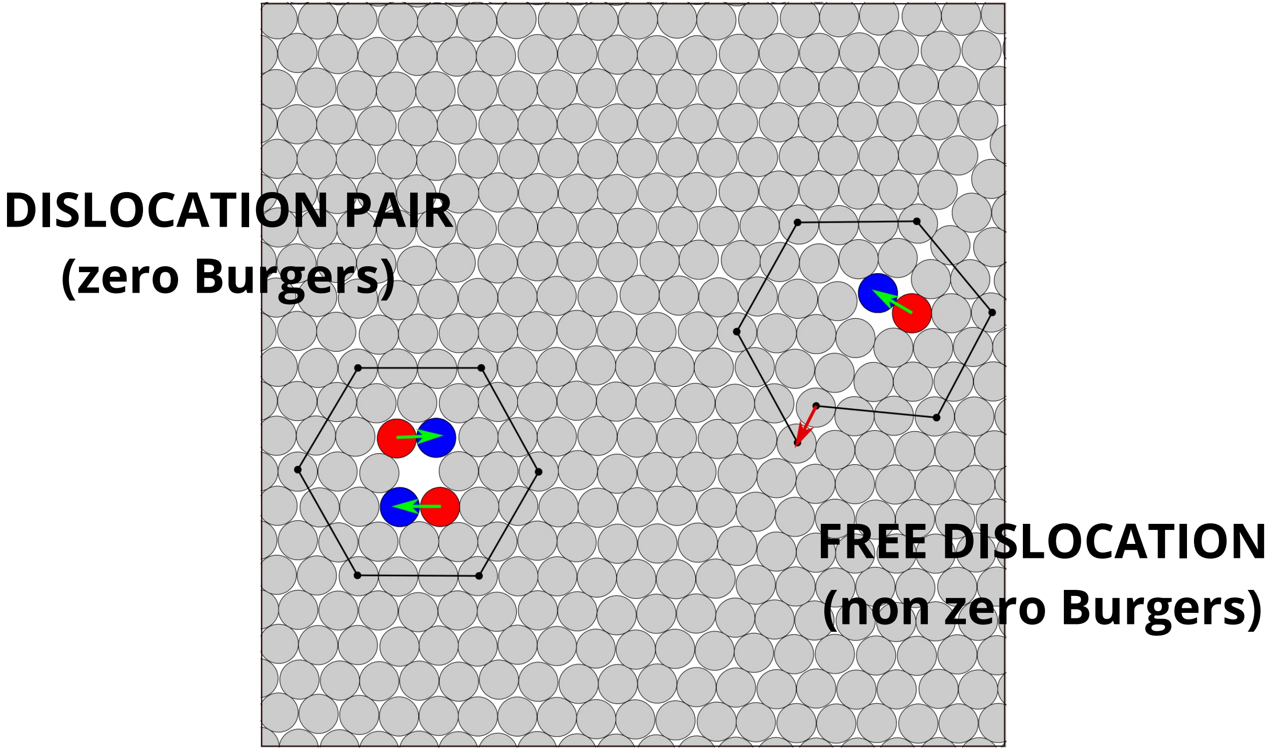
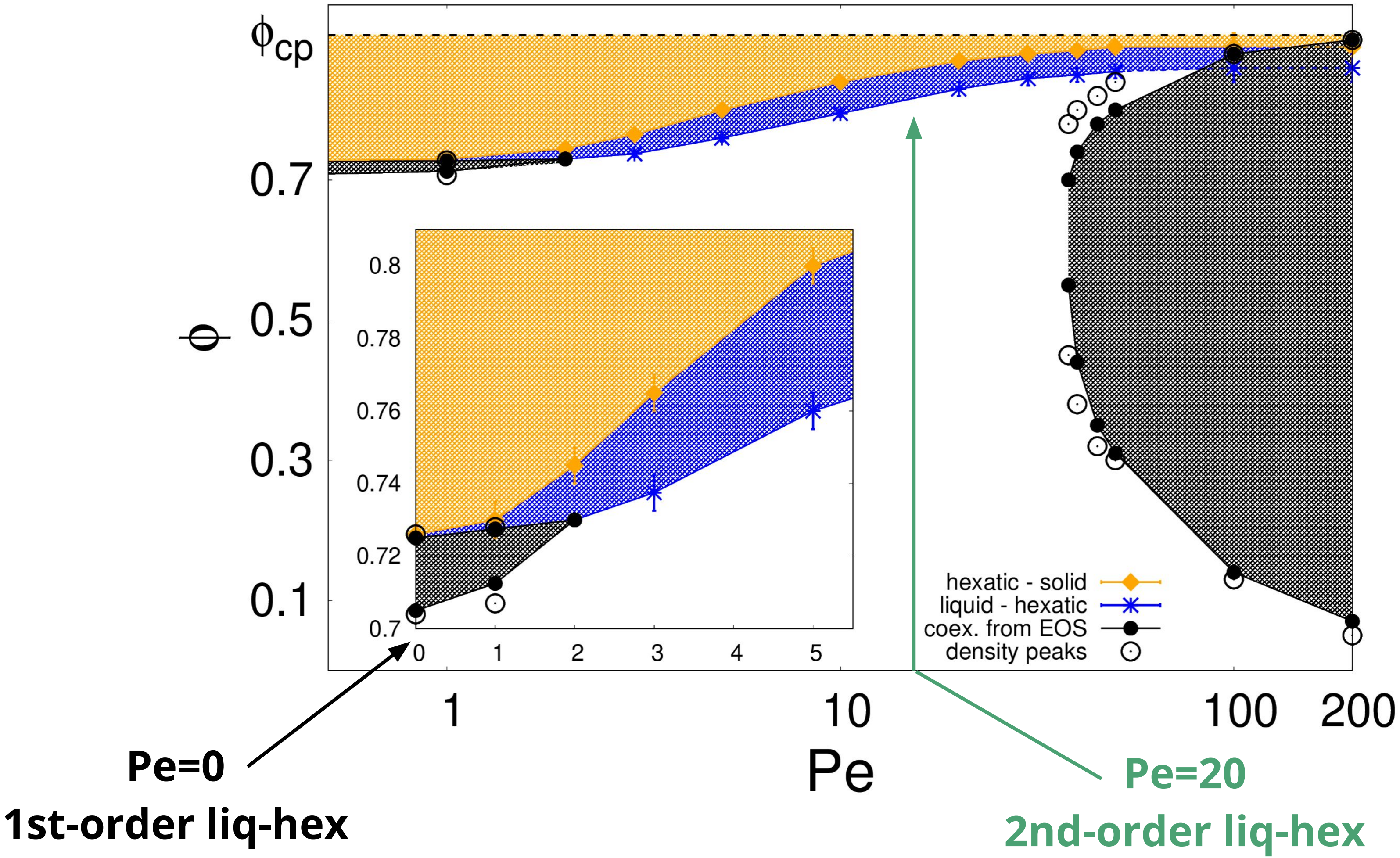
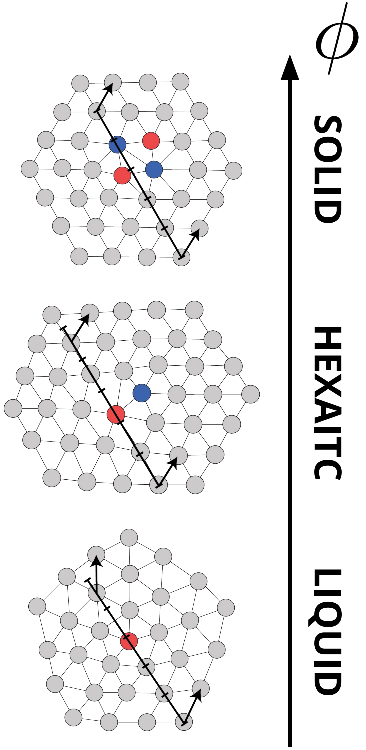


