# Topological defects in 2d passive & active matter

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Work in collaboration with

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**P. Digregorio** (Bari , Italia & Lausanne, Suisse)

**47th MECO Erice 2022**

# Results

## Summary

- **Solid** - **hexatic** à la BKT-HNY even quantitatively ($\nu$ value) and independently of the activity (Pe). *Universality.*

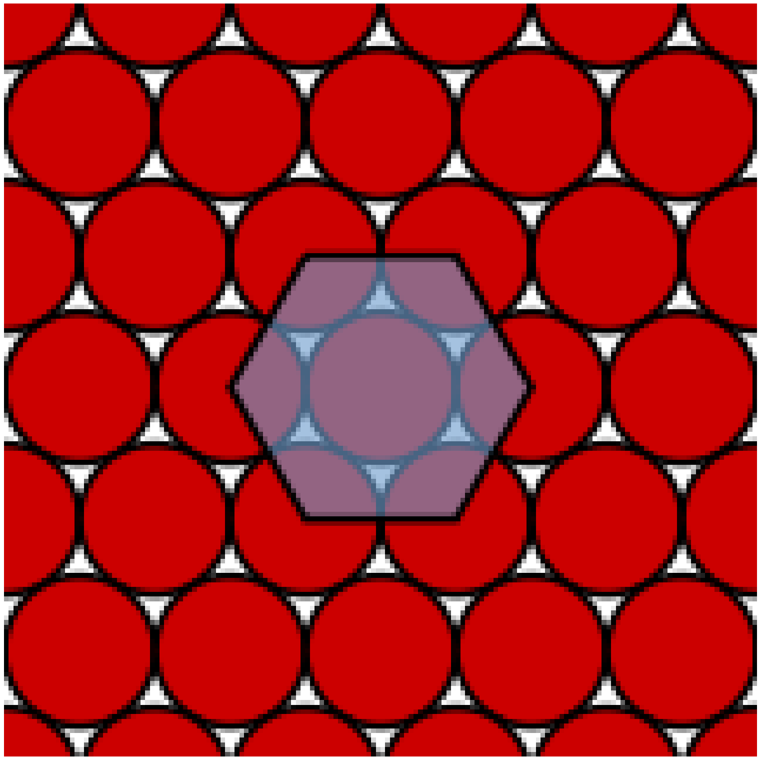
- **Hexatic** - **liquid** very few disclinations and not even free. *Breakdown of the BKT-HNY picture for all Pe (even zero).*

- Close to, but in the liquid, **percolation** of clusters of defects, with properties of uncorrelated critical percolation ($d_{\rm f}, \tau$).

- In **MIPS**, network of defects on top of the interfaces between hexatically ordered regions, interrupted by the *gas bubbles in cavitation.*

# Hard disks in $2d$

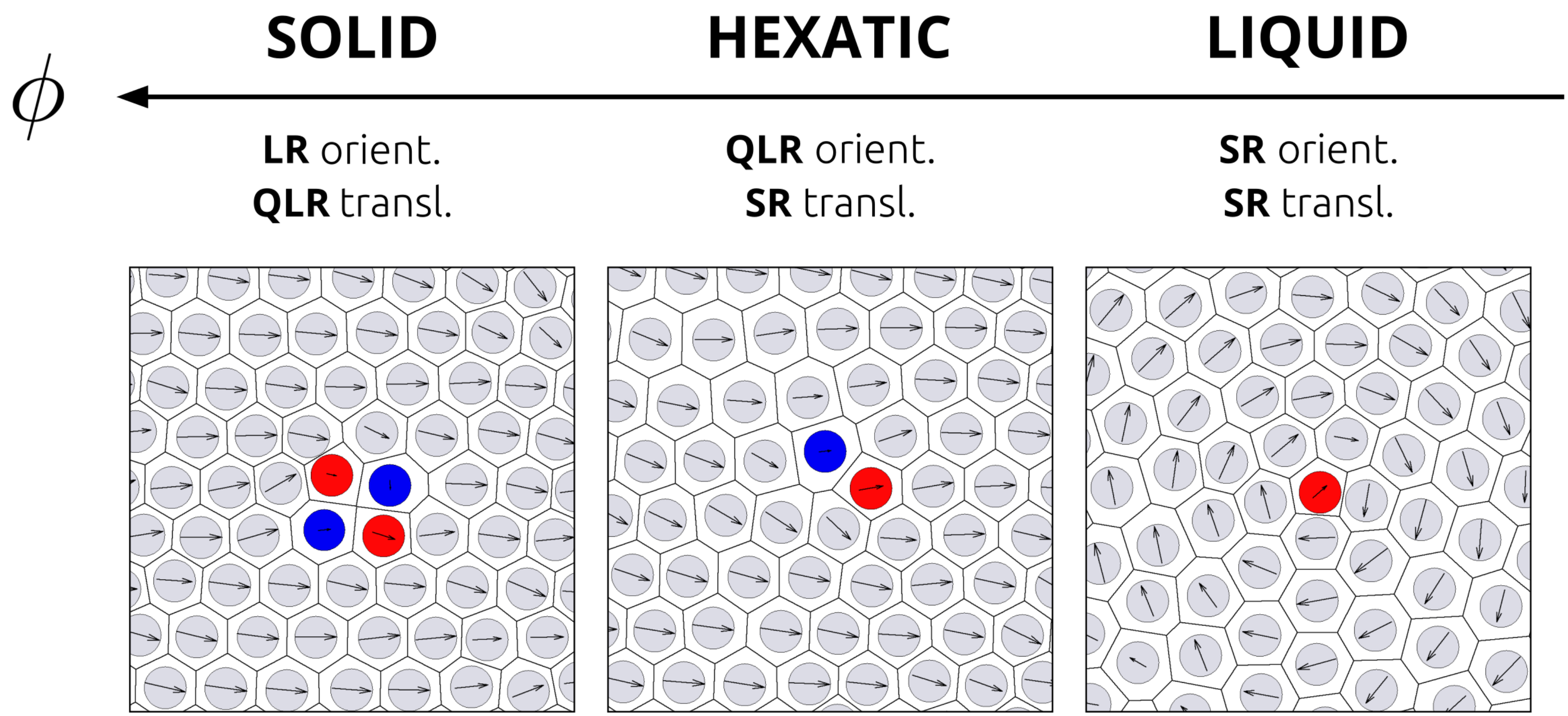
**$T = 0$ crystal at $\phi_{\rm cp}$: triangular lattice w/6 nearest neighbours**



$d = 2$ packing fraction $\phi = S_{\rm occupied}/S$. At close packing $\phi_{\rm cp} \approx 0.91$

# Freezing/Melting

## Mechanisms in $2d$ passive systems




Arrows oriented (LR) less oriented (QLR) order lost

● five neighbours ● seven neighbours

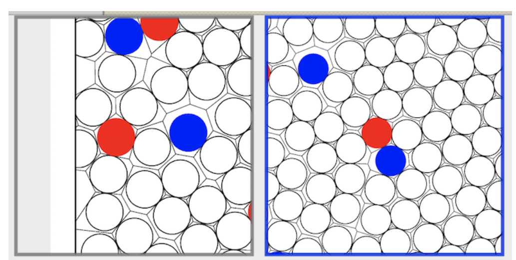
Voronoi tesselation

# BKT-HNY theory

## Transitions in passive systems

Exponential decrease of the number density of free defects at the transitions coming from the disordered sides

$$\rho_d \sim a \ \exp\left[-b\left(\frac{\phi_c}{\phi_c-\phi}\right)^{\nu}\right]$$



with $\nu = 0.37$ for dislocations at the **solid** - **hexatic** transition

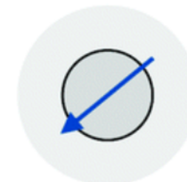
and $\nu = 0.5$ for disclinations at the **hexatic** - **liquid** transition

**Kosterlitz-Thouless, Halperin-Nelson, Young, 70s**

# Active Brownian disks

## The standard model

Active force $\mathbf{F}_{\text{act}}$ along $\mathbf{n}_i = (\cos\theta_i(t), \sin\theta_i(t))$



$$m\ddot{\mathbf{r}}_i + \gamma\dot{\mathbf{r}}_i = F_{\text{act}}\mathbf{n}_i - \boldsymbol{\nabla}_i \sum_{j(\neq i)} U_{\text{Mie}}(r_{ij}) + \boldsymbol{\xi}_i \,, \qquad \dot{\theta}_i = \eta_i \,,$$

$\mathbf{r}_i$ position of $i$th part & $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ inter-part distance, $m/\gamma \ll 1$

short-ranged repulsive truncated Mie potential $\approx (\frac{r}{\sigma_d})^{-2n} - (\frac{r}{\sigma_d})^{-n} \quad n = 32$

Zero-mean Gaussian white noises with $\xi_i^a \propto \sqrt{2\gamma k_B T}$ and $\eta_i \propto \sqrt{2D_\theta}$

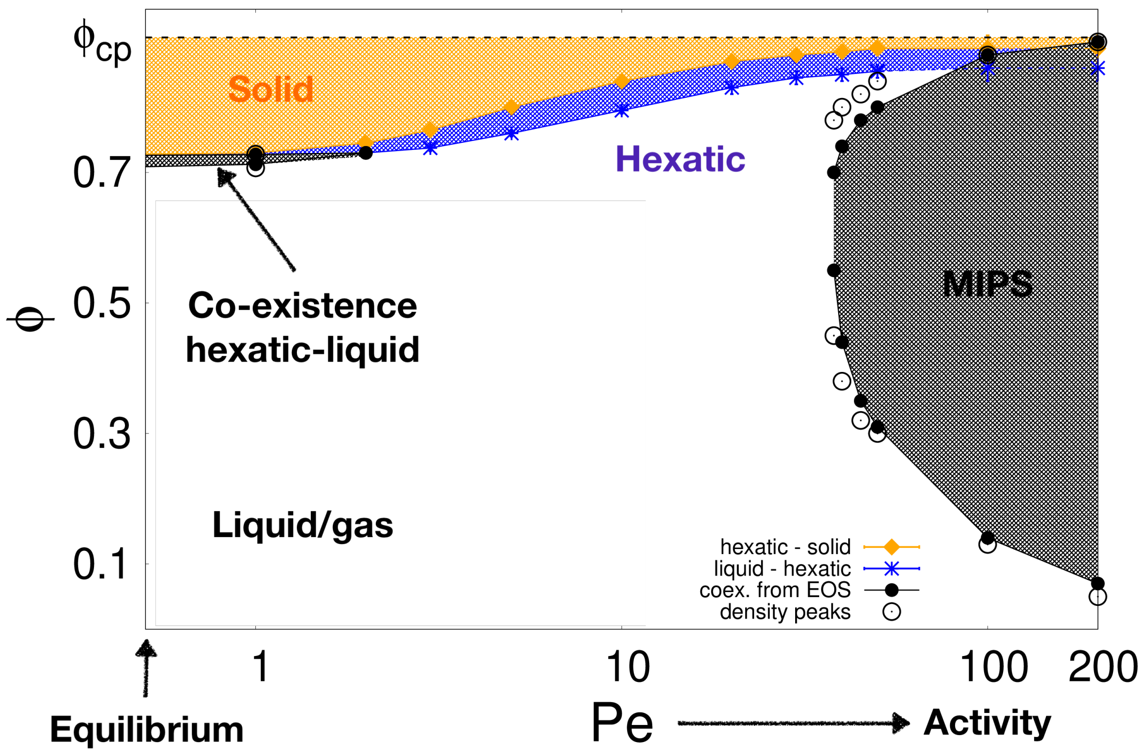
The time-scale $\tau_p = D_\theta^{-1}$ with $D_\theta = 3k_BT/(\gamma\sigma_d^2)$ sets crossover from ballistic to enhanced diffusive motion ($\approx$ persistent random walk) $\ell_p \sim \text{Pe}\,\sigma_d/3$

Péclet number Pe = $F_{\text{act}}\sigma_d/(k_BT)$ and packing fraction $\phi = \pi\sigma_d^2 N/(4S)$

