Active Brownian Particles under shear

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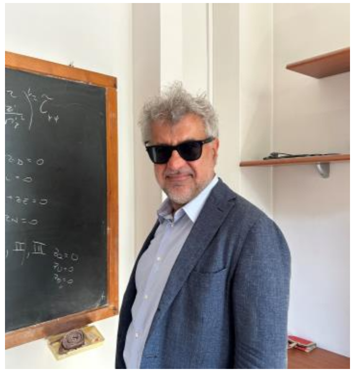
TURBFIELD group – Sezione di Bari



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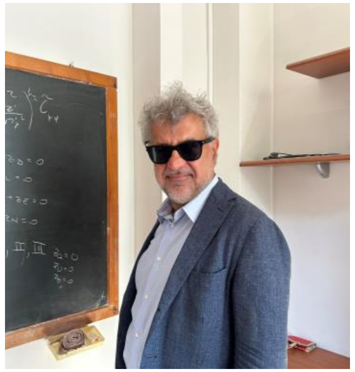

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P.I.

Associated Professor

Post-Doc Researchers

Ph.D. Students

Active Matter

- *Active matter systems* are composed by particles that can gain energy from their environment and can auto-propel.

- *Active systems* range from biological extracts to groups of animals, and exist at different length scales and time scales.

- Self-propulsion strongly affects the **diffusion** and the **aggregation** properties of these systems.

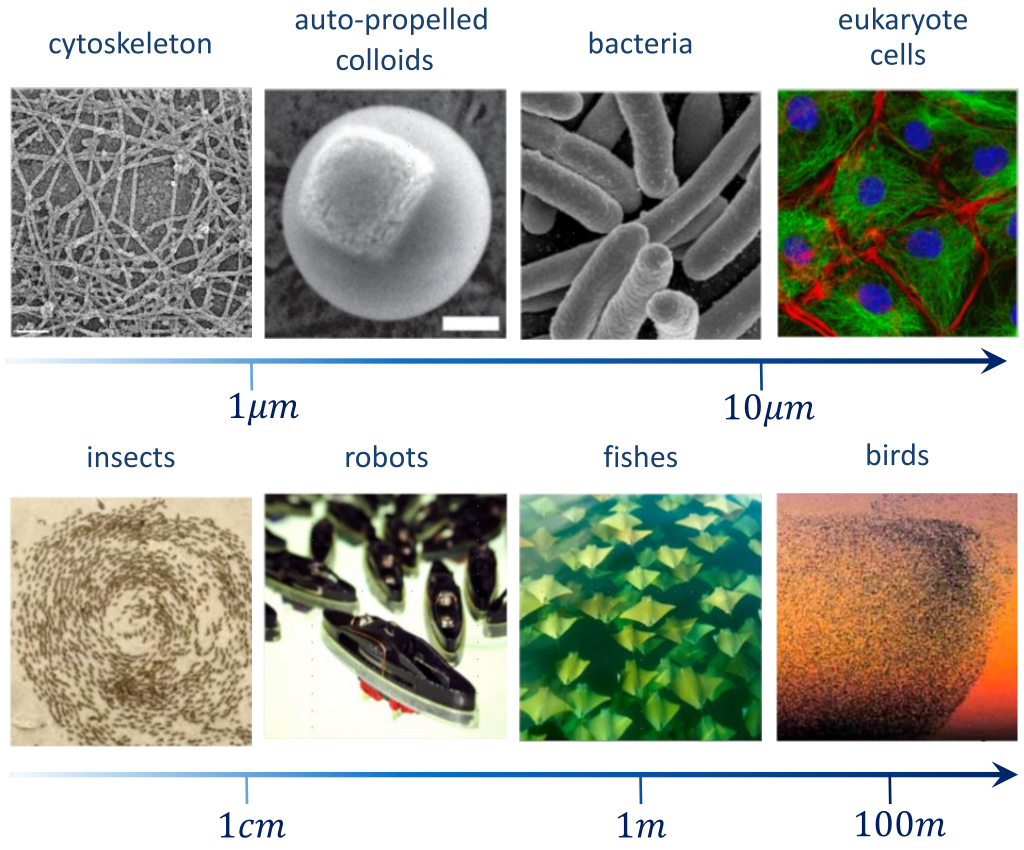
- Auto-propulsion is quantified by the **Péclet number.**