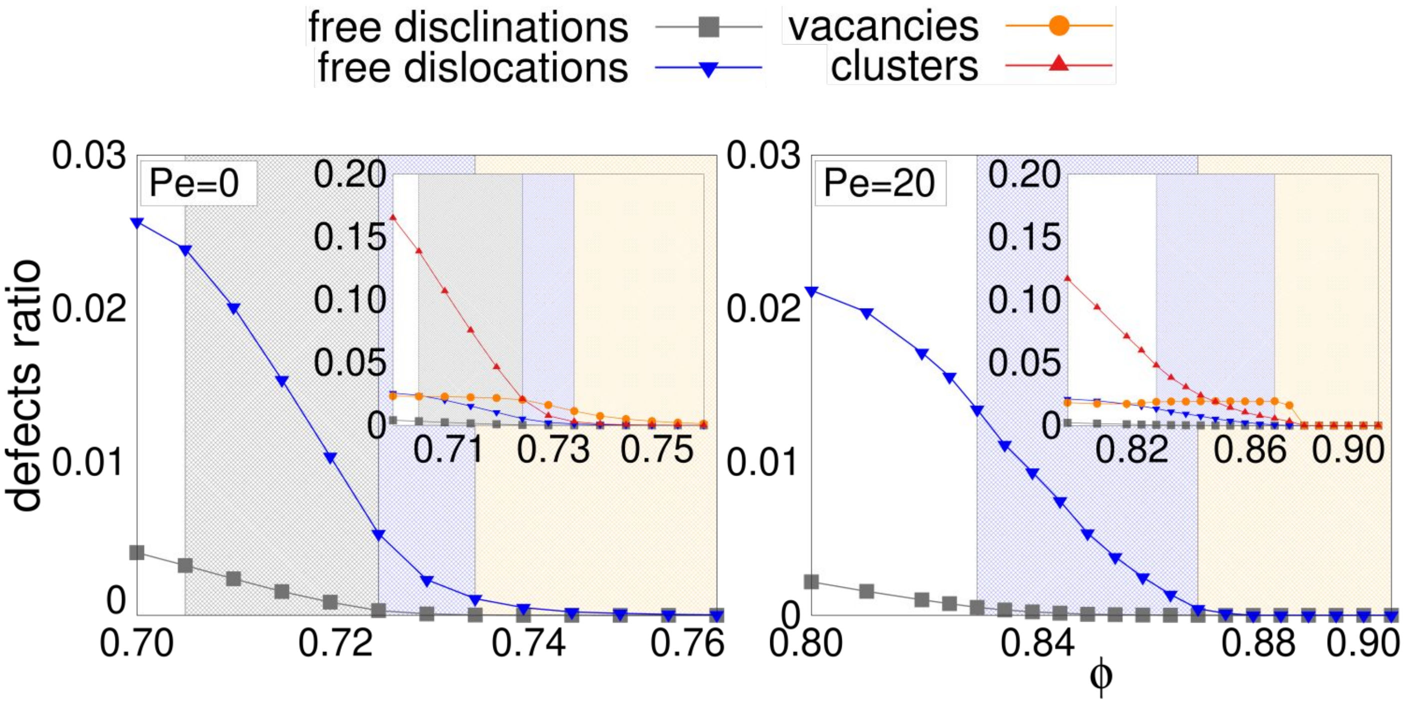




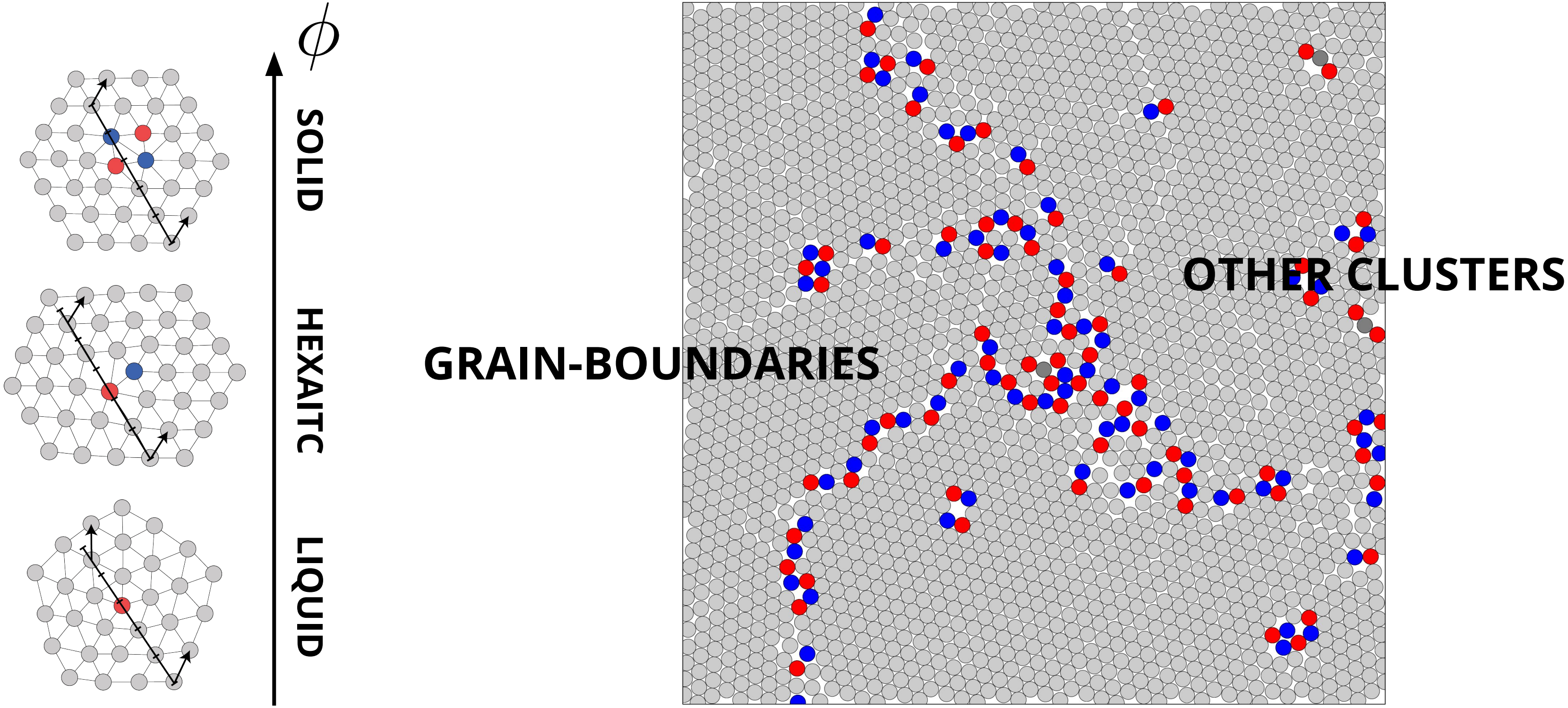
ϕ_{cp}
0.7
0.5
0.3
0.1
ϕ
1
10
100
200
Pe
0.8
0.78
0.76
0.74
0.72
0.7
0
1
2
3
4
5
hexatic - solid
liquid - hexatic
coex. from EOS
density peaks
Pe=0
1st-order liq-hex
Pe=20
2nd-order liq-hex

Equilibrium-like KTHN defects unbinding mechanism for the active system?

