# Hexatic and microemulsion phases in a 2D quantum Coulomb gas

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# Outline

- Model (one component quantum Coulomb gas)
- Phase diagram
- Wigner crystal melting
  - ★ Hexatic phase
  - ★ Microemulsion phase

# The model

$$H = -\frac{\hbar^2}{2m} \sum_{i=1,N} \nabla_i^2 + \sum_{i<j} \frac{e^2}{r_{ij}} + V_{\text{background}}$$

- One component system of charges (e) interacting via a **long-range $1/r$ potential in 2D**
- **Rigid** background (total charge is neutral)
- **Quantum effects** included through the kinetic term
- No statistics ("**Bolzmannons**") (distinguishable particles)

# The model (II)

Effective dimensionless parameters:

- Wigner-Seitz radius $r_s = r/a_0$ with $r = 1/\sqrt{\rho\pi}$
- Temperature dependent coupling $\Gamma = e^2/rk_BT$

Units Rydberg $a_0 = 1,\ e^2 = 2,\ m = 1/2,\ k_B = 1$

$$H = -1/r_s^2 \sum_{i=1,N} \nabla_i^2 + 1/r_s \sum_{i<j} 1/r_{ij} + V_{\text{background}}$$

Small $r_s$
weakly interacting regime
**liquid**

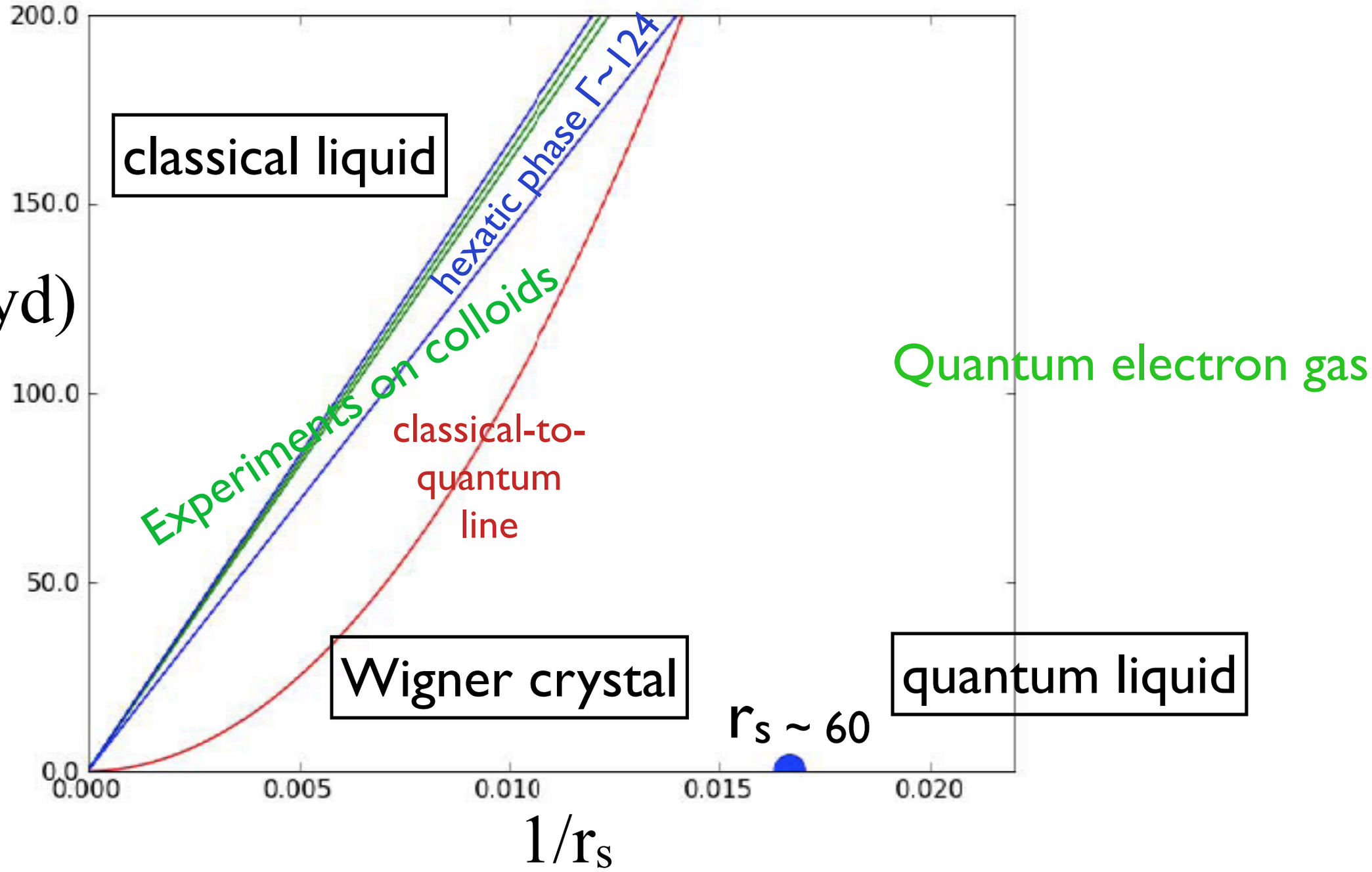
Large $r_s$
strongly interacting regime
**Wigner crystal**

# (some) Experimental realizations

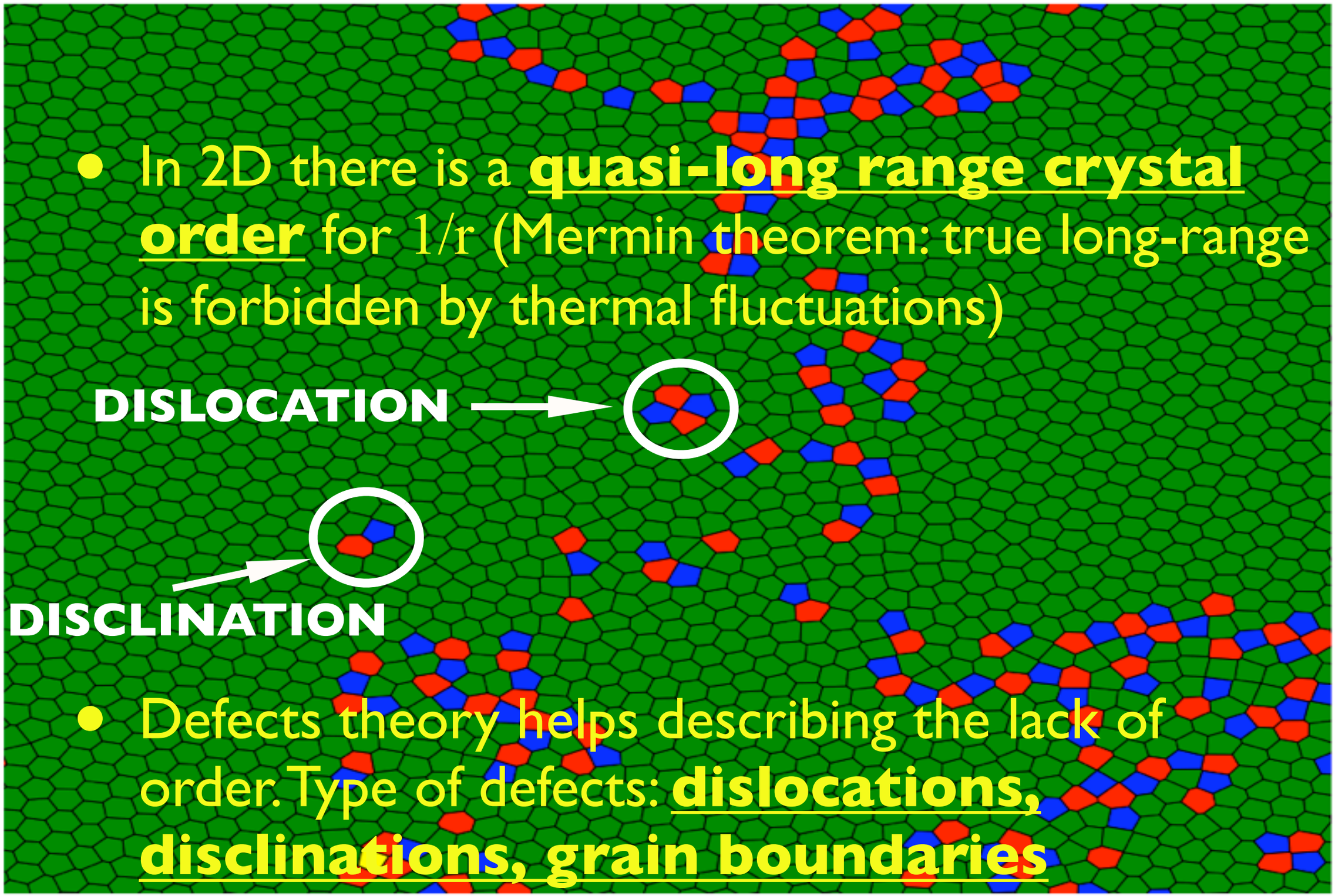
- X. H. Zheng and R. Grieve (PRB **73**, 064205 (2006), charged millimeter-sized steel balls
- Keim, Maret, and von Grunberg (cond-mat/0610332, PRL **95**, 185502 (2005)), magnetically oriented colloids
- Quinn and Goree (PRE **64**, 051404 (2001)), charged microspheres suspended in plasma
- Electrons on liquid helium (Grimes and Adams, 1979) and in MOSFET.... they are fermions, but by studying our model (computationally easier) we can infer some properties also in the charge sector of electronic 2D systems (particularly at low density where statistics is less relevant)

# Phase diagram

## (up to now)



# Defects in the Wigner crystal




- In 2D there is a **quasi-long range crystal order** for $1/r$ (Mermin theorem: true long-range is forbidden by thermal fluctuations)

- Defects theory helps describing the lack of order. Type of defects: **dislocations, disclinations, grain boundaries**

# Melting of a 2D crystal according to the Kosterliz-Thouless transition

- Halperin and Nelson explain the melting as a two-step process: dislocation unbinding, and disclination unbinding
- **Dislocation unbinding**: crystal-to-hexatic transition (loss of translational order, a quasi long-range hexatic orientational order survives)
- **Disclination unbinding**: hexatic-to-liquid transition (loss of orientational order, isotropic liquid)
- The two phase transitions are **second order and of KT type** (namely the critical exponents can be determined universally)
- **Classical one component plasma** with $1/r$ shows hexatic phase sandwiched between crystal and liquid around $\Gamma \sim 123$ (although there is no consensus)

# T=0 melting with Coulomb interaction (microemulsion theory)

- Direct liquid-to-crystal first order transition with phase separation forbidden by the long-range Coulomb interaction and the rigid background.

