# Active brownian particles and topological phase transitions

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Work in collaboration with
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Isabella Petrelli (UniBa)

# Summary

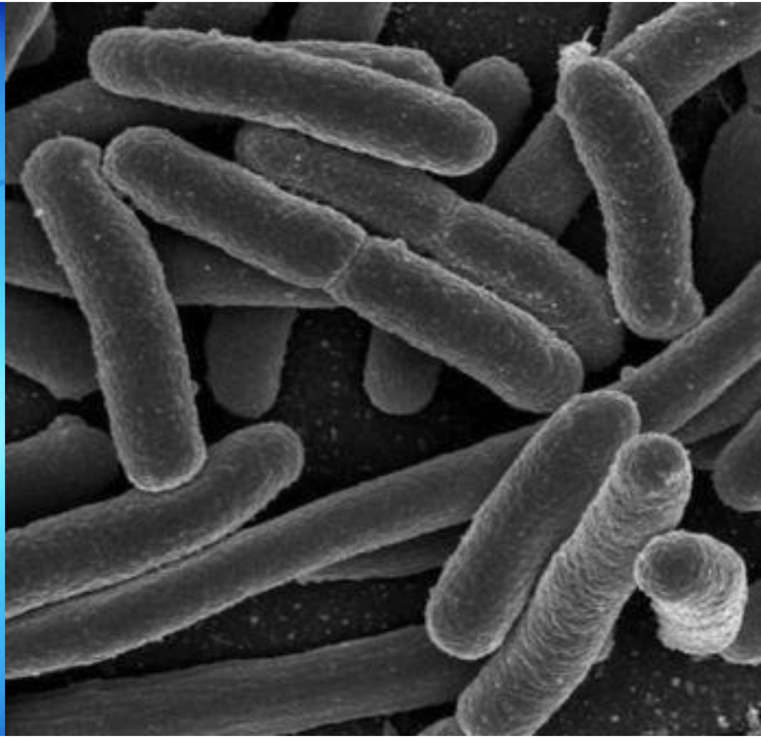
- Active matter. Aggregation phenomena out of thermal equilibrium
- Active brownian particles
- Melting in 2D. Phase transitions in low-dimensional systems and KTHNY theory of topological phase transitions
- Phase diagram of active disks and dumbbells
- Conclusions and outlooks

# Active matter

# Active systems in nature

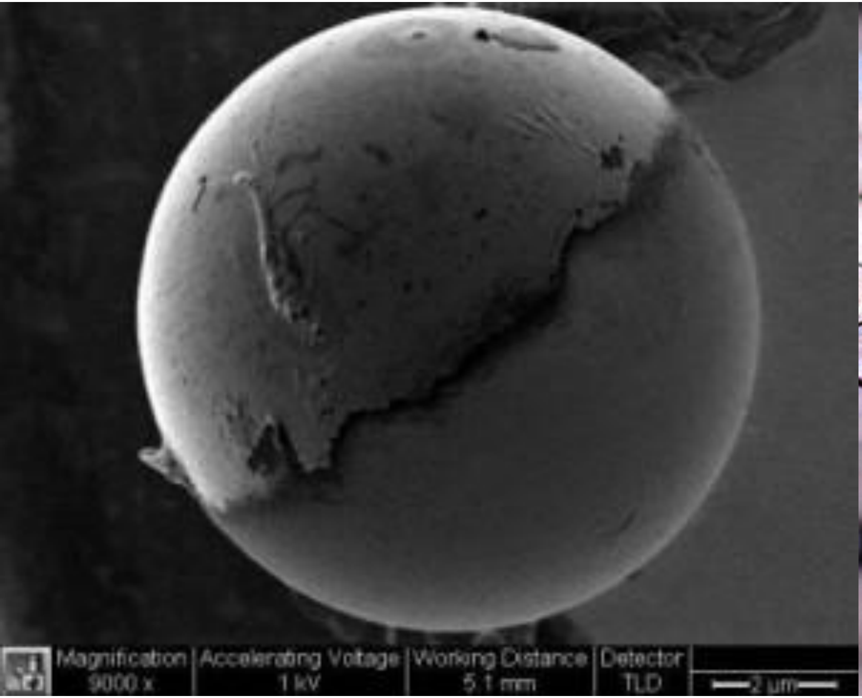
**Birds flocking**

**Fish schools**



**Bacteria**

# In experiments




**Janus particles**

**Buttinoni I., *et al.,*** Phys.Rev.Lett., 110 238301, (2013)
**Ginot F., et al.**, Phys. Rev. X, 5 011004, (2015)

**Polar disks**

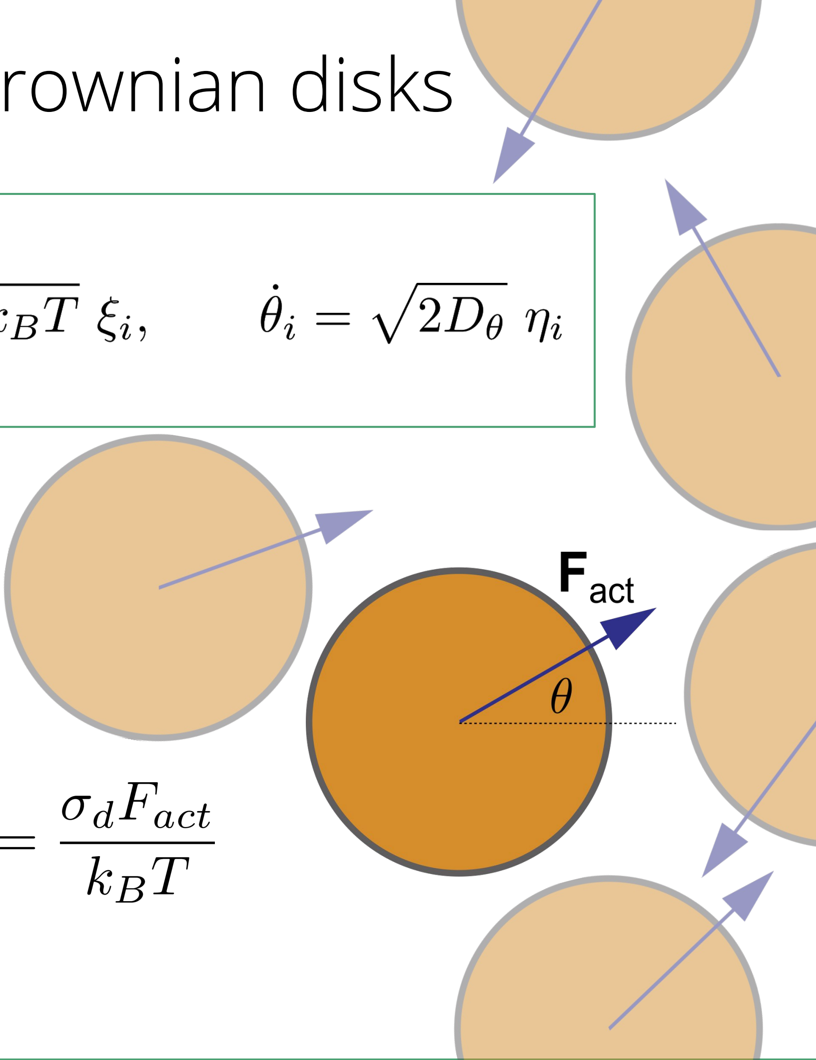
**Dauchot O., *et al.*** Phys. Rev. Lett., 105 098001, (2010)