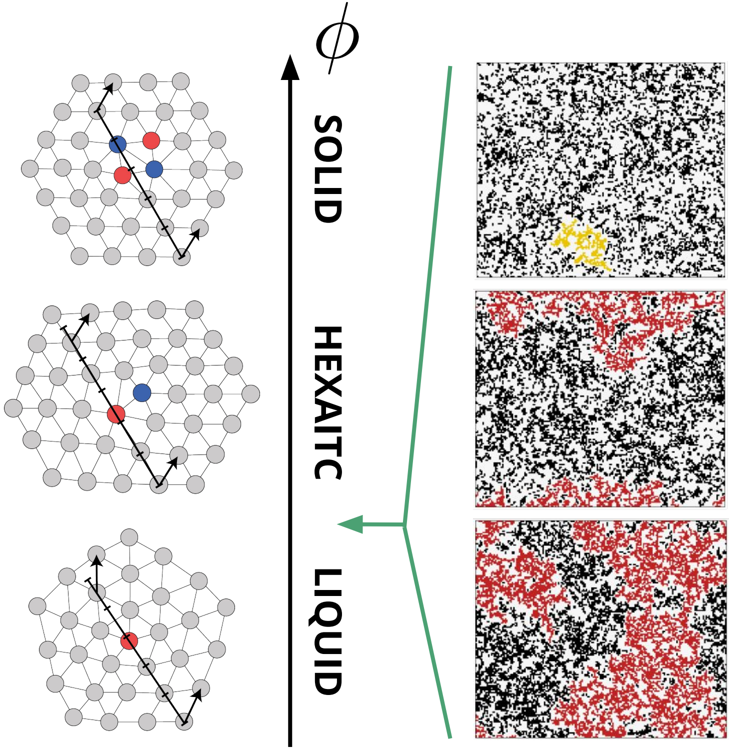


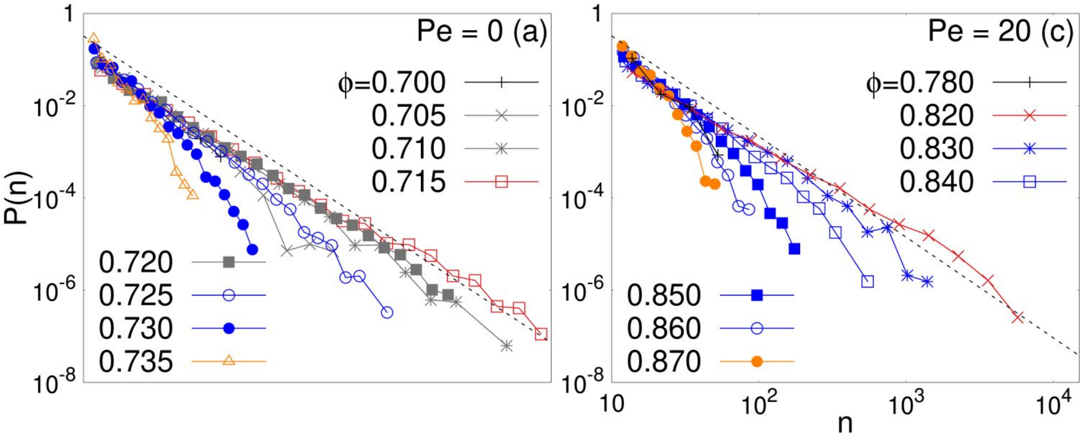


Clusters of defects



Clusters of defects - **PERCOLATION**





Publications

- L.F. Cugliandolo, PD, G. Gonnella, A. Suma, *“Phase Coexistence in Two-Dimensional Passive and Active Dumbbell Systems”*, Phys. Rev. Lett., 119, **Dec 2017**
- G. Negro, L.N. Carenza, PD, G. Gonnella, A. Lamura, *”Morphology and flow patterns in highly asymmetric active emulsions”,* Physica A: Statistical Mechanics and its Applications, 503, **Mar 2018**
- PD, D. Levis, A. Suma, L.F. Cugliandolo, G. Gonnella, I. Pagonabarraga, *“Full Phase Diagram of Active Brownian Disks: From Melting to Motility-Induced Phase Separation”*, Phys. Rev. Lett., 121, **Ago 2018**
- Petrelli, PD, L.F. Cugliandolo, G. Gonnella, A. Suma, *“Active dumbbells: dynamics and morphology in the coexisting region”*, Eur. Phys. J. E (2018) 41: 128, **Oct 2018**
- PD, Levis D.,Suma A., Cugliandolo L.F., Gonnella G., Pagonabarraga I., *“2D melting and motility induced phase separation inActive Brownian Hard Disks and Dumbbells”* J. Phys.: Conf. Ser.1163 012073, **2019**

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- L.F. Cugliandolo, PD, G. Gonnella, A. Suma, *"Phase Coexistence in Two-Dimensional Passive and Active Dumbbell Systems"*, Phys. Rev. Lett., 119, **Dec 2017**
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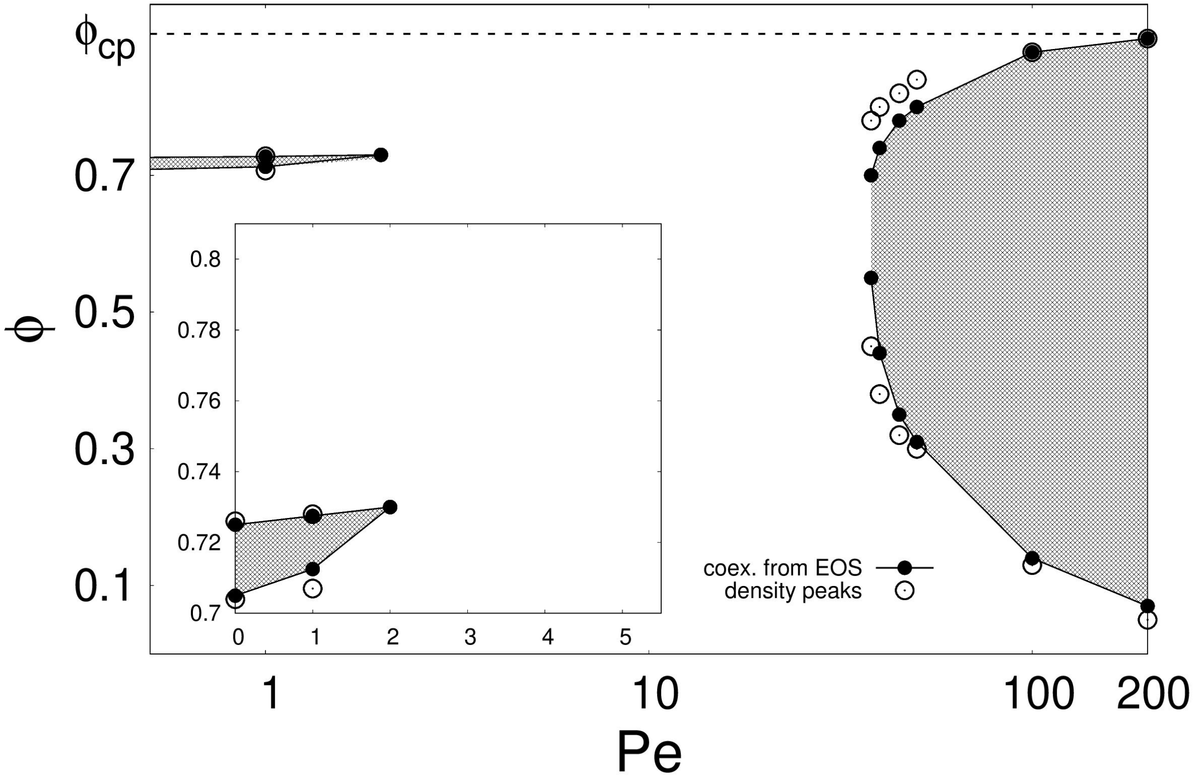
Thank you!

Thank you!