auto-propulsion → F_a

linear dimension of particles → σ

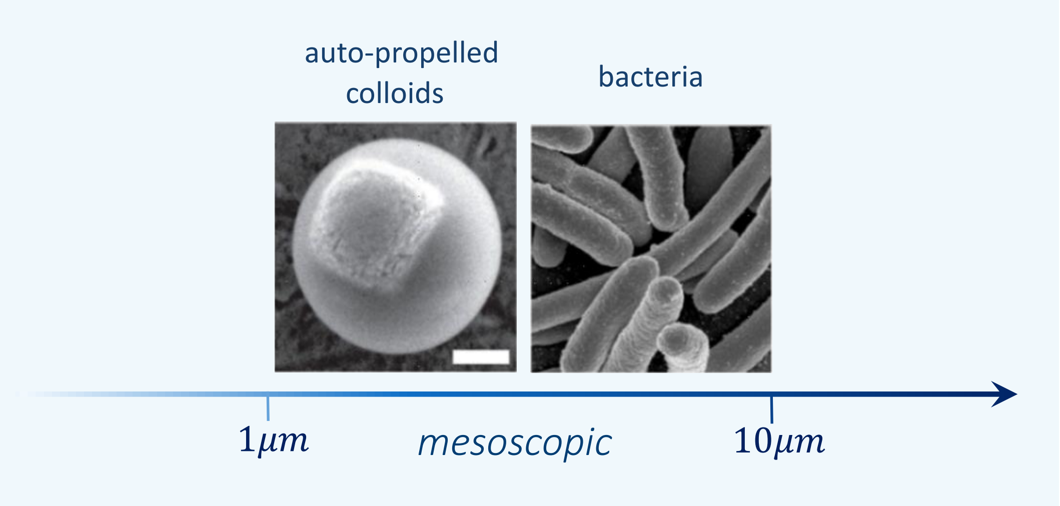
$$Pe = \frac{F_a \, \sigma}{k_B T}$$

temperature → $k_B T$

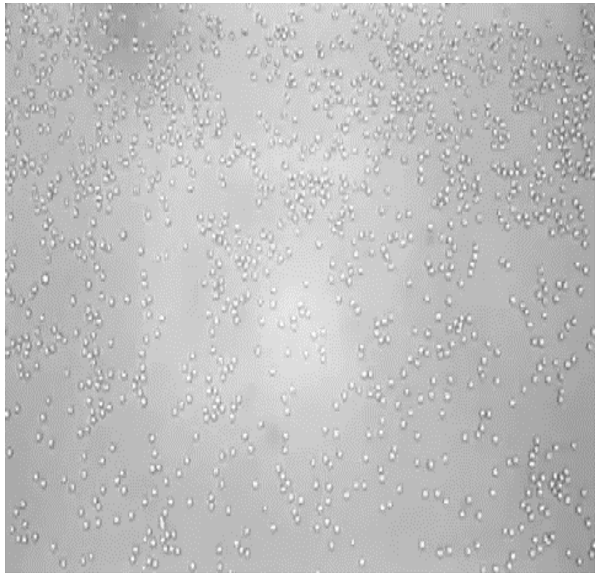


Active Matter

- We are interested in the *mesoscopic* scale.
  - In this regime, the interactions are comparable with the typical energy scales of the environment.



- An experimental realization of colloidal self-propelled particles.
  - light OFF → no chemical reactions occur, and particles are "passive".
  - light ON → chemical reactions take place, and particles begin to move.