**Bialké, Speck & Löwen, PRL 108, 168301 (2012), Fily & Marchetti, *ibid* 235702.**

# Active hard disks

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




Motility induced

phase separation

gas & dense

**Cates & Tailleur**

**Ann. Rev. CM 6, 219 (2015)**

**Farage, Krinninger & Brader**

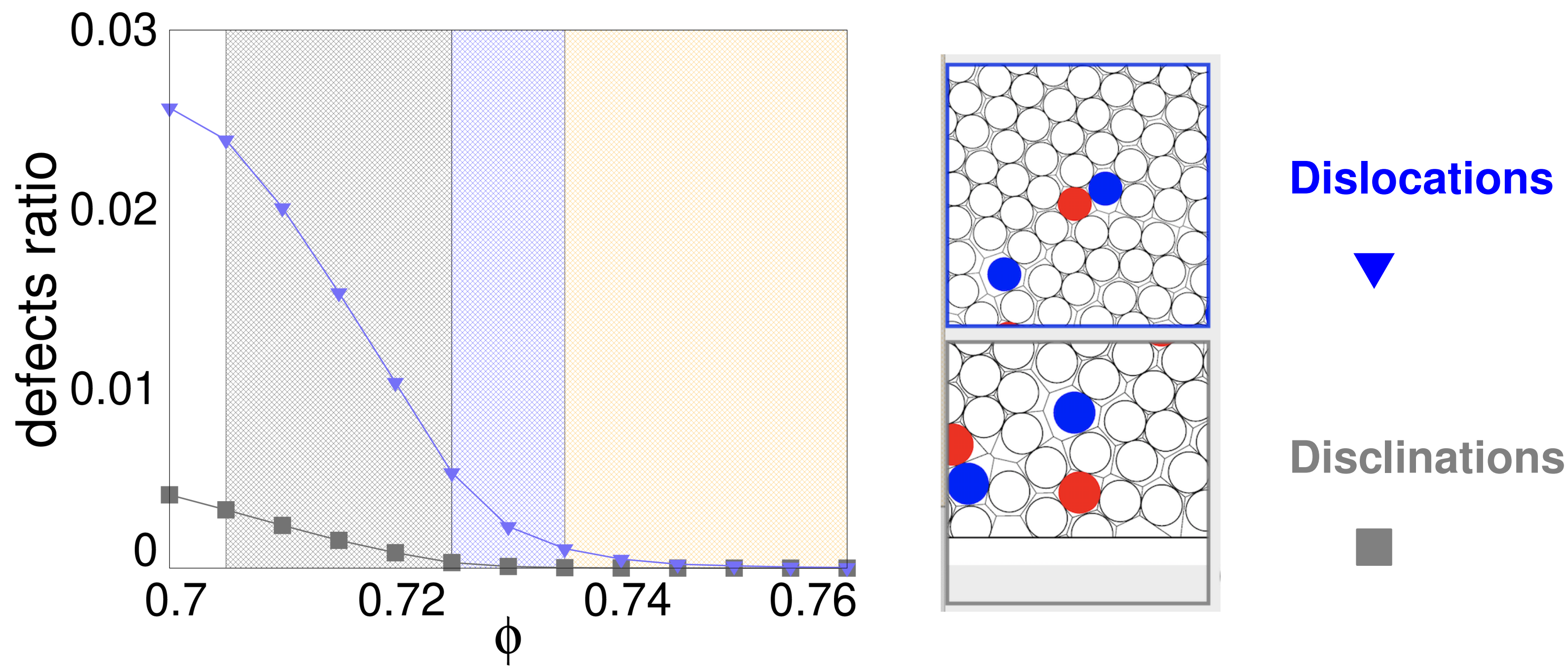
**PRE 91, 042310 (2015)**

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

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

# Unbinding of defects

**Solid-hexatic transition & the emergence of the liquid at Pe = 0**




**Dislocations** ▼ unbind at the **solid** - **hexatic** transition as in BKT-HNY

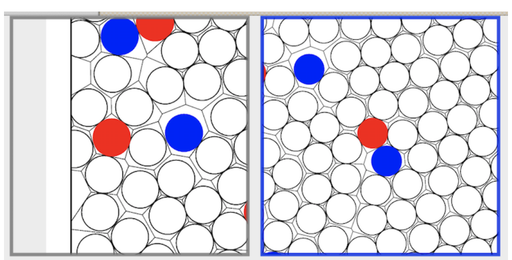
**Disclinations** ■ unbind when the **liquid** appears in the co-existence region

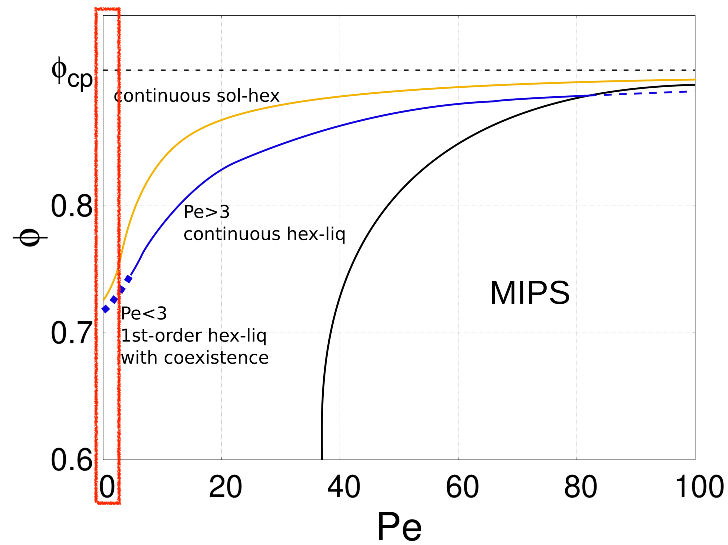
# BKT-HNY theory

**Solid-hexatic transition & the emergence of the liquid at Pe = 0**

In the passive case : Exponential decrease of the number density of free defects at the transition coming from the disordered side

$$\rho_d \sim a \ \exp\left[-b\left(\frac{\phi_c}{\phi_c-\phi}\right)^{\nu}\right]$$



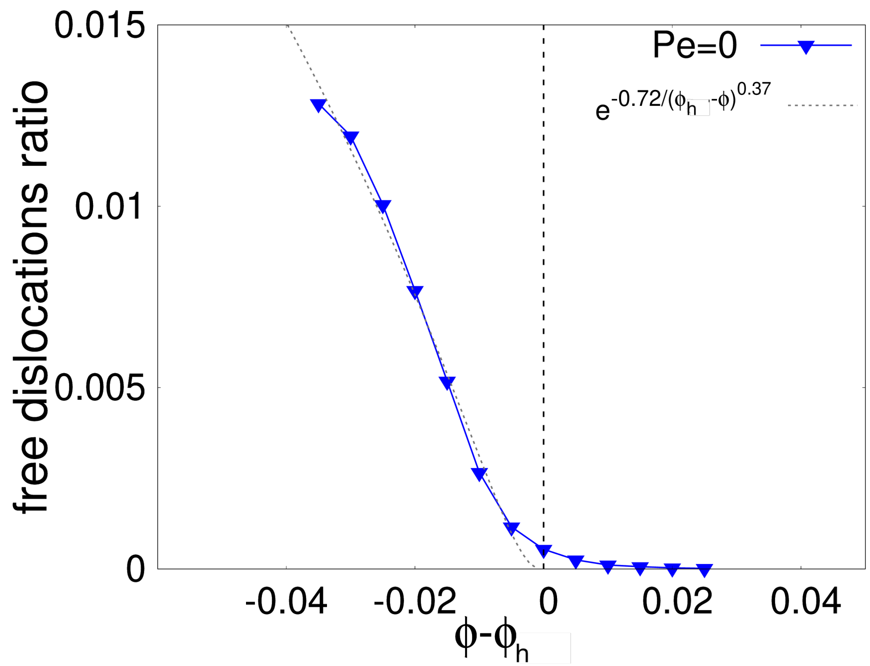



with $\nu = 0.37$ for dislocations at the **solid** - **hexatic** transition

and $\nu = 0.5$ for disclinations at the **hexatic** - **liquid** transition

# Dislocations

## At the Pe = 0 solid-hexatic transition



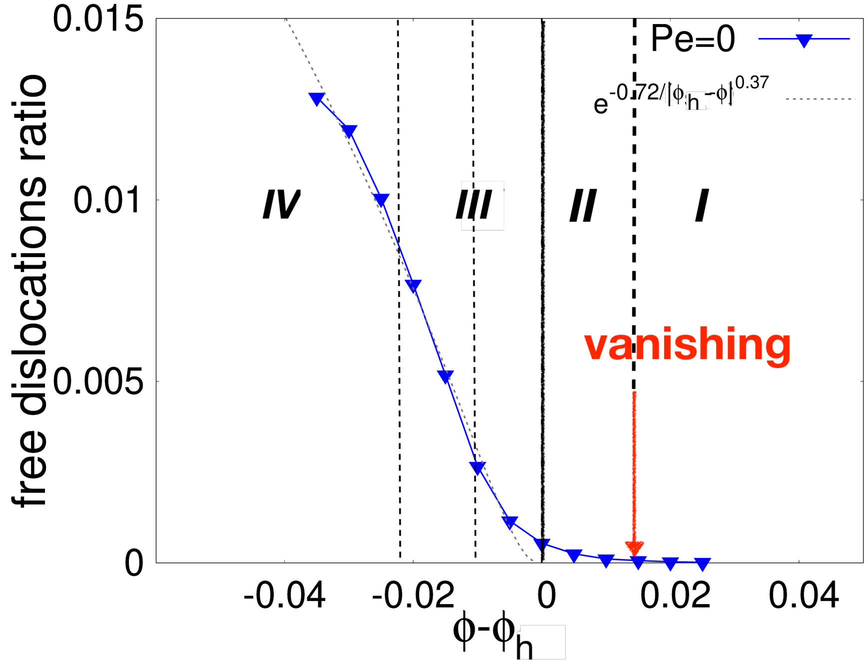

**Dislocations** ▼ unbind close to the **solid** - **hexatic** transition

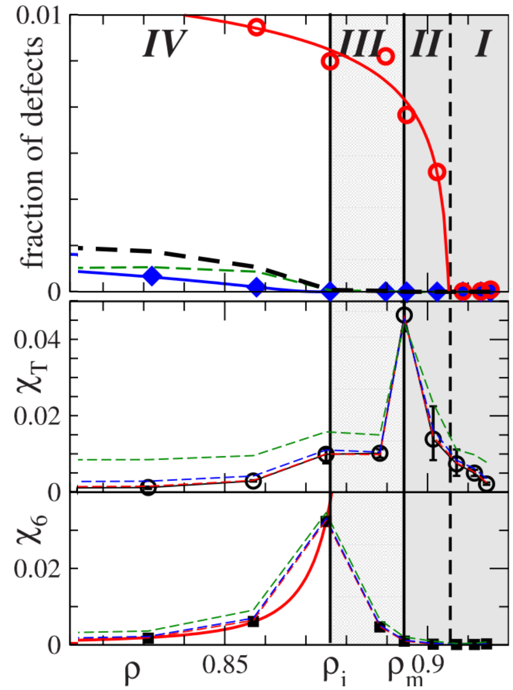
$\phi_h$ from the measurement of correlation functions and other observables,

Dotted line exponential form with $\nu = 0.37$ and $\rho_d$ forced to vanish at $\phi_h$

# Dislocations

## At the Pe = 0 solid-hexatic transition




Do **dislocations** ▼ really unbind at the **solid** - **hexatic** transition $\phi_h$ ?

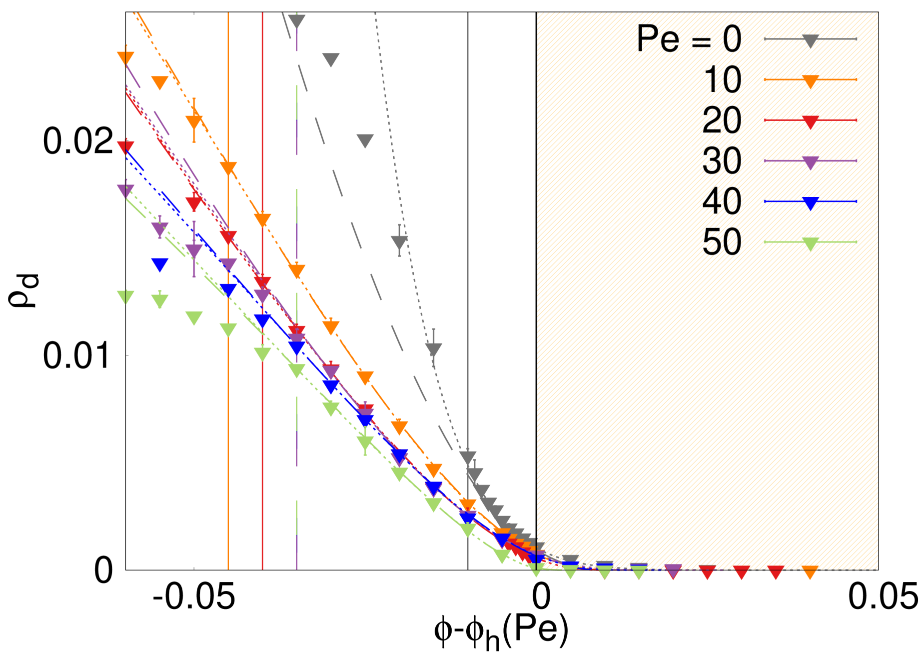
Even experimentally $\phi_c > \phi_h$ & $\rho_d(\phi > \phi_c)$ is much larger than for us

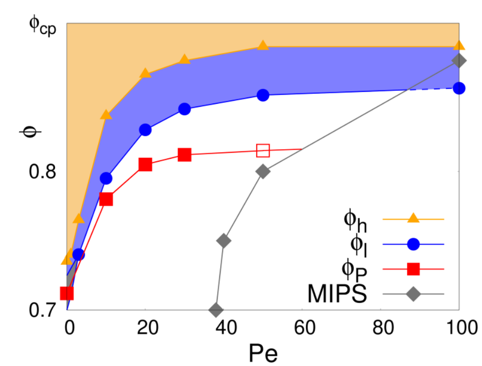
though $\nu = 0.37$ is acceptable (effect of parameter $b$ quite large)