Phase diagram of active disks

Phase diagram for active disks

- Liquid-hexatic coexistence at low Pes
- MIPS at high Pes



DP, Levis D., Suma A., Cugliandolo L.F., Gonnella G., Pagonabarraga I., Phys. Rev. Lett., 121 098003 (2018)

Phase diagram for active disks

- Local density pdfs
- Local hexatic parameter

DP, Levis D., Suma A., Cugliandolo L.F., Gonnella G., Pagonabarraga I., Phys. Rev. Lett., 121 098003 (2018)

Phase diagram for active disks

- Local density pdfs
- Local hexatic parameter
- **Equation of state**

$$P = \frac{N k_B T}{V} + \frac{1}{4V} \sum_{i,j} \sum_{u_x, u_y \in \mathbb{Z}} \langle \mathbf{f}_{ij} \cdot (\mathbf{r}_i - \mathbf{r}_j - \mathbf{R}_\mathbf{u}) \rangle + \frac{F_{act}}{2V} \sum_i \langle \mathbf{n}_i \cdot \mathbf{r}_i \rangle$$

DP, Levis D., Suma A., Cugliandolo L.F., Gonnella G., Pagonabarraga I., Phys. Rev. Lett., 121 098003 (2018)

Phase diagram for active disks

- Local density pdfs
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- **Equation of state**

$$P = \boxed{\frac{N k_B T}{V}} + \frac{1}{4V} \sum_{i,j} \sum_{u_x, u_y \in \mathbb{Z}} \langle \mathbf{f}_{ij} \cdot (\mathbf{r}_i - \mathbf{r}_j - \mathbf{R}_{\mathbf{u}}) \rangle + \frac{F_{act}}{2V} \sum_i \langle \mathbf{n}_i \cdot \mathbf{r}_i \rangle$$

- **Ideal gas**

