Fluids and Structures: interaction and modeling

May 23, Napoli

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PHASE COEXISTENCE IN BIDIMENSIONAL PASSIVE AND ACTIVE DUMBBELL SYSTEMS

SUMMARY

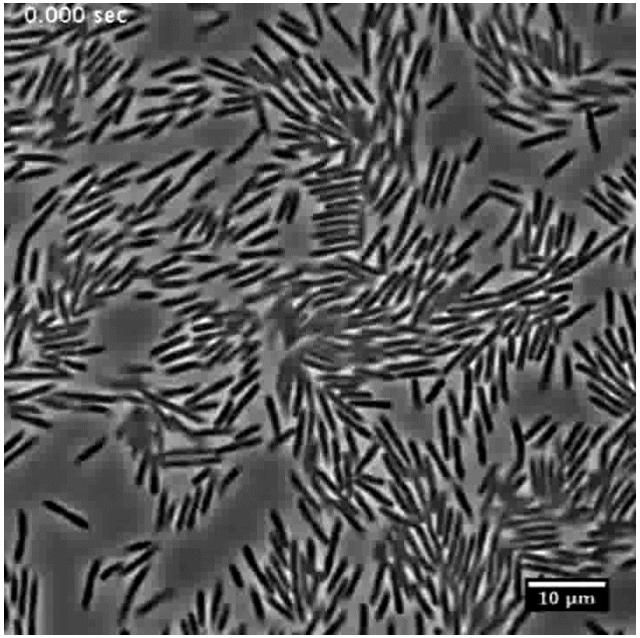
- Introduction
- The dumbbell model
- The 2D passive system
- Simulation results
- Conclusions

ACTIVE MATTER

Active matter systems are out of equilibrium systems in which constituents consume internal energy to move or make work on the environment.

Active particles display:

- Aggregation, favored by elongated shape (bacteria)
- Activity-induced phase separation



ACTIVE DUMBBELLS

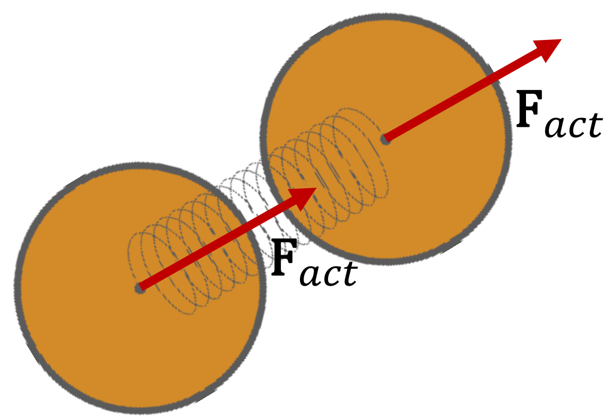
THE 2D DUMBBELL MODEL

$$m\,\ddot{\boldsymbol{r}}_i(t) = -\gamma\dot{\boldsymbol{r}}_i(t) - \frac{\partial U_{FENE}}{\partial r_{i,i+1}}\hat{\boldsymbol{r}}_{i,i+1} - \sum_{j\neq i}^{2N}\frac{\partial U_{WCA}}{\partial r_{ij}}\hat{\boldsymbol{r}}_{i,j} + \sqrt{2\gamma k_B T}\,\boldsymbol{\eta}_i + \mathbf{F}_{act,i}$$

- γ friction, $\boldsymbol{\eta}$ uncorrelated Gaussian noise;
- $F_{FENE}(r)$ finite extensible non-linear force;
- $U_{WCA}(r)$ generalized repulsive potential;
- $\mathbf{F}_{act,i}$ active force, constant in magnitude and directed along the main axis.

$$U_{WCA}(r) = 4\epsilon\left[\left(\frac{r}{\sigma}\right)^{-2n} - \left(\frac{r}{\sigma}\right)^{-n}\right] + U_{WCA}(r_c)$$

$$n = 6\ (\mathrm{LJ}), 32$$



[1] A. Suma, G. Gonnella, *et al.*, Phys. Rev. E, 2014.

