Nonequilibrium analysis on two dimensional melting

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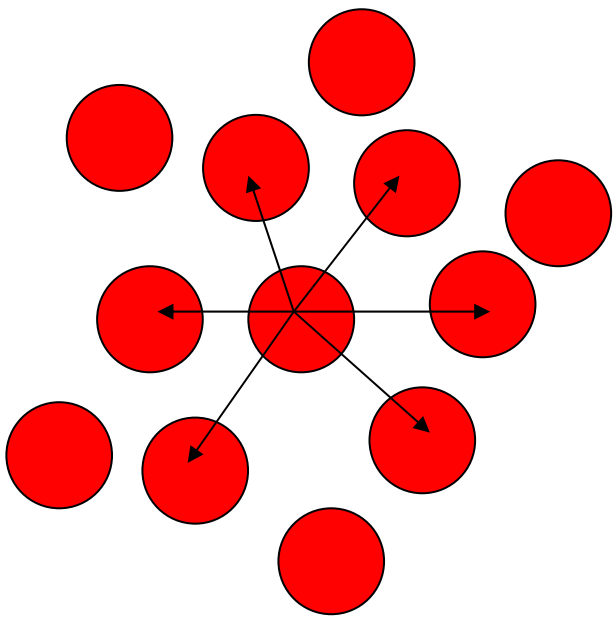
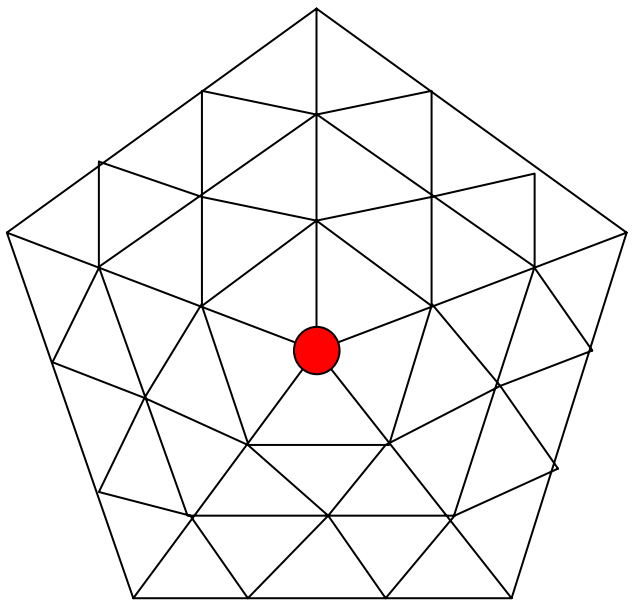
複雑系科学専攻多自由度システム情報論講座

渡辺宙志





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Introduction: What is Phase Transition?

Phase Transition is competition between energy and entropy.

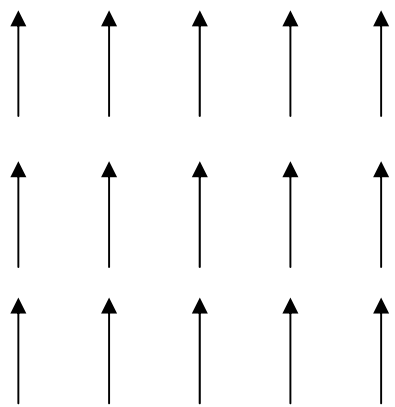
Minimize Free Energy!