# Active brownian hard disks

# The simplest model of active brownian disks

$$\mathbf{n}_i = (\cos\theta_i(t), \sin\theta_i(t))$$

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



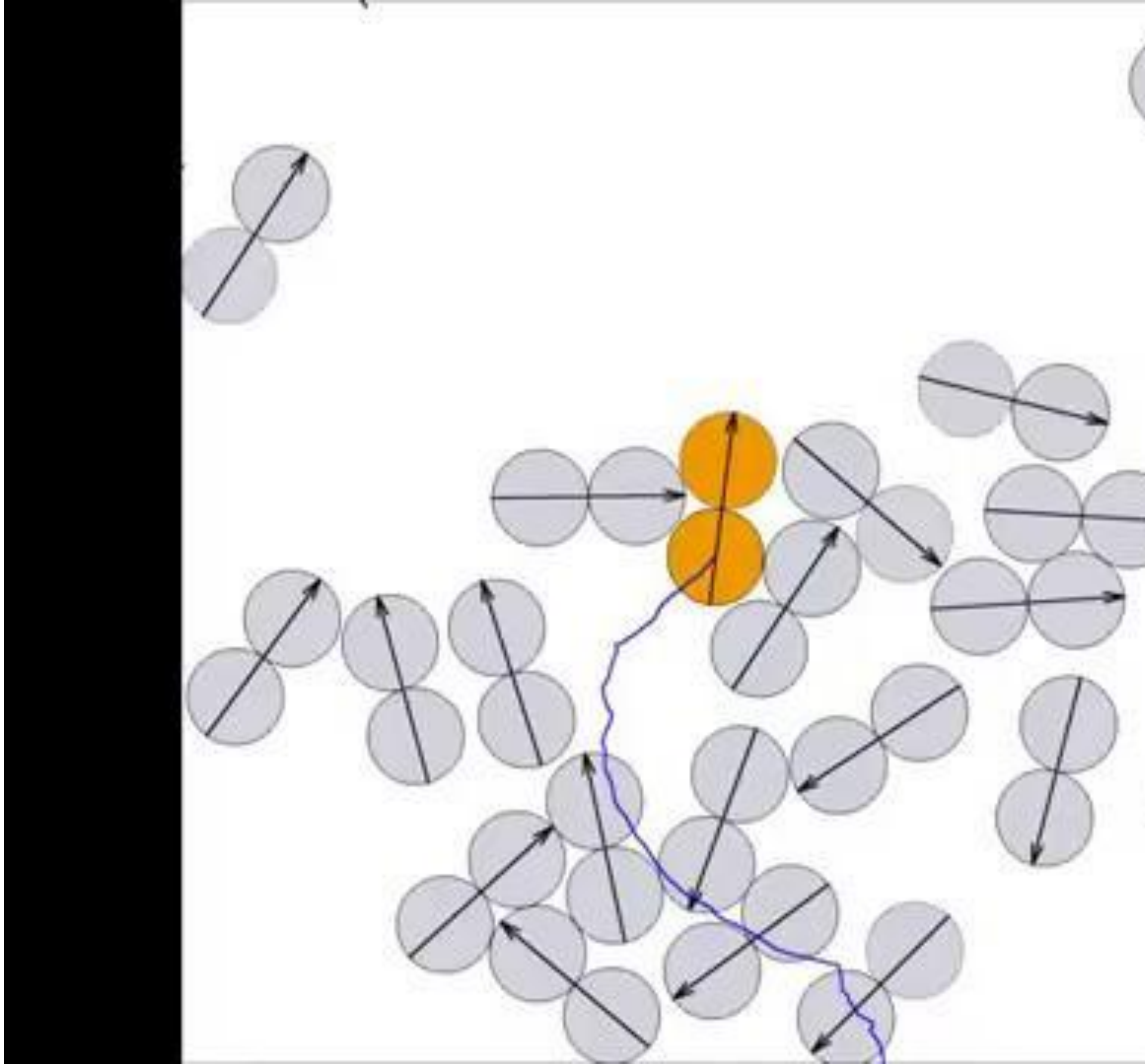

- Surface fraction: $\phi = N\dfrac{\pi\sigma_d^2}{4S}$
- Advective: $Lv_{act} = \sigma_d \dfrac{F_{act}}{\gamma}$
- Diffusive: $D = \dfrac{k_B T}{\gamma}$