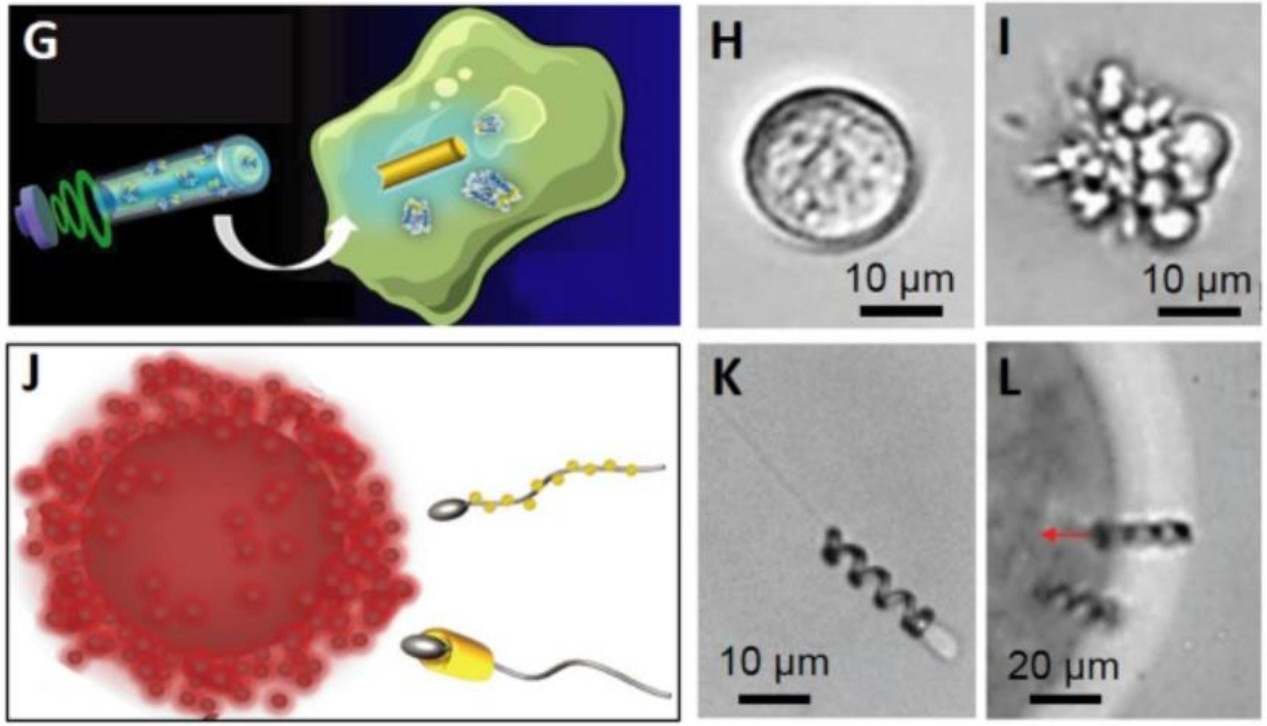


J. Palacci et al, Science, 2013

Active Matter: application to drug delivery

nanomotor-based intracellular delivery of an enzyme to induce apoptosis.

sperm cell-based hybrid microswimmers.



healthy human gastric adenocarcinoma before and after nanomotor delivery.

transport of an immotile sperm from a microhelix onto the oocyte.

schemes

experimental realizations

A.Ghosh et al, Nano Today, 2020

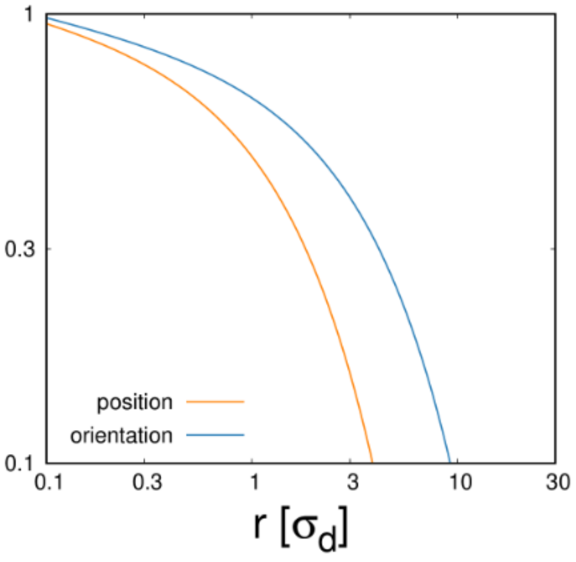
Phase transitions in 2D

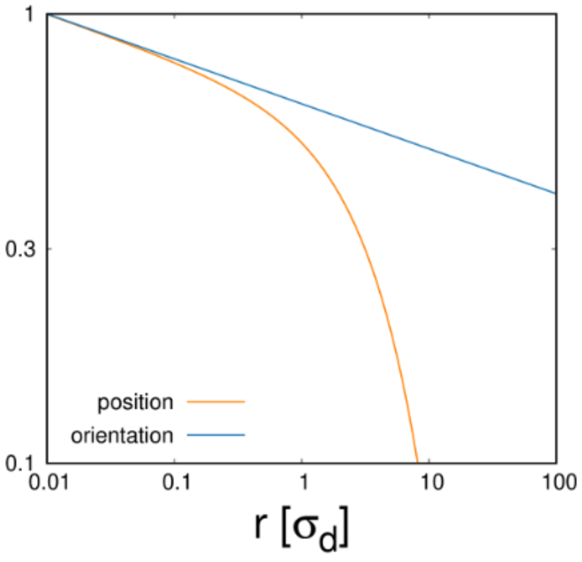
- In passive systems, phase transitions are described by the Kosterlitz-Thouless-Halperin-Nelson (KTHNY) theory.

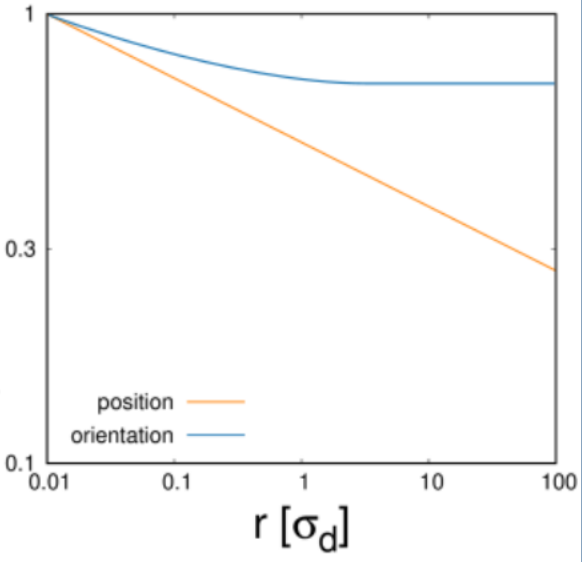
ϕ →

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

Pair correlations







Active Brownian Particle model

THE MODEL

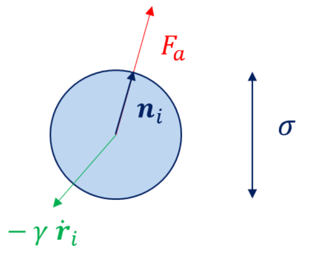
- The setup is a two-dimensional system of *Active Brownian Particles* (ABP) in a box with periodic boundary conditions.