ACTIVE DUMBBELLS

N dumbbells on a surface of area S

- Surface fraction

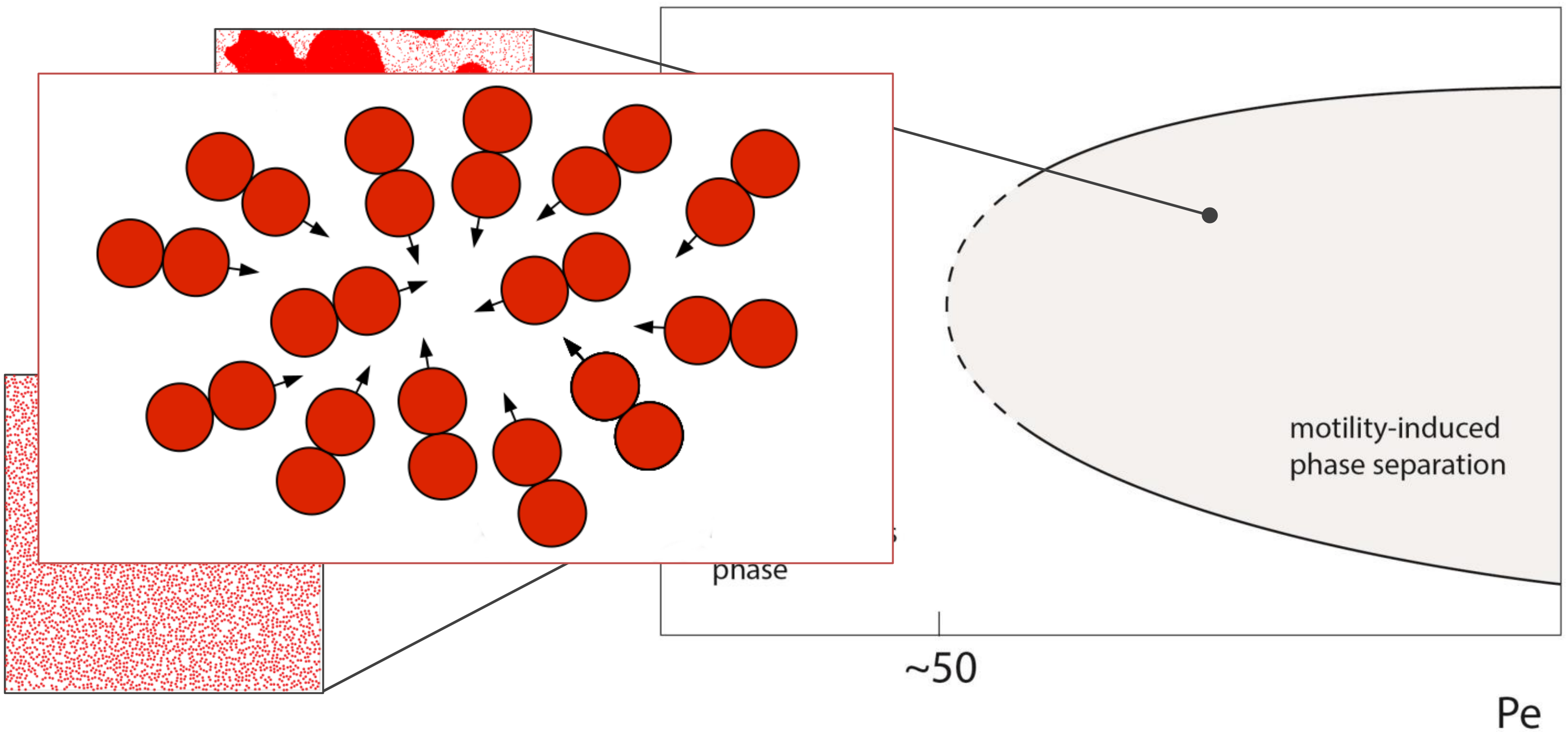
$$\phi = N\,\frac{\pi\sigma^2}{2S}$$

- Active and diffusive transport relative rates

$$\mathrm{Pe} = \frac{L v_a}{D} = \frac{2\sigma F_{act}}{k_B T}$$

PECLET NUMBER

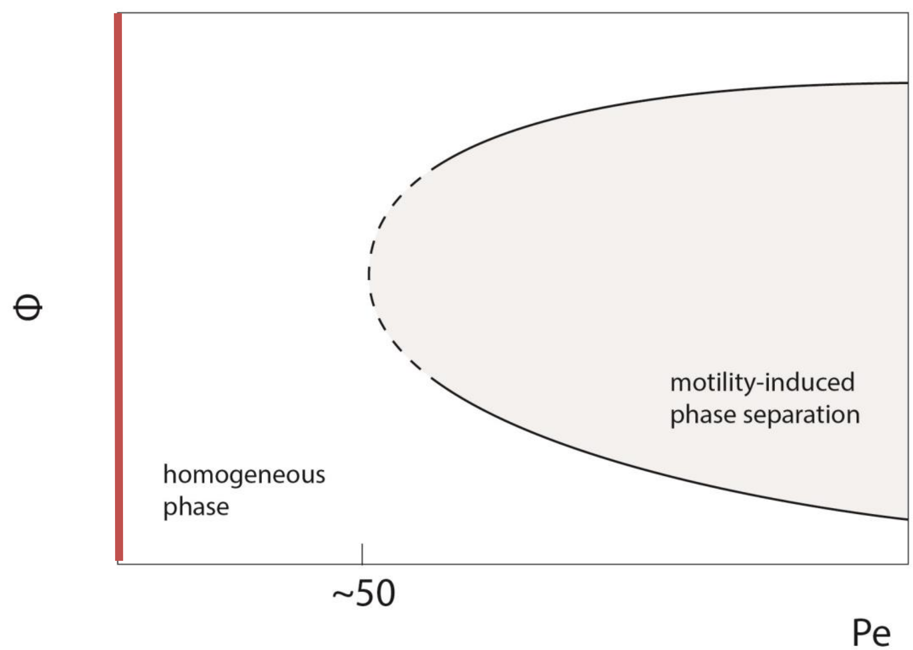
ACTIVE DUMBBELLS



[1] A. Suma, D. Marenduzzo, G. Gonnella, and E. Orlandini, **EPL** 108, 56004 (2014).
[2] J. Siebert, J. Letz, T. Speck, P. Virnau, **arXiv** (2016).

PURPOSE OF OUR WORK

We want to relate phase separation of active dumbbells to the behavior of the system at Pe=0.



KTHN TRANSITIONS SCENARIO FOR 2D HARD-DISK SYSTEMS

ϕ

SOLID
- quasi-long-range positional order
- long-range orientational order

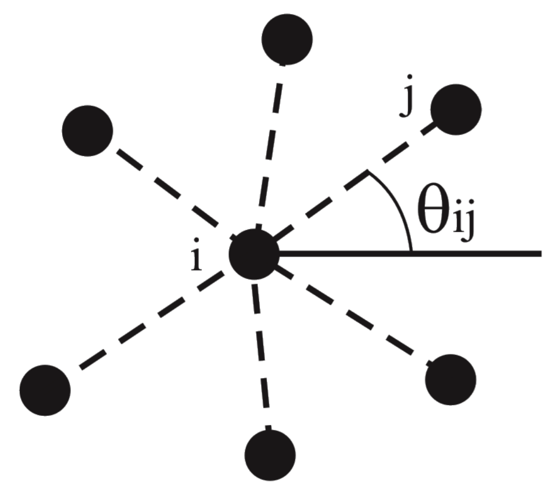
II order

HEXATIC
- short-range positional order
- quasi-long-range orientational order

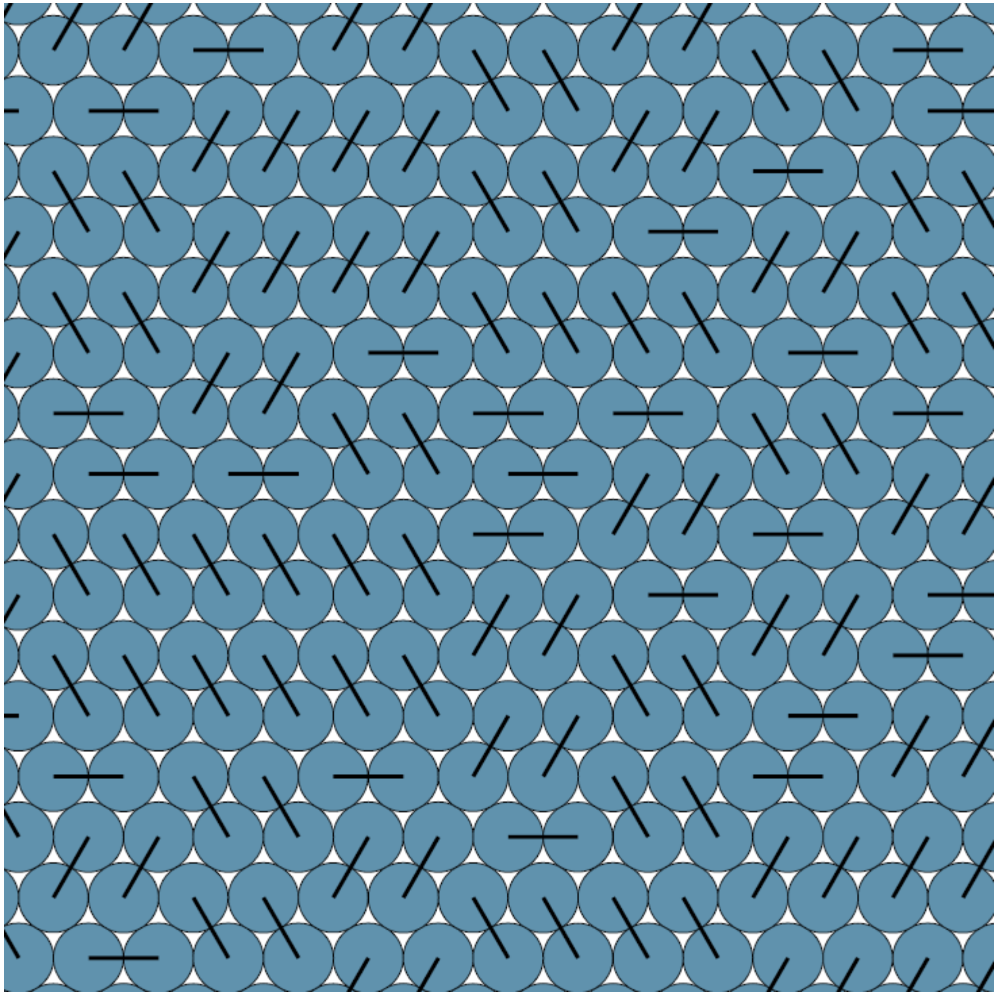
II order

LIQUID
- short-range order

$$\psi_{6,i} = \frac{1}{N_i} \sum_{j=0}^{N_i} e^{i6\theta_{ij}}$$

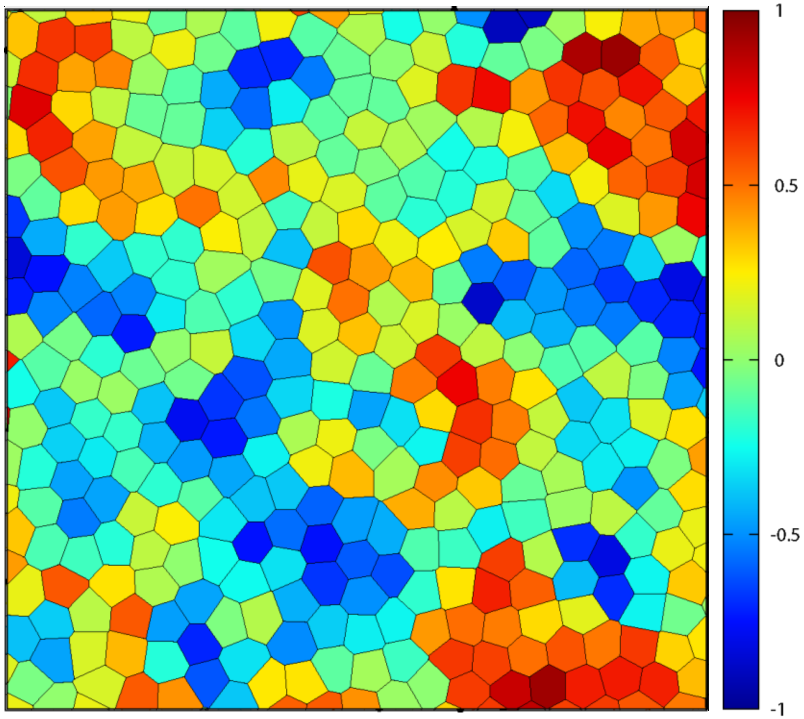


[1] J. M. Kosterlitz , D. J. Thouless, Journal of Physics C, 1973
[2] B. I. Halperin and David R. Nelson. Phys. Rev. Lett., 1978.
[3] S. C. Kapfer and W. Krauth, Phys. Rev. Lett., 2015.

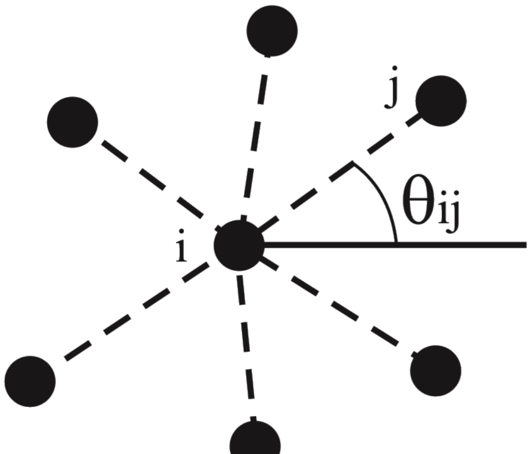


Close-packed configuration of dumbbells

KTHN TRANSITIONS SCENARIO FOR 2D HARD-DISK SYSTEMS



$$\psi_{6,i} = \frac{1}{N_i}\sum_{j=0}^{N_i} e^{i6\theta_{ij}}$$



[1] J. M. Kosterlitz , D. J. Thouless, **Journal of Physics C,** 1973

[2] B. I. Halperin and David R. Nelson. **Phys. Rev. Lett.**, 1978.