$$F = E - TS$$

$$S = k \ln W$$

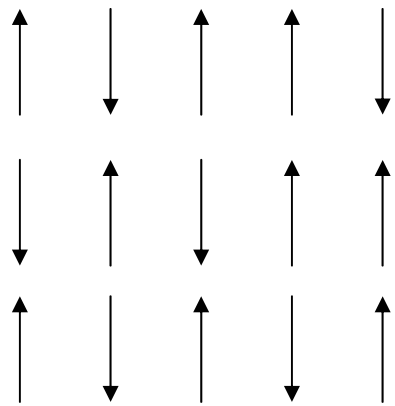
W: Number of States

For example: 2D Ising Model



Low Temperature

$$W = 2$$

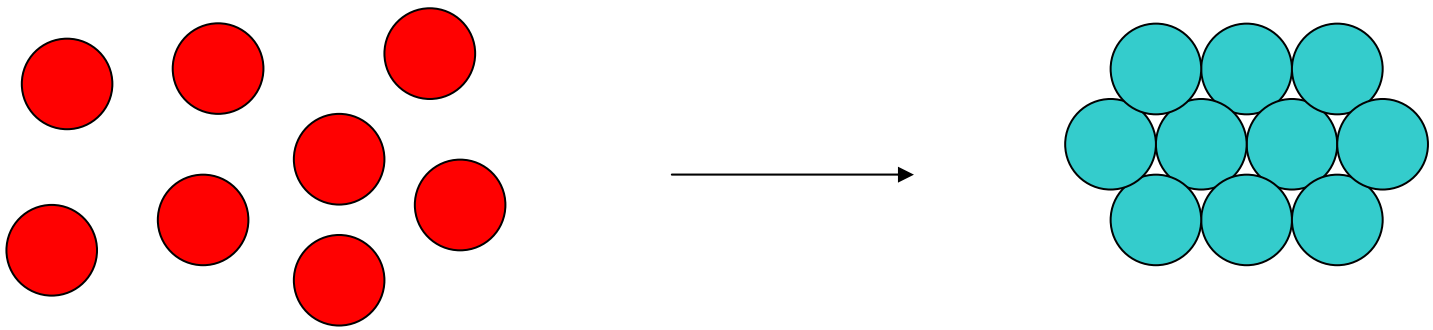


High Temperature

$$W = 2^N$$

Introduction: What is melting?

Our image : Attractive Particle Model



Fluid

Solid

High temperature

Kinetic Energy >> Attractive Interaction

Low temperature

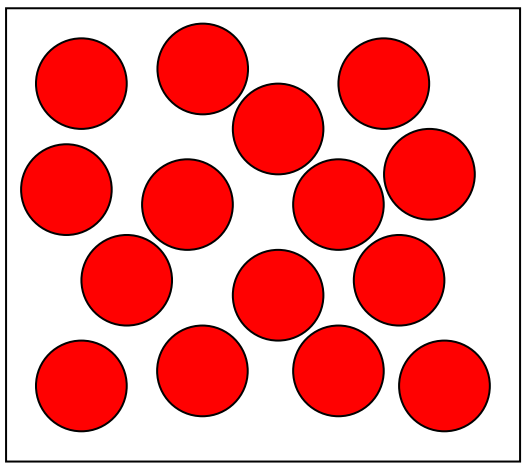
Kinetic Energy << Attractive Interaction

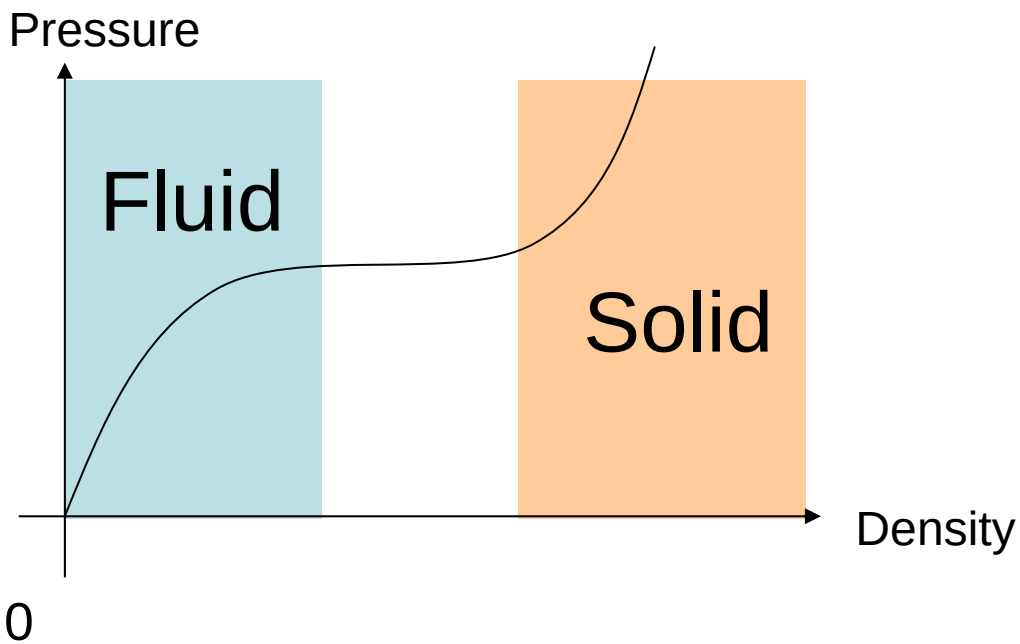
It is not TRUE!