- Jamei, Kivelson and Spivak [Phys. Rev. Lett. **94**, 056805 (2005)] showed (with mean field techniques) that a 2D charged system does not make a direct transition from crystal to liquid

- A stripe phase between liquid and crystal has lower energy at the mean field level

- Other phases (like bubbles) are also possible. Alternating crystal and liquid patches with a finite characteristic length ("microemulsions"). For stripes, the mean field optimal width is [Jamei et al, and Ortix et al. PRB **75**, 195107 (2007)]:

$$a \exp\left(4\pi^2 e^2 \sigma / \Delta\mu_c^2\right)$$

# Quantum Monte Carlo methods

- Finite T: **Path Integral Monte Carlo** (PIMC)
- T=0: **Diffusion Monte Carlo** (DMC)
- General properties of the two algorithms in the case of Bosons and Bolzmannons: **no sign problem**, so they are "formally" exact!
- With Bolzmannons, the PIMC sampling is even faster, no need to include permutations

# Path integral MC

Thermal density matrix $\hat{\rho} = e^{-\beta(\hat{T}+\hat{V})}$

Trotter decomposition $\hat{\rho} = \lim_{M\to\infty}[e^{-\tau(\hat{T}+\hat{V})}]^M \qquad \tau = \beta/M$

Partition function $Z = \int dR_1 \ldots dR_M e^{-\sum_{i=1}^{M} S(R_{i-1},R_i,\tau)}$

Primitive action

$$S(R_0, R_1, \tau) = (R_1 - R_0)^2/4\lambda\tau + \frac{\tau}{2}(V(R_0) + V(R_1))$$

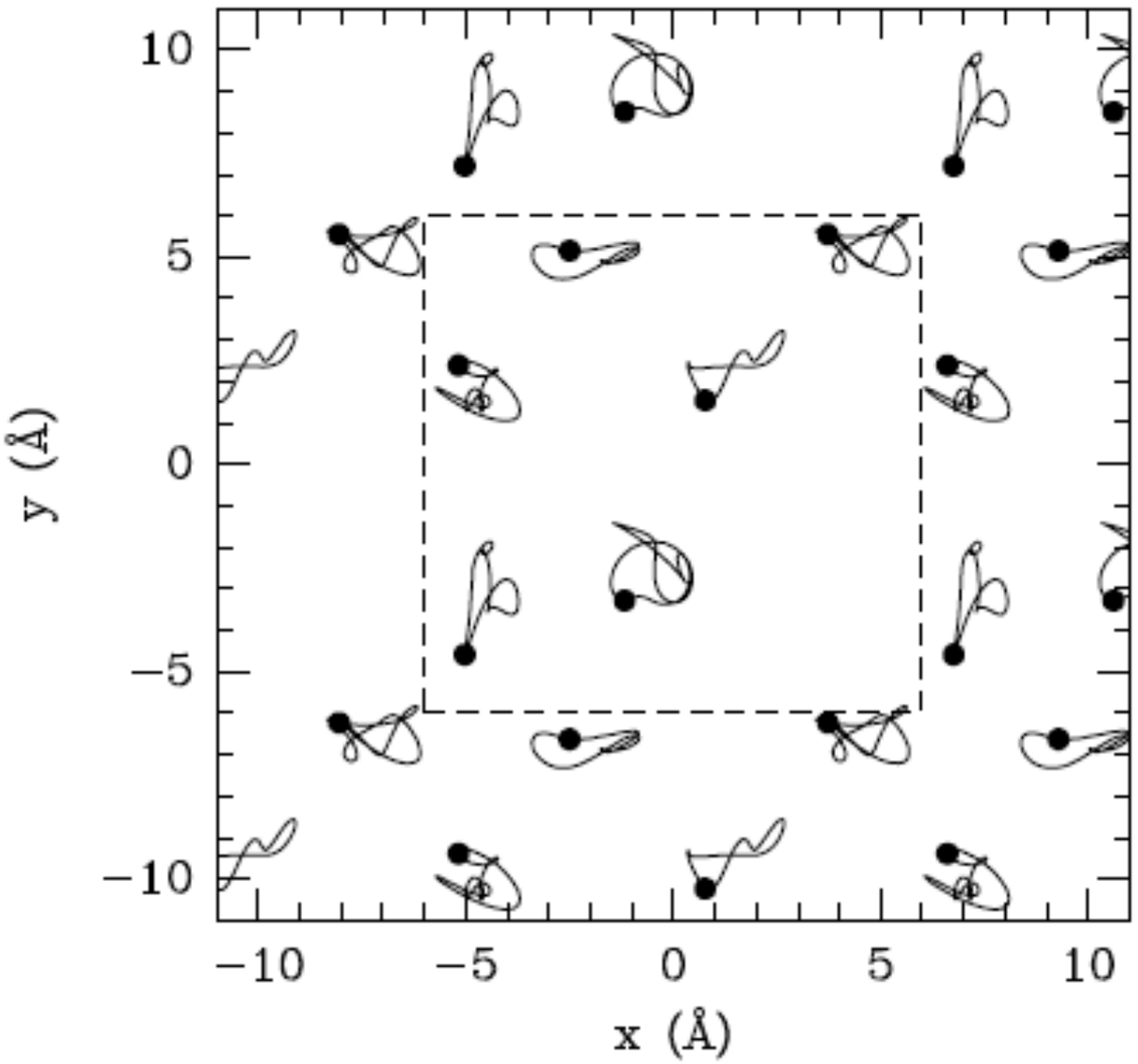
# Sampling the partition function

Each particle is a polymer

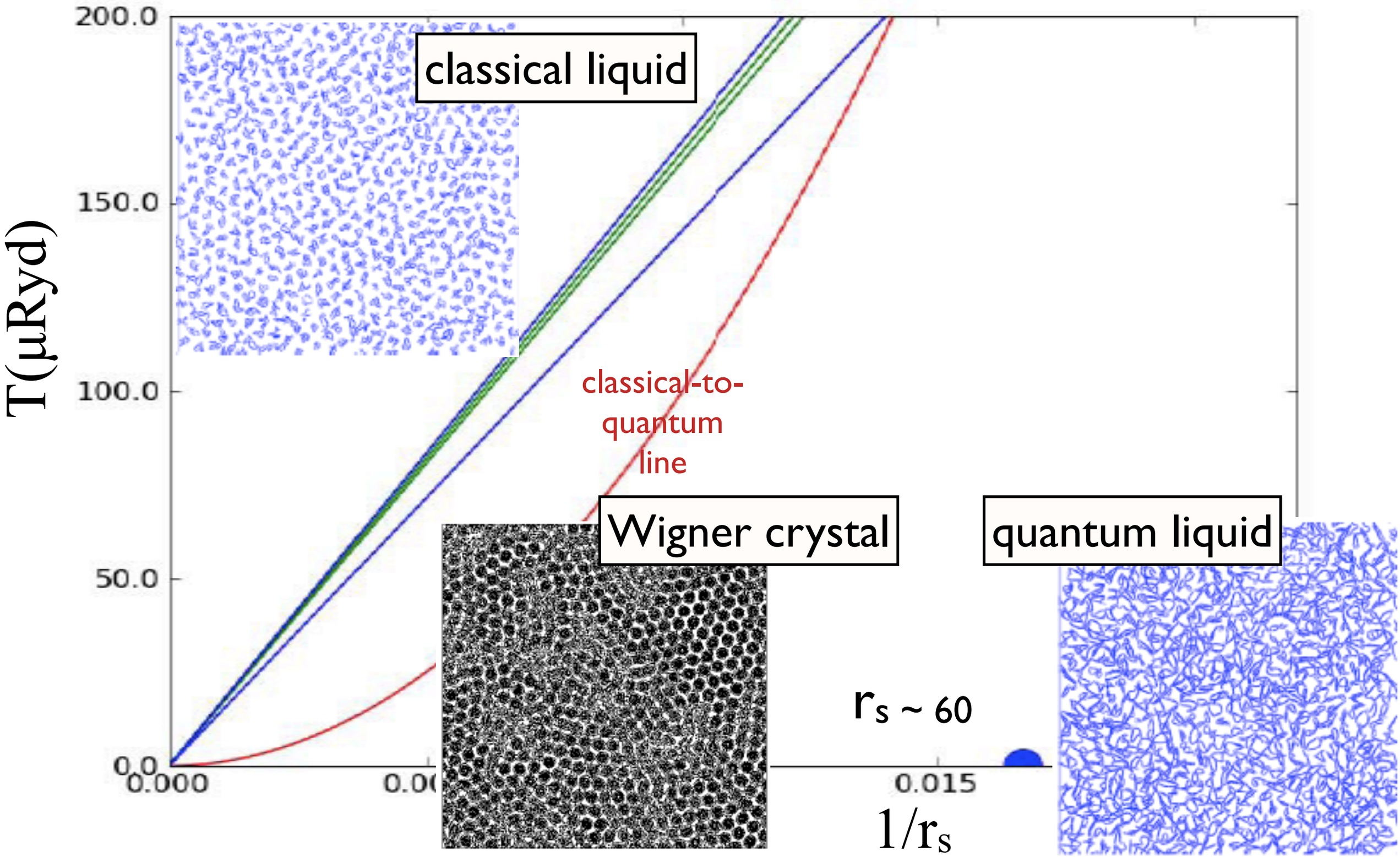
The trace implies close paths

The extension of the path is due to the quantum nature of the wave packet

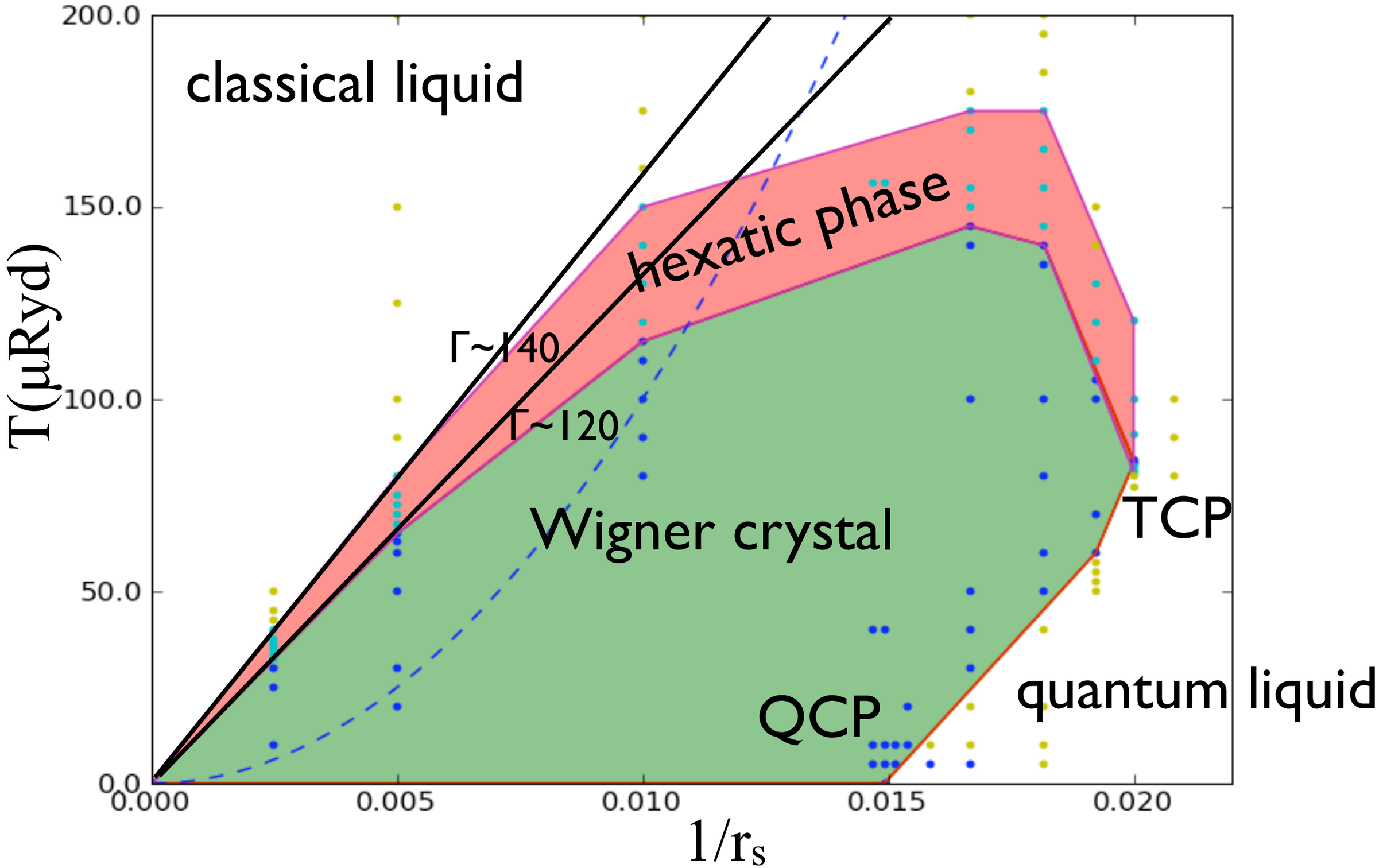
The lower the temperature, the longer the polymer