[3] S. C. Kapfer and W. Krauth, **Phys. Rev. Lett.,** 2015.

2D PASSIVE TRANSITIONS FOR DUMBBELLS

ϕ

SOLID

- quasi-long-range positional order
- long-range orientational order

II order

HEXATIC

- short-range positional order
- quasi-long-range orientational order

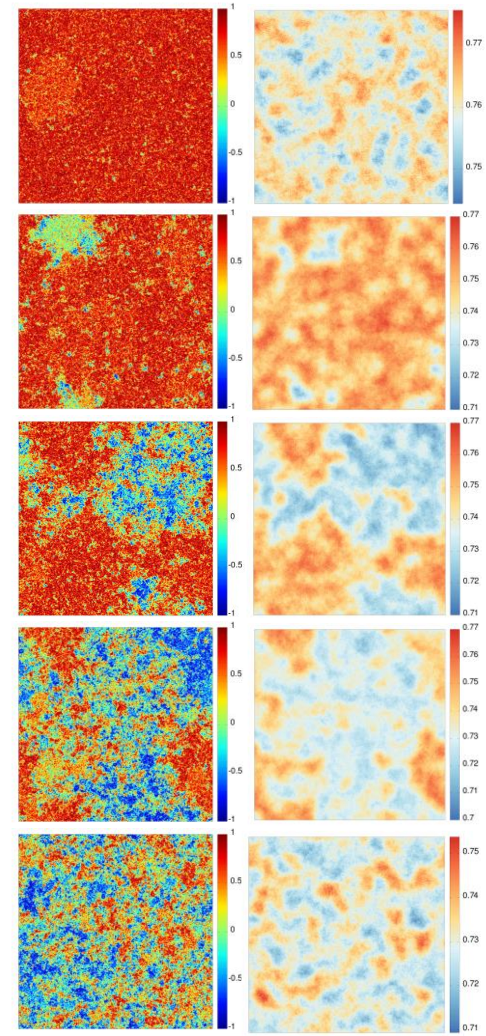
$\phi = 0.756$

II order

$\phi = 0.730$

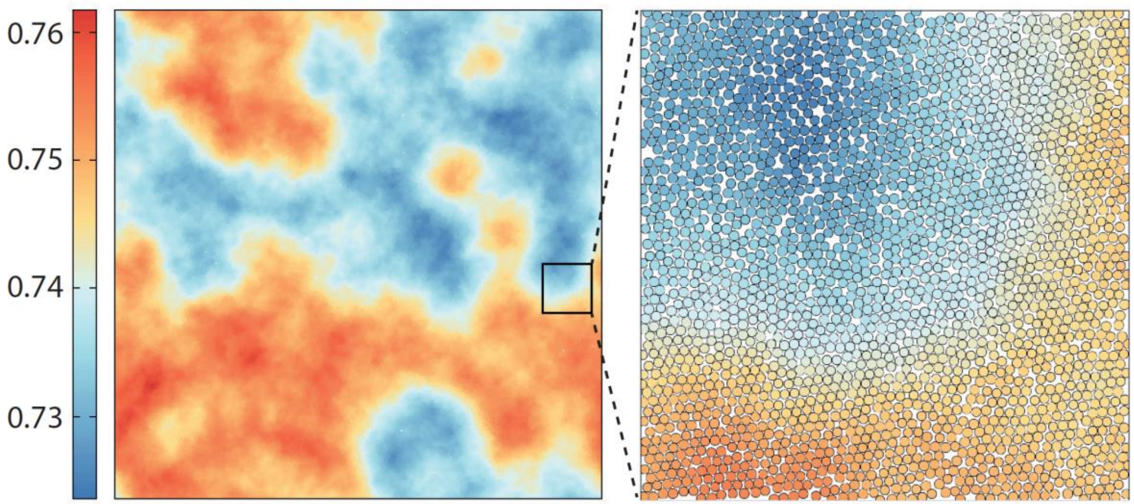
LIQUID

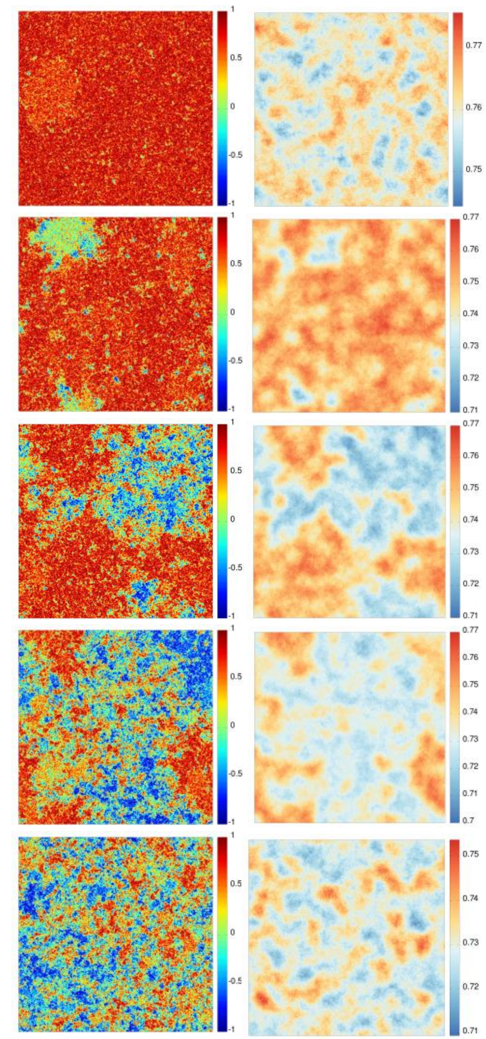
- short-range order



[1] L.F. Cugliandolo, P. Digregorio, G. Gonnella, A. Suma, arXiv, 2016.

2D PASSIVE TRANSITIONS FOR DUMBBELLS





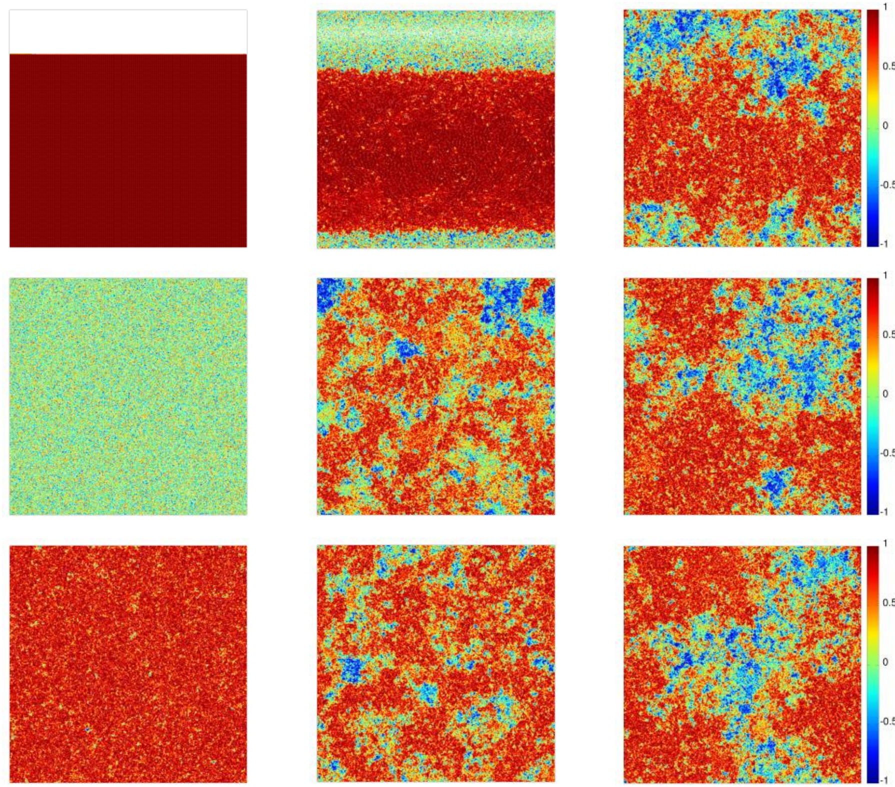
[1] L.F. Cugliandolo, P. Digregorio, G. Gonnella, A. Suma, arXiv, 2016.