DP, Levis D., Suma A., Cugliandolo L.F., Gonnella G., Pagonabarraga I., Phys. Rev. Lett., 121 098003 (2018)

Phase diagram for active disks

- Local density pdfs
- Local hexatic parameter
- **Equation of state**

$$P = \frac{Nk_BT}{V} + \boxed{\frac{1}{4V}\sum_{i,j}\sum_{u_x,u_y\in\mathbb{Z}}\langle \mathbf{f}_{ij}\cdot(\mathbf{r}_i-\mathbf{r}_j-\mathbf{R}_\mathbf{u})\rangle} + \frac{F_{act}}{2V}\sum_i \langle \mathbf{n}_i\cdot\mathbf{r}_i\rangle$$

- Ideal gas
- **internal virial (interactions)**

DP, Levis D., Suma A., Cugliandolo L.F., Gonnella G., Pagonabarraga I., Phys. Rev. Lett., 121 098003 (2018)

Phase diagram for active disks

- Local density pdfs
- Local hexatic parameter
- **Equation of state**

$$P = \frac{N k_B T}{V} + \frac{1}{4V} \sum_{i,j} \sum_{u_x, u_y \in \mathbb{Z}} \langle \mathbf{f}_{ij} \cdot (\mathbf{r}_i - \mathbf{r}_j - \mathbf{R}_{\mathbf{u}}) \rangle + \boxed{\frac{F_{act}}{2V} \sum_i \langle \mathbf{n}_i \cdot \mathbf{r}_i \rangle}$$

- Ideal gas
- internal virial (interactions)
- **active non-conservative virial (swim pressure)**

DP, Levis D., Suma A., Cugliandolo L.F., Gonnella G., Pagonabarraga I., Phys. Rev. Lett., 121 098003 (2018)

Phase diagram for active disks

- Local density pdfs
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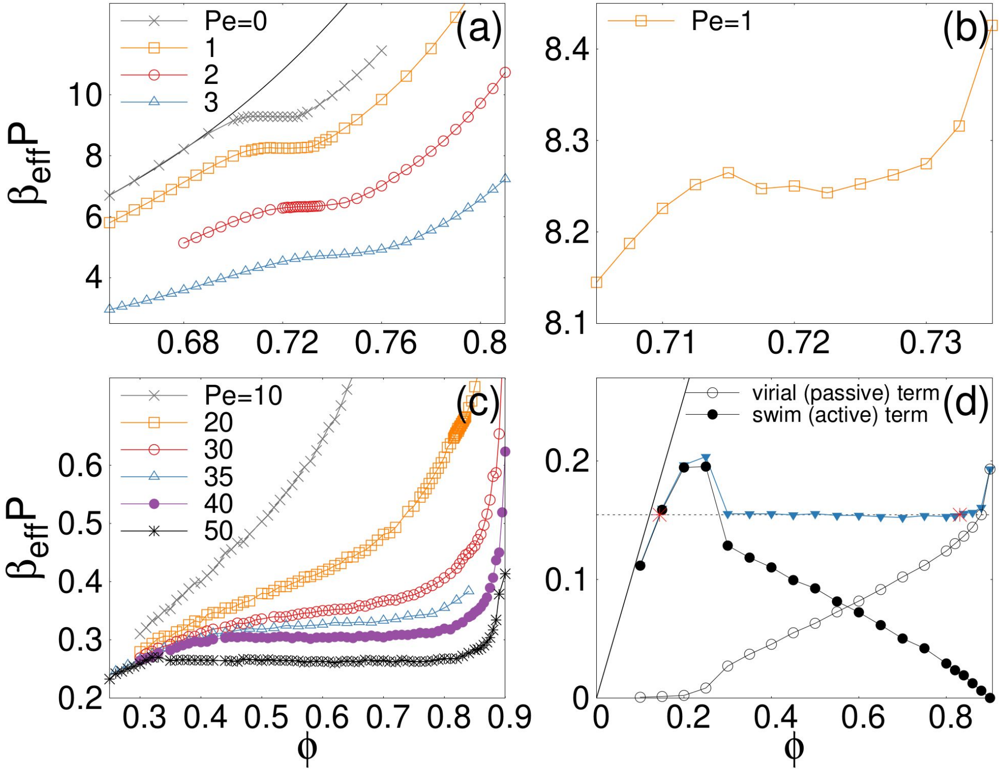
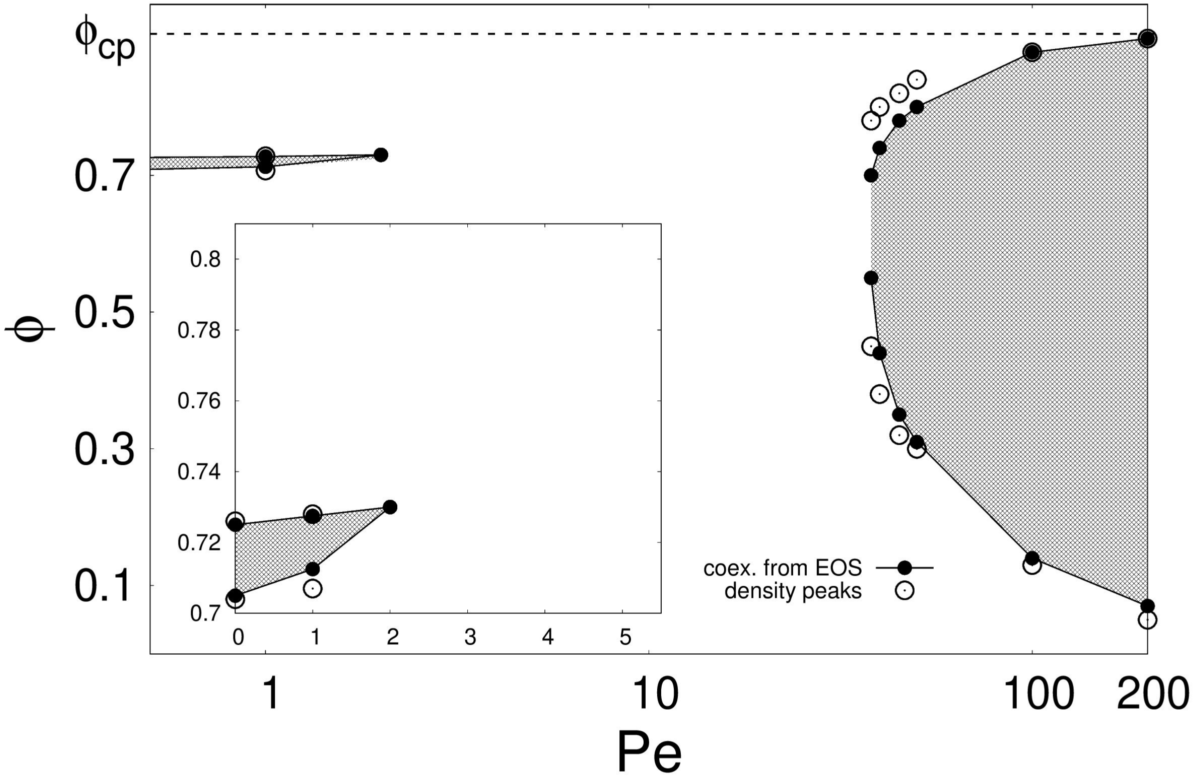
- **Equation of state**