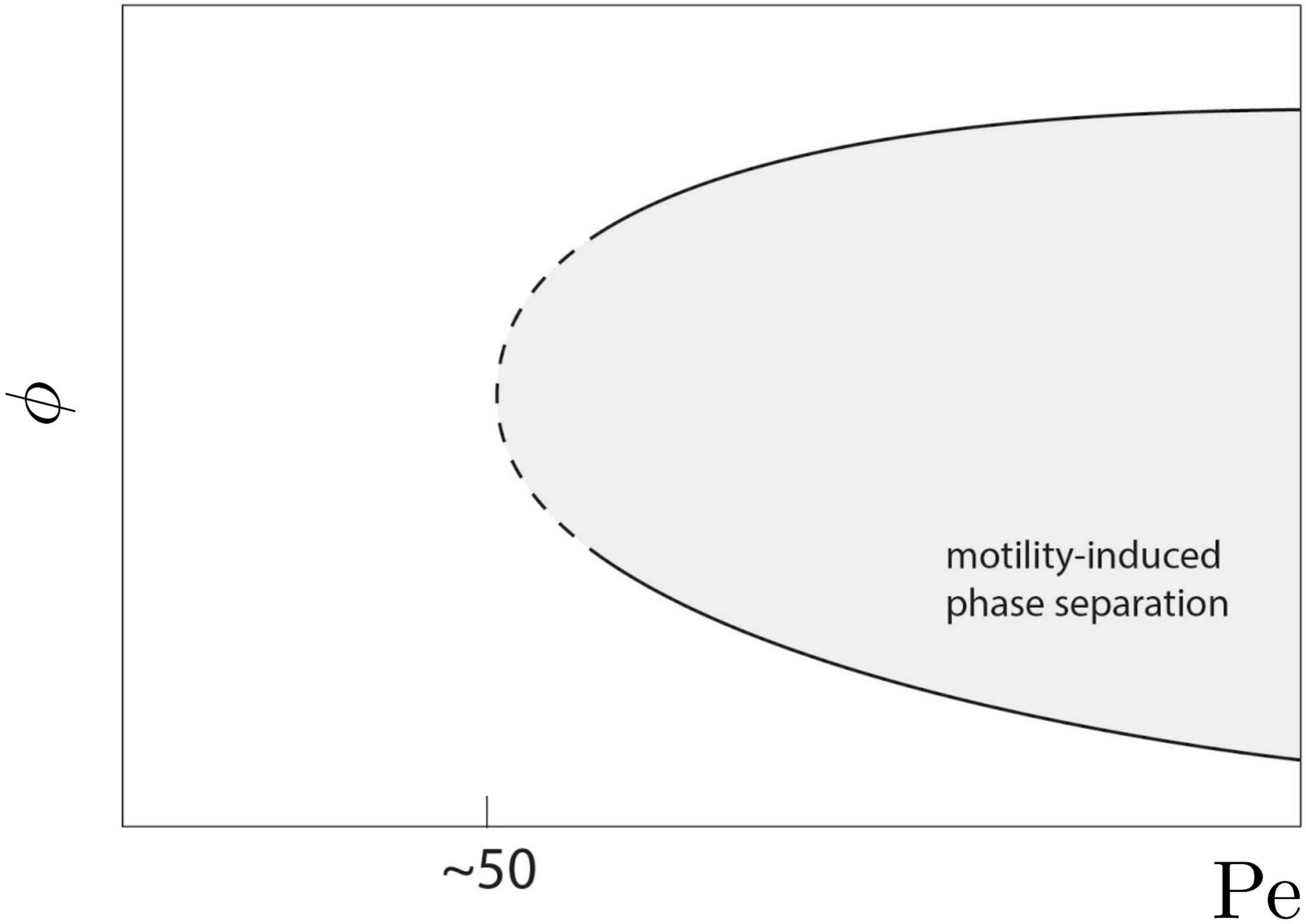
Péclet number

$$\mathrm{Pe} = \frac{Lv_{act}}{D} = \frac{\sigma_d F_{act}}{k_B T}$$

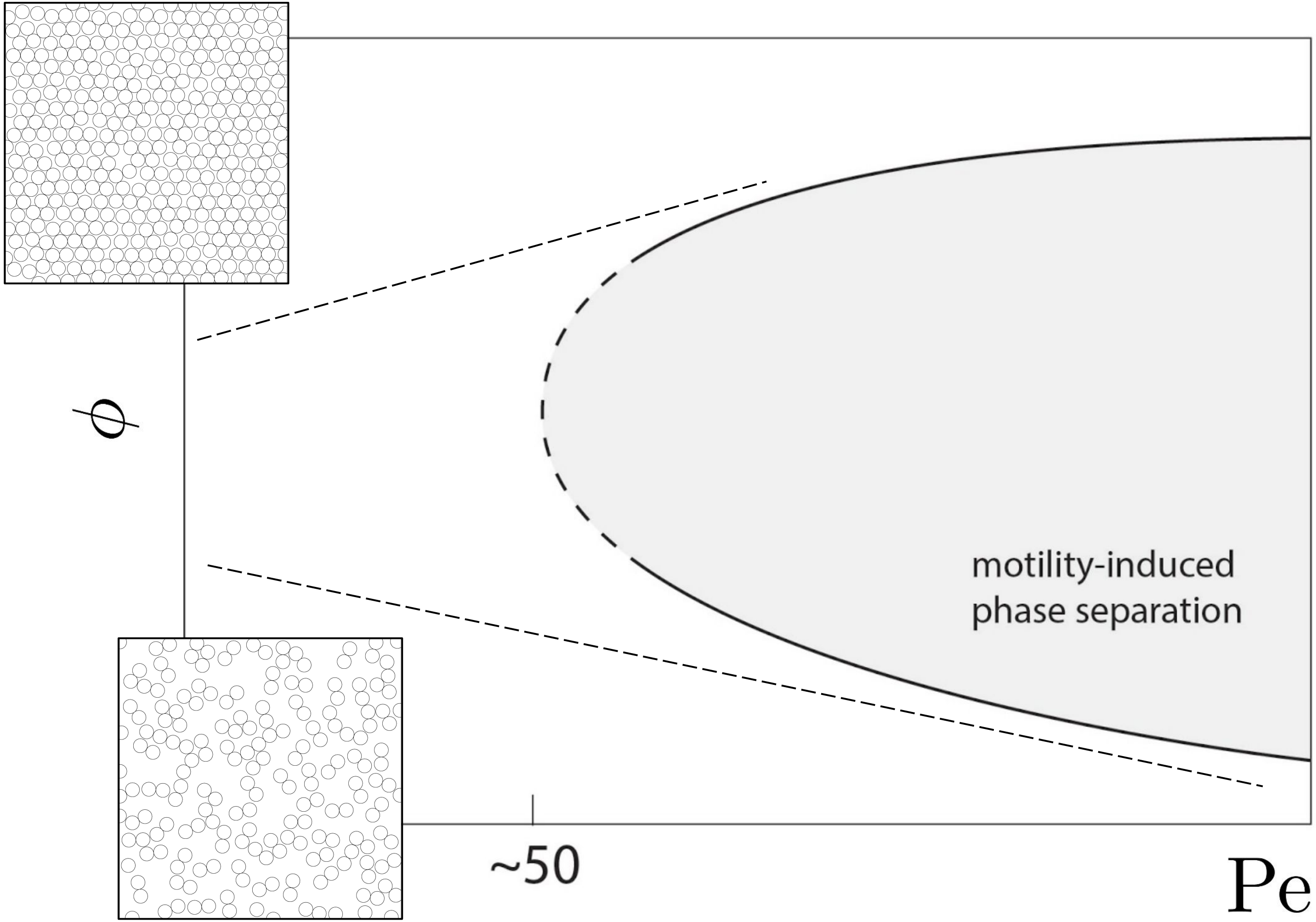
# **P**ersistent BM and aggregation

- Self-propelled particles accumulate where they move more slowly.
- They may also slow down at high density.
- Positive feedback which can lead to motility-induced phase separation (MIPS) between dense (ordered) and dilute (fluid/gas) phases