DIFFERENT STARTS

FROM STRIPED

FROM RANDOM

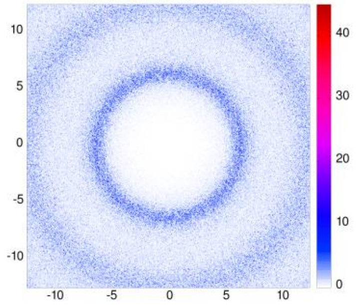
FROM ORDER



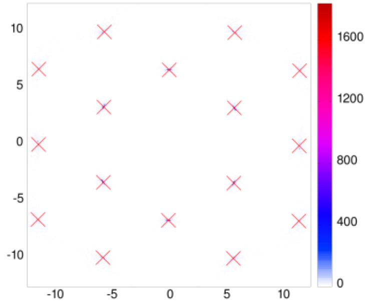
[1] L.F. Cugliandolo, P. Digregorio, G. Gonnella, A. Suma, arXiv, 2016.

THE STATIC STRUCTURE FACTOR

$\phi = 0.66$ (liquid phase)



$\phi = 0.76$ (solid phase)



$$S(\vec{k}) = \frac{1}{2N}\left\langle \sum_{i=1}^{2N}\sum_{j=1}^{2N} e^{i\,\vec{k}(\vec{r}_i - \vec{r}_j)} \right\rangle$$

Bragg peaks

$$\vec{k}_1 = \frac{4\pi}{a\sqrt{3}}\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right) \ ; \ \vec{k}_2 = \frac{4\pi}{a\sqrt{3}}(0,1)$$

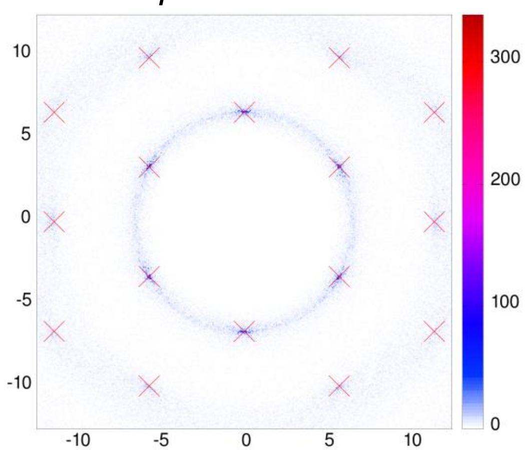
where

$$a = \left(\frac{\pi}{2\sqrt{3}\phi}\right)^{1/2} \sigma_d$$

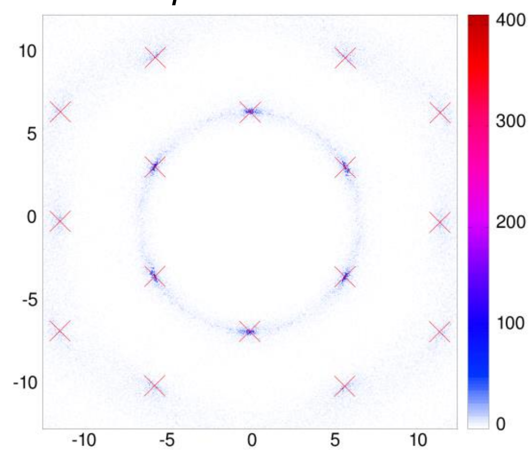
THE STATIC STRUCTURE FACTOR

in the co-existence region

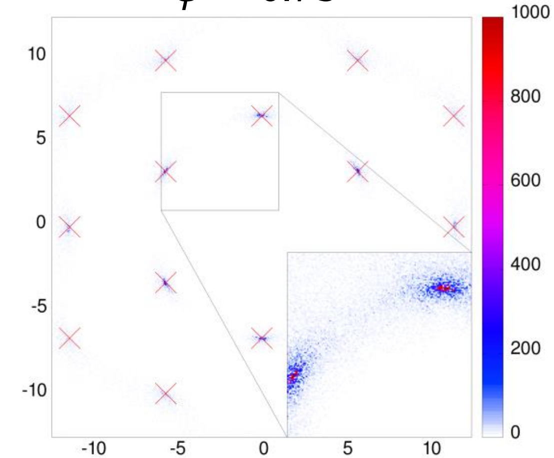
$\phi = 0.734$



$\phi = 0.74$



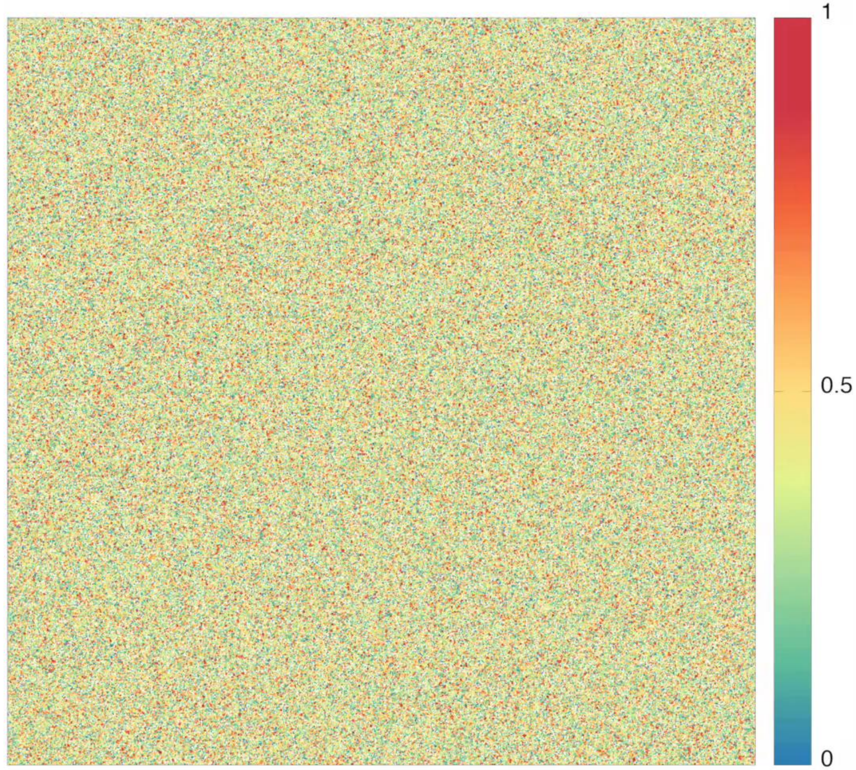
$\phi = 0.75$



BACK TO THE ACTIVE DUMBBELLS

LOW-PE ACTIVE DUMBBELLS

Pe=2

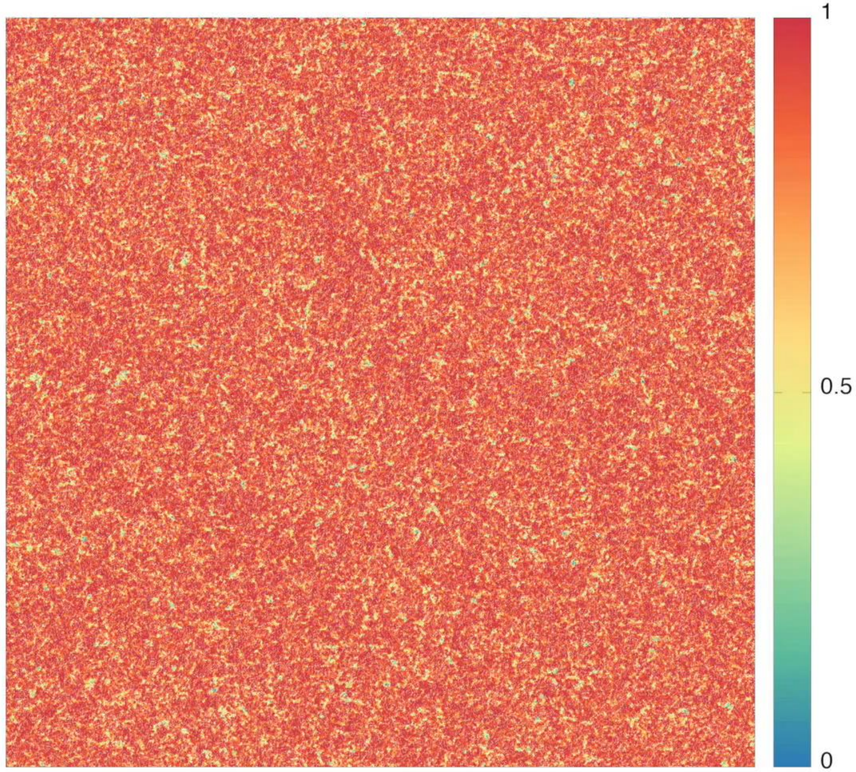


$|\psi_{6,i}|$

[1] L.F. Cugliandolo, P. Digregorio, G. Gonnella, A. Suma, arXiv, 2016.