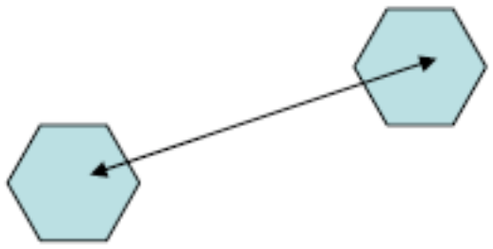
# Toward our QMC phase diagram



# PIMC phase diagram



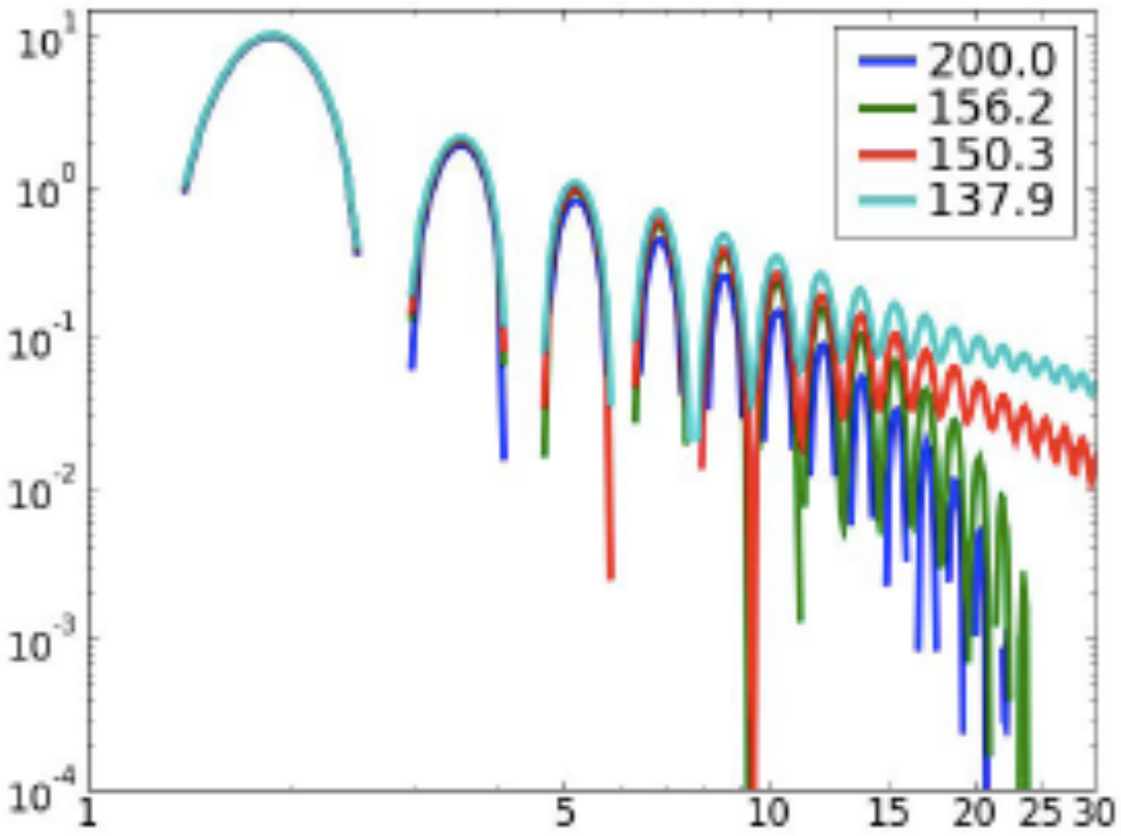
# Hexatic order parameter

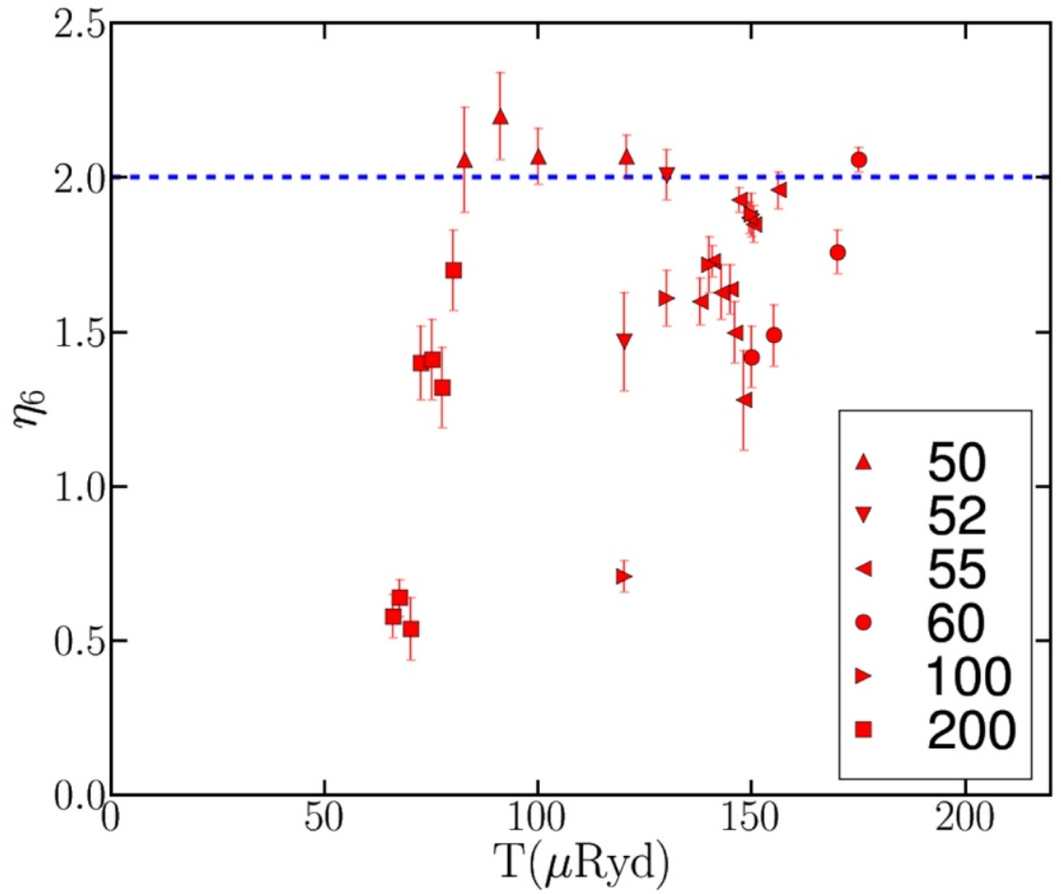


$$g_6(r) = \left\langle \varphi^*(r)\varphi(0) \right\rangle \quad \sim 1/r^{\eta}$$

$$\varphi(r_i) = \sum_{<j>} e^{i6\theta_{ij}}$$

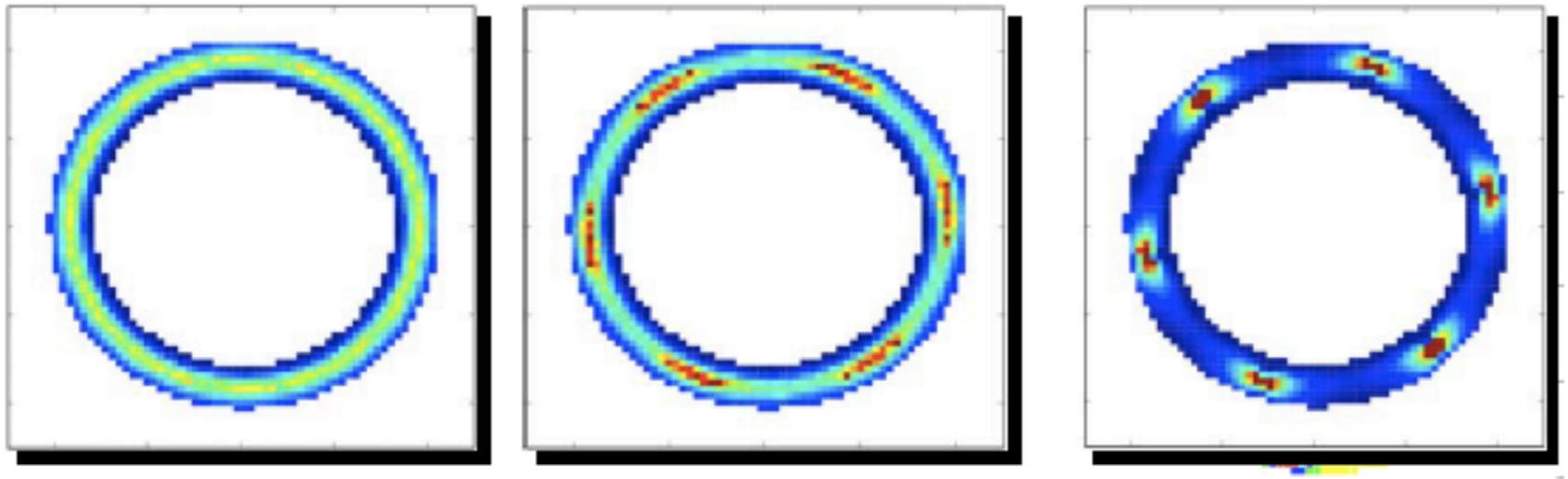
We found $\eta \sim 2$
(while in the KT $\eta = 1/4$)



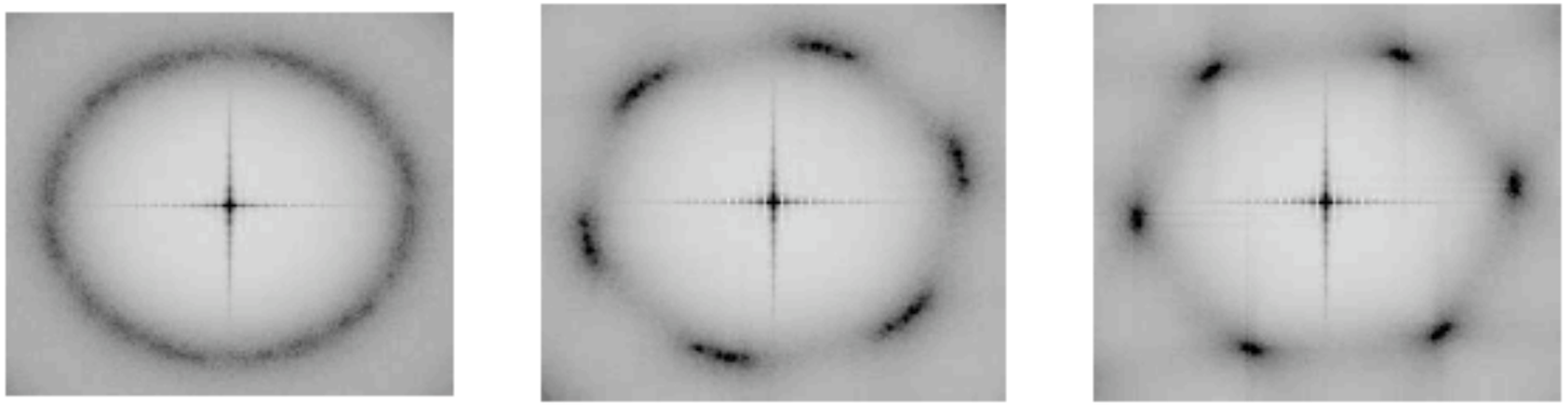
# Structure factors

PIMC



Exper.