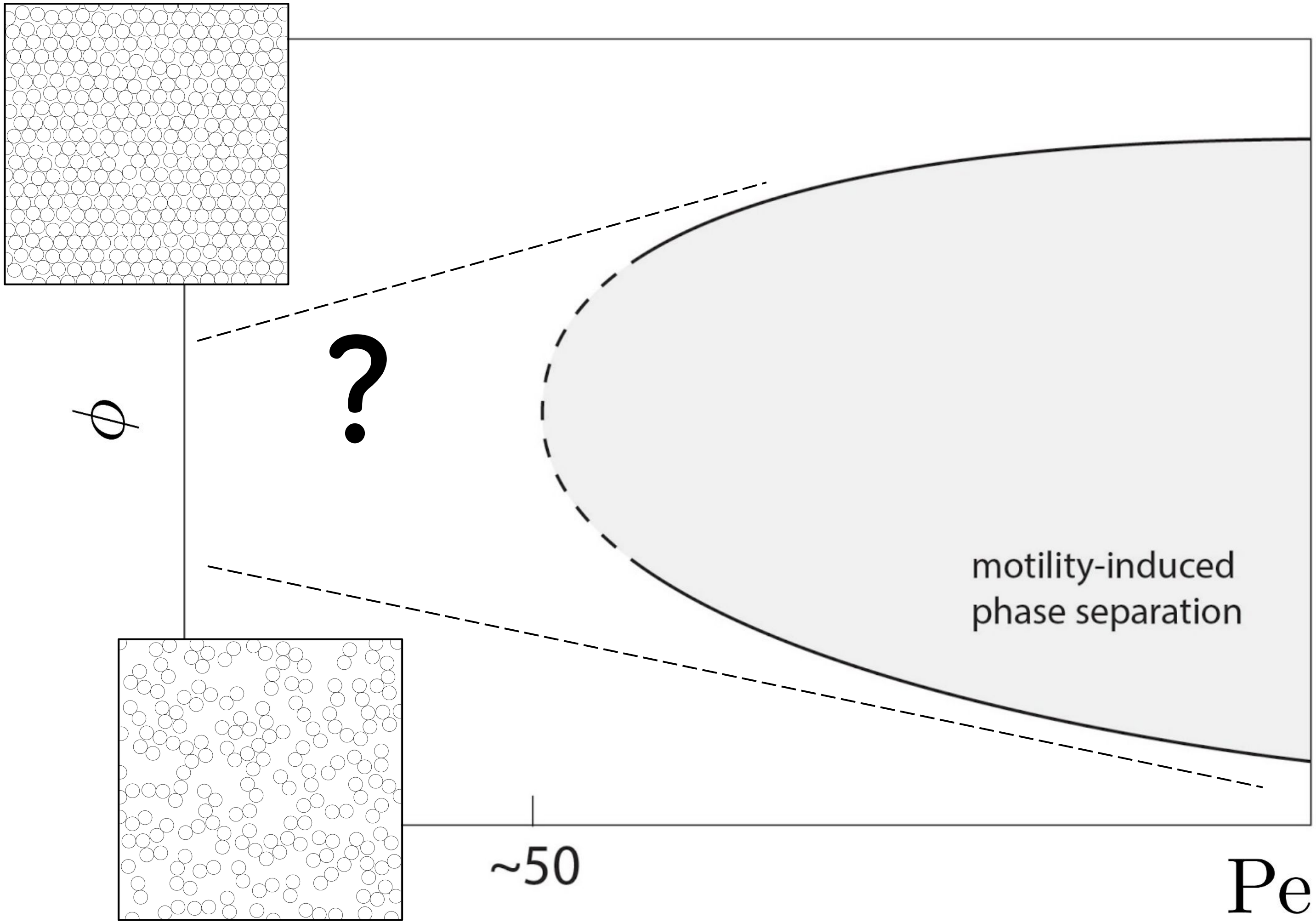




$\phi$
motility-induced
phase separation
~50
Pe



φ
motility-induced
phase separation
~50
Pe



?
$\phi$
motility-induced
phase separation
~50
Pe

# Phase transitions in 2D

## KTHN melting transitions

# **N**o crystals in 2D

Order-disorder transitions have long been known to have different properties at different space dimensionality (Peierls **1934**, Landau **1937**).

# **N**o crystals in 2D

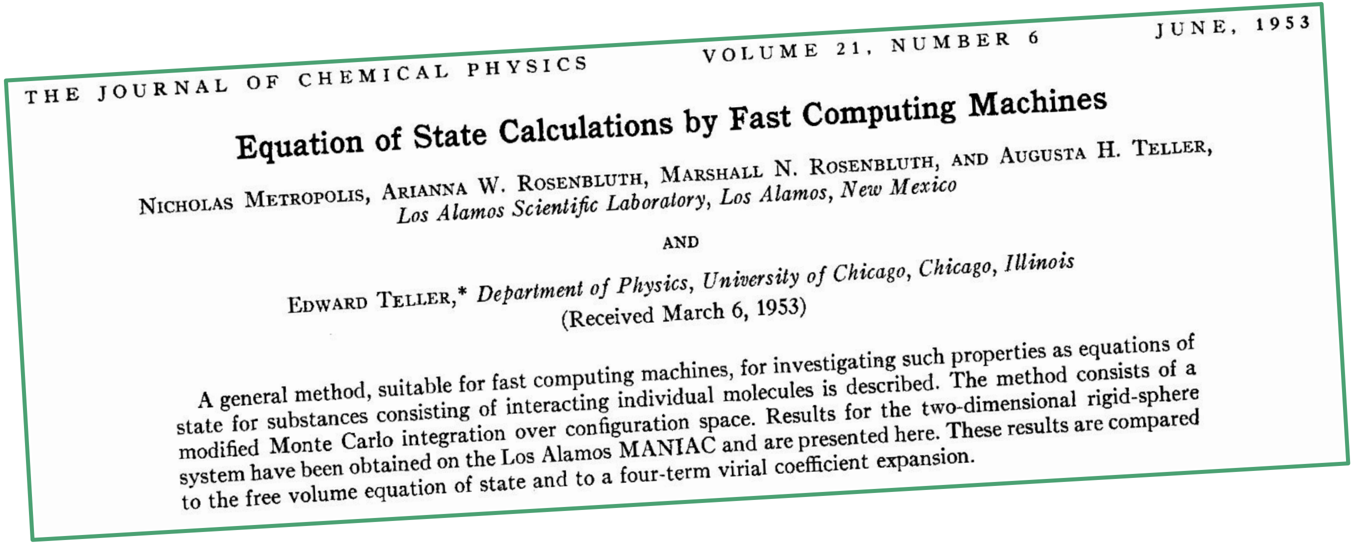
Order-disorder transitions have long been known to have different properties at different space dimensionality (Peierls **1934**, Landau **1937**).