repulsive interaction — auto-propulsion

$$\gamma \dot{\boldsymbol{r}}_i(t) = -\boldsymbol{\nabla} U + \boldsymbol{F}_{\boldsymbol{a},i} + \boldsymbol{\xi}_{\boldsymbol{i}}(t)$$

$$\dot{\theta}_i = \sqrt{2D_\theta}\,\eta_i$$

Gaussian noises



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

RESULTS

Digregorio et al, Phys. Rev. Lett. **121**, 098003

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repulsive interaction → $-\boldsymbol{\nabla} U$

auto-propulsion → $\boldsymbol{F}_{a,i}$

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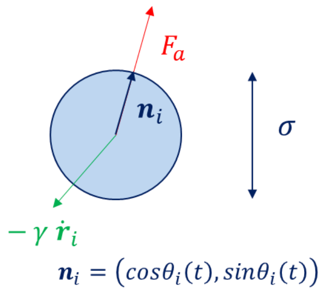
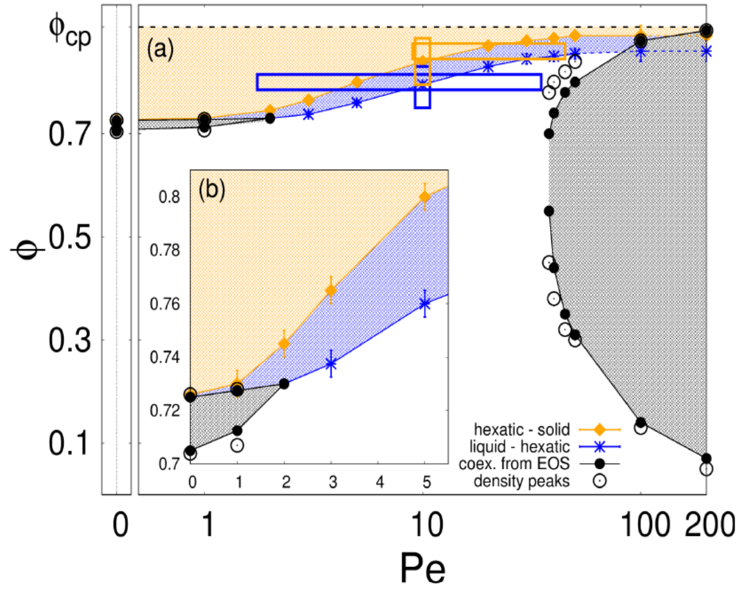
$$\dot{\theta}_i = \sqrt{2D_\theta}\,\eta_i$$

Gaussian noises → $\boldsymbol{\xi}_i(t)$, η_i





RESULTS

- From phase diagram $\phi - Pe$:
  activity destabilizes the ordered phases.
  at higher densities, a solid *active* phase exists for any Pe.

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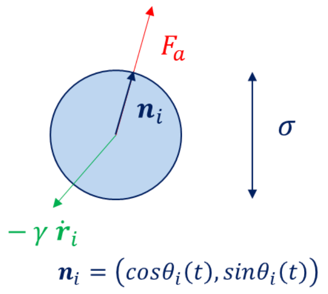
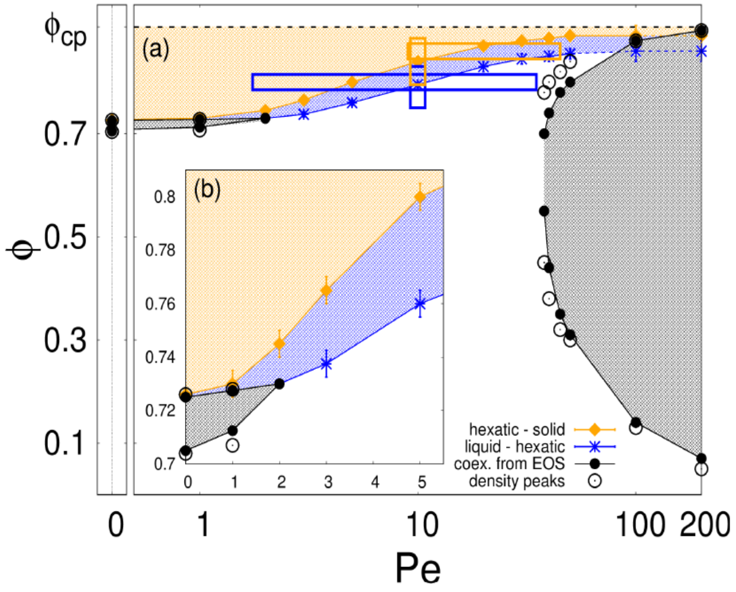
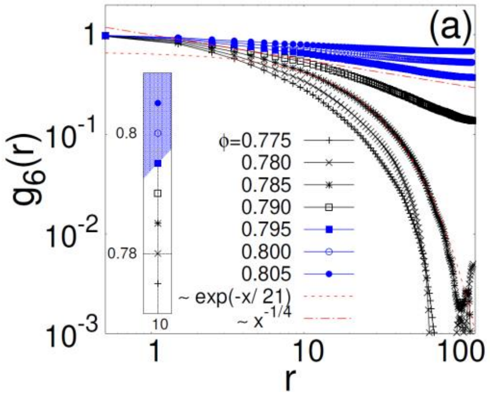