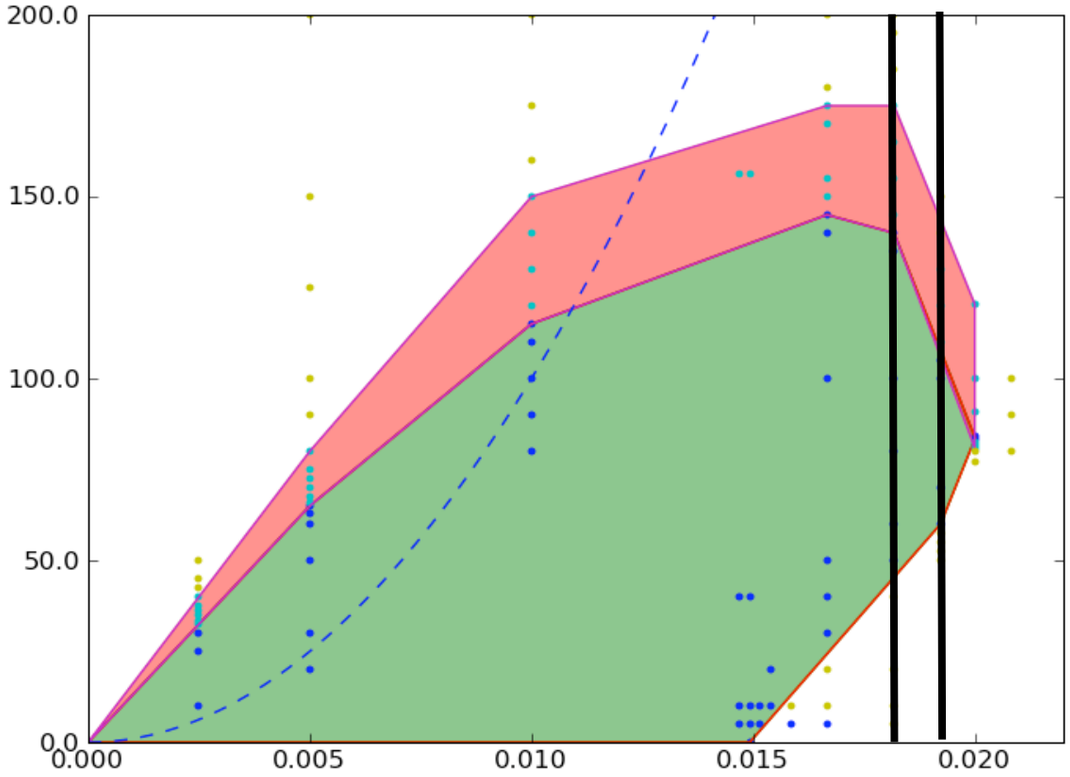
Keim, Maret, von Grunberg.

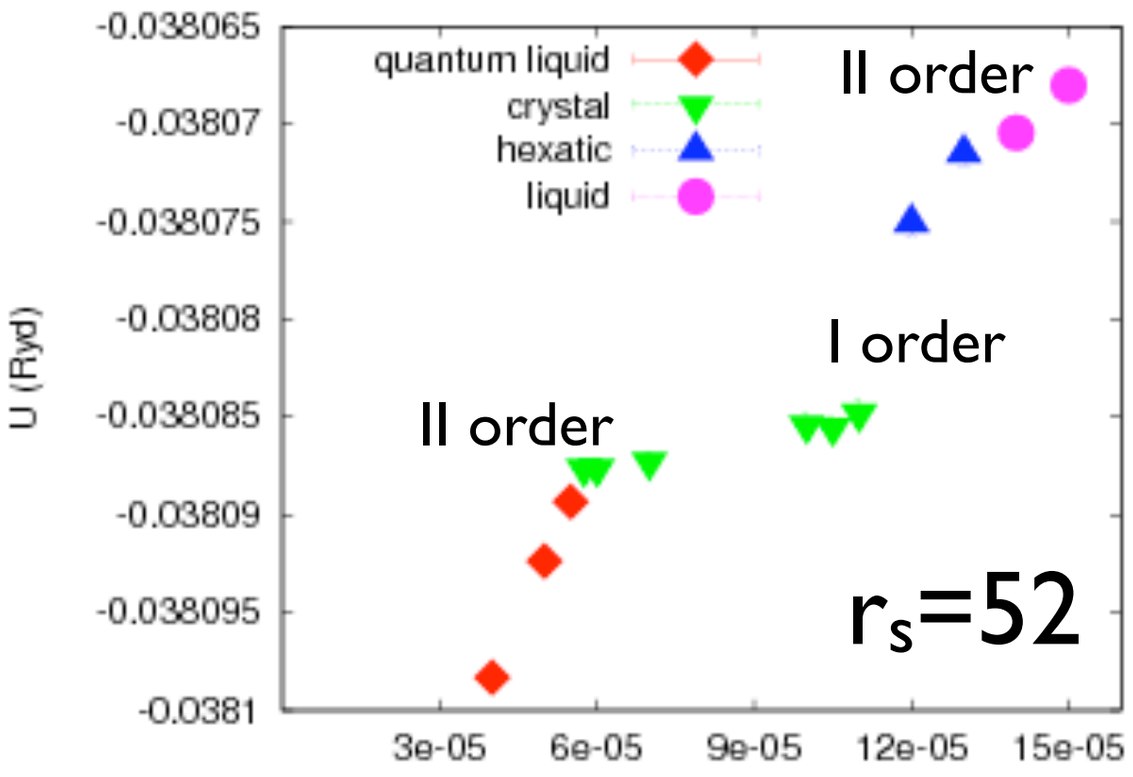


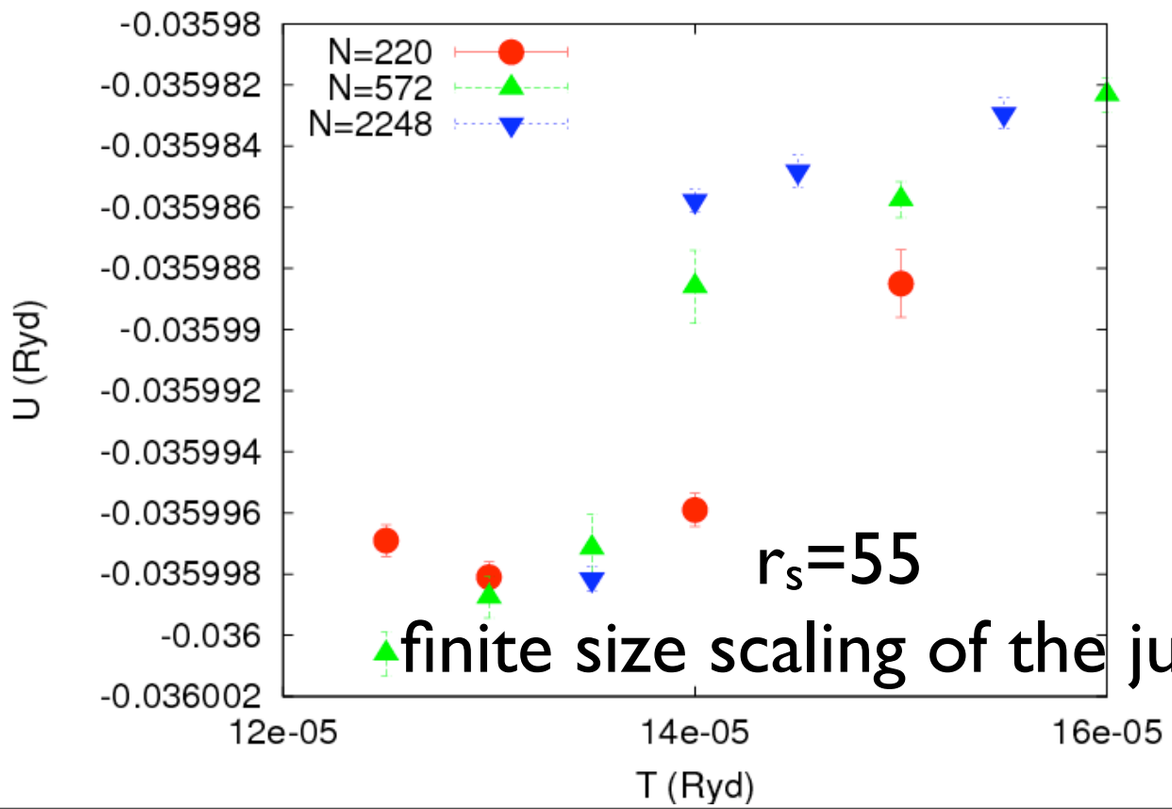
Classical MC

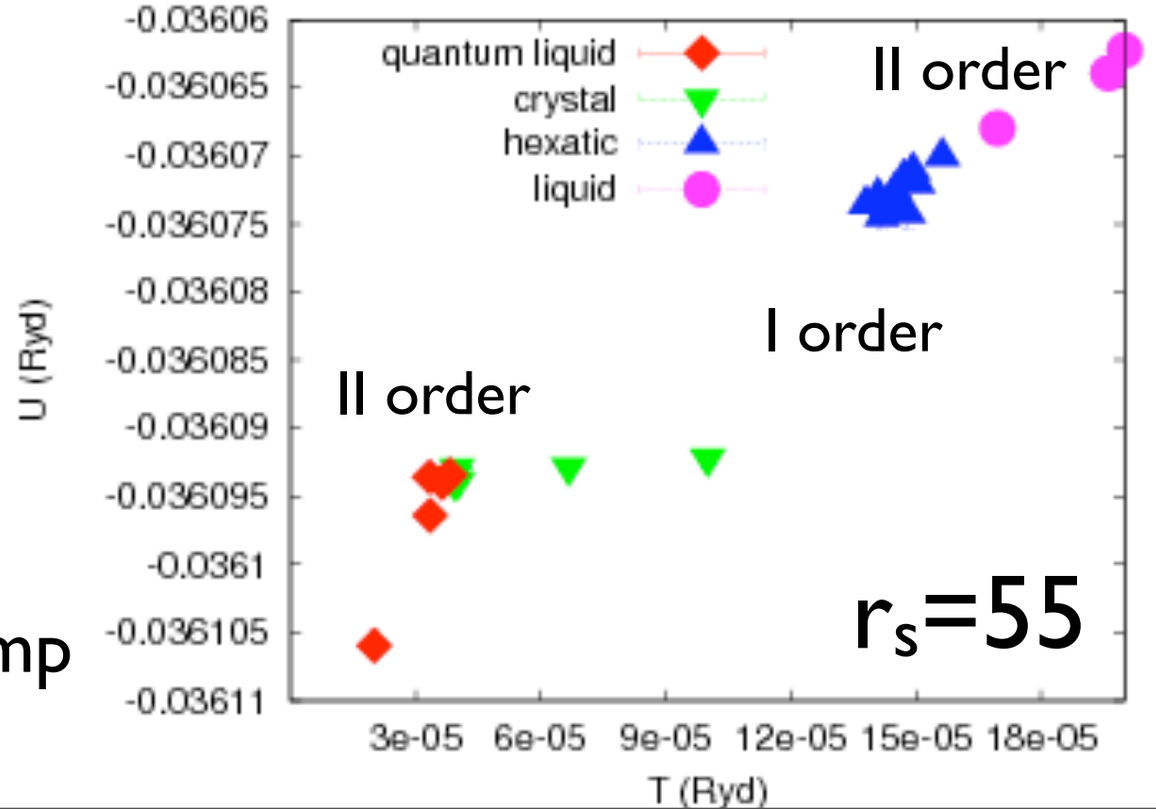
(a) $\Gamma = 100$ (b) $\Gamma = 123$ (c) $\Gamma = 150$