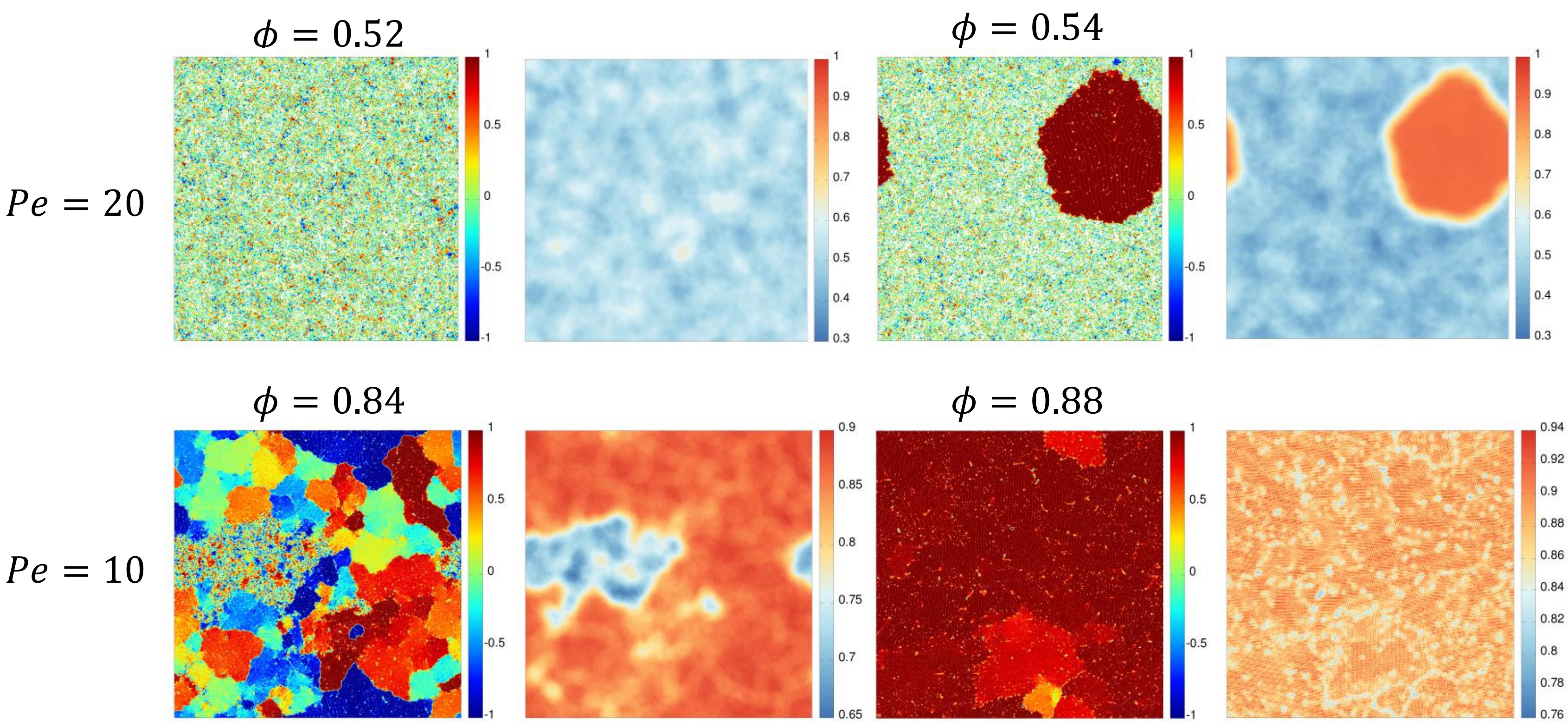
LOW-PE ACTIVE DUMBBELLS

Pe=10

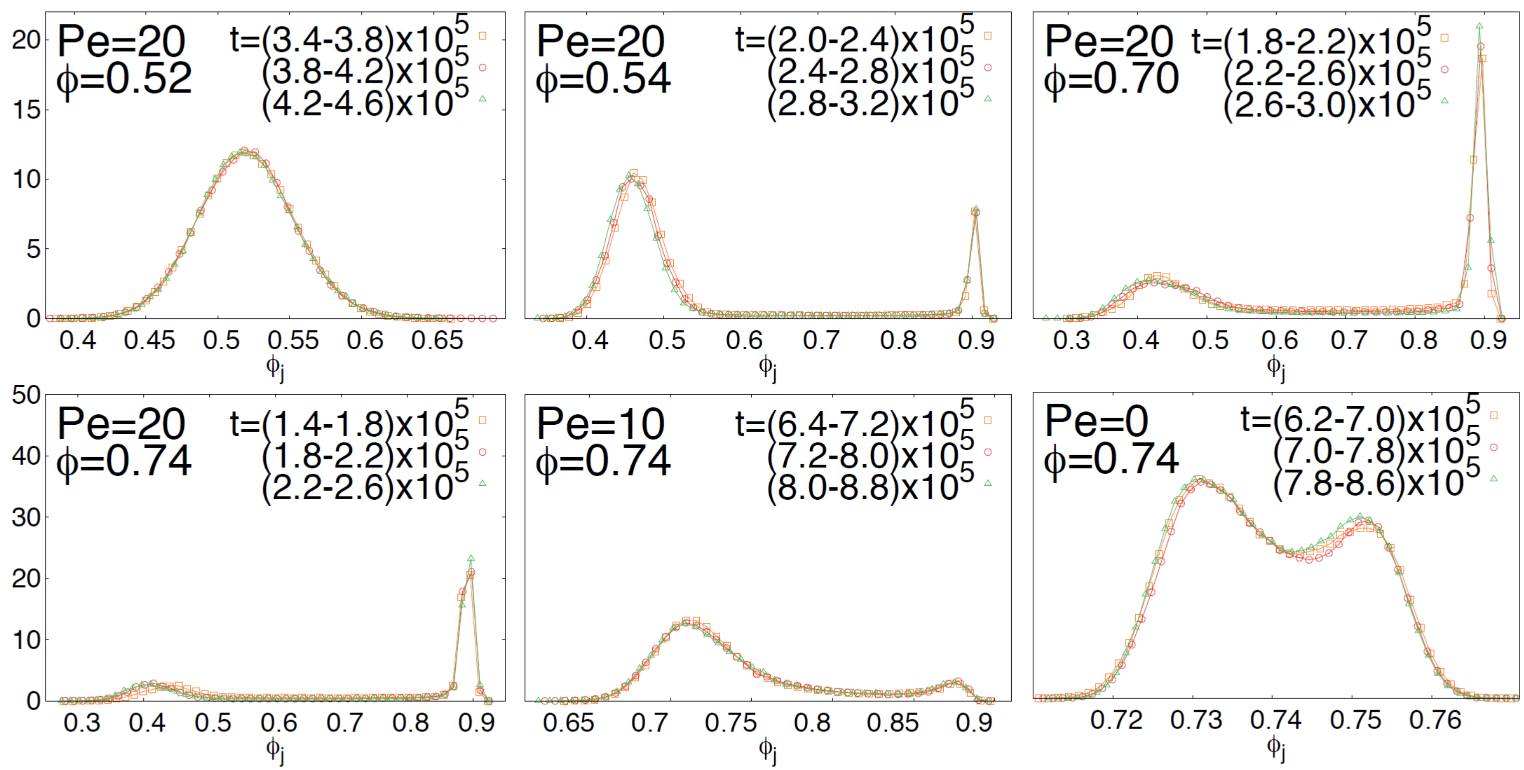


[1] L.F. Cugliandolo, P. Digregorio, G. Gonnella, A. Suma, arXiv, 2016.