**Han, Ha, Alsayed, & Yodh, PRE 77, 041406 (2008)** Short-range & repulsive microgel

# Dislocations

**At the solid-hexatic transition in the active case $\nu = 0.37$**




Four ($\phi_c, \nu, a, b$ dotted) vs. three ($\phi_c, \nu = 0.37, a, b$ dashed) parameter fits on data in the hexatic & solid phases only. Criteria to support $\nu = 0.37$:

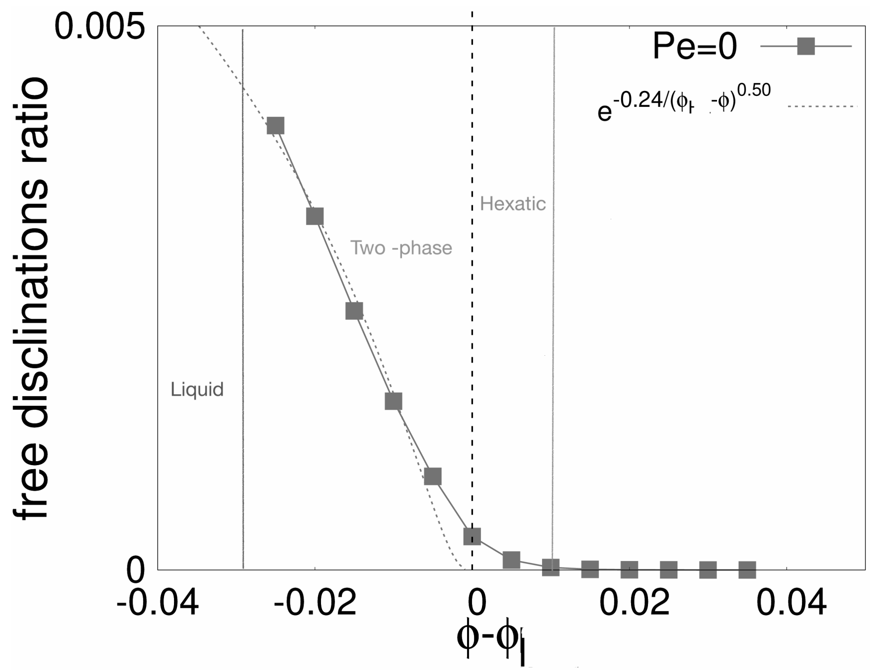
– $\chi^2$

– not crazy values for $a$, $b$ but crazy values for $\nu$ if let to be fitted

– the closeness between $\phi_c$ and $\phi_h$ *cfr.* **Batrouni et al** for $2d$XY

# Disclinations

**At Pe = 0 close to the 1st order hexatic - liquid transition**

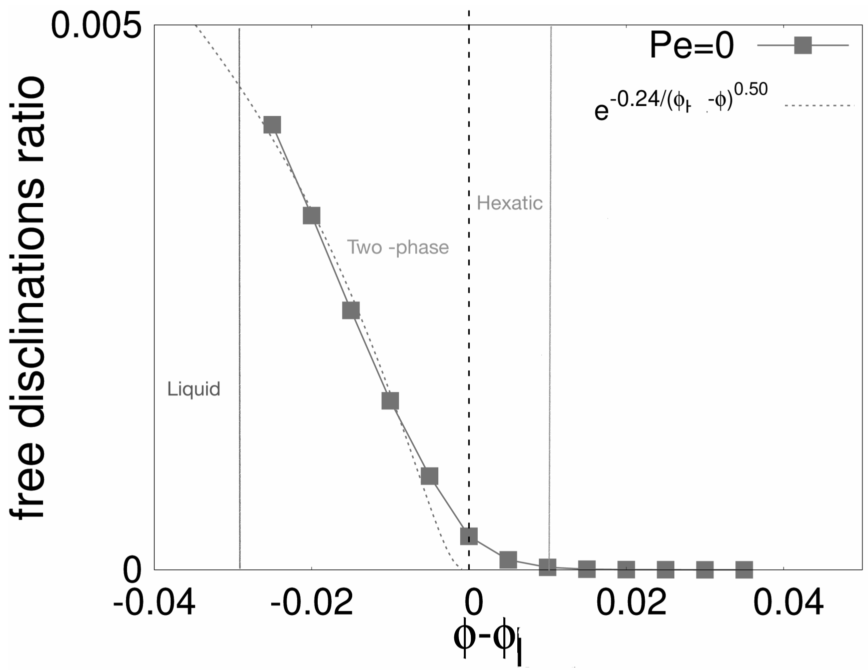


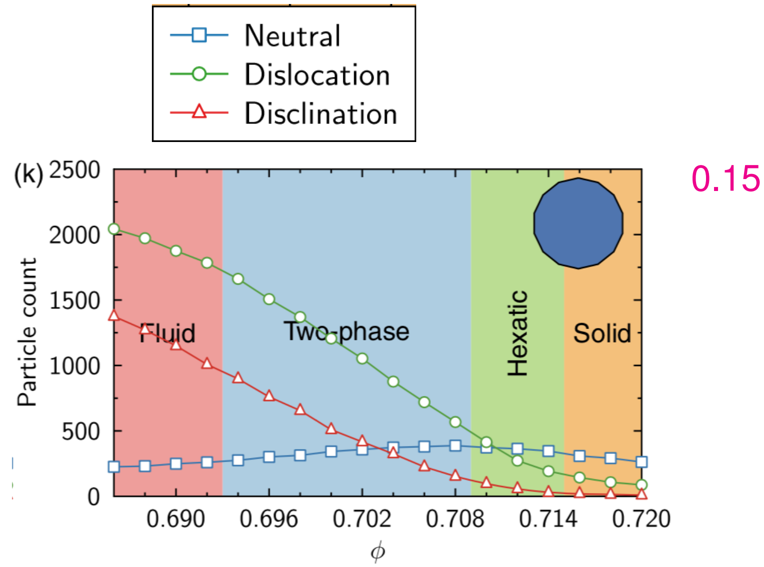

**Disclinations** ■ unbind close to where the **liquid** appears in co-existence at $\phi_l$

Dotted line with $\nu = 0.5$ and $\rho_d$ forced to vanish at $\phi_l$, the upper limit of the co-existence region

# Disclinations

## At Pe = 0 close to the 1st order hexatic-liquid




**Disclinations** ■ unbind close to where the **liquid** appears in co-existence at $\phi_l$

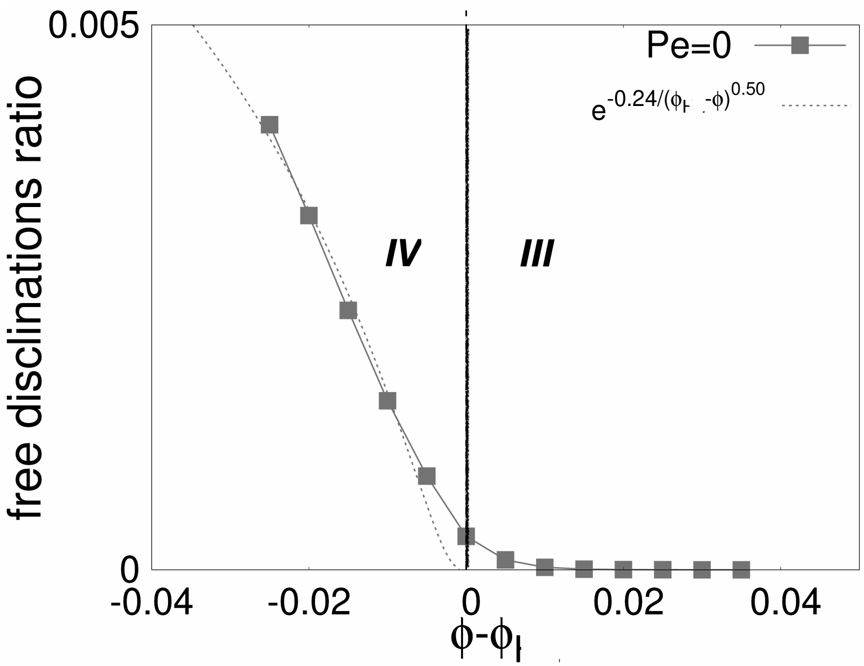
Dotted line with $\nu = 0.5$ forced to vanish at $\phi_l$ (upper co-existence)

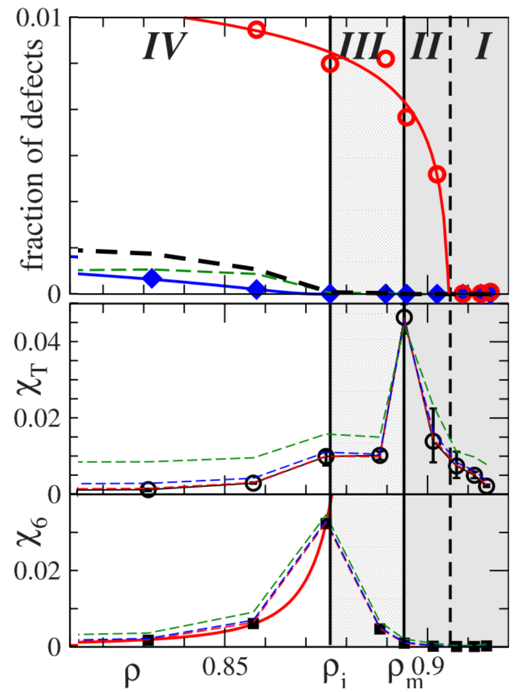
**Anderson, Antonaglia, Millan, Engel & Glotzer, PRX 7, 021001 (2017)** MC hard

$N = 16384 \implies \rho_d \sim 0.01$ at $\phi_l$ also more than us but we use $N = 260000$

# Disclinations

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




**Disclinations** ■ unbind close to where the **liquid** appears in co-existence at $\phi_l$

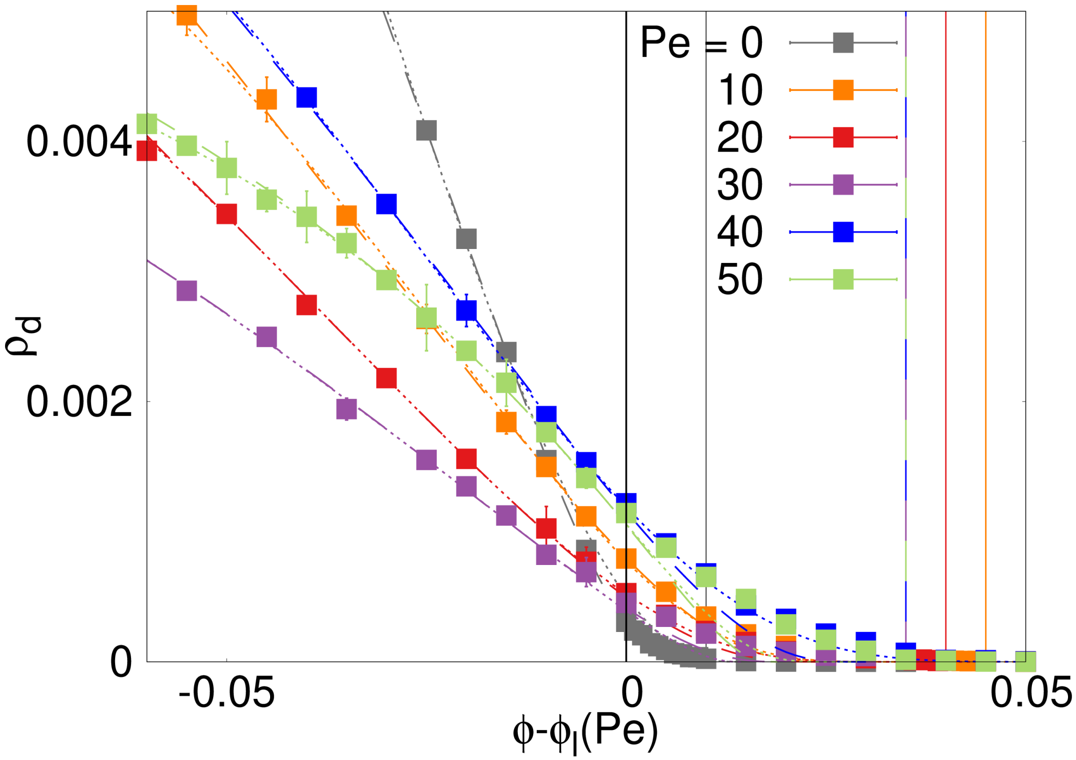
Dotted line with $\nu = 0.5$ forced to vanish at $\phi_l$

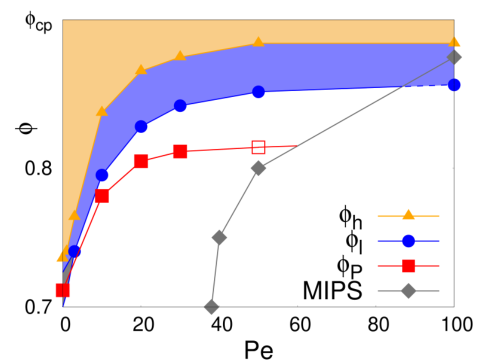
**Han, Ha, Alsayed, & Yodh, PRE 77, 041406 (2008)** Short-range & repulsive microgel