Alder Transition

Alder and Wainright reported a melting transition with using a particle dynamics(ED).

Hard disk Only exclusive volume effect





They concluded the transition is the first order.

Mermin-Wagner's theorem ruled out a positional order

Historical Background

1962 Alder and Wainright

They reported the transition of hard-disk system with MD.

Alder transition

1966 Mermin and Wagner

There are no positional order in the two-dimensional system with finite temperature.

1972 Kosterlitz and Thouless

New phase with quasi-long-range order → KT transition

1978 Halperin, Nelson and Young

They explaned the two-dimensional solid based on the KT transition.

KTHNY Theory

Another theory of first order transition was proposed by Chui.
This problem is still devative.

問題の難しさの整理

- 物が凍るのに、構成粒子に引力相互作用はいらない
  - 融解相転移は、エントロピーによるanomalyのみ
  - 2次元、3次元ともにAlder転移はおきる
- 二次元系では結晶を作れない(Mermin-Wagner)
  - 3次元では結晶ー液体の一次転移
  - 2次元ではKT転移(連続転移)
- ただし、Merminの証明は有限の相互作用のみ
  →剛体円盤系については良く分からない

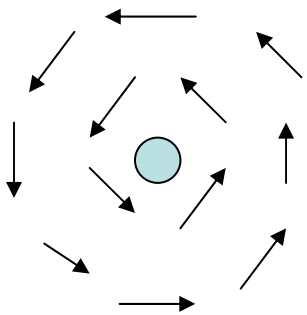
Kosterlitz-Thouless Transition(1)

Mermin-Wagner's Theorem

Two-dimensional systems with short-range interaction cannot break continuous symmetry spontaneously at finite temperature.

No magnetization in spin systems
No positional order in particle systems

Kosterlitz-Thouless Transition



Defects: Vortices (Excitation)

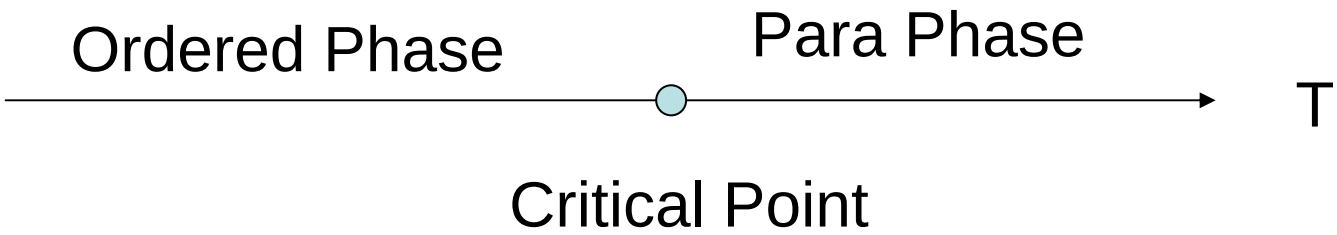
Vortex has charge (Plus and Minus).
Vortices make pairs at low temperature.

Low Temperature :The system is almost uniform.

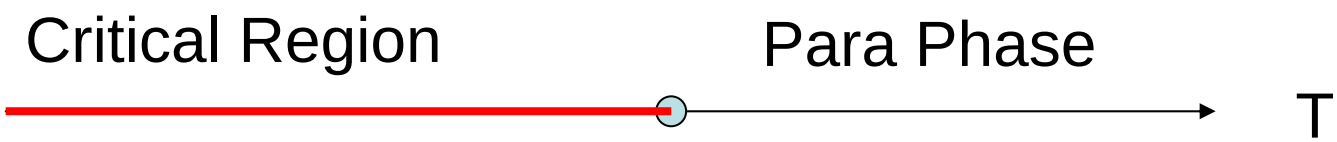
High Temperature: There are many vortices.

Kosterlitz-Thouless Transition(2)

Ordinary continuous transition(2nd order)



Kosterlitz-Thouless Transition



KTHNY Theory (1)

They treated two defects independently.