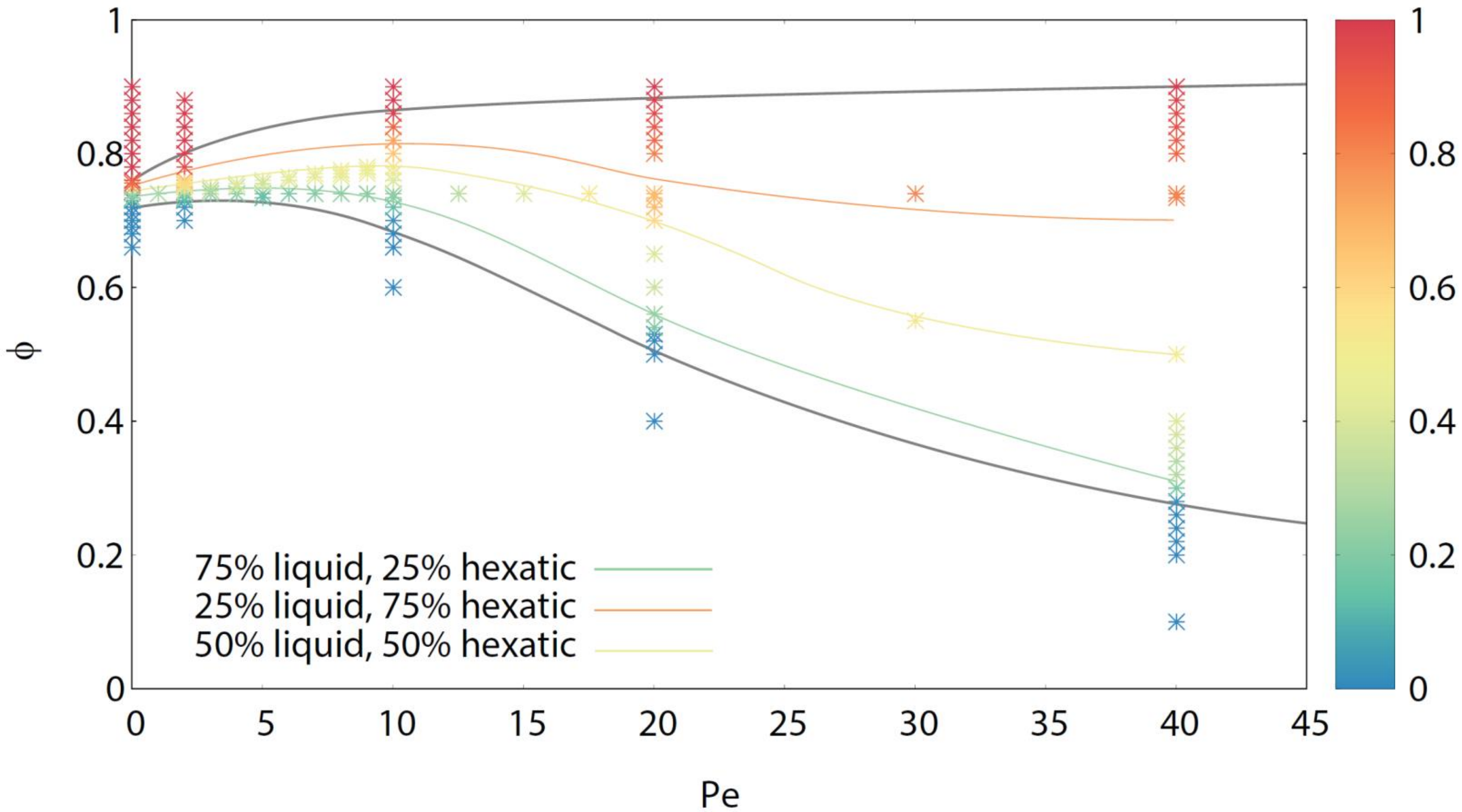
BOUNDARY OF THE CO-EXISTENCE REGION



LOCAL DENSITY BEHAVIOR IN THE CO-EXISTENCE REGION

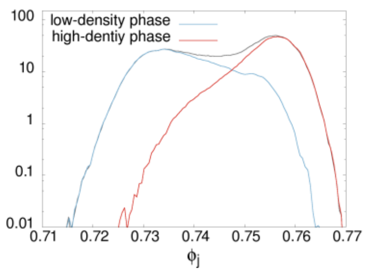


PHASE DIAGRAM

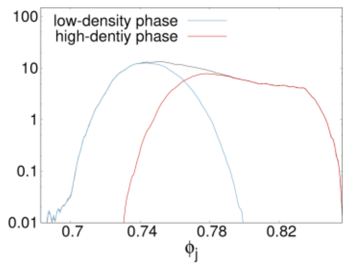


FURTHER CHARACTERIZATION OF THE COEXISTENCE REGION: DENSITY BEHAVIOR

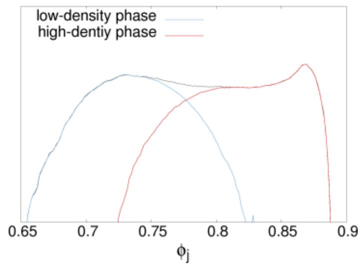
$Pe = 0, \phi = 0.744$



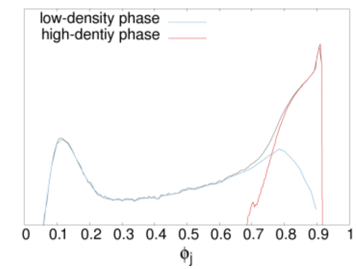
$Pe = 5, \phi = 0.765$

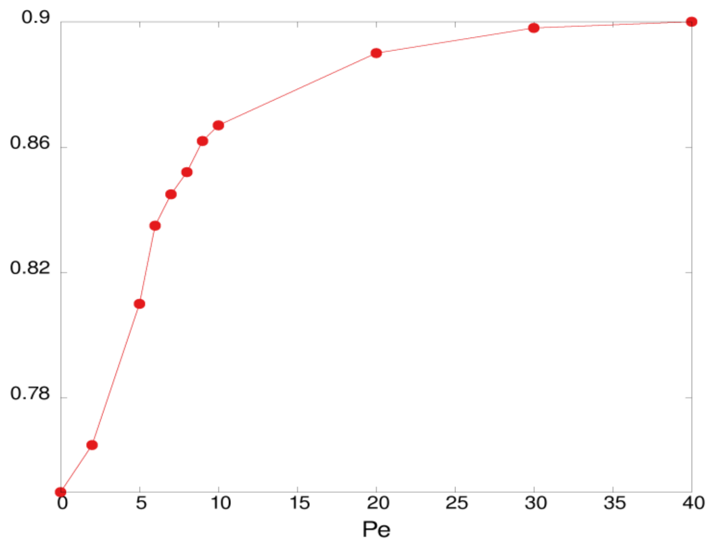


$Pe = 10, \phi = 0.78$



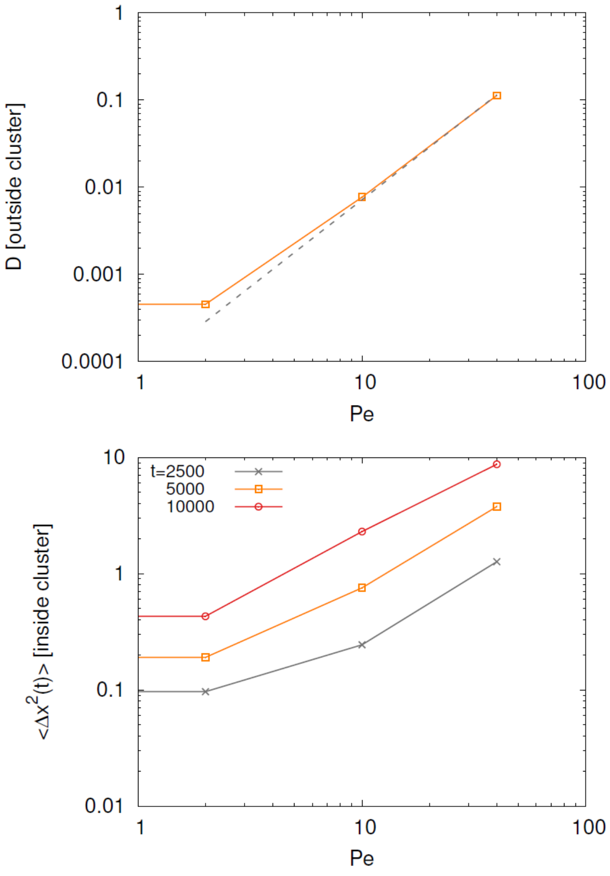
$Pe = 40, \phi = 0.50$



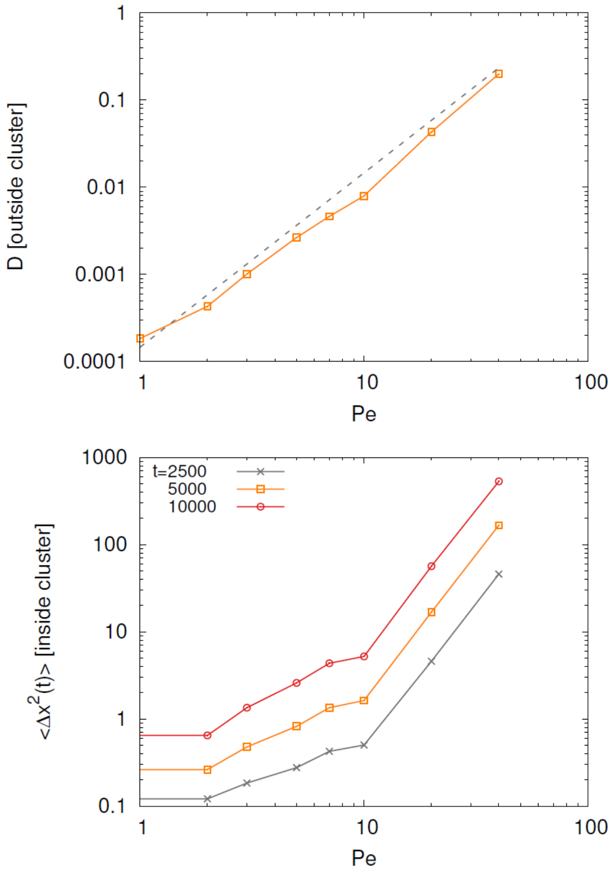


DIFFUSION CONSTANT

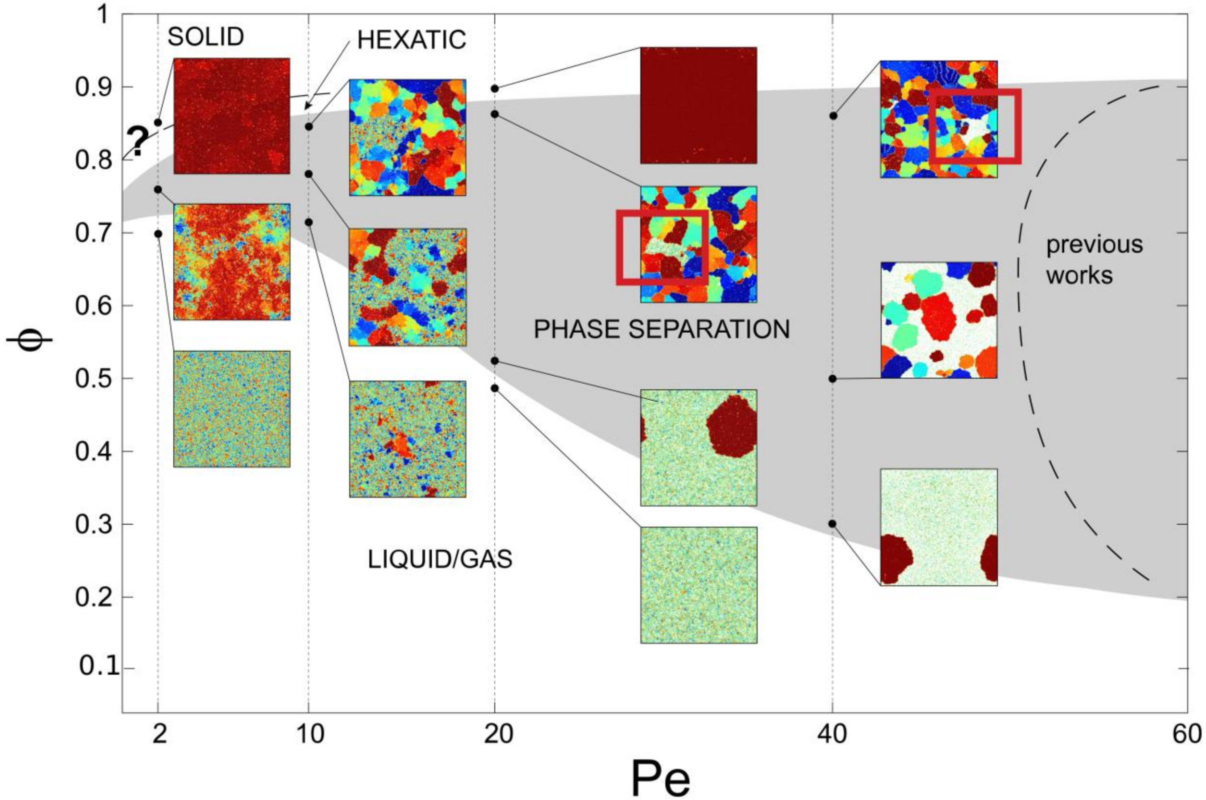
75% hexatic - 25% liquid



50% hexatic - 50% liquid



PHASE DIAGRAM



[1] L.F. Cugliandolo, P. Digregorio, G. Gonnella, A. Suma, arXiv, 2016.

CONCLUSION