# Order of the transitions

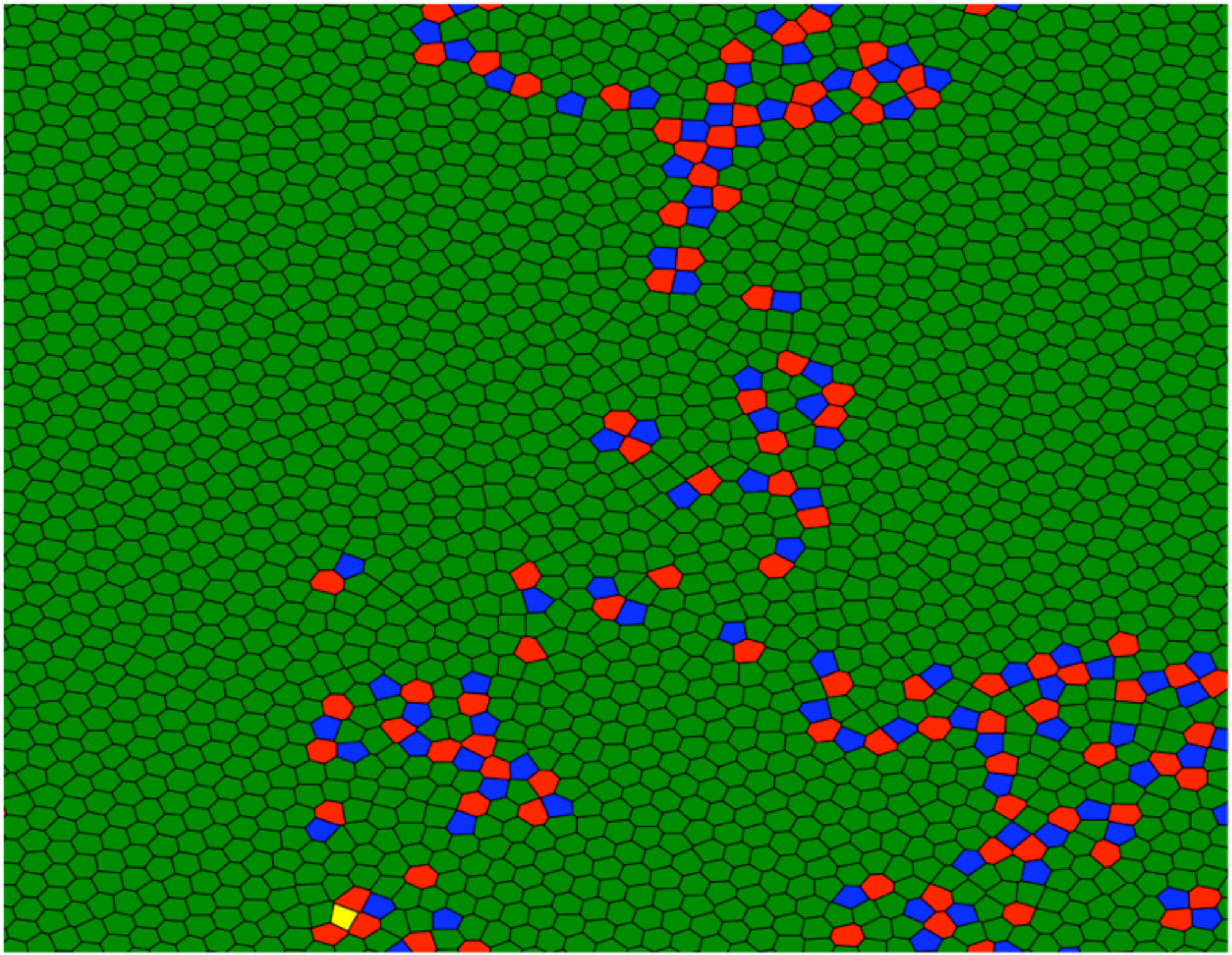


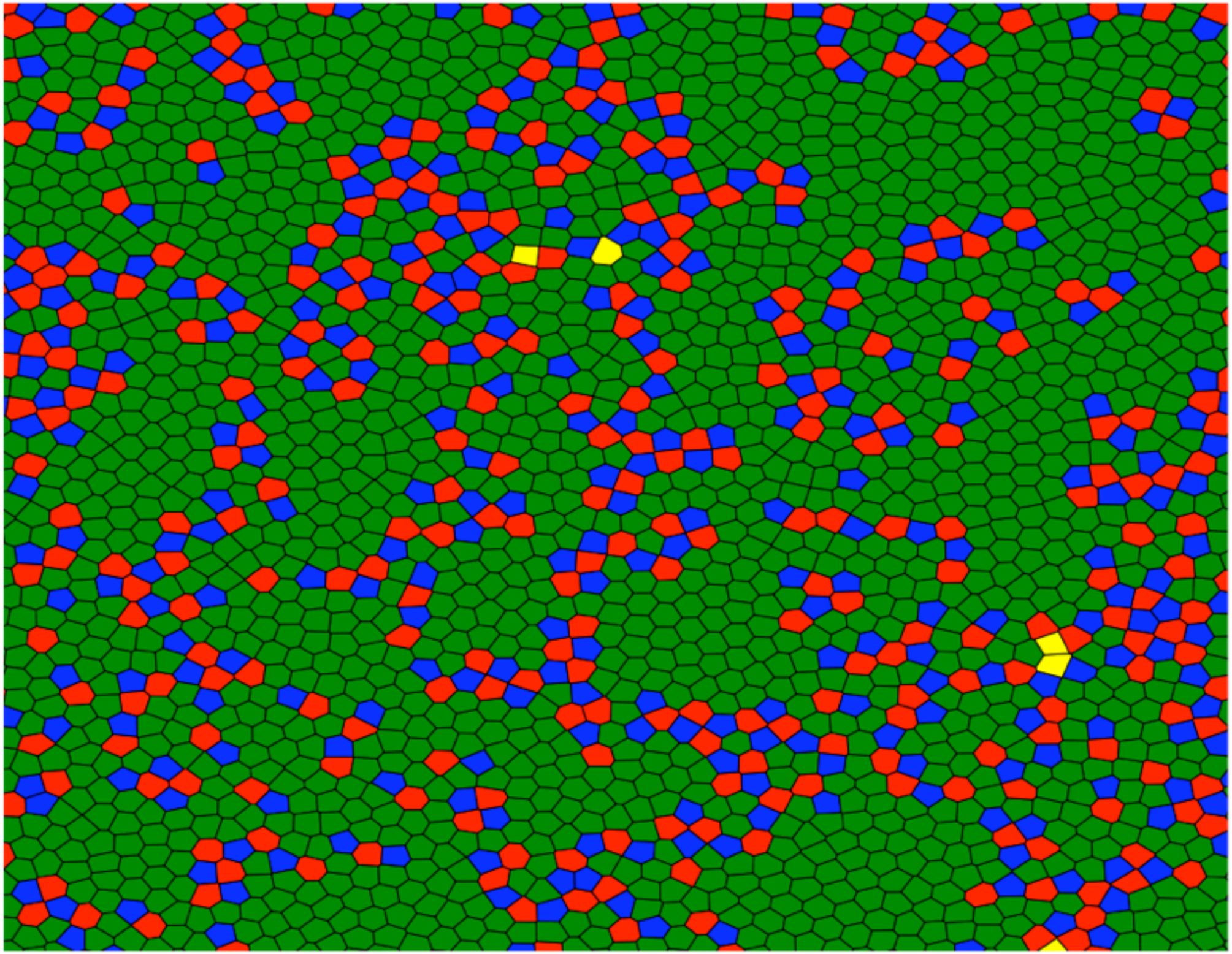



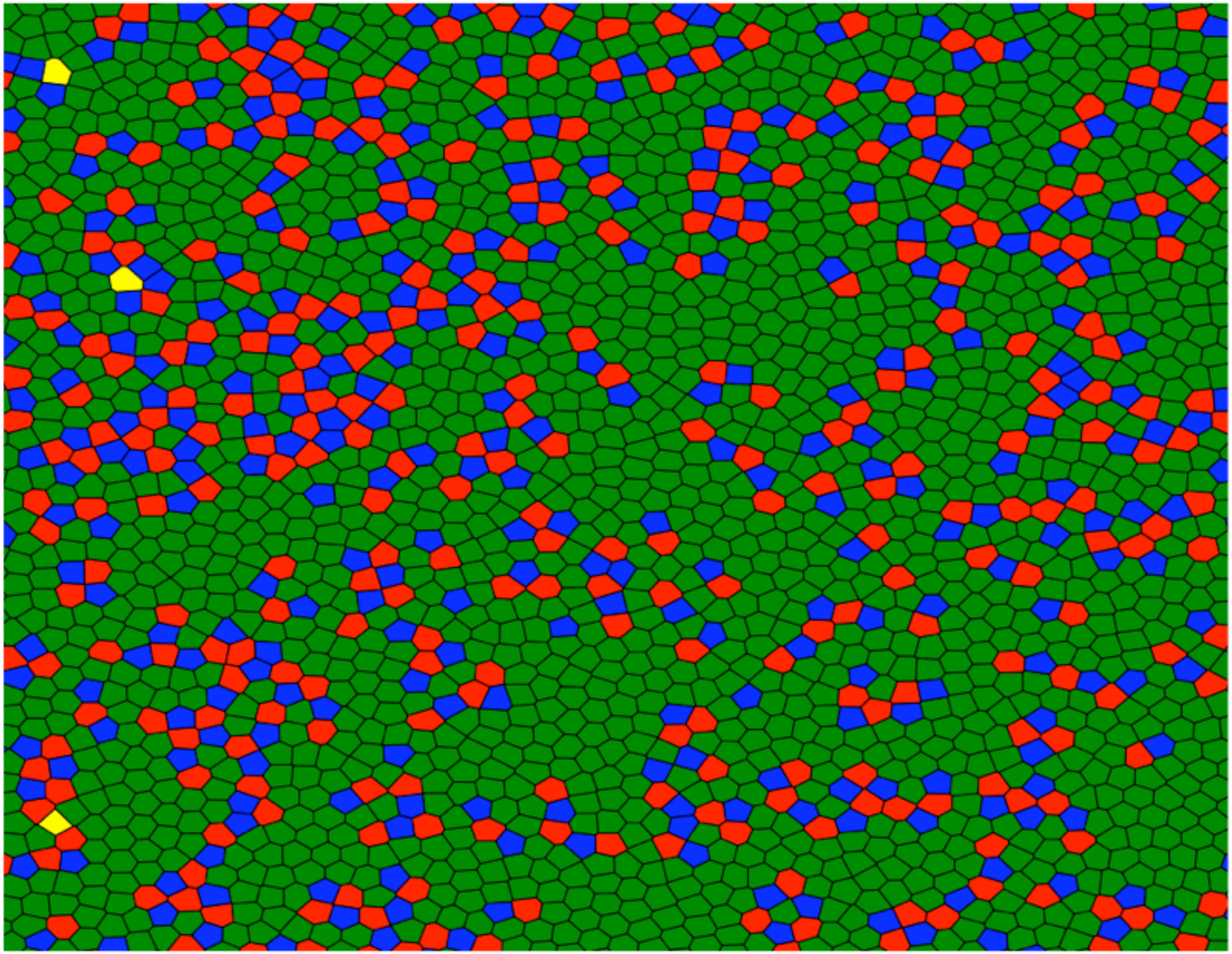
# Voronoi (crystal) $r_s$=55



# Voronoi (hexatic) $r_s$=55

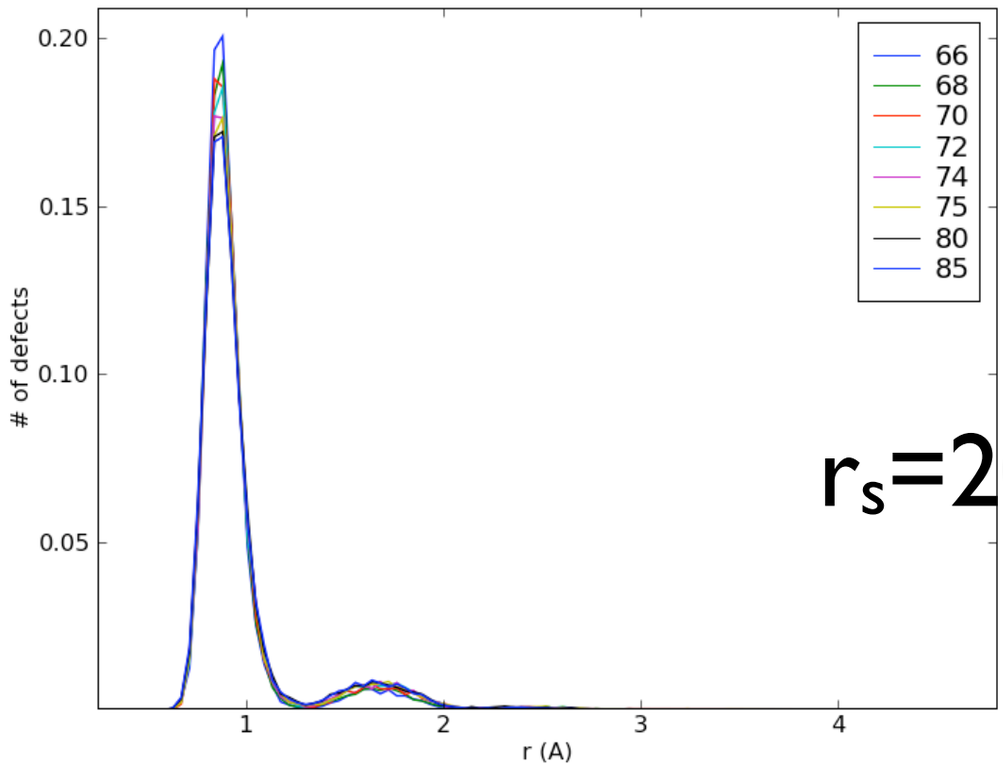


# Voronoi (liquid) $r_s$=55

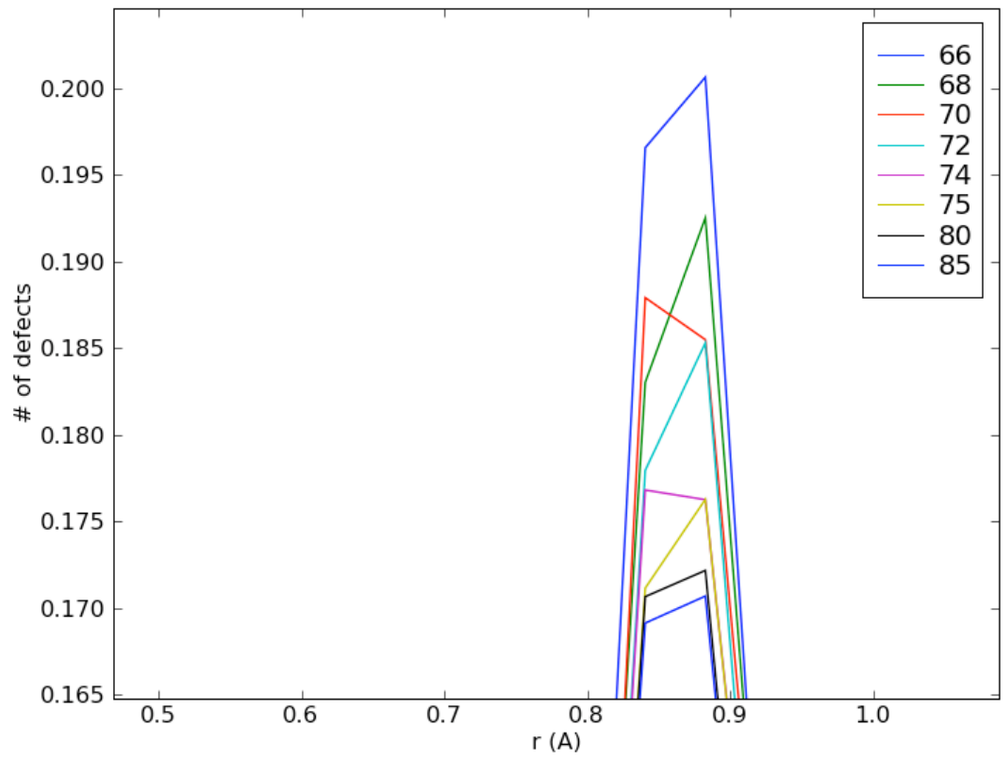


# Grain boundaries and disclination unbinding

- First order crystal-to-hexatic explained by grain boundaries (PRB **28**, 178 (1983))
- Hexatic-to-liquid "standard" KT (disclination unbinding)




$r_s$=200



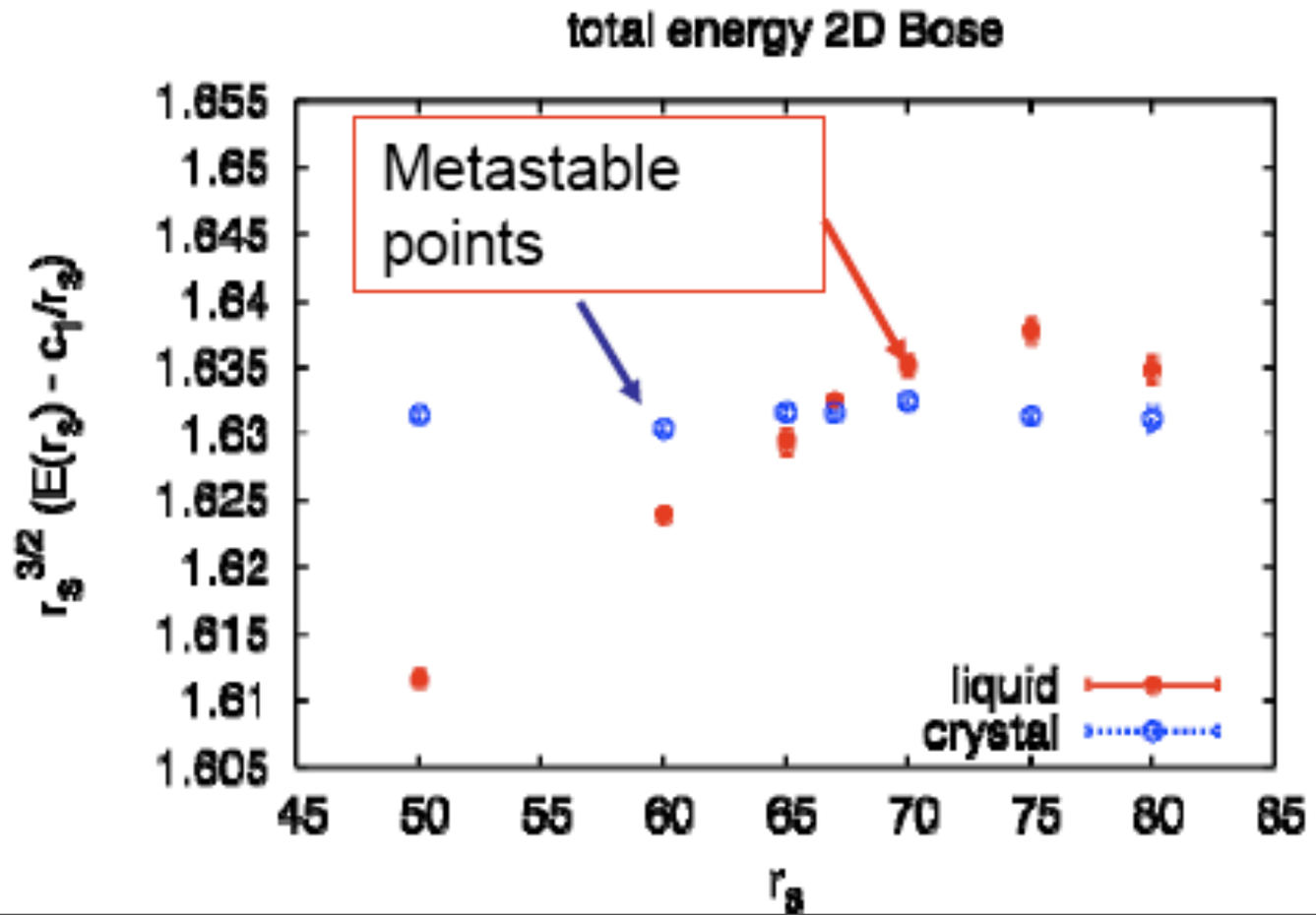