Two Defects

Disclinations (Line defects)
Dislocations (Point defects)

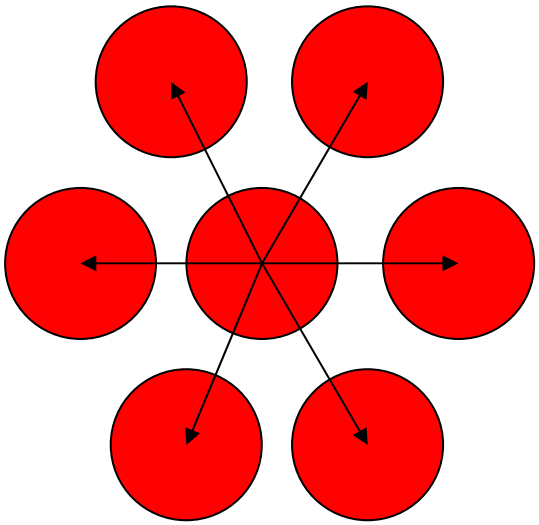
$$H = \frac{J}{2}\sum_{i \neq j} q_i q_j \log \frac{\left| r_i - r_j \right|}{r_0} + E_c$$

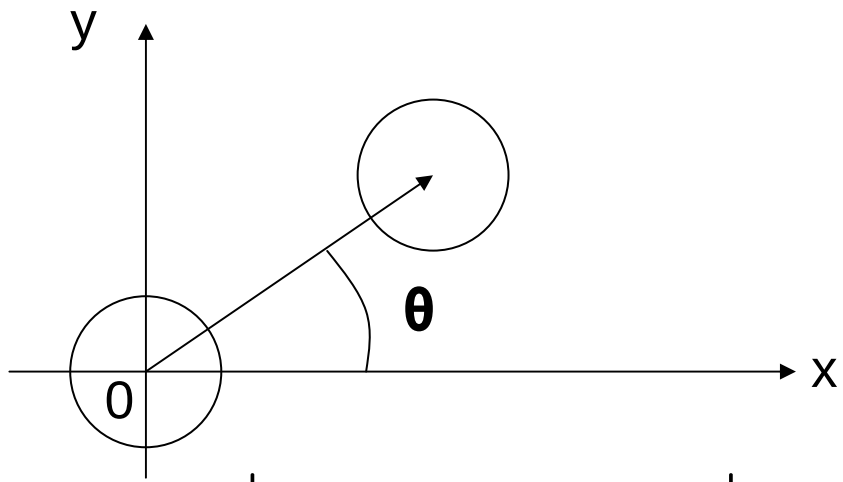
Renormalization analysis like as KT, the coupling constant J becomes relevant to irrelevant at the critical density.

They predicted two KT transitions.

A new phase, named a hexatic phase is introduced.

Bond-orientational Order





$$\phi_6 = \left| \sum_j \exp(6 i \theta_j) \right|$$

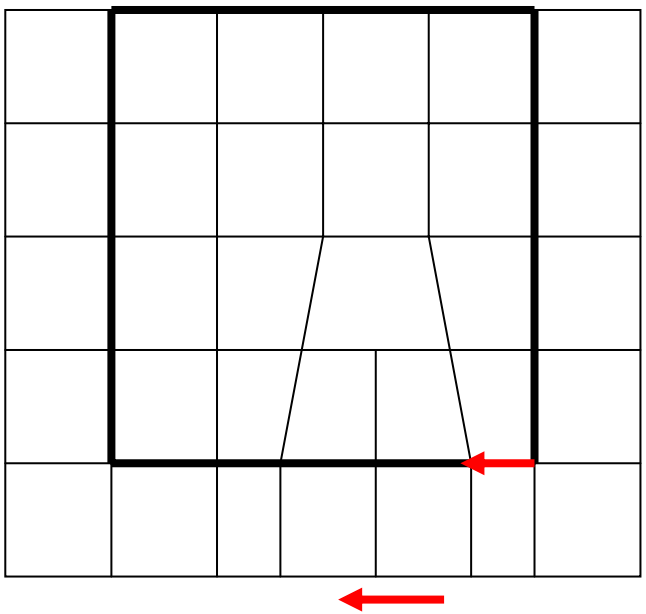
Perfect Hexagonal Packed $\phi_6 = 1$

Completely Disordered $\phi_6 = 0$

Index to describe how close the system is to hexagonal ordering.