DP, Levis D., Suma A., Cugliandolo L.F., Gonnella G., Pagonabarraga I., Phys. Rev. Lett., 121 098003 (2018)

Phase diagram for active disks

- Liquid-hexatic coexistence at low Pes
- MIPS at high Pes
- **No coexistence in the middle !!**



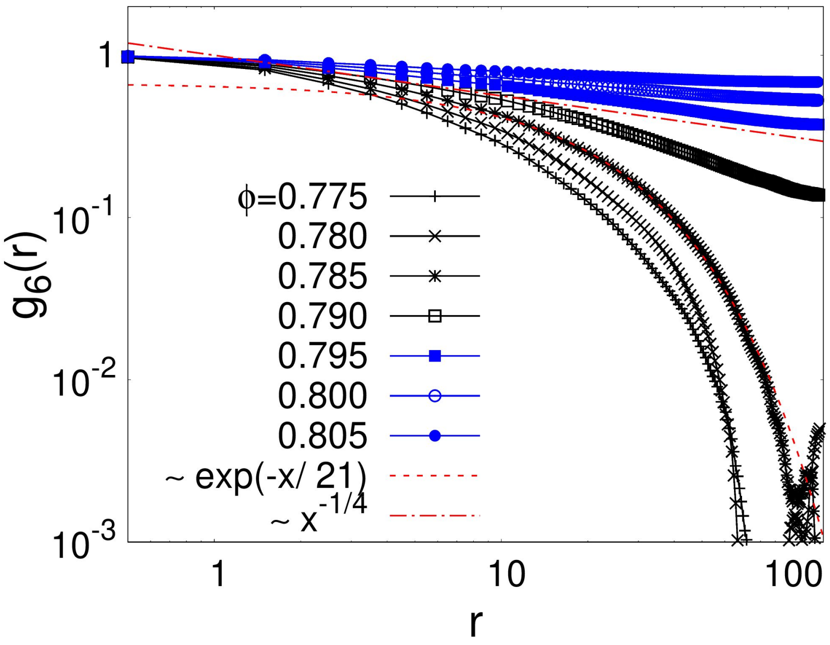
DP, Levis D., Suma A., Cugliandolo L.F., Gonnella G., Pagonabarraga I., Phys. Rev. Lett., 121 098003 (2018)

Phase diagram for active disks

- Spatial correlations of local hexatic

$$\psi_{6i} = \frac{1}{N_i}\sum_{j=1}^{N_i} e^{\mathrm{i}6\theta_{ij}}$$

$$g_6(r) = \frac{\langle \psi_{6i}\psi_{6j}^{*}\rangle_{r_{ij}=r}}{\langle |\psi_{6i}|^2\rangle}$$