# Diffusion MC

- Imaginary time evolution to project out the higher energy components of an initial state
- The initial state is called "trial wave function" and it is also used to guide particles during diffusion
- DMC more accurate/efficient than PIMC but potentially more biased by the trial wave function
- Liquid wave function $\Psi_{\rm liquid}(R) = \exp[-\sum_{i<j} u_{\rm rpa}(r_{ij})]$
- Crystal wave function

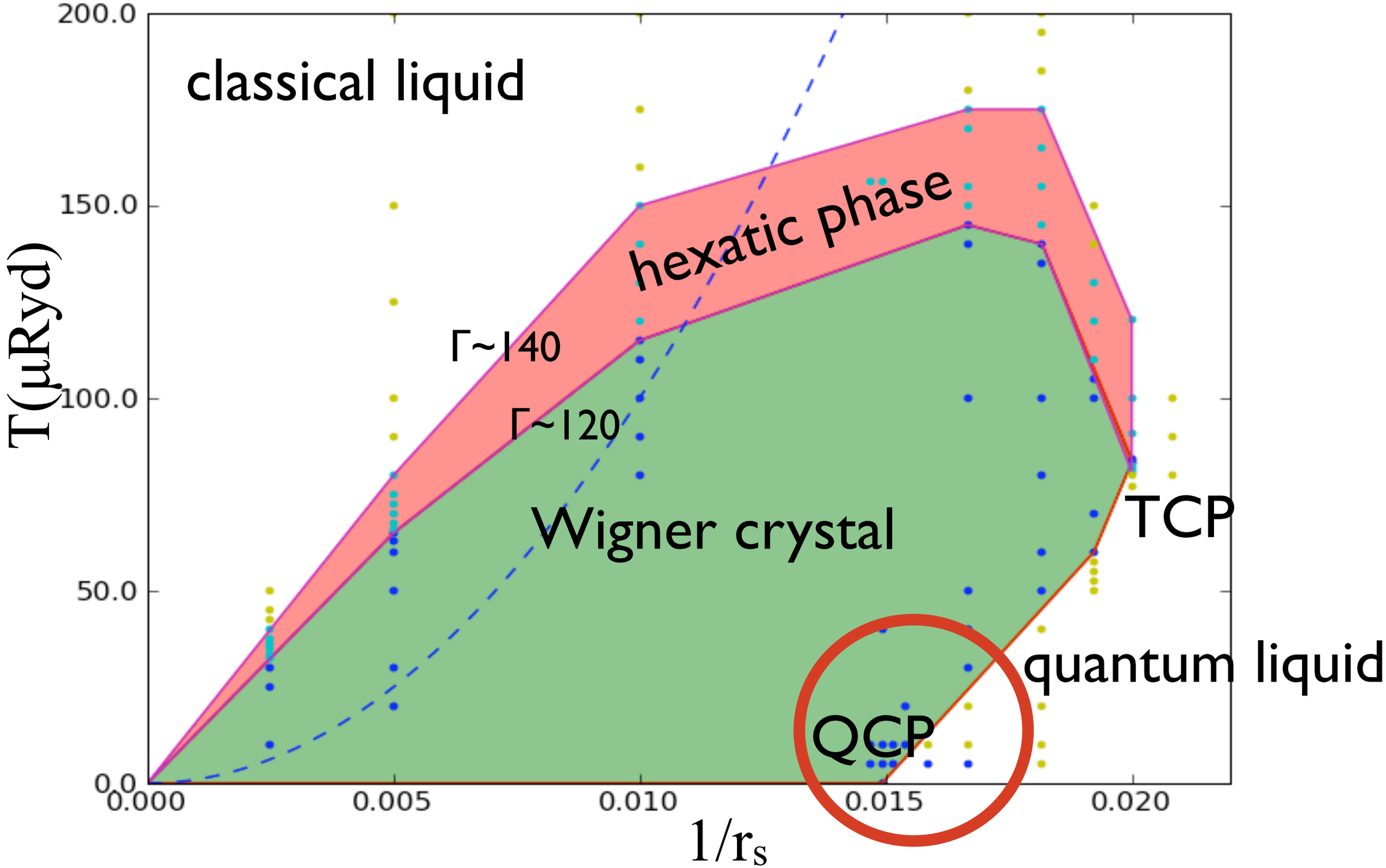
$$\Psi_{\rm solid}(R) = \Psi_{\rm liquid}(R) \exp[-\sum_i \alpha (r_i - I_i)^2]$$