RESULTS

- From phase diagram $\phi - Pe$:
  activity destabilizes the ordered phases.
  at higher densities, a solid *active* phase exists for any Pe.

- At fixed activity $Pe = 10$:
  at $\phi = 0.795$ a phase transition in the orientation correlations occurs.



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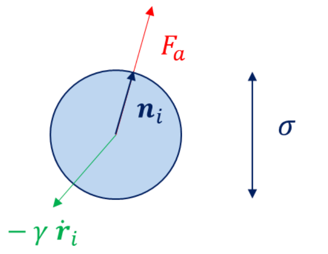
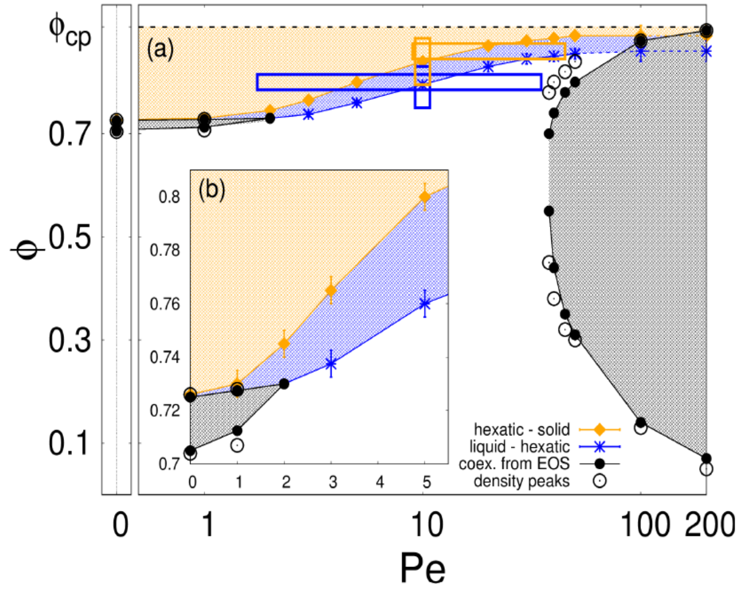
$$\dot{\theta}_i = \sqrt{2D_\theta}\eta_i$$

Gaussian noises



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



RESULTS

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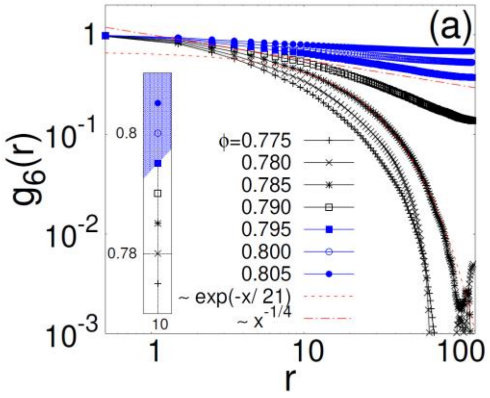
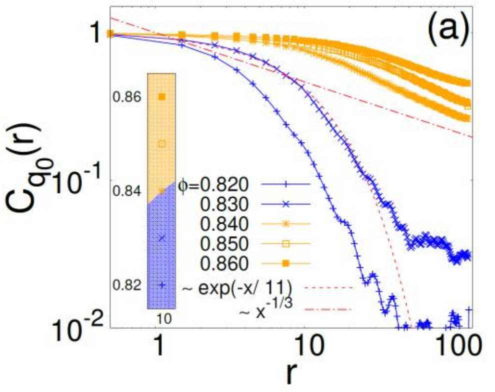
  activity destabilizes the ordered phases.
  at higher densities, a solid *active* phase exists for any Pe.

- At fixed activity $Pe = 10$:
  at $\phi = 0.795$ a phase transition in the orientation correlations occurs.
  at $\phi = 0.830$ a phase transition in the positional correlations occurs.