Do not identify a 1st order transition

# Disclinations

## At the hexatic - liquid transition at all Pe




Messier than for dislocations

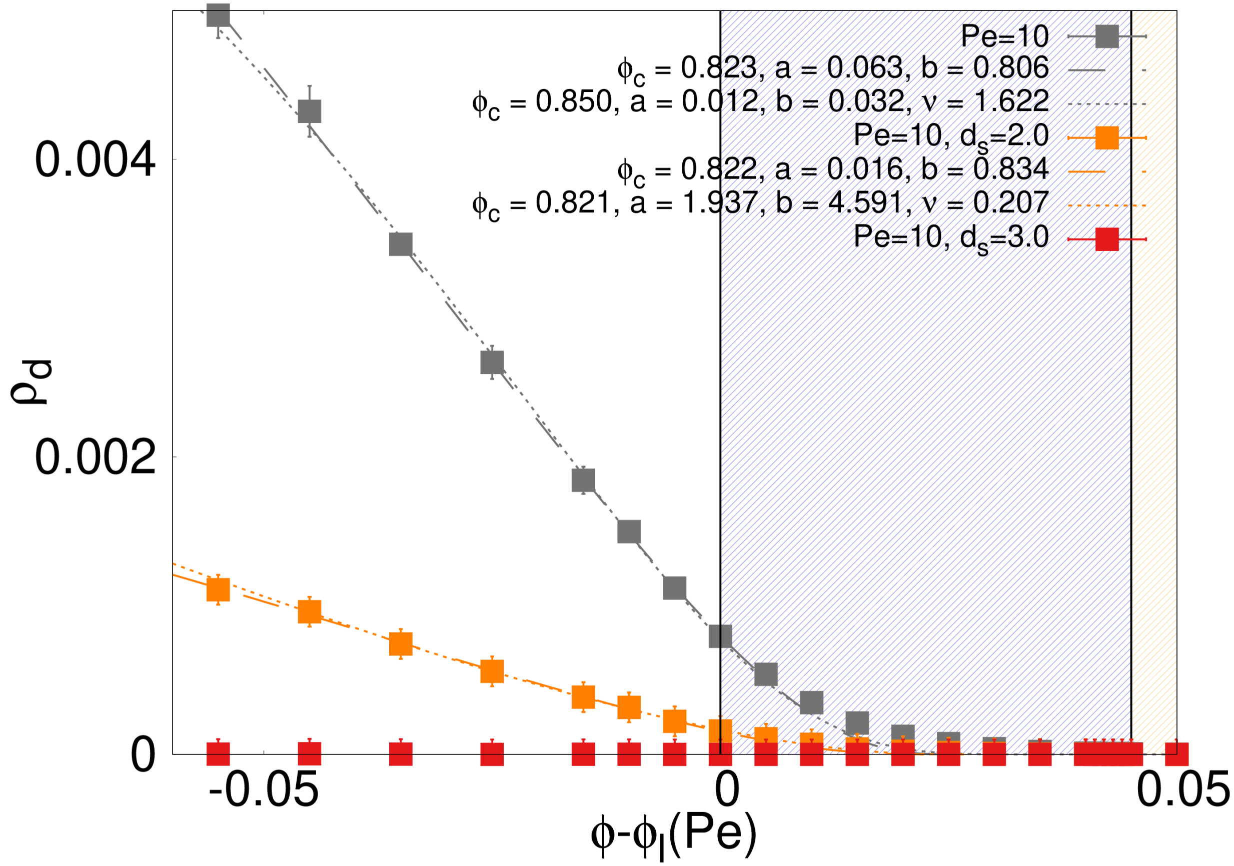
$\phi_l$ upper limit of co-existence at Pe = 0 & critical **hexatic** - **liquid** at Pe $\neq 0$

Dotted and broken lines show three ($a$, $b$, $\phi_c$) and four (also $\nu$) parameter fits.

Vertical lines are at $\phi_h$ (end of the hexatic phase)

# Disclinations

**Effect of coarse-graining : basically, no free disclinations**




Pe = 10

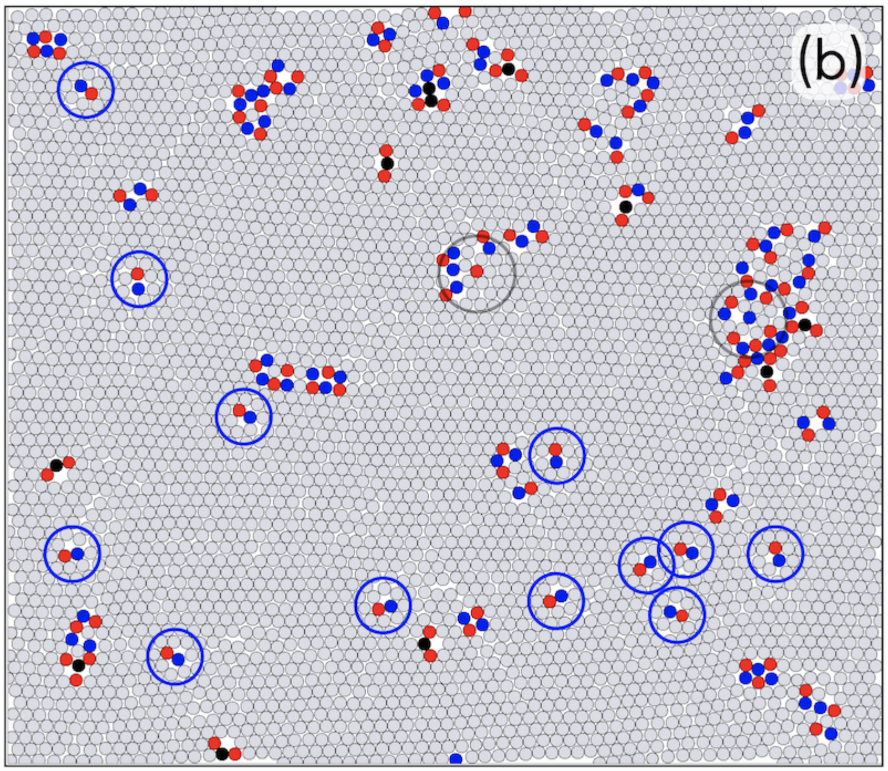
$\phi_l = 0.795$

| $d_s$ | $\phi_c$ |
|---|---|
| 0 | 0.823 |
| 2 | 0.822 |
| 3 | 0.821 |

No more

# Disclinations

**At the hexatic - liquid transition $\phi_l$ at all Pe**



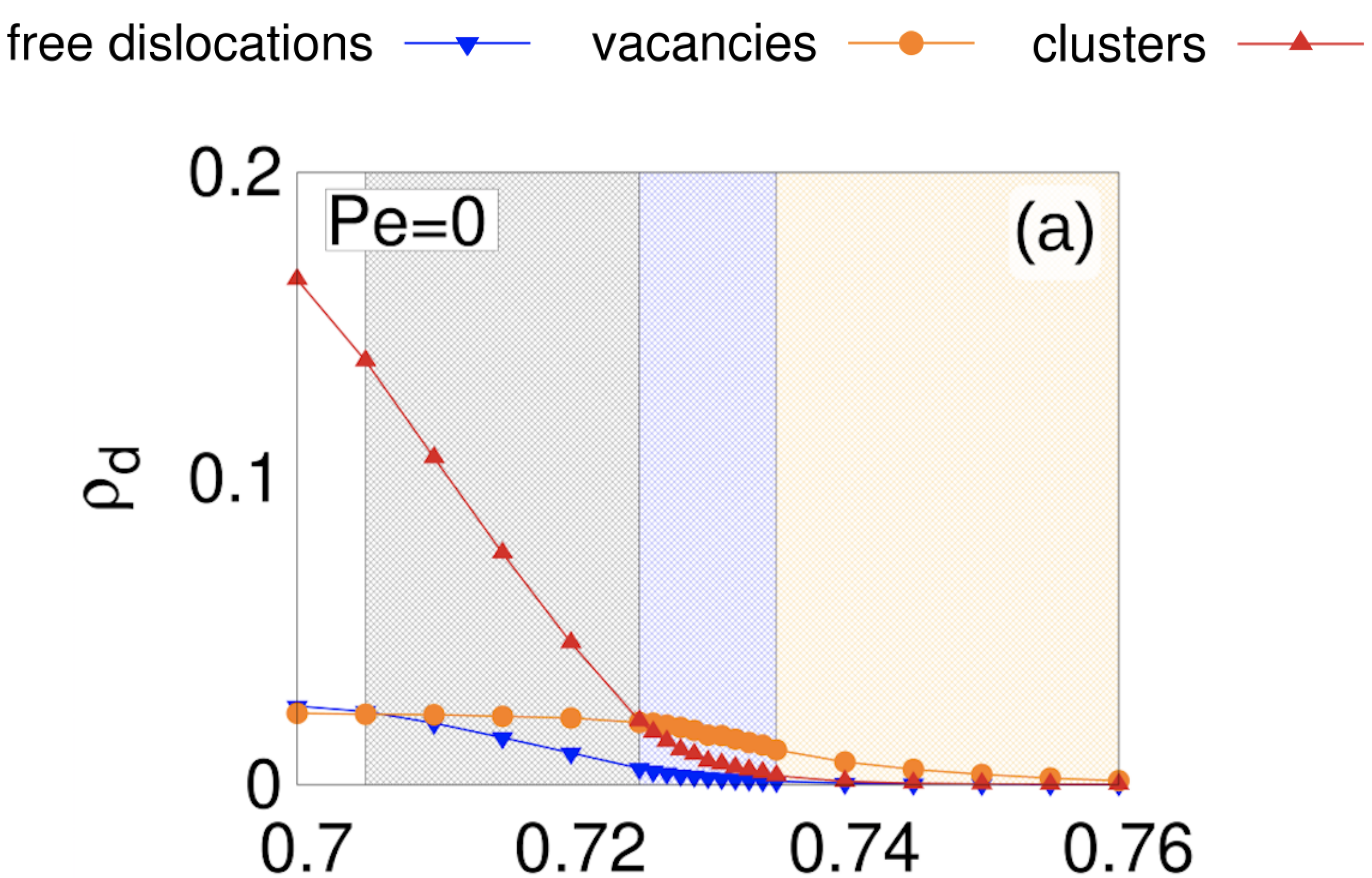

dislocations

disclinations

Very few disclinations, and always very close to other defects, so **not free**

# Clusters

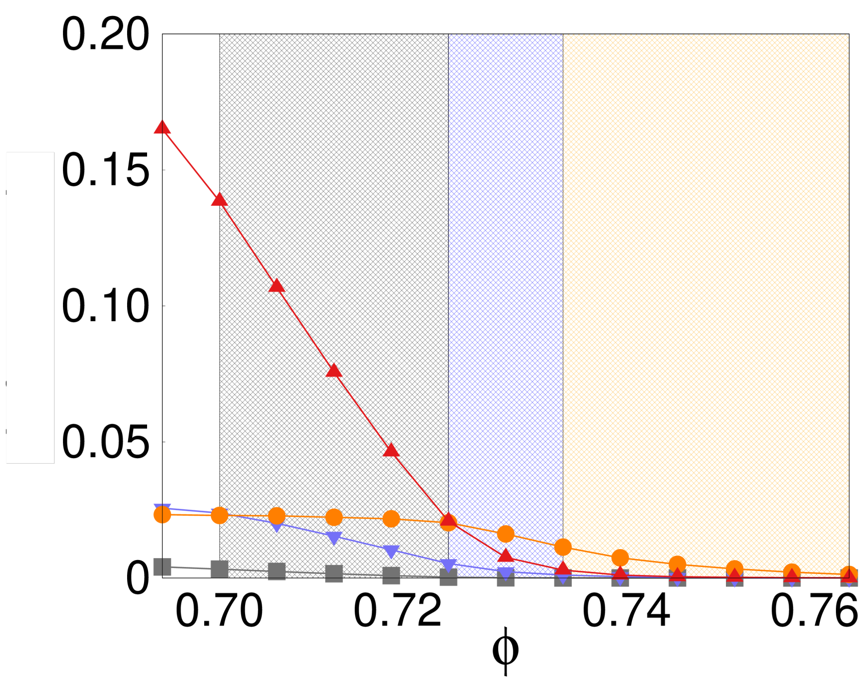
**Close to the hexatic - liquid transition**