- Active dumbbells phase separate for any value of activity.
- There is no discontinuity between the passive and active regions in the coexistence region.

ACTIVE DUMBBELLS

THE 2D DUMBBELL MODEL[1]

N dumbbells on a surface of area S

- Surface fraction $\phi = N\,{}^{\pi\sigma^2}/_{2S}$
- Advective transport $Lv_a = {}^{\sigma F_{act}}/_{\gamma}$
- Diffusive transport $D = {}^{k_B T}/_{2\gamma}$
- Active force $Lv_a = {}^{\sigma F_{act}}/_{\gamma}$
- Viscous force $\mu = {}^{\gamma\sigma^2}/_{m}$

PECLET NUMBER

$$\mathrm{Pe} = \frac{Lv_a}{D} = \frac{2\sigma F_{act}}{k_B T}$$

REYNOLDS NUMBER

$$\mathrm{Re}^{(\mathrm{act})} = \frac{mF_{act}}{\sigma\gamma^2}$$

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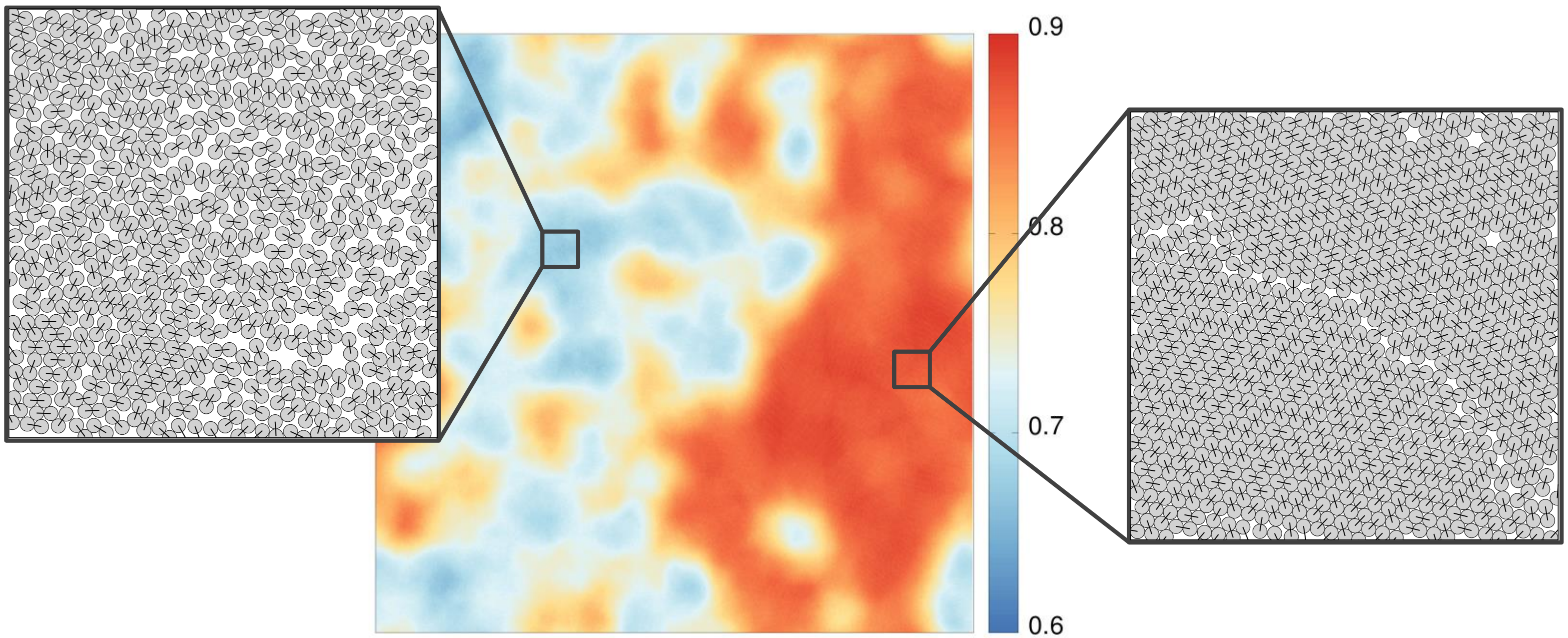
[1] A. Suma, G. Gonnella, *et al.*, **Phys. Rev. E**, 2014.