Digregorio et al, Phys. Rev. Lett. **121**, 098003

Active Brownian Particle under shear

THE MODEL

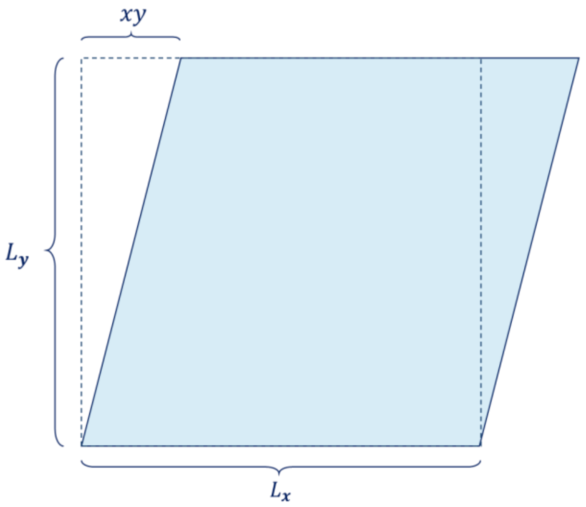
- We generalize the ABP model introducing in the equation a **velocity profile linearly growing** with the height.

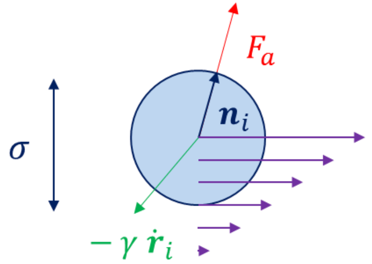
repulsive interaction — auto-propulsion — shear

$$\gamma \dot{\boldsymbol{r}}_i(t) = -\boldsymbol{\nabla} U + \boldsymbol{F}_{\boldsymbol{a},i} + \dot{\gamma}\boldsymbol{e}_{\boldsymbol{x}} y_{\boldsymbol{i}} + \boldsymbol{\xi}_{\boldsymbol{i}}(t)$$

$$\dot{\theta}_i = \sqrt{2D_\theta}\,\eta_{\boldsymbol{i}}$$

Gaussian noise





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

AIM OF OUR WORK

We want to characterize:

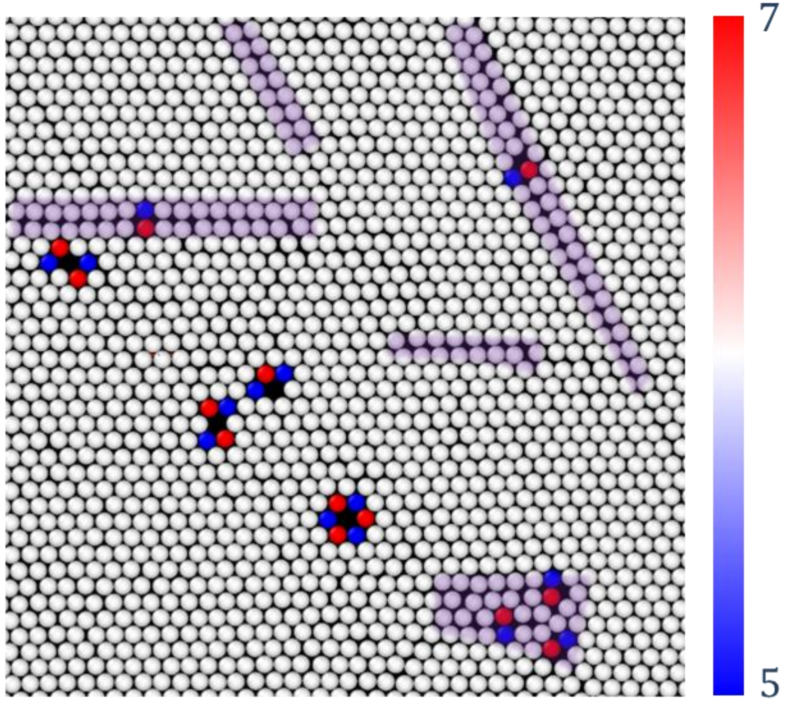
- the phase diagram of the system.
- the role played by shear in the exponents of the phase transition.

Active Brownian Particle under shear

To characterize the phase of the system, the following must be evaluated

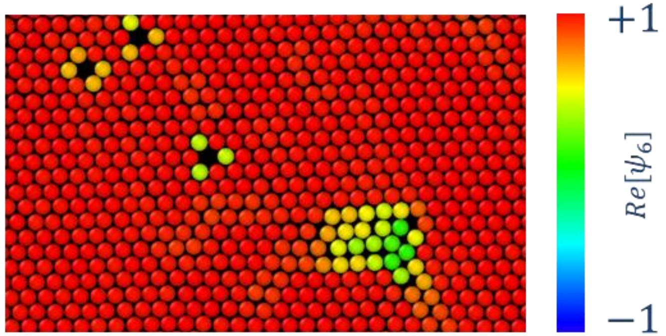
- ψ_6 (hexatic order)

  order parameter providing a quantitative definition of the local (or the global) order between adjacent particles.



$$\psi_{6,glob} = \frac{1}{N}\sum_{j=1}^{N} \psi_{6,j}$$

$$\psi_{6,j} = \frac{1}{n_j}\sum_{k=1}^{n_j} e^{i6\vartheta_{jk}}$$



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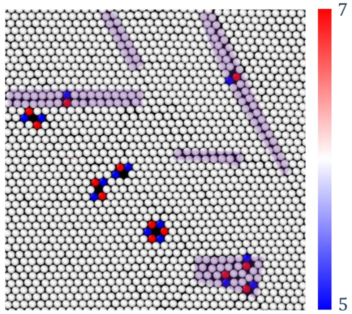