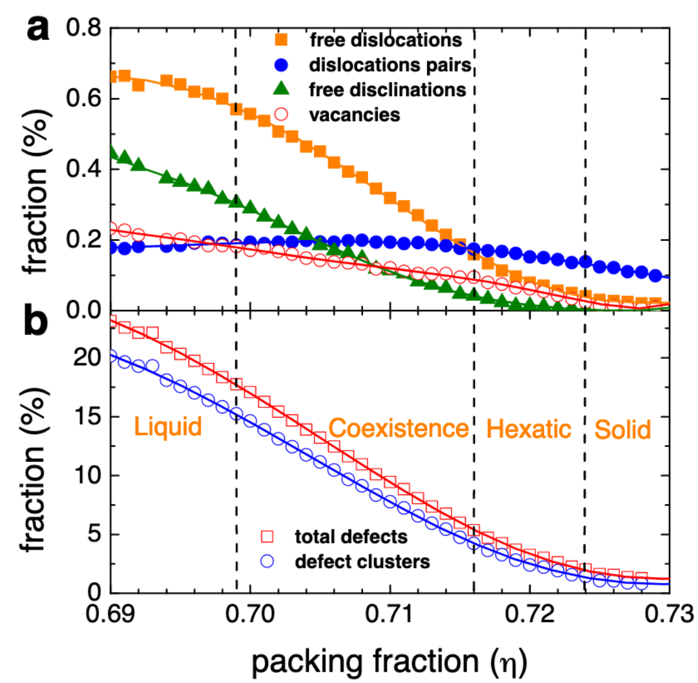



As soon as the liquid appears in co-existence, **defects in clusters dominate**

# Clusters

**Within the co-existence region at Pe = 0**




**Clusters ▲** proliferate within the co-existence region

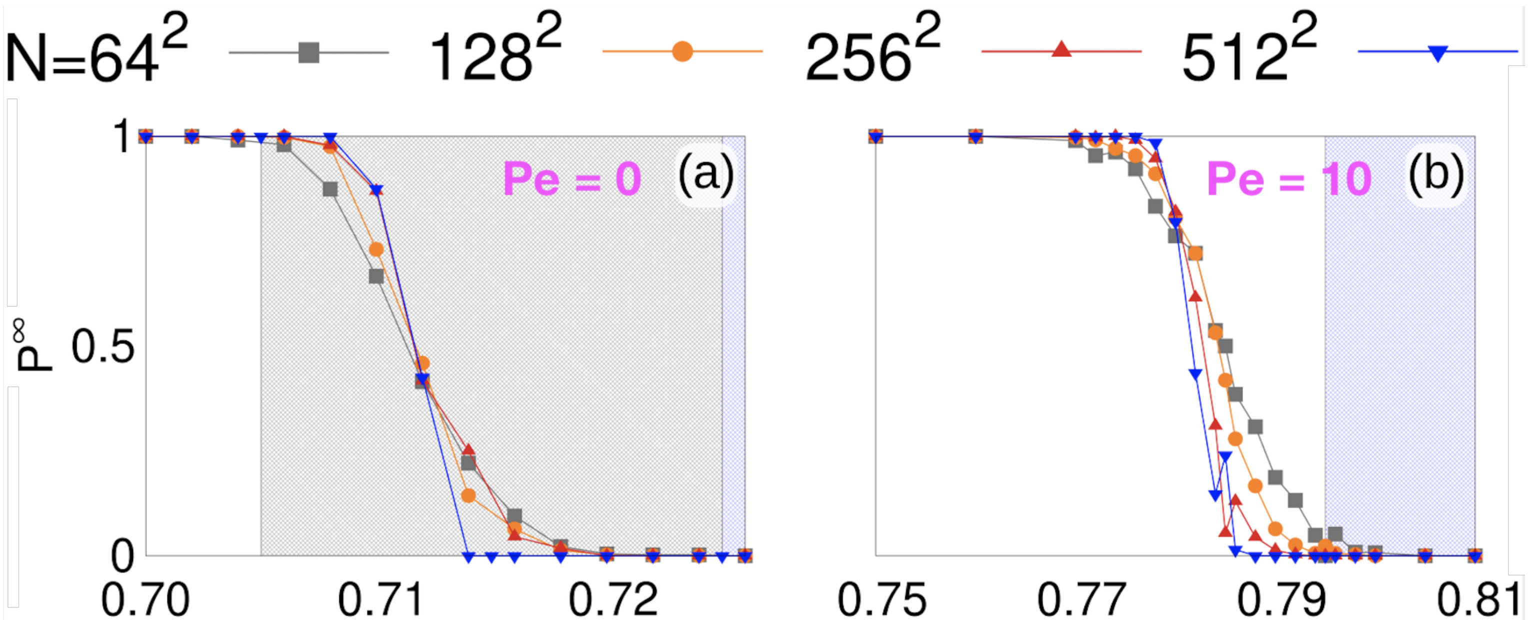
**Vacancies ●** remain approximately constant within the co-existence region

**Qi, Gantapara & Dijkstra, Soft Matter 10, 5419 (2014)** Event drive MD hard disks

# Clusters

## Percolation : finite size scaling

The probability of there being a wrapping cluster ($d_s = 3\sigma_d$)

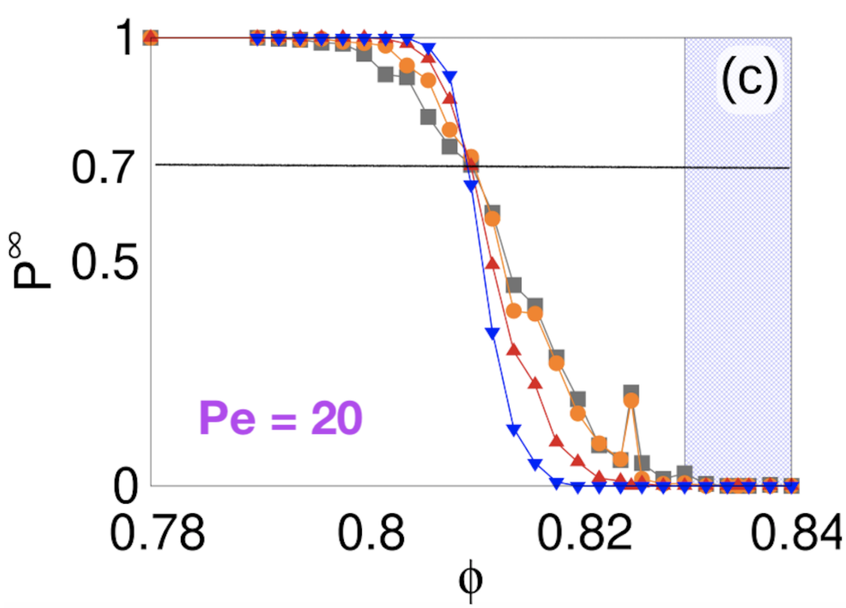


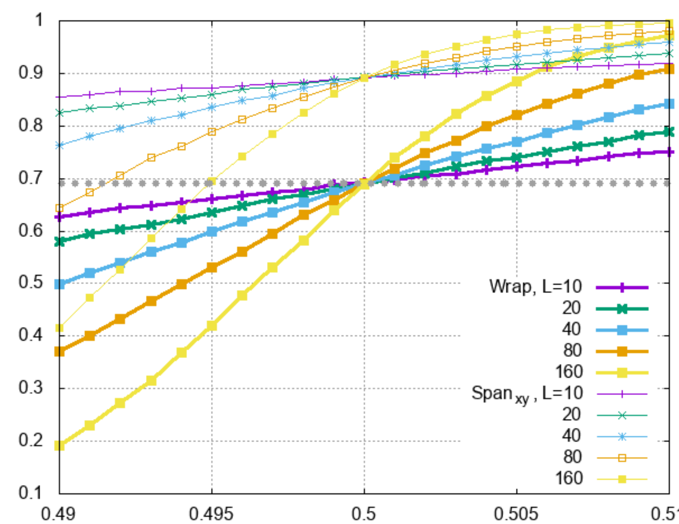

At $\phi_p$ close but below the $\phi_l$ where the **liquid** first appears.

# Clusters

## Percolation : finite size scaling

The probability of there being a wrapping cluster ($d_s = 3\sigma_d$)



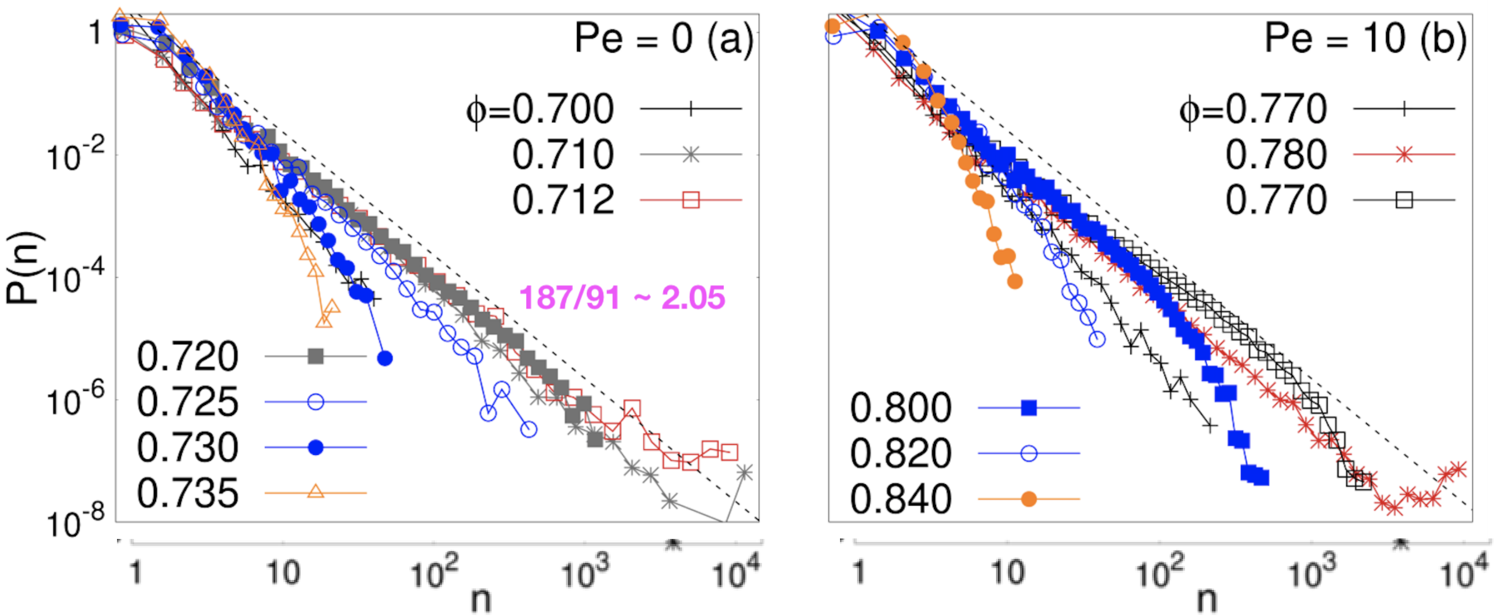

At $\phi_p$ close but below the $\phi_l$ where the **liquid** first appears.

Critical site percolation **M. Picco**

# Clusters

## Percolation : cluster size distribution

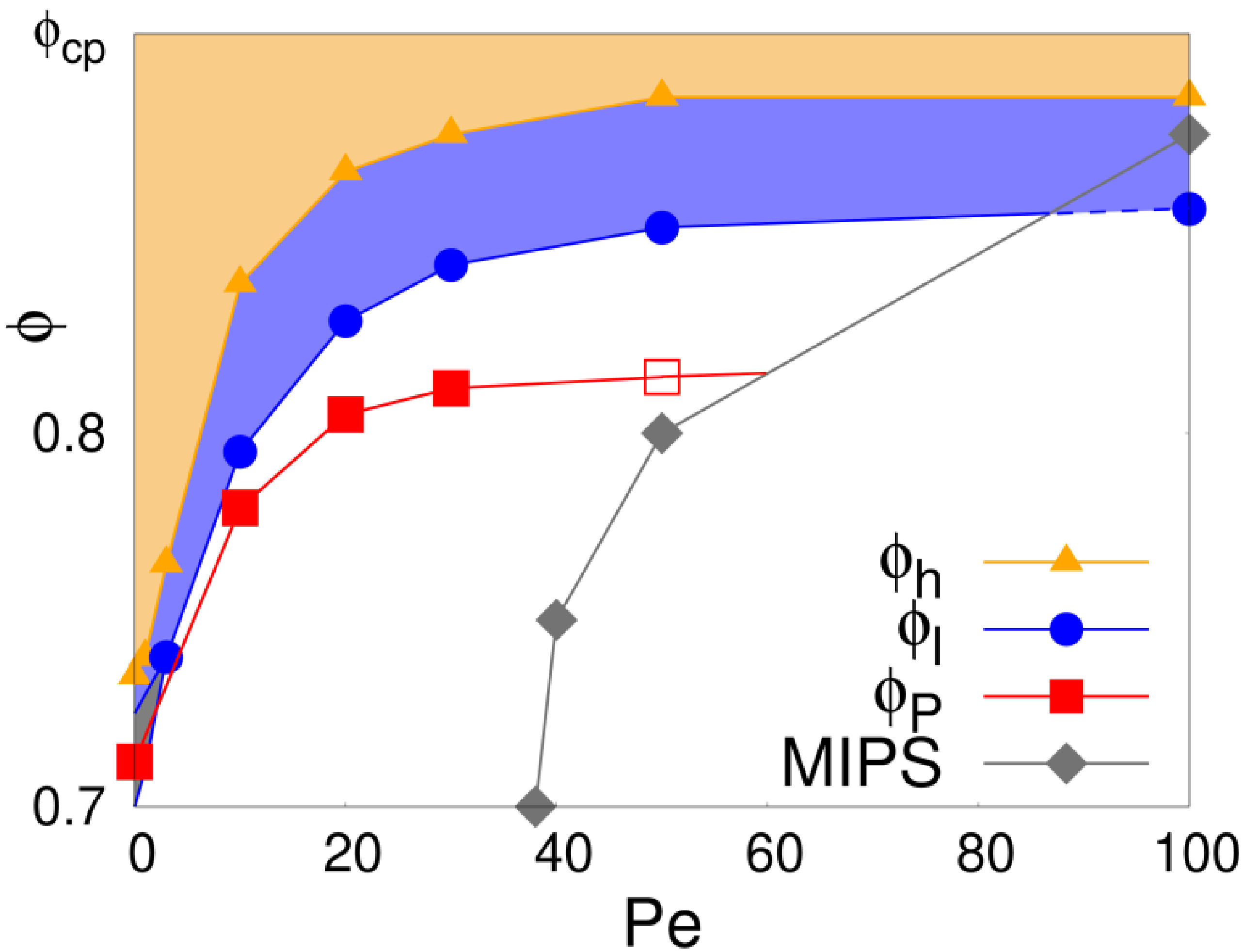
$P(n) \sim n^{-\tau}$ with $\tau = 1 + d/d_f = 187/91 \sim 2.05$




Red data points at $\phi_p$ within the co-existence region at Pe = 0, and slightly below $\phi_l$ at Pe $\neq 0$.