# Ground state liquid-crystal transition

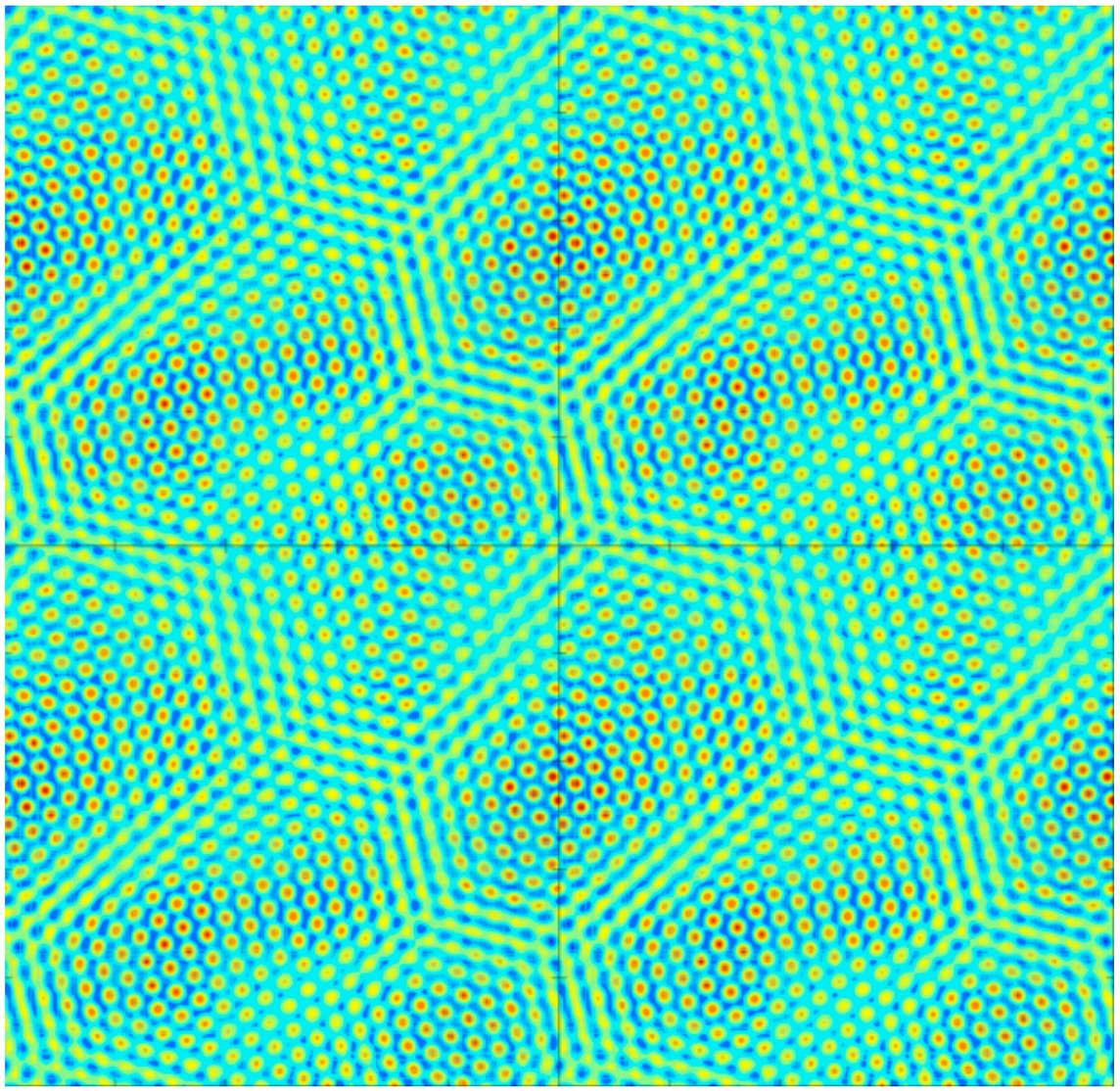
- We have established a much more accurate estimation of the transition at $r_s$=66.5 (old reference *S. De Palo, S. Conti, and S. Moroni, Phys. Rev. B* ***69****, 035109 (2004)*.
- Accurate finite size corrections based on the method in *S. Chiesa at al., Phys. Rev. Lett* **97**, 076404(2006)