## Mermin-Wagner theorem (**1966**)

Continuous symmetries cannot be spontaneously broken at finite temperatures with sufficiently short-range interactions in dimensions $\mathrm{d} \leqslant 2$.

**D**oes an equilibrium ordered phase exist for 2d system with short-range interactions?

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



THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

**Equation of State Calculations by Fast Computing Machines**

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
*Los Alamos Scientific Laboratory, Los Alamos, New Mexico*

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

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

### VI. CONCLUSION

The method of Monte Carlo integrations over configuration space seems to be a feasible approach to statistical mechanical problems which are as yet not analytically soluble. At least for a single-phase system a sample of several hundred particles seems sufficient. In the case of two-dimensional rigid spheres, runs made with 56 particles and with 224 particles agreed within statistical error. For a computing time of a few hours with presently available electronic computers, it seems possible to obtain the pressure for a given volume and temperature to an accuracy of a few percent.

In the case of two-dimensional rigid spheres our results are in agreement with the free volume approximation for $A/A_0<1.8$ and with a five-term virial expansion for $A/A_0>2.5$. There is no indication of a phase transition.

Work is now in progress for a system of particles with Lennard-Jones type interactions and for three-dimensional rigid spheres.

VOLUME 21, NUMBER 6 JUNE, 1953

; by Fast Computing Machines

MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
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VI. CONCLUSION

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statistical mechanical p...
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a sample of several hun...
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VOLUME 21, NUMBER 6 JUNE, 1953

...Machines

PHYSICAL REVIEW VOLUME 127, NUMBER 2 JULY 15, 1962

## Phase Transition in Elastic Disks*

B. J. ALDER AND T. E. WAINWRIGHT
*University of California, Lawrence Radiation Laboratory, Livermore, California*

(Received October 30, 1961)

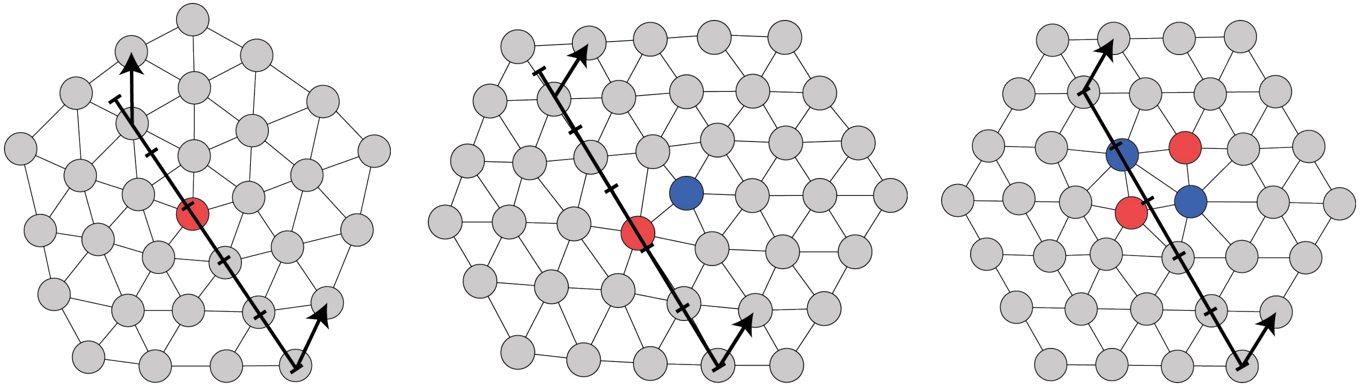
The study of a two-dimensional system consisting of 870 hard-disk particles in the phase-transition region has shown that the isotherm has a van der Waals-like loop. The density change across the transition is about 4% and the corresponding entropy change is small.