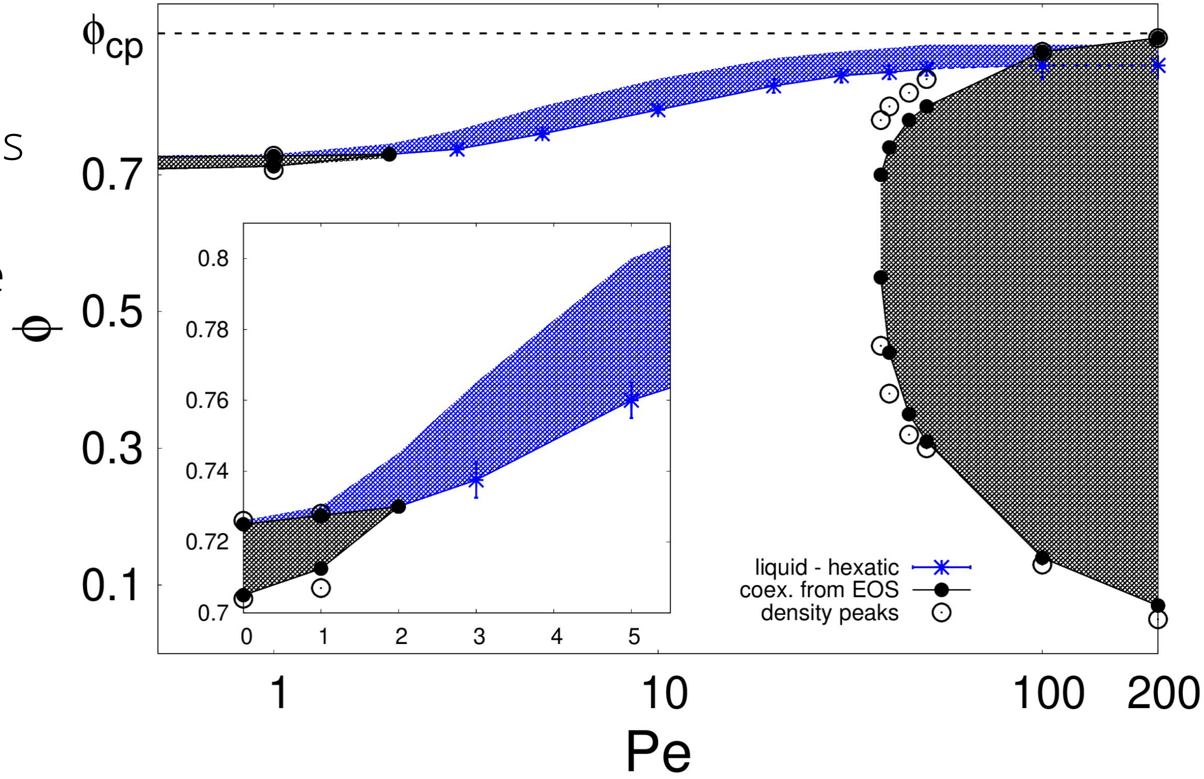


DP, Levis D., Suma A., Cugliandolo L.F., Gonnella G., Pagonabarraga I., Phys. Rev. Lett., 121 098003 (2018)

Phase diagram for active disks

- Liquid-hexatic coexistence at low Pes
- MIPS at high Pes
- No coexistence in the middle

- **Liquid-hexatic transition**



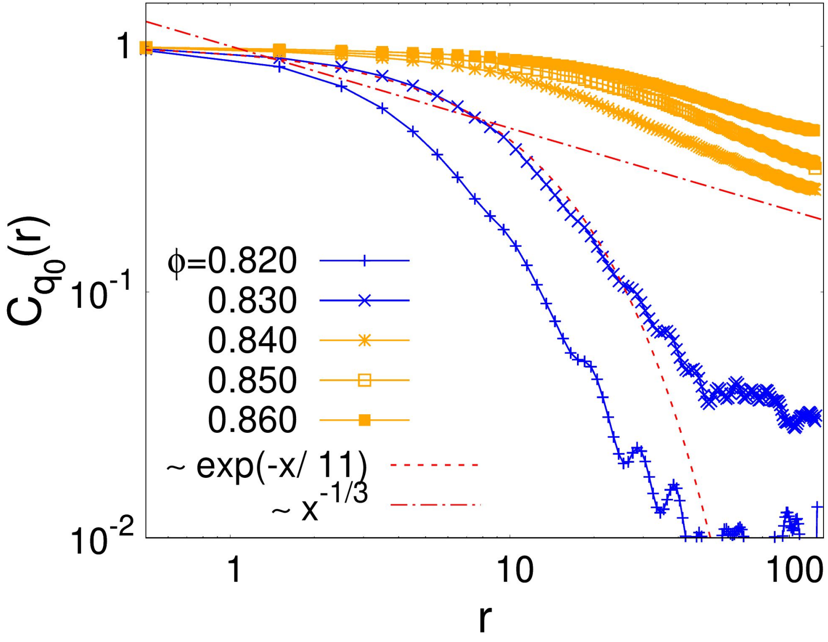
DP, Levis D., Suma A., Cugliandolo L.F., Gonnella G., Pagonabarraga I., Phys. Rev. Lett., 121 098003 (2018)

Phase diagram for active disks

- Spatial correlations of disks positions

$$C_{\mathbf{q}_0}(r) = \langle e^{\mathbf{i}\mathbf{q}_0\cdot(\mathbf{r}_i-\mathbf{r}_j)}\rangle$$