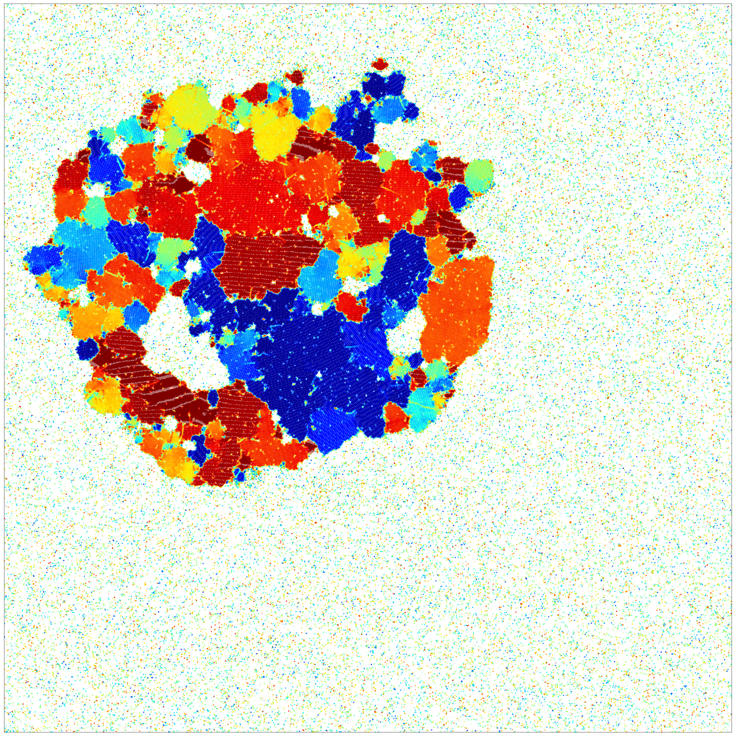
# Clusters

**Percolation : the critical curve**



# MIPS

## Stationary state



Dense/dilute separation[1]

For low packing fraction $\phi$

a single round droplet.

A mosaic of different

hexatic orders[2] with

gas bubbles[2,3,4]

Defects ?

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

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

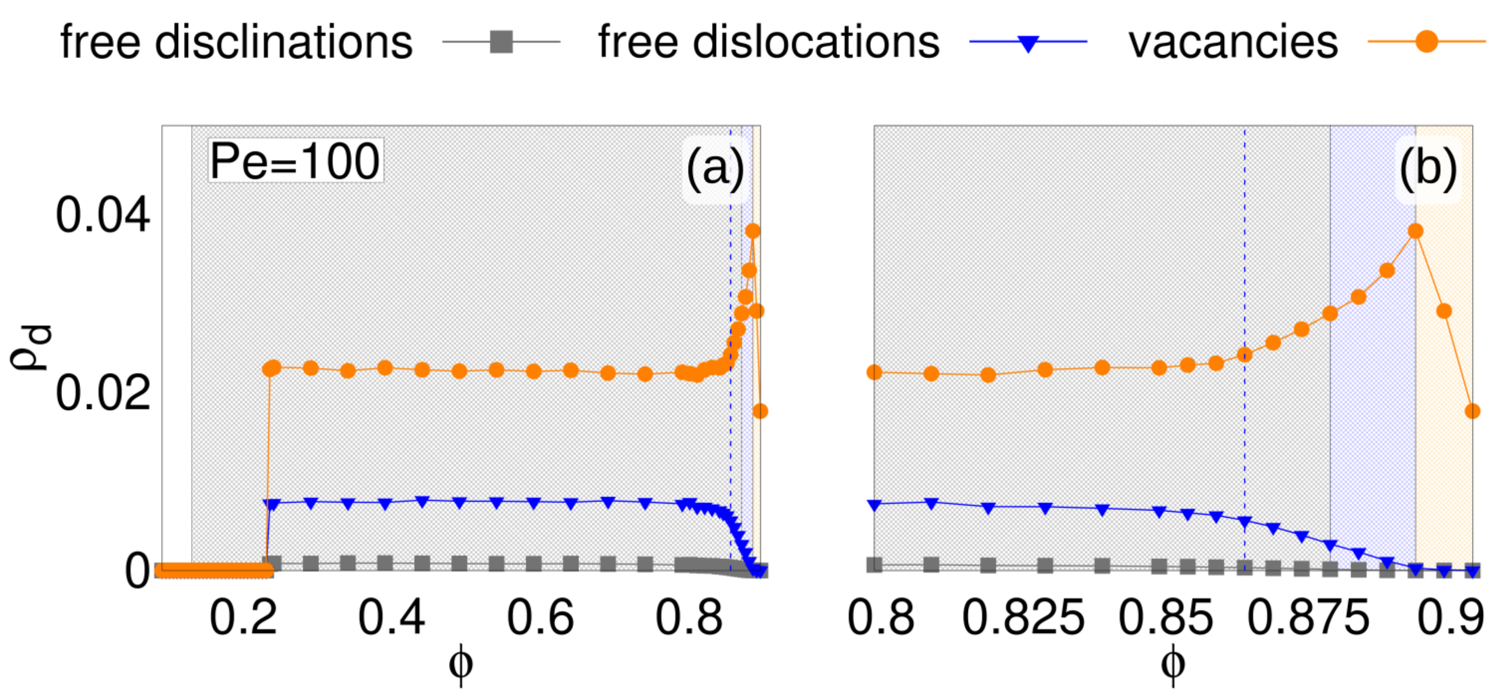
[3] **Tjhung, Nardini & Cates, PRX 8, 031080 (2018)**

[4] **Shi, Fausti, Chaté, Nardini & Solon, PRL 125, 168001 (2020)**

# MIPS

## Point-like defects - constant density at fixed Pe

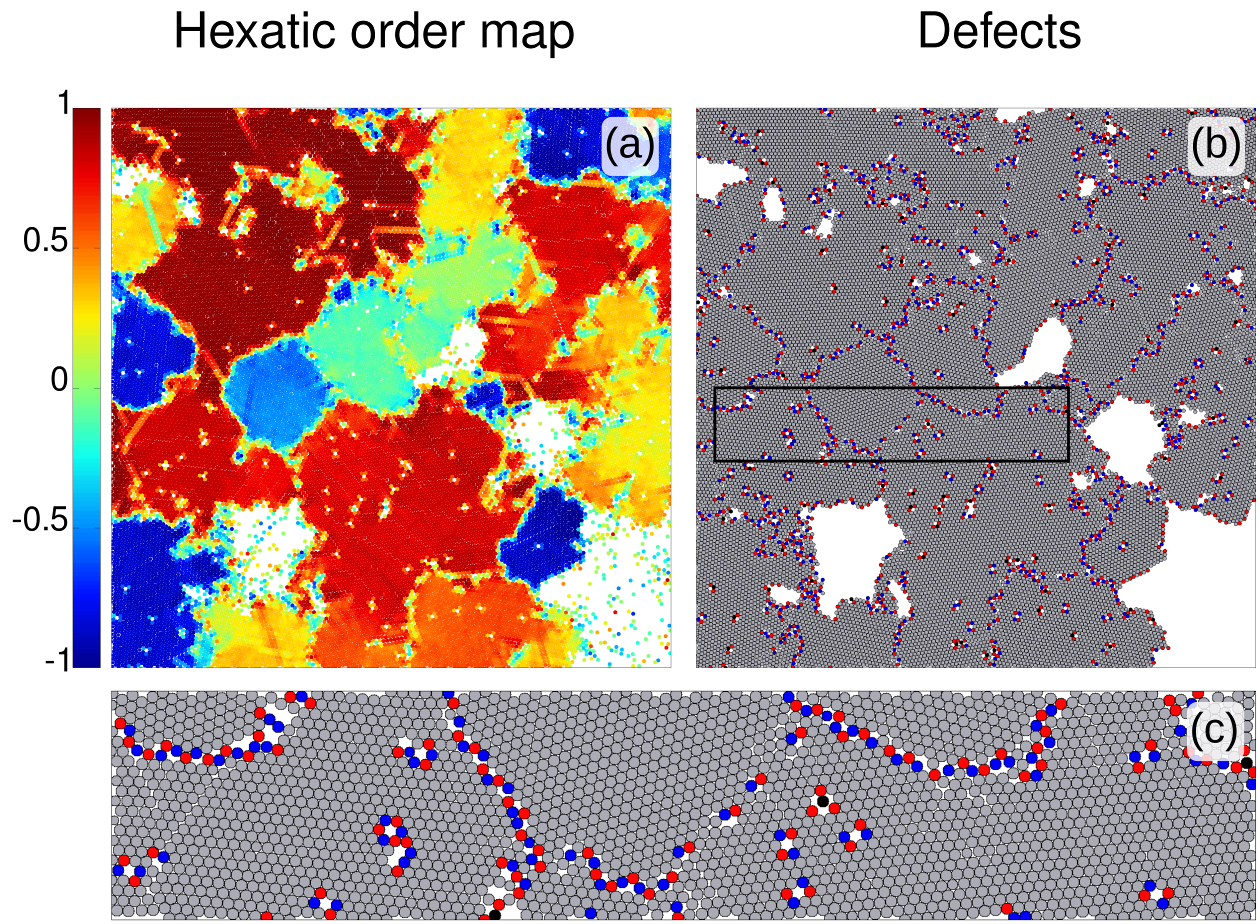
A zoom over high $\phi$




Densities $\rho_d$ are quite independent of $\phi$ in the bulk of the **MIPS** phase

# MIPS

## Defects along boundaries between hexatically ordered patches




Zoom over the rectangular selection

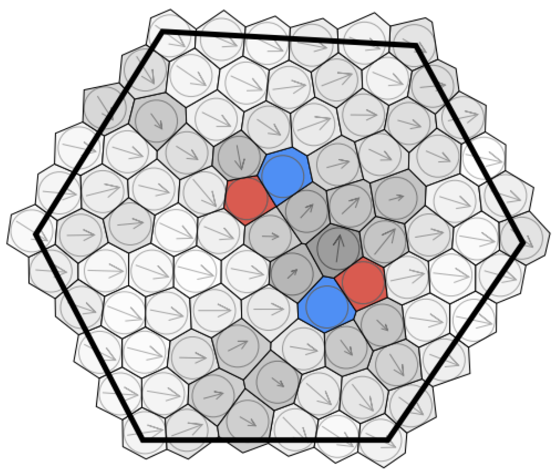
# Results

## Summary

- **Solid** - **hexatic** à la BKT-HNY even quantitatively ($\nu$) and independently of Pe. Universality.
- **Hexatic** - **liquid** very few disclinations and not even free. Breakdown of the BKT-HNY picture for all Pe.
- Close to, but in the liquid, **percolation** of clusters of defects, with properties of uncorrelated critical percolation ($d_{\mathrm{f}}, \tau$).
- In **MIPS**, network of defects on top of the interfaces between hexatically ordered regions, interrupted by the gas bubbles in cavitation.