# **P**hase transitions in 2d short-range interacting particles: Halperin-Nelson

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

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

$\longrightarrow \phi$



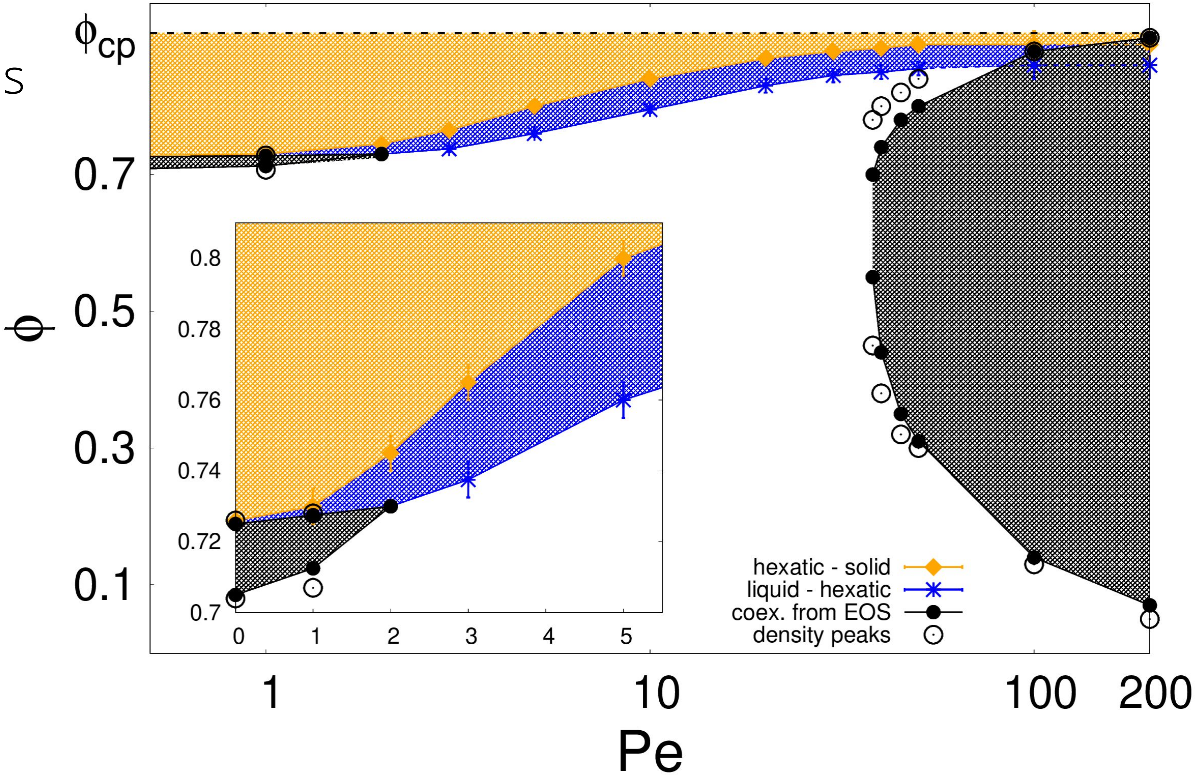
# Phase diagram of hard disks

# Phase diagram for active disks

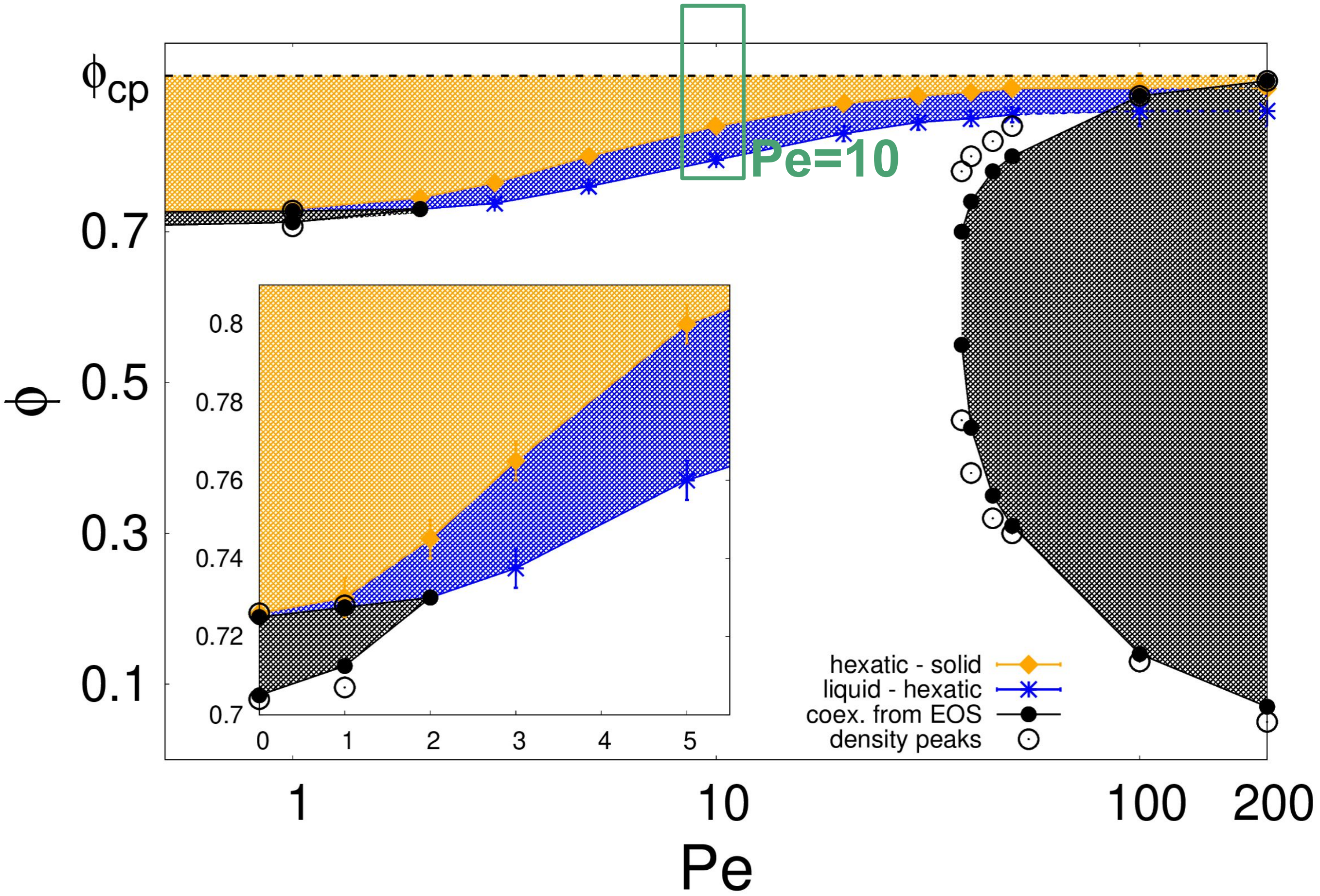
- Coexistence at low Pes
- MIPS at high Pes