$\mathbf{q}_0$ maximum diffraction peak



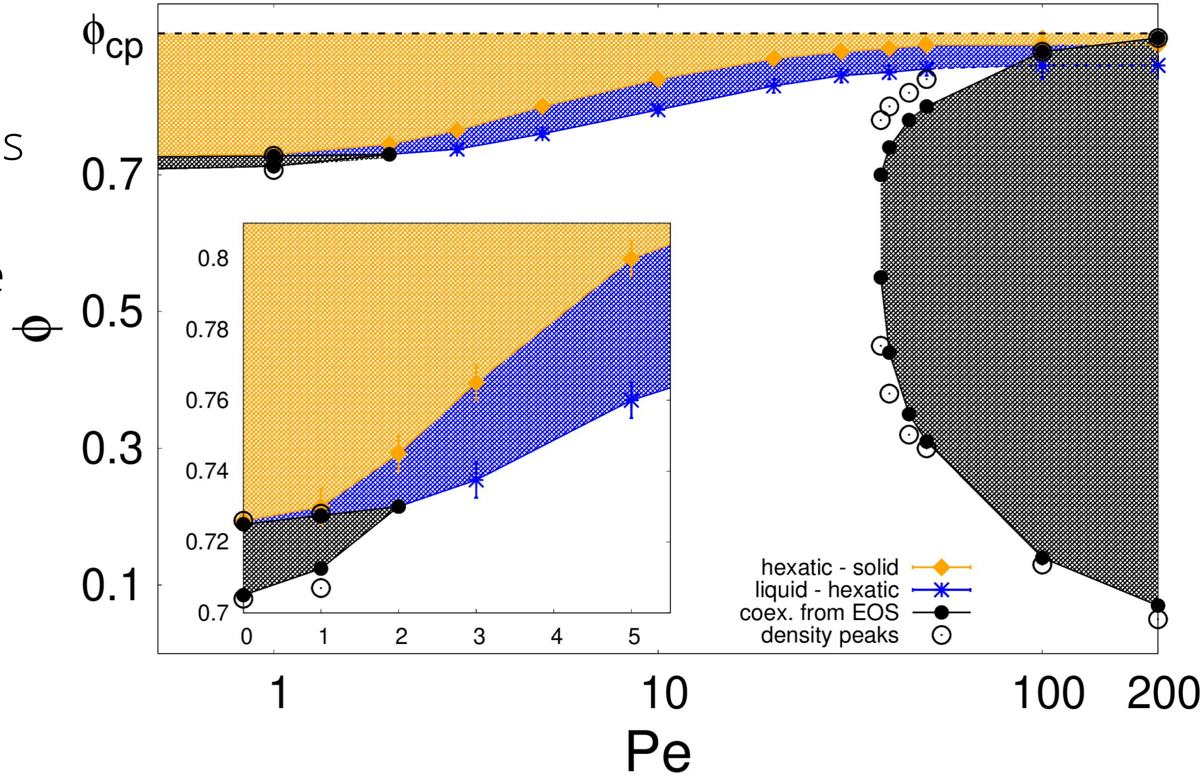
DP, Levis D., Suma A., Cugliandolo L.F., Gonnella G., Pagonabarraga I., Phys. Rev. Lett., 121 098003 (2018)

Phase diagram for active disks

- Liquid-hexatic coexistence at low Pes
- MIPS at high Pes
- No coexistence in the middle

- Liquid-hexatic transition

- **Hexatic-crystal transition**



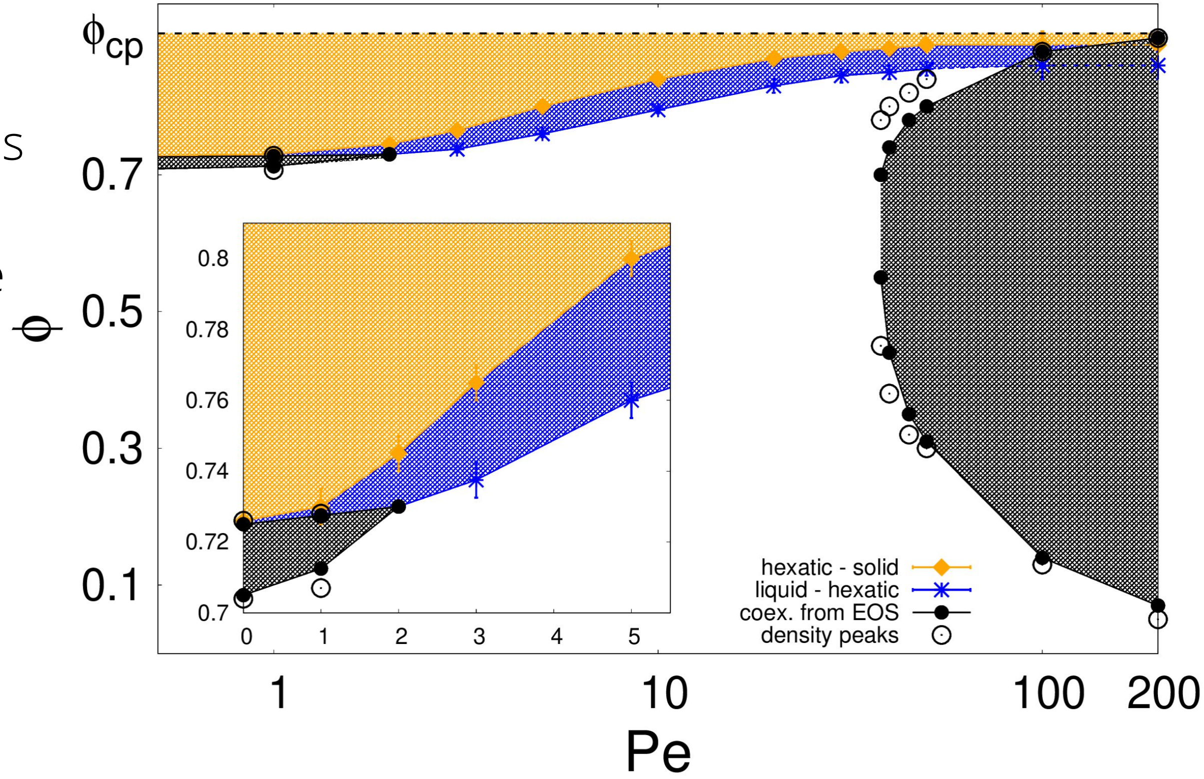
DP, Levis D., Suma A., Cugliandolo L.F., Gonnella G., Pagonabarraga I., Phys. Rev. Lett., 121 098003 (2018)

Phase diagram for active disks

- Liquid-hexatic coexistence at low Pes
- MIPS at high Pes
- No coexistence in the middle

- Liquid-hexatic transition

- Hexatic-crystal transition



DP, Levis D., Suma A., Cugliandolo L.F., Gonnella G., Pagonabarraga I., Phys. Rev. Lett., 121 098003 (2018)