# Defects

## Unbinding of dislocations: from the solid to the hexatic



A bound pair of dislocations

A free dislocation

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

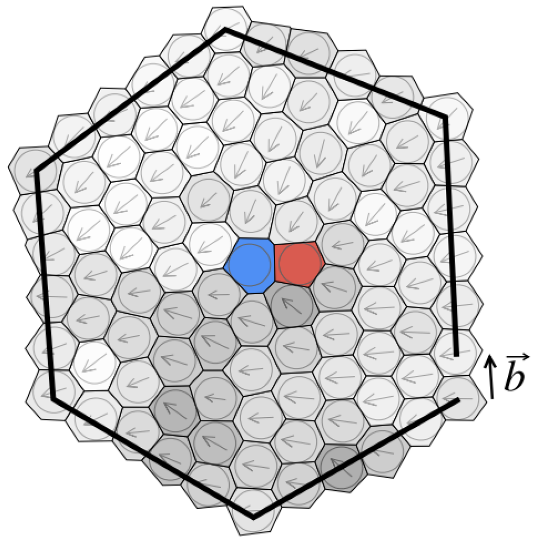
The **blue** disks have seven neighbours and the **red** ones have five.

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

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

# Defects

## Unbinding of dislocations : from the solid to the hexatic




A bound pair of dislocations

A free dislocation

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

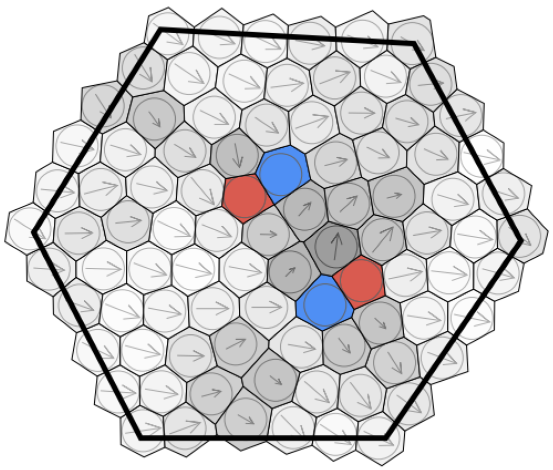
The **blue** disks have seven neighbours and the **red** ones have five.

**On the right image** : the external path fails to close, no perfect hexagon.

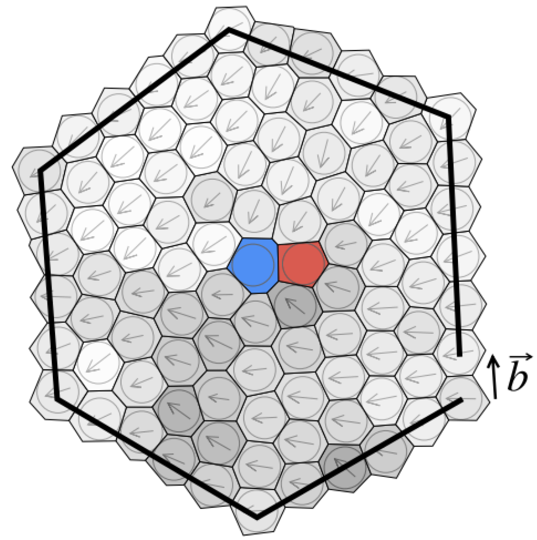
The effect of the defects spreads & kills translation order : **hexatic** phase.

# Defects

## Unbinding of dislocations: from the solid to the hexatic



A bound pair of dislocations




A free dislocation

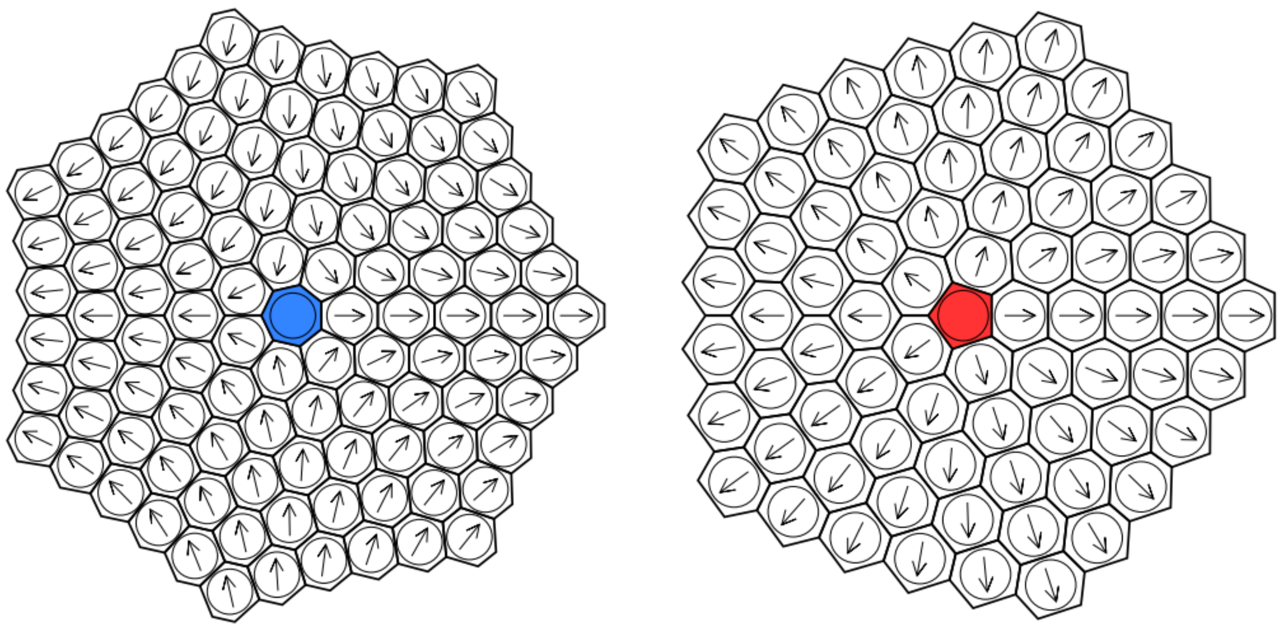
In the crystal the centres of the disks form a triangular lattice

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

The underlying arrows are roughly aligned in both images. The hexatic phase keeps quasi long-range orientational order.

# Defects

## Unbinding of disclinations: from the hexatic to the liquid



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**.

# Dislocations

## At the solid-hexatic transition at all Pe

$\nu = 0.37$

| Pe | $\nu$ | $a$ | $b$ | $\phi_c$ | $\phi_h$ | $\chi^2/\text{ndf}$ |
|---|---|---|---|---|---|---|
| 0 | 0.37 | 8 | 2 | 0.75 | 0.735 | 1.61 |
| 10 | 0.37 | 1.5 | 1.61 | 0.853 | 0.840 | 2.76 |
| 20 | 0.37 | 1.2 | 1.59 | 0.883 | 0.870 | 1.34 |
| 30 | 0.37 | 2 | 1.9 | 0.897 | 0.880 | 2.08 |
| 40 | 0.37 | 0.81 | 1.47 | 0.898 | 0.885 | 0.791 |
| 50 | 0.37 | 0.38 | 1.17 | 0.895 | 0.890 | 0.493 |

✓

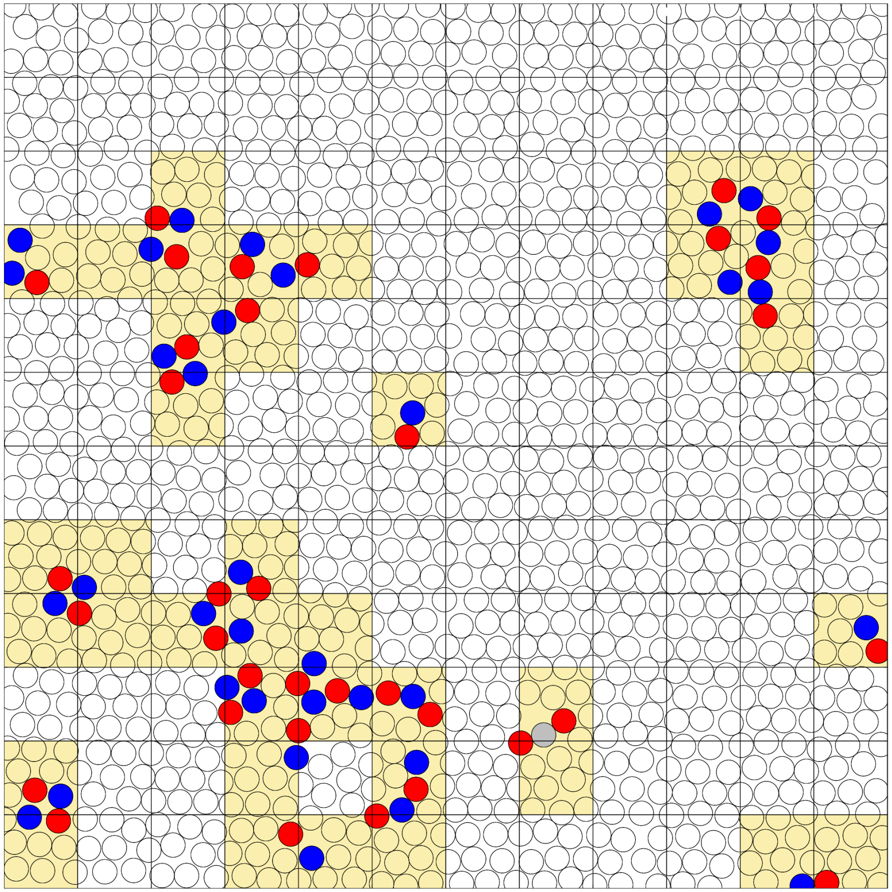
$\nu$ free

| Pe | $\nu$ | $a$ | $b$ | $\phi_c$ | $\phi_h$ | $\chi^2/\text{ndf}$ |
|---|---|---|---|---|---|---|
| 0 | 9 | 13 | 0.002 | 1 | 0.735 | 0.920 |
| 10 | 0.6 | 0.4 | 0.7 | 0.857 | 0.840 | 2.89 |
| 20 | 0.3 | 5 | 3 | 0.881 | 0.870 | 1.39 |
| 30 | 0.8 | 0.2 | 0.3 | 0.909 | 0.880 | 2.08 |
| 40 | 0.7 | 0.2 | 0.4 | 0.90 | 0.885 | 0.924 |
| 50 | 0.2 | 7 | 3 | 0.892 | 0.890 | 0.461 |

✗

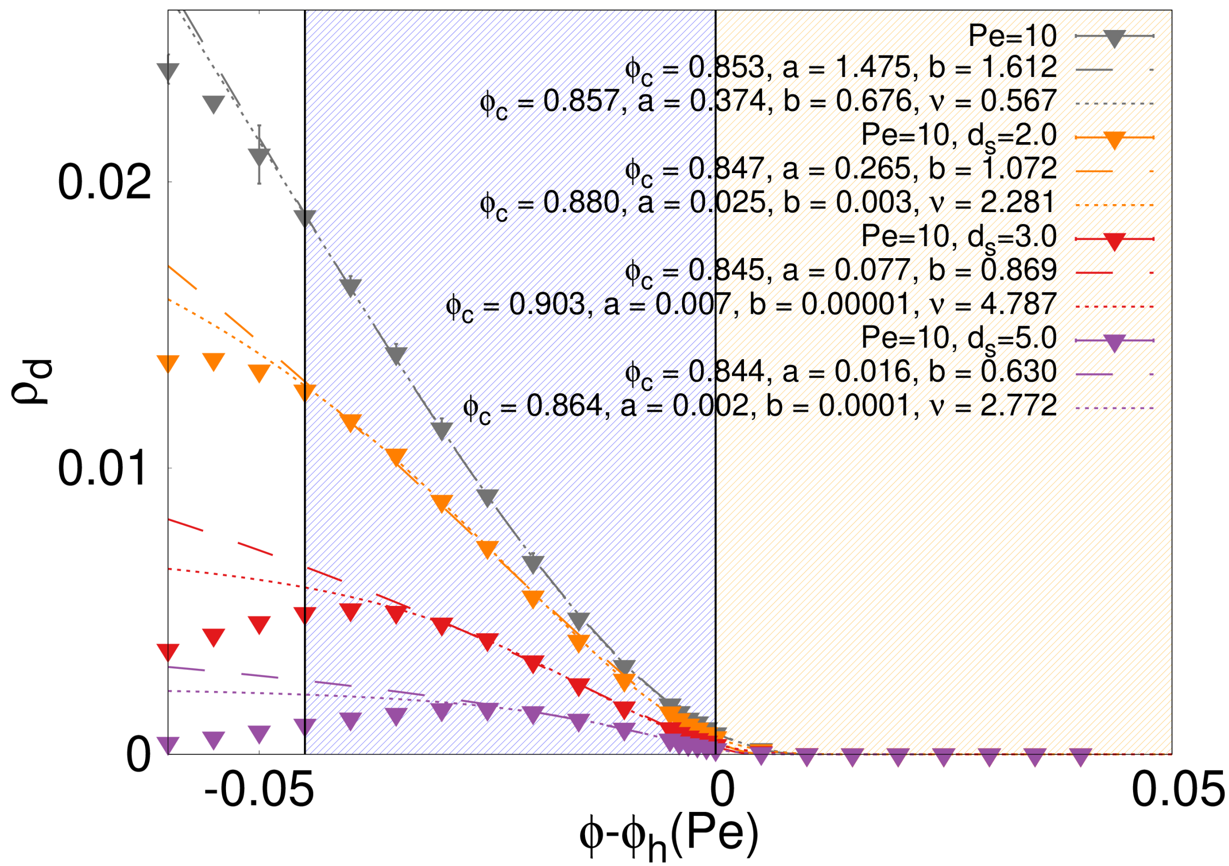
# Coarse graining

**Square boxes with $\ell = 3\sigma_d$**



# Dislocations

## Effect of coarse-graining: the notion of freedom




Pe = 10

$\phi_h = 0.84$

$\phi_c = 0.853 \;\; (0)$

$\phi_c = 0.847 \;\; (2)$

$\phi_c = 0.845 \;\; (3)$

$\phi_c = 0.844 \;\; (5)$

# Disclinations

**At the hexatic - liquid transition at all Pe**

$\nu = 0.50$

| Pe | $\nu$ | $a$ | $b$ | $\phi_c$ | $\phi_l$ | $\chi^2$/ndf |
|---|---|---|---|---|---|---|
| 0 | 0.5 | 0.072 | 0.62 | 0.734 | 0.725 | 0.430 |
| 10 | 0.5 | 0.06 | 0.81 | 0.823 | 0.795 | 1.09 |
| 20 | 0.5 | 0.05 | 0.8 | 0.857 | 0.830 | 0.710 |
| 30 | 0.5 | 0.025 | 0.64 | 0.866 | 0.845 | 0.895 |
| 40 | 0.5 | 0.053 | 0.71 | 0.880 | 0.850 | 0.809 |
| 50 | 0.5 | 0.016 | 0.41 | 0.874 | 0.855 | 0.233 |