- Liquid-hexatic transition

- Hexatic-crystal transition




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



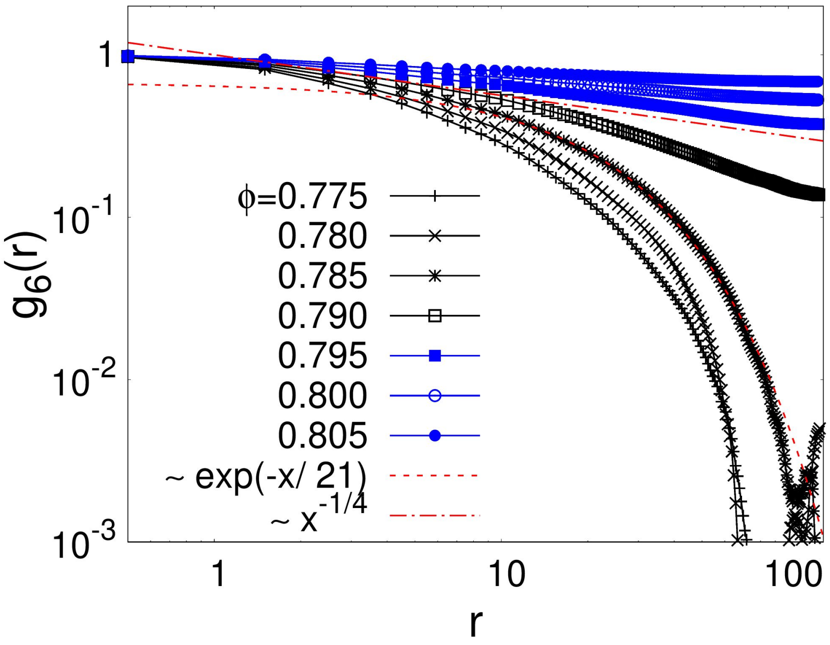
Pe=10
ϕcp
0.7
0.5
0.3
0.1
ϕ
1
10
100
200
Pe
0.8
0.78
0.76
0.74
0.72
0.7
0
1
2
3
4
5
hexatic - solid
liquid - hexatic
coex. from EOS
density peaks

# Liquid-hexatic transition

- Spatial correlations of local hexatic

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

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

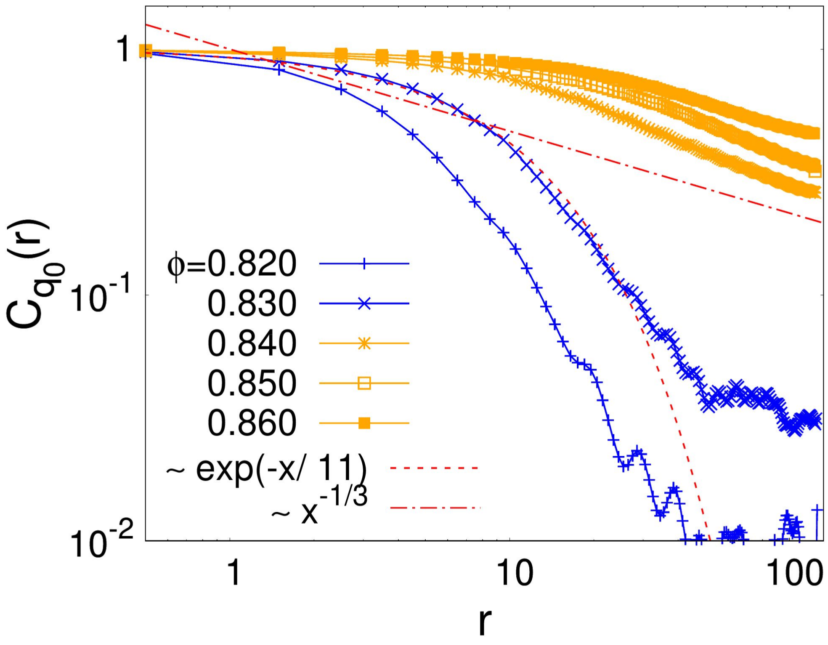


# **H**exatic-solid transition

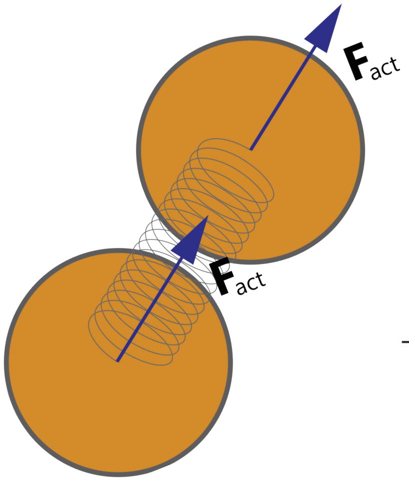
- Spatial correlations of disks positions

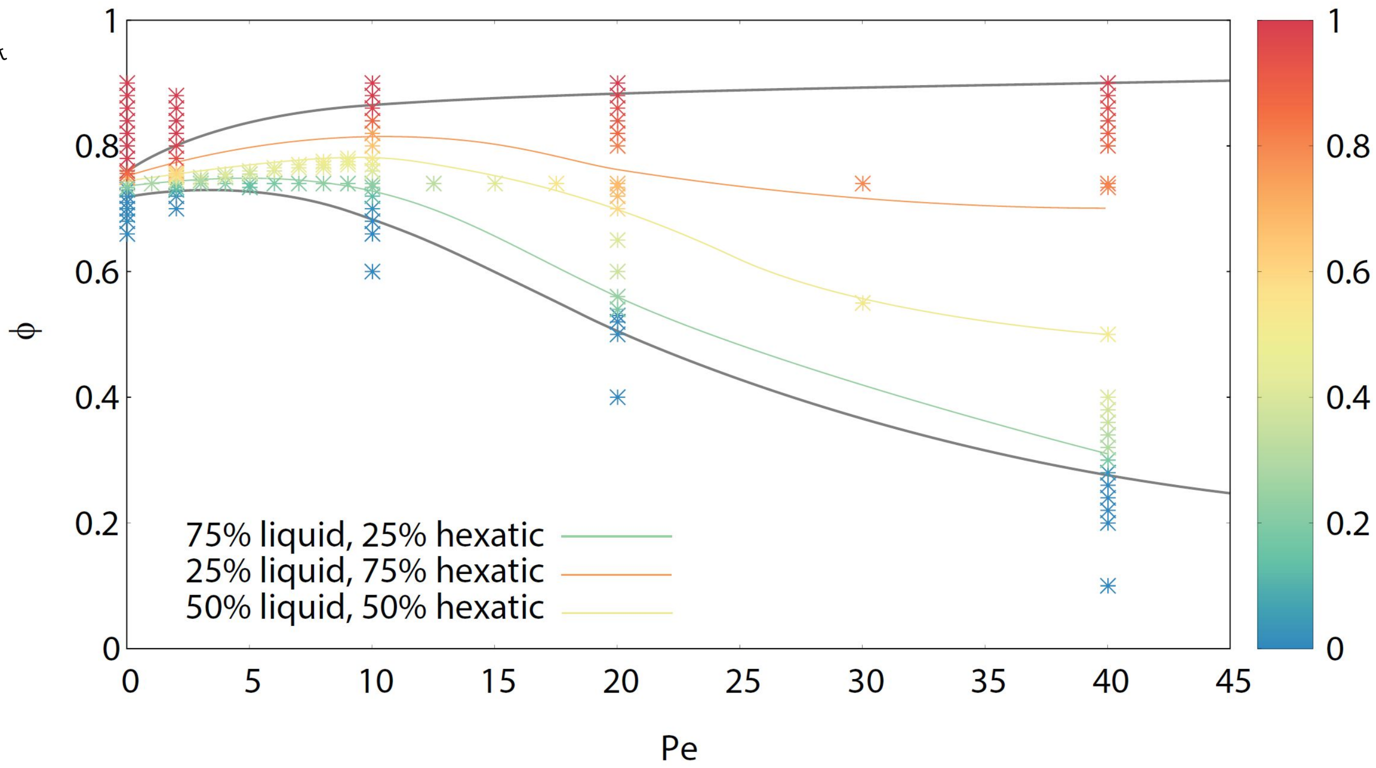
$$C_{\mathbf{q}_0}(r) = \langle e^{\mathbf{i}\mathbf{q}_0 \cdot (\mathbf{r}_i - \mathbf{r}_j)} \rangle$$