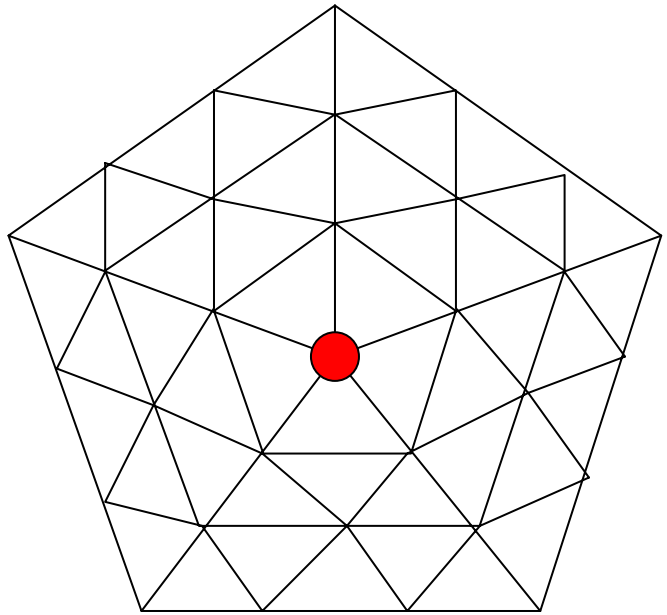
Two kinds of defects

Dislocation



Burgers Vector

Disclination



Singular Point

Defect type	Vector
bond-orientational order	don't destroy
Influence	local

Defect type	Scalar
bond-orientational order	destroy
Influence	global

KTHNY Theory (2)

	Solid	Hexatic	Fluid
Dislocation	Pair	Free	Free
Disclination	Quartet	Pair	Free
Positional Correlation	Quasi-long-range	Short range	Short range
Bond-orientational Correlation	Long range	Quasi-long-range	Short range

Point!

Quasi-long-range order is power law decay.

We can determine the three phases with the bond-orientational order

Points of the Alder transition

- The simplest particle model has such a complicated behavior.

- What is the nature of the melting transition?
  - It is pure entropic effect (Packing Entropy).

- Strong finite-size effects.
  - It make the problem difficult.

Recent Studies

1962	B. J. Alder et. al.	MD(NVT)	first order	N=870	PR 127,359
1982	S. T. Chui	Analytic arguments	first order	Collective excitations of dislocations	PRL 48,933
1992	J. A. Zollweg G. V. Chester	MC(NVT)	week first order	Strong finite-size dependence	PRB 46 11186
1995	J. Lee K. J. Strandburg	MC(NpT)	first order	Double peeked V	PRB 46, 11190
1995	J. F. Fernandez et. al.	MC	One-stage continuous	Bond-orientational ord.	PRL 75, 3477
1994	S. Todo and M. Suzuki	Analytic arguments	first order	Padé approximation coherent anomaly	JPSJ 63,3552
1995	H. Weber et. al.	MC	first order	Finite-size scaling	PRB 51,14636
1999	A. Jaster	MC	KTHNY	divergence of B.O.O.	PRE 59 2594
2000	S. Sengupta et.al.	MC	first order	Renormalization analysis	PRE 61, 6294

The points of our study

1) To confirm the KTHNY theory.

2) Use the particle-dynamics simulations
(Other studies use the Monte Carlo method)

3) Observe non-equilibrium relaxation(NER) processes of the bond-orientational order.
(Other people studied equilibrium state.)

4) Finite-time scaling analysis
(Other studies use finite-size scaling analysis.)

Non-equilibrium Relaxation Method

By analyzing non-equilibrium relaxation(NER) process, we can study equilibrium properties of systems.

Points

1) Save much computational time
   It requires only relaxation processes.