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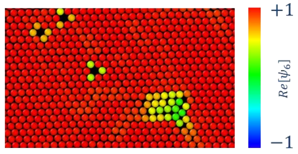
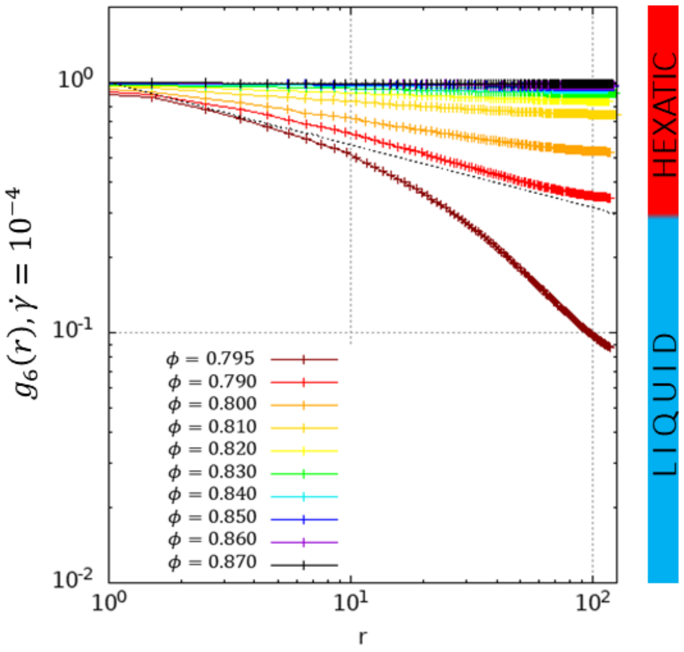


- $g_6(r)$ **hexatic correlations**

  This quantity measures how well the local hexatic order of particle arrangements is preserved over distance.

$$g_6(r = |r_j - r_k|) = \frac{\langle \psi_{6,j}(r_j)\psi_{6,j}(r_j)\rangle}{\langle \psi_{6,j}(r_j)^2\rangle}$$



The decay of the hexatic correlations:

- *hexatic phase* → algebraic, with exponent $\eta = 0.25$ prescript by the KTHNY theory;
- *liquid phase* → exponential.

The exponents of the phase transition correspond to the ones predicted by the KTHNY theory!

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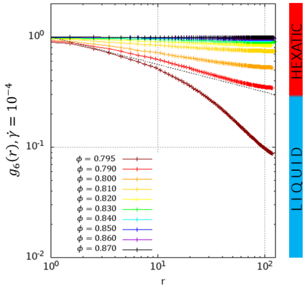

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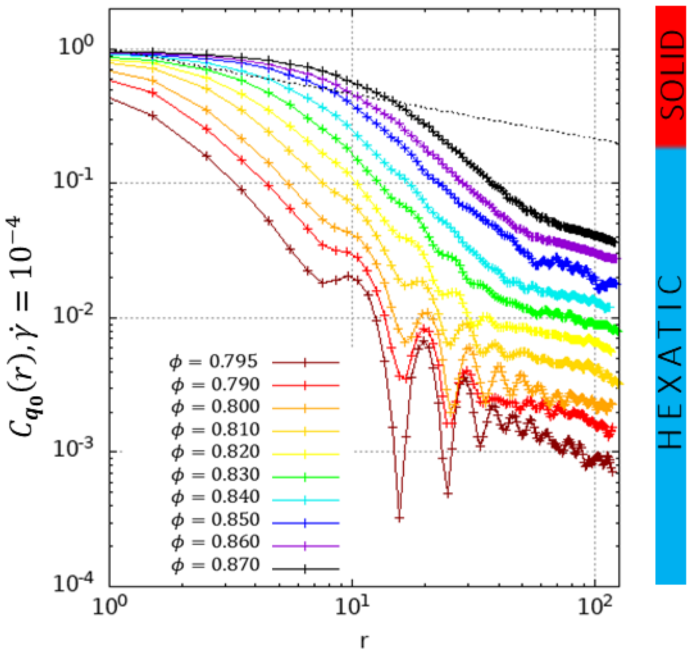
- $C_{q_0}(r)$ positional correlations

  This quantity describes how the positions of particles are related to each other over distance in the real space.

$$C_{q_0}(r) = \langle e^{i q_0 (r_i - r_j)} \rangle$$



The decay of the positional correlations:

- *solid phase* → algebraic, with exponent $\eta = 0.33$ prescript by the KTHNY theory;
- *hexatic phase* → exponential.

As soon as there is shear rate $\dot{\gamma}$, there is no solid phase!