✓

| $\phi_h$ |
|---|
| 0.735 |
| 0.840 |
| 0.870 |
| 0.880 |
| 0.885 |
| 0.890 |

$\nu$ free

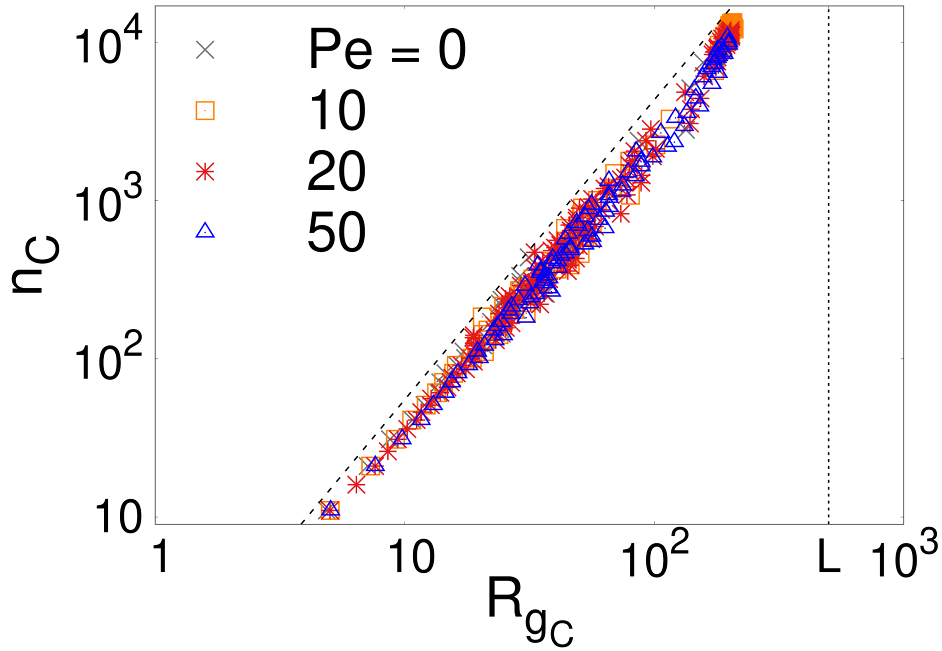
| Pe | $\nu$ | $a$ | $b$ | $\phi_c$ | $\phi_l$ | $\chi^2$/ndf |
|---|---|---|---|---|---|---|
| 0 | 0.4 | 0.4 | 2 | 0.7 | 0.725 | 3.24 |
| 10 | 2 | 0.012 | 0.03 | 0.85 | 0.795 | 0.859 |
| 20 | 1 | 0.02 | 0.2 | 0.9 | 0.830 | 0.858 |
| 30 | 0.3 | 0.09 | 2 | 0.86 | 0.845 | 0.965 |
| 40 | 2 | 0.013 | 0.01 | 0.96 | 0.850 | 0.661 |
| 50 | 0.9 | 0.008 | 0.1 | 0.88 | 0.855 | 0.288 |

✗

# Clusters

## Percolation : fractality

Binned scatter plot of the mass of each cluster $n_C$ against its radius of gyration $R_{g\,C}$

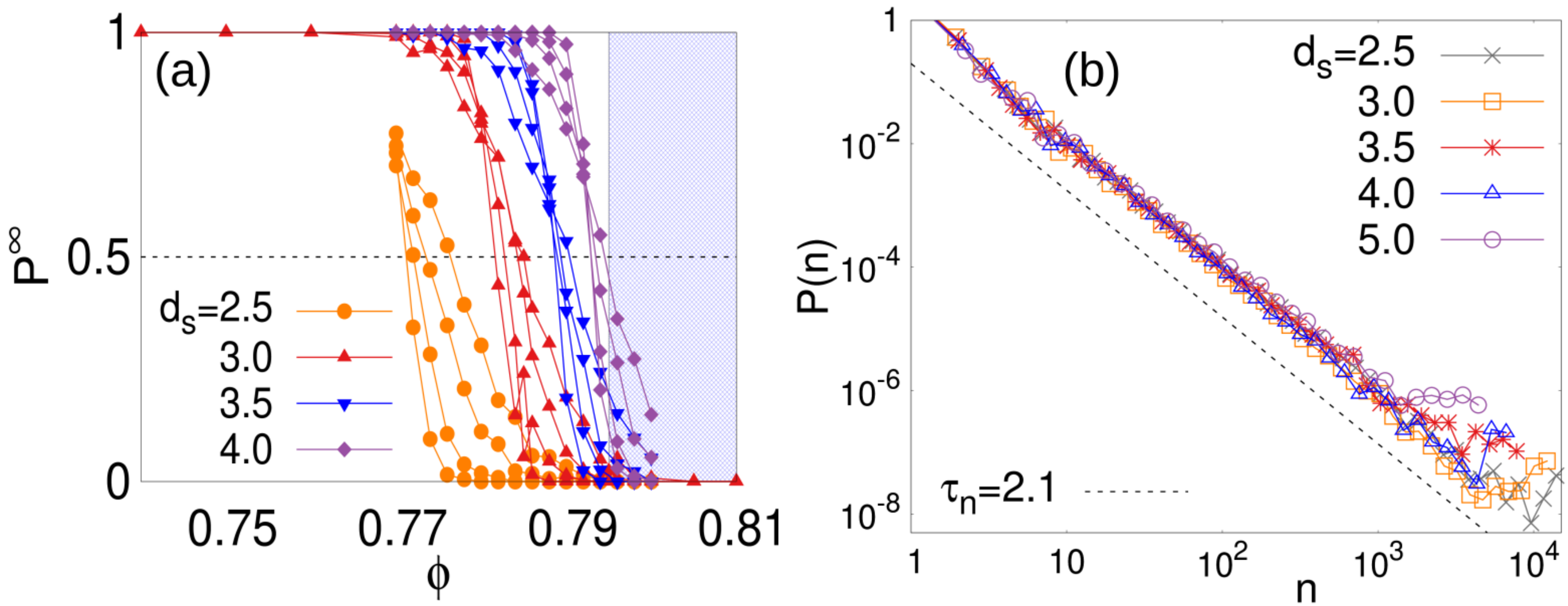



At $\phi_p$ close but below $\phi_l$ where the **liquid** first appears.

Dashed inclined line $n_C \sim R_{g\,C}^{\,d_\mathrm{f}}$ with $d_\mathrm{f} \sim 1.90$

# Clusters

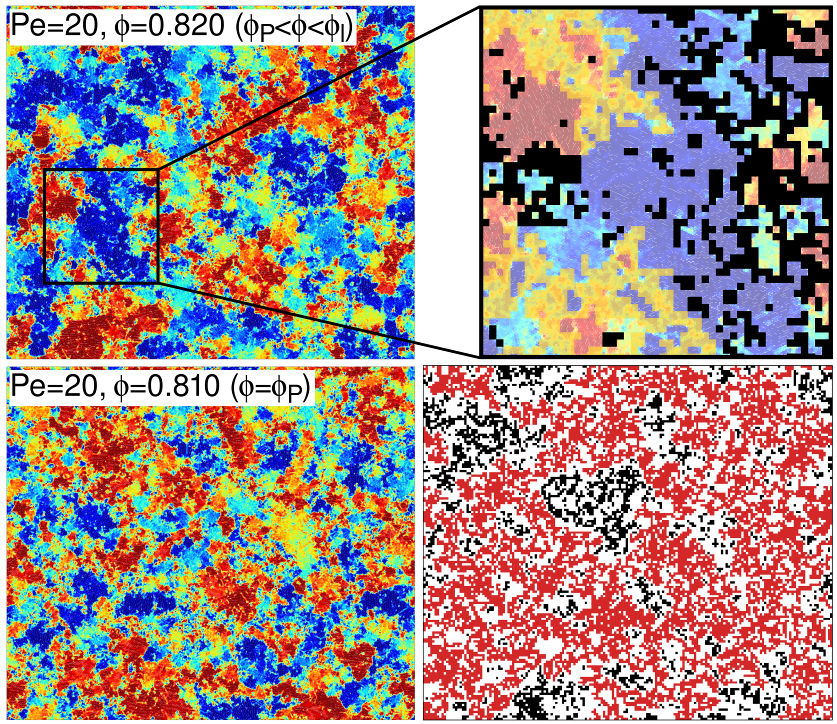
**Percolation: (in)dependence on coarse-graining Pe = 10**




$\phi_p$ displaces towards larger values with increasing $d_s$ but $d_\mathrm{f}, \tau$ do not change.

# Clusters

## Percolation : hexatic color maps & clusters



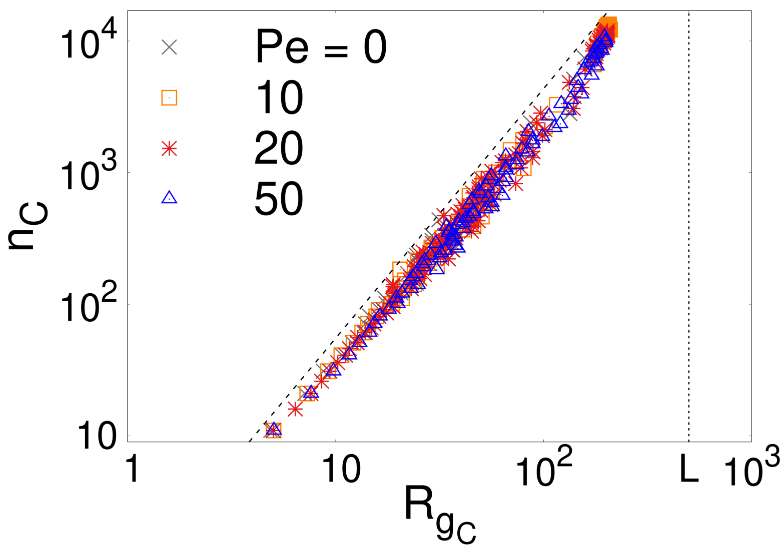

The liquid permeates the sample through the interfaces between local hexatically ordered patches

But, are these the most relevant critical clusters ? Recall Fortuin-Kasteleyn

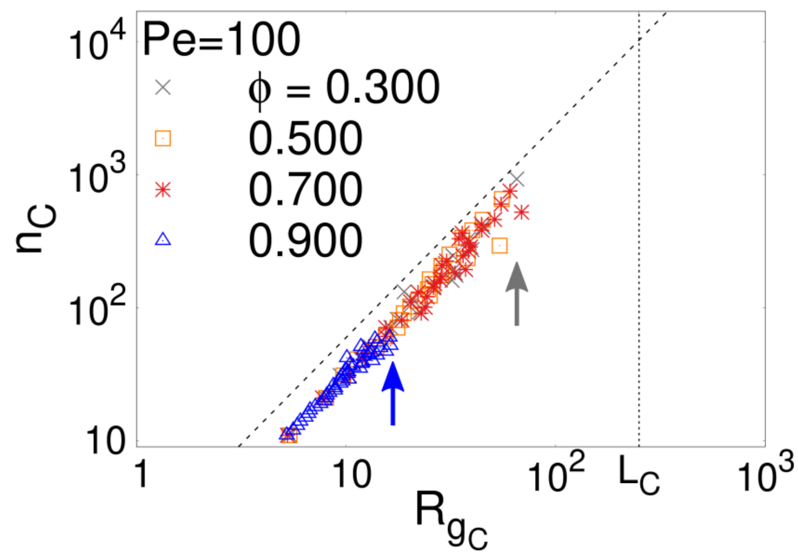
# MIPS

**No criticality due to gas bubbles in cavitation**

**Percolation transition**




**MIPS**




No $\phi$ dependence in MIPS

$L_C$ estimated linear size of dense phase