$\mathbf{q}_0$ maximum diffraction peak



# Phase diagram for active dumbbells

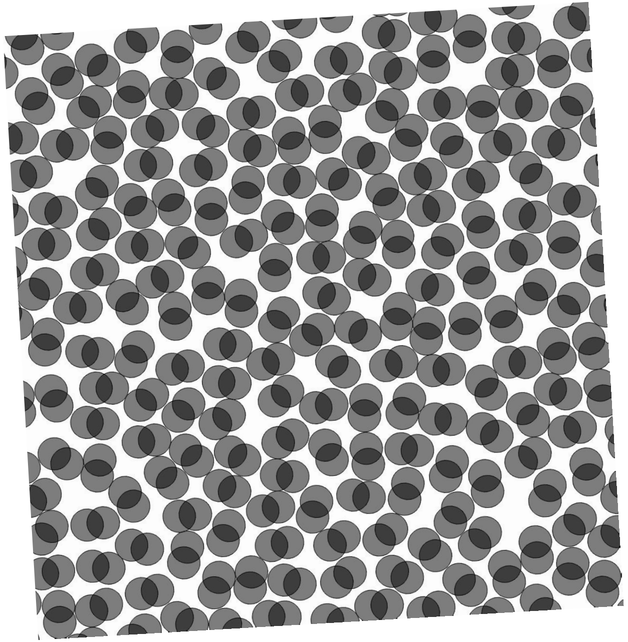



**Cugliandolo L.F., Digregorio P., Gonnella G., Suma A.,** Phys. Rev. Lett., 119 268002 (2017)

# **N**ext year

- Can the phase transitions between active phases be explained in term of structural properties?
- Do the out-of-equilibrium aggregation phenomena strongly depend on the underlying order?
- Which are the laws for the kinetics of the clustering phenomena? Are they affected by the shape of the particles?



# Next year

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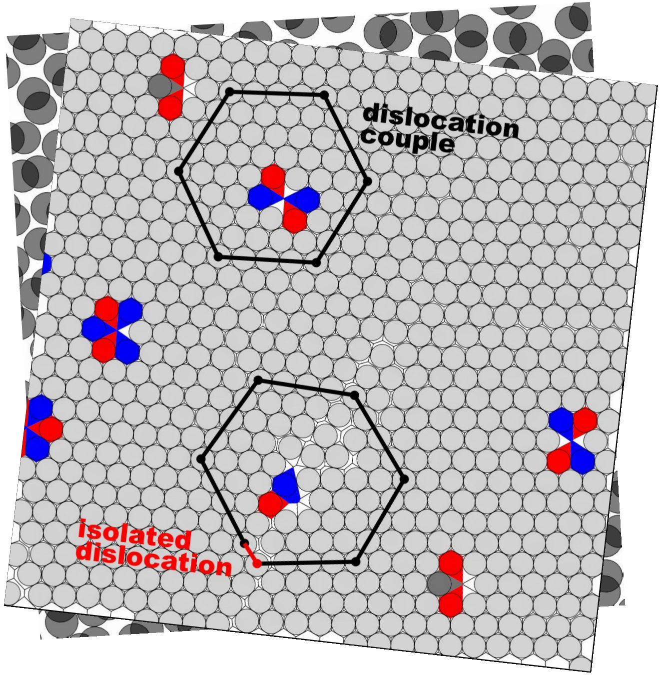

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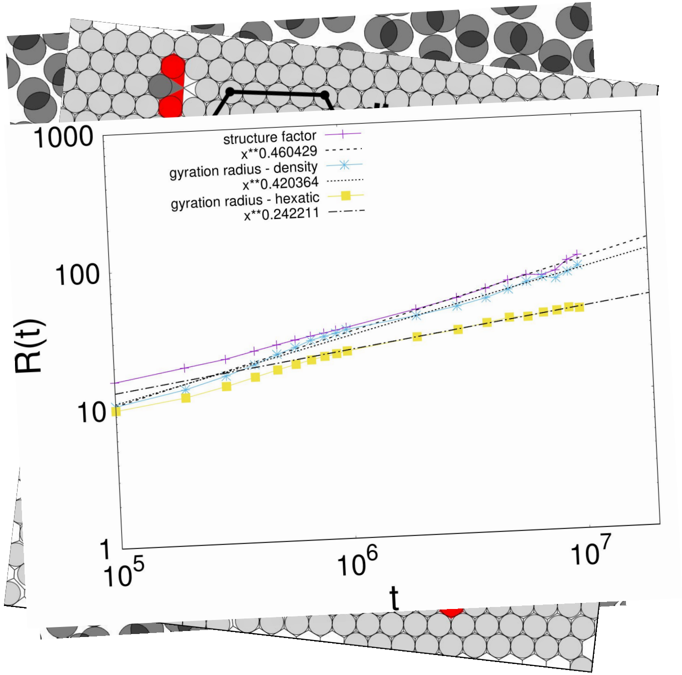

# Publications

- 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"*, arXiv 1805.06683., accepted on EPJE, **Oct 2018**

# **P**ublications

- 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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# **T**hank you!