Active Brownian Particle under shear

To characterize the phase of the system, the following must be evaluated

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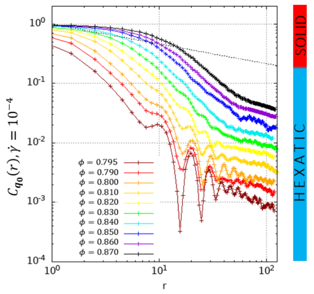

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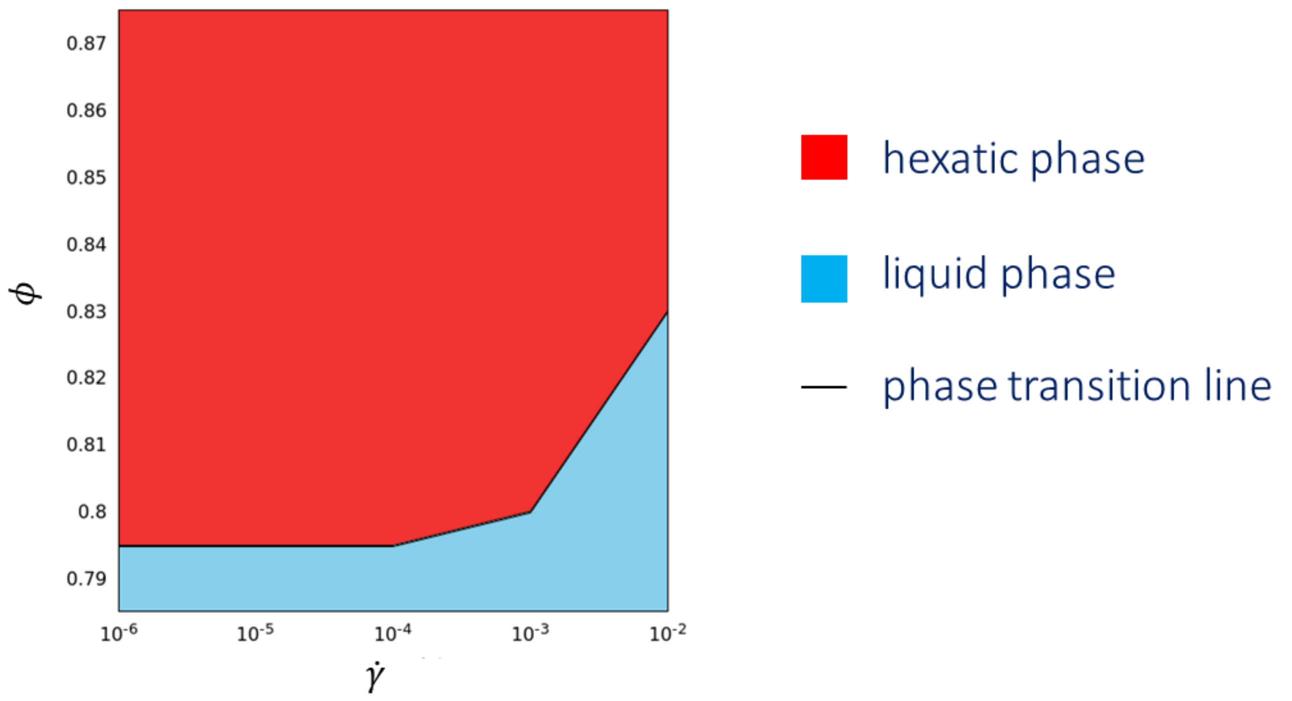
- **Phase Diagram**

It maps out the different collective states, i.e. the phases of the system, emerging as a function the of control parameters: density ϕ, and shear rate $\dot{\gamma}$.



Conclusions and future studies

RESULTS SUMMARY

- The global hexatic order showed a rearranging tendency of the system.
- From the structure factor, a periodic behaviour of the system and the typical correlation length were found.
- The presence of the shear seems to “liquify” the system.
- We determined the phase diagram for ABP under shear at a fixed Pe.

- Phase Diagram

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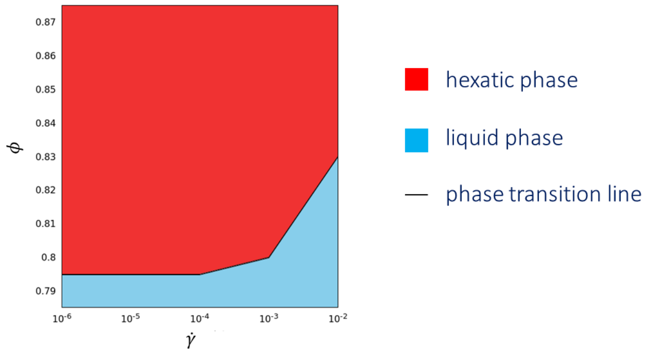

WHAT IS NEXT?

- Is there an interplay between activity and shear?
- Does the shear modify the critical exponents of the KTHNY theory? If so, in which way?
- How do defects behave under shear? Does their density change in different parts of the phase diagram?

Thank you for your attention!

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