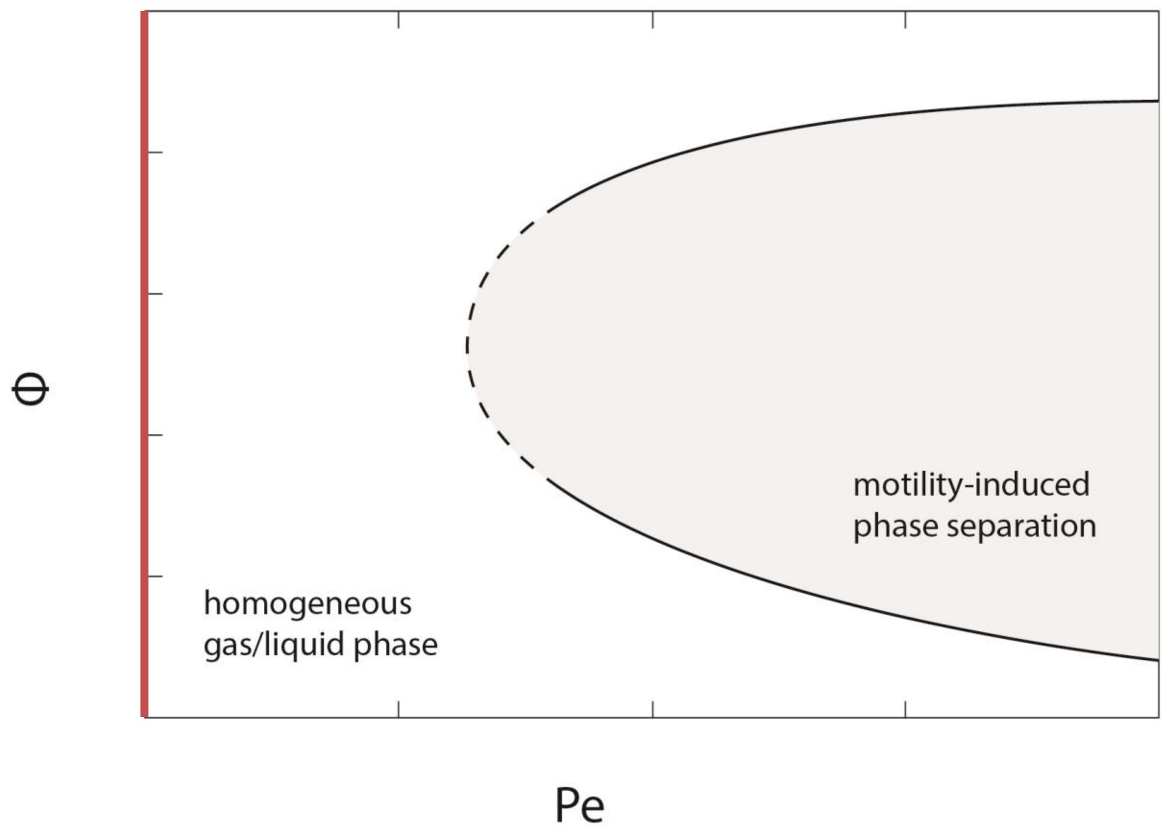
LOW-PE ACTIVE DUMBBELLS

PHASE SEPARATION IN THE DUMBBELL MODEL[1]



[1] L.F. Cugliandolo, P. Digregorio, G. Gonnella, A. Suma, arXiv, 2016.

In our work we want to connect phase separation of active particles to what happens at Pe=0.



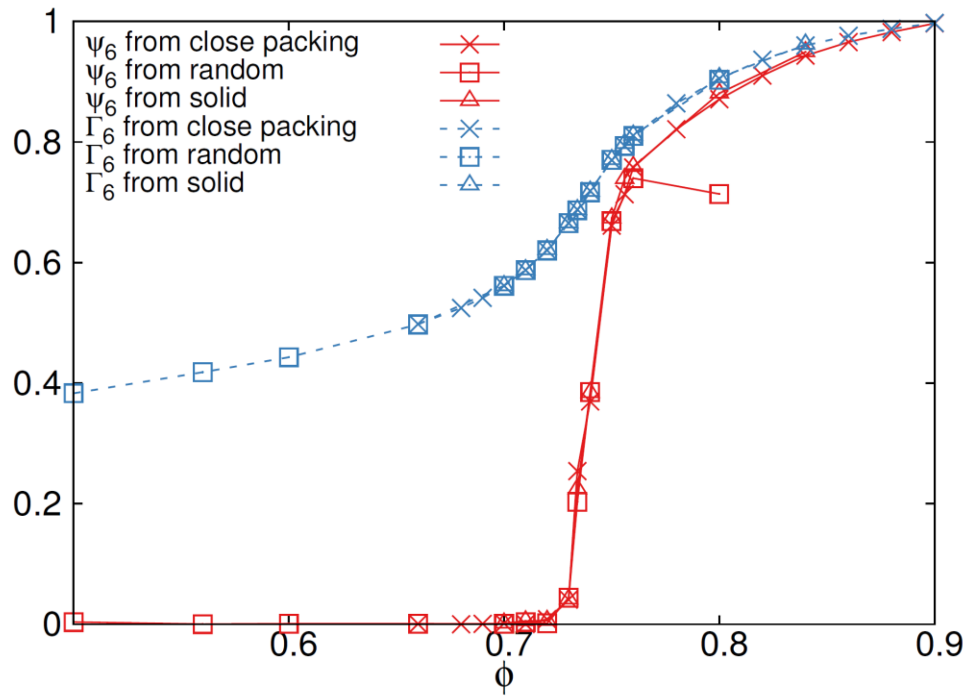
THE STATIC STRUCTURE FACTOR

$$S(\vec{k}) = \frac{1}{2N}\left\langle \sum_{i=1}^{2N}\sum_{j=1}^{2N} e^{i\,\vec{k}(\vec{r}_i-\vec{r}_j)} \right\rangle$$

2D PASSIVE TRANSITIONS

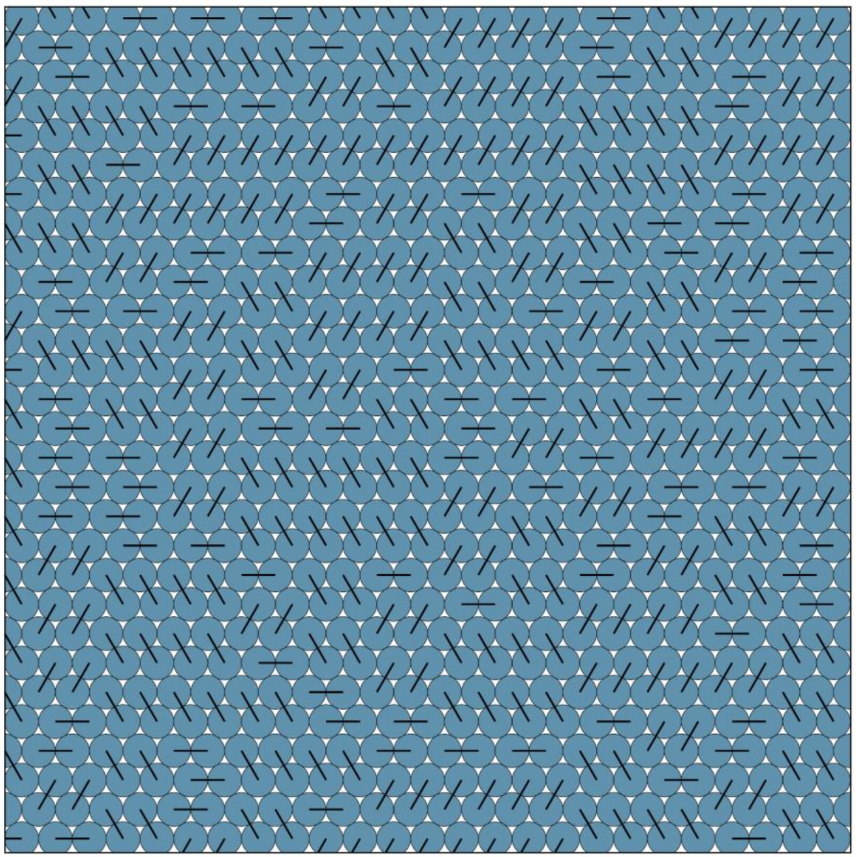
GLOBAL PARAMETERS

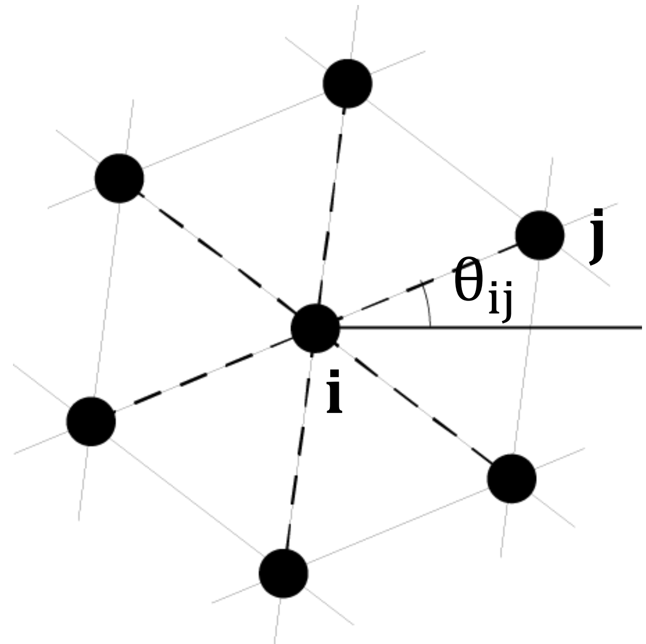
- $\Psi_6 = \frac{1}{N}\sum_{i=1}^{N} \psi_{6,i}$
- $\Gamma_6 = \frac{1}{N}\sum_{i=1}^{N} |\psi_{6,i}|$



[1] L.F. Cugliandolo, P. Digregorio, G. Gonnella, A. Suma, **arXiv**, 2016.

KTHN TRANSITIONS SCENARIO FOR 2D HARD-DISKS SYSTEMS





$$|\psi_{6,i}| = 1$$