# Where to look for inhomogeneous phases?

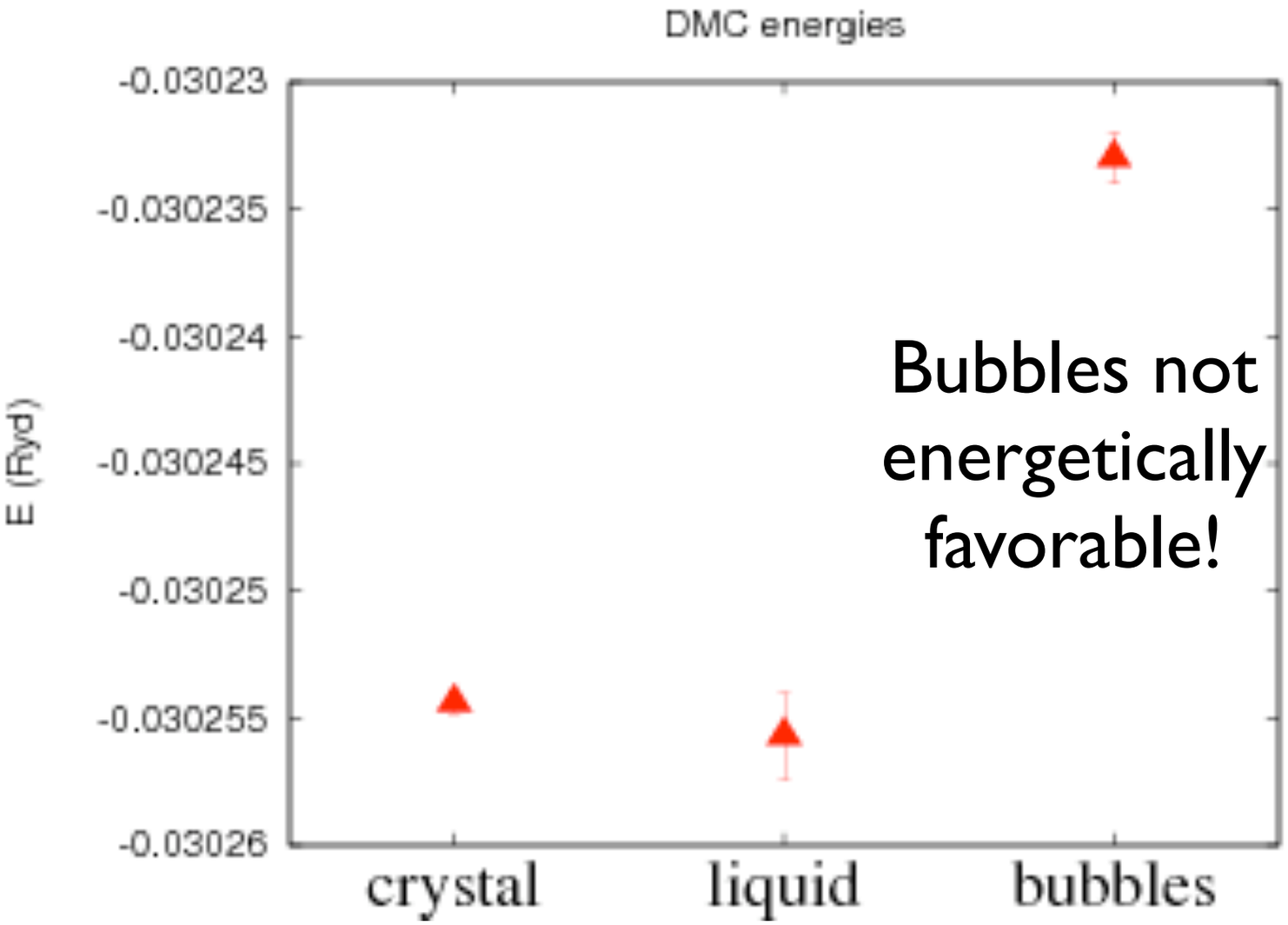


# Metastable bubbles

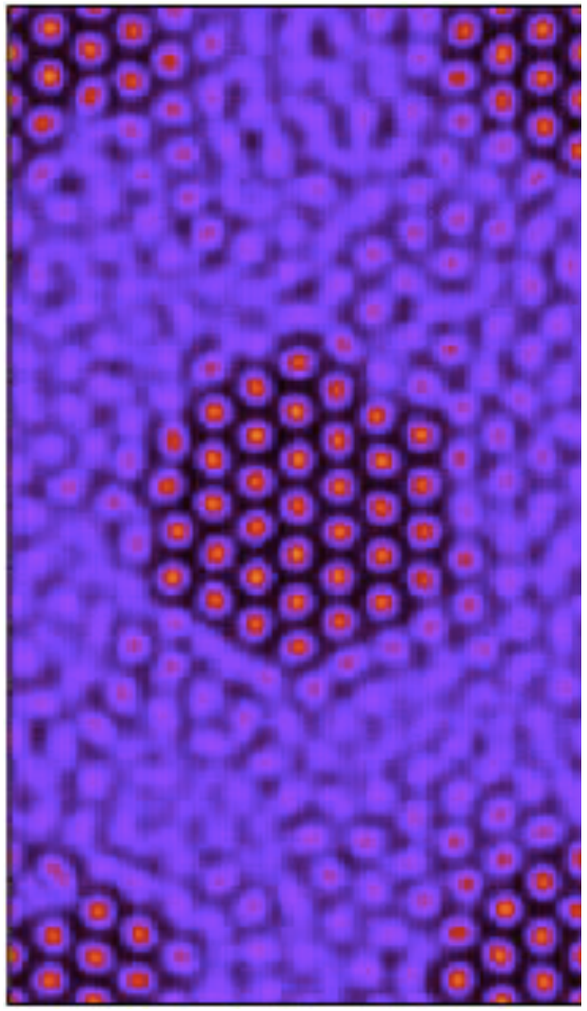


**PIMC** Very low T (< 10 micro Ry)

# Non-homogeneous bubble phases

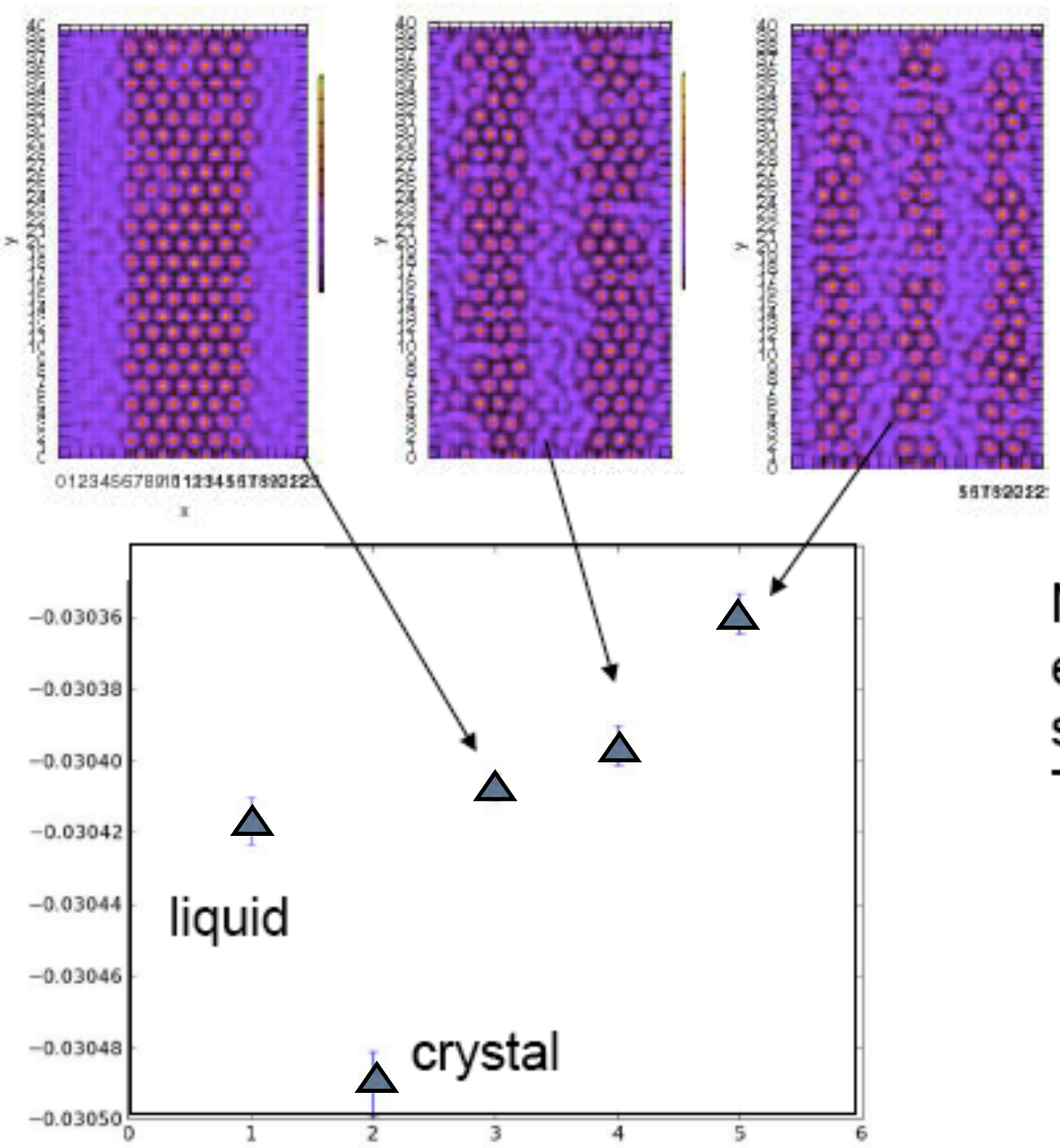



**DMC** T=0



density contour plot

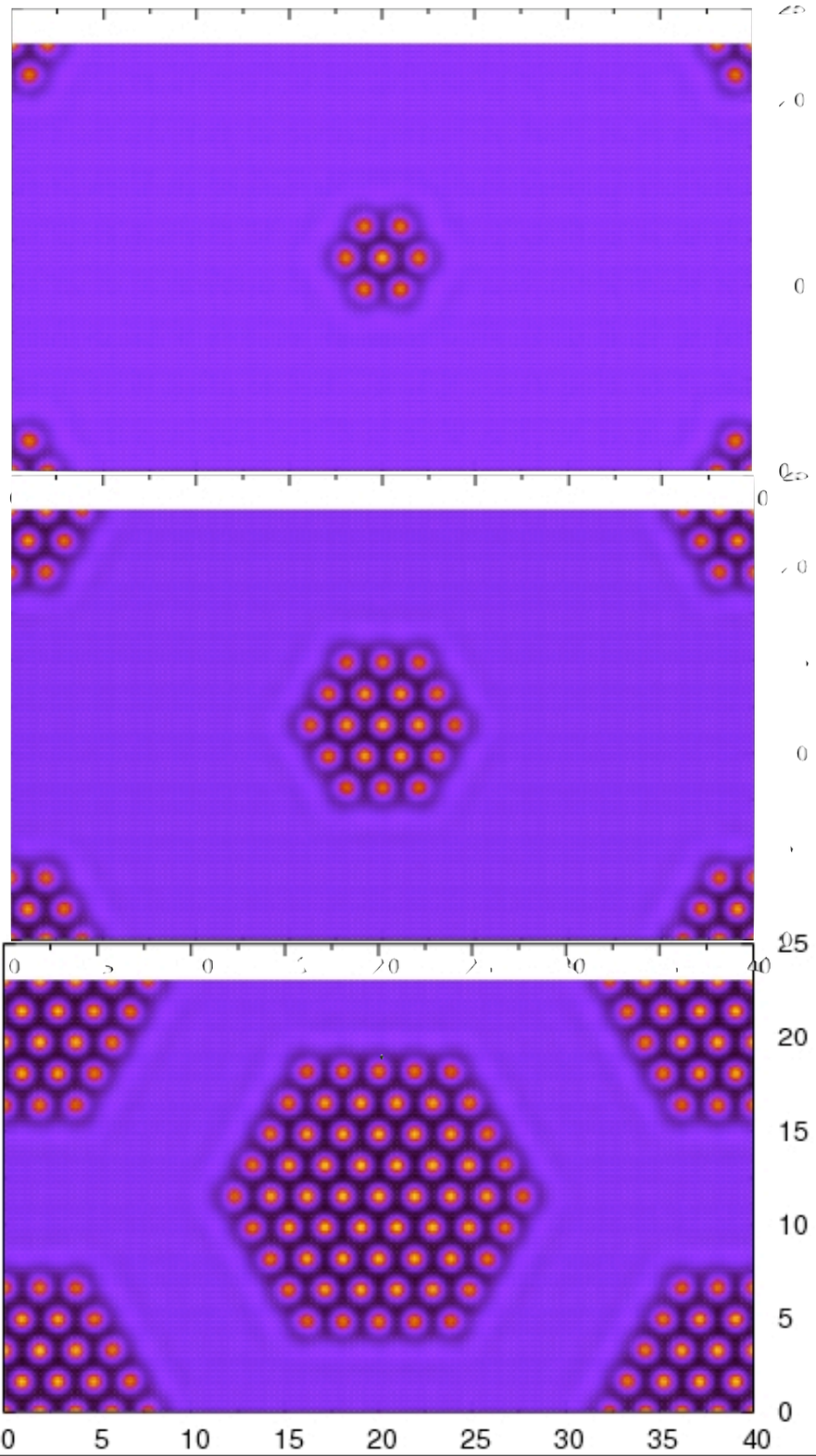
# Stripes

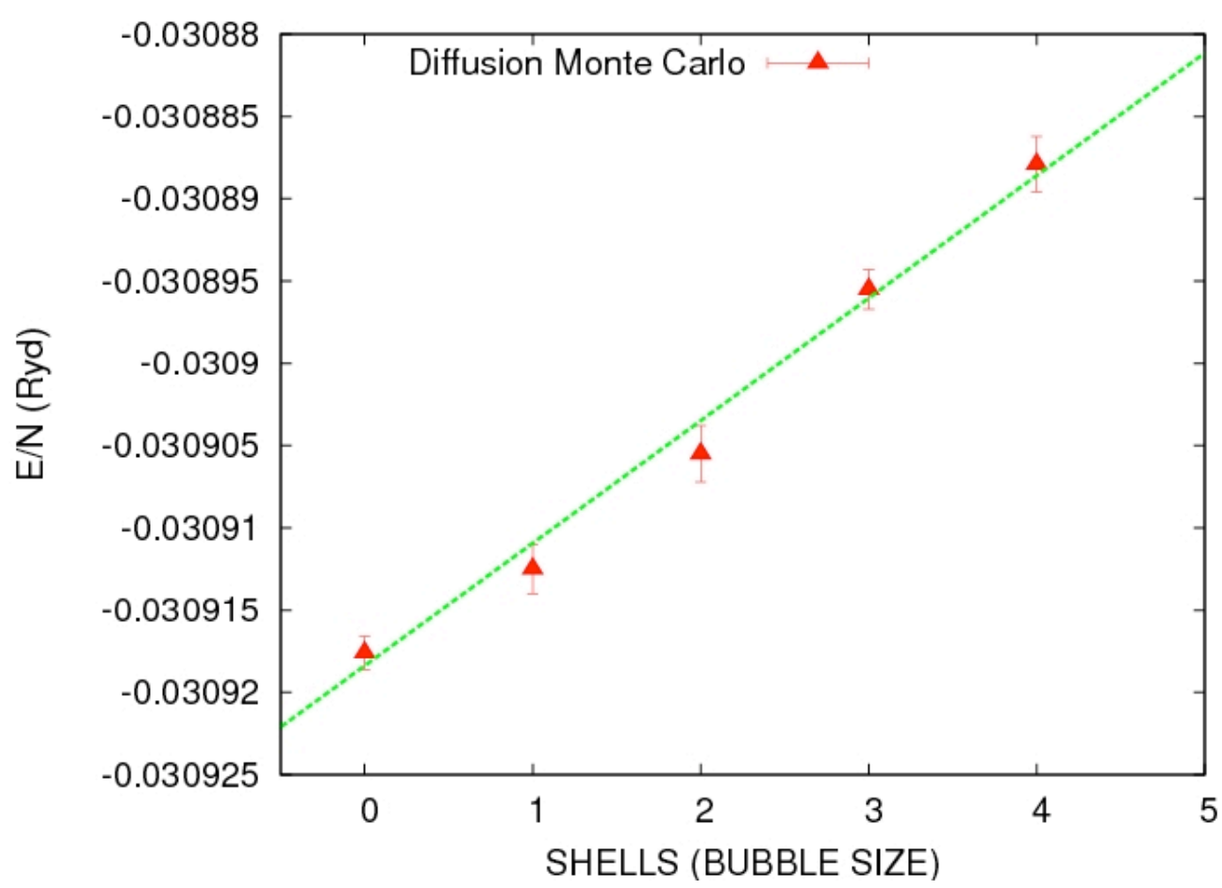



Energy

No evidence for stripes at T=0

# Bubbles




By fitting different bubble sizes we estimate the surface tension

**DMC** T=0

# Using microscopics and mean field

- From the dependence of the stripe and bubble energies on their size we can estimate the surface energy σ
- From the "pure" liquid and crystal calculations we can estimate the free energy of the homogeneous phases and the chemical potential μ
- We obtain: σ~1.5 μRyd/a.u., Δμ~59.8 μRyd
- This implies a mean field characteristic length

$$a \exp\left(4\pi^2 e^2 \sigma / \Delta\mu_c^2\right) \sim \exp(3\ 10^5)$$

- The **very small chemical potential difference** between the two homogeneous phases makes the mean field **characteristic length of microemulsion exceedingly large**, impossible to see in any experimental setup or in simulations

# Conclusions

We have established the outline of the phase diagram for a quantum one component plasma with Coulomb interactions

We see a sandwiched region of hexatic phase where quantum effects are marginal

Some discrepancy with KTHNY (order, critical exponents)

If inhomogeneous phases exist their characteristic length is larger than any feasible experimental setup or simulation cell

Reference: PRL in press, and arXiv:0905.4515

Future work: inclusion of disorder, Bose and Fermi statistics