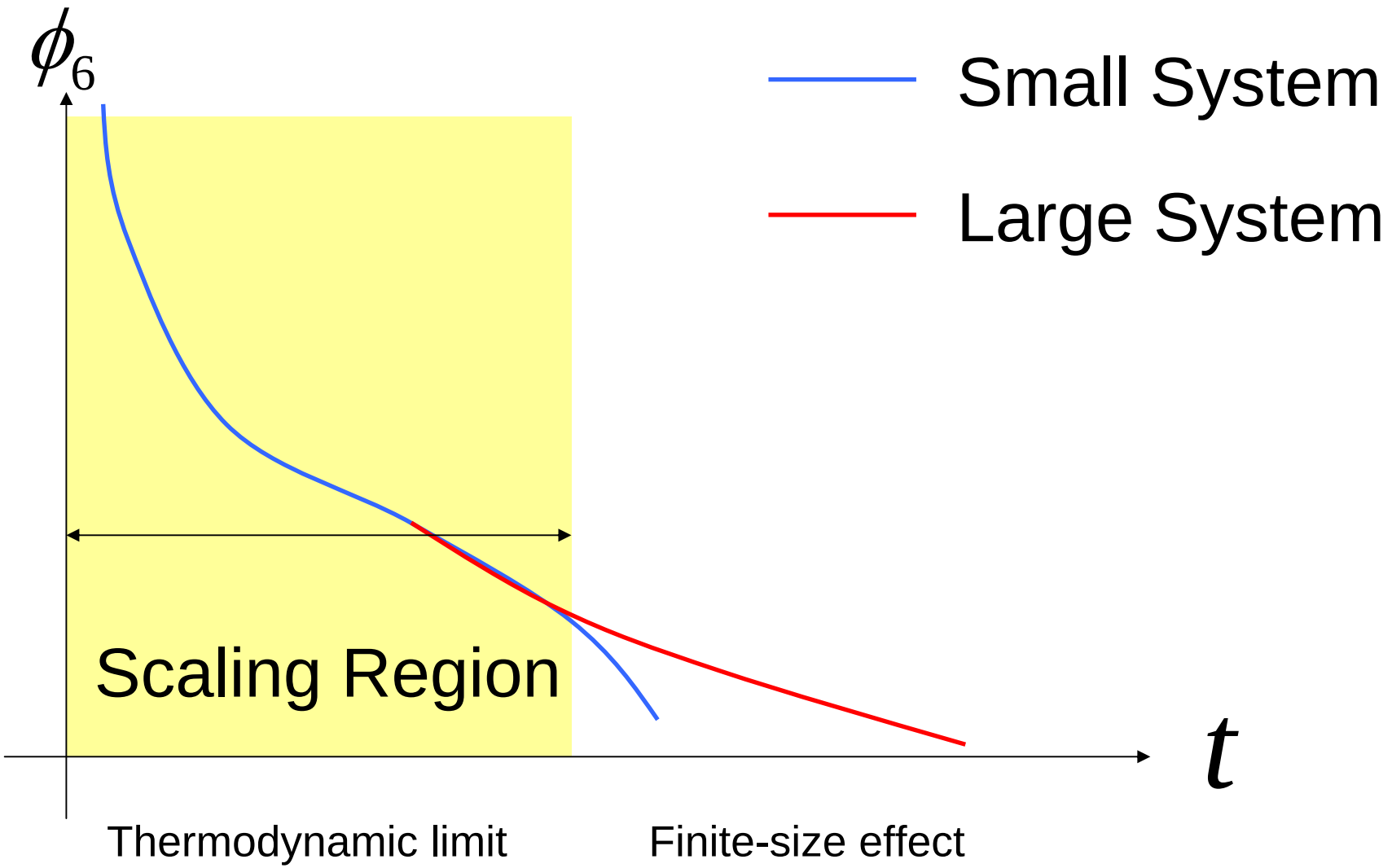
2) Less influenced by the finite-size effects.

3) Based on a finite time scaling hypothesis

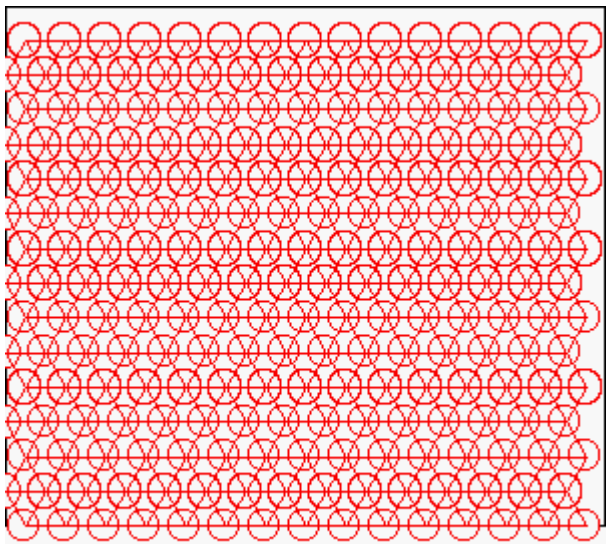
$$F(\varepsilon, h, L, t) = L^{-d}\overline{F}(\varepsilon L^{y_H}, hL^{y_H}, tL^{-z})$$
$$\tau = \xi^{z}$$

There are many studies which use the NER method with MC simulations. In this study, we apply the NER method for a particle dynamics simulation for the first time.

Finite-size effect



Numerical Simulations



1) Initial State — the perfect hexagonal order
2) density — controlled by particle size
3) the range of density — 0.85 to 0.95
4) Time evolution — particle dynamics
5) The number of particles — 23288
6) Total steps — 1,300,000,000

The behavior of the bond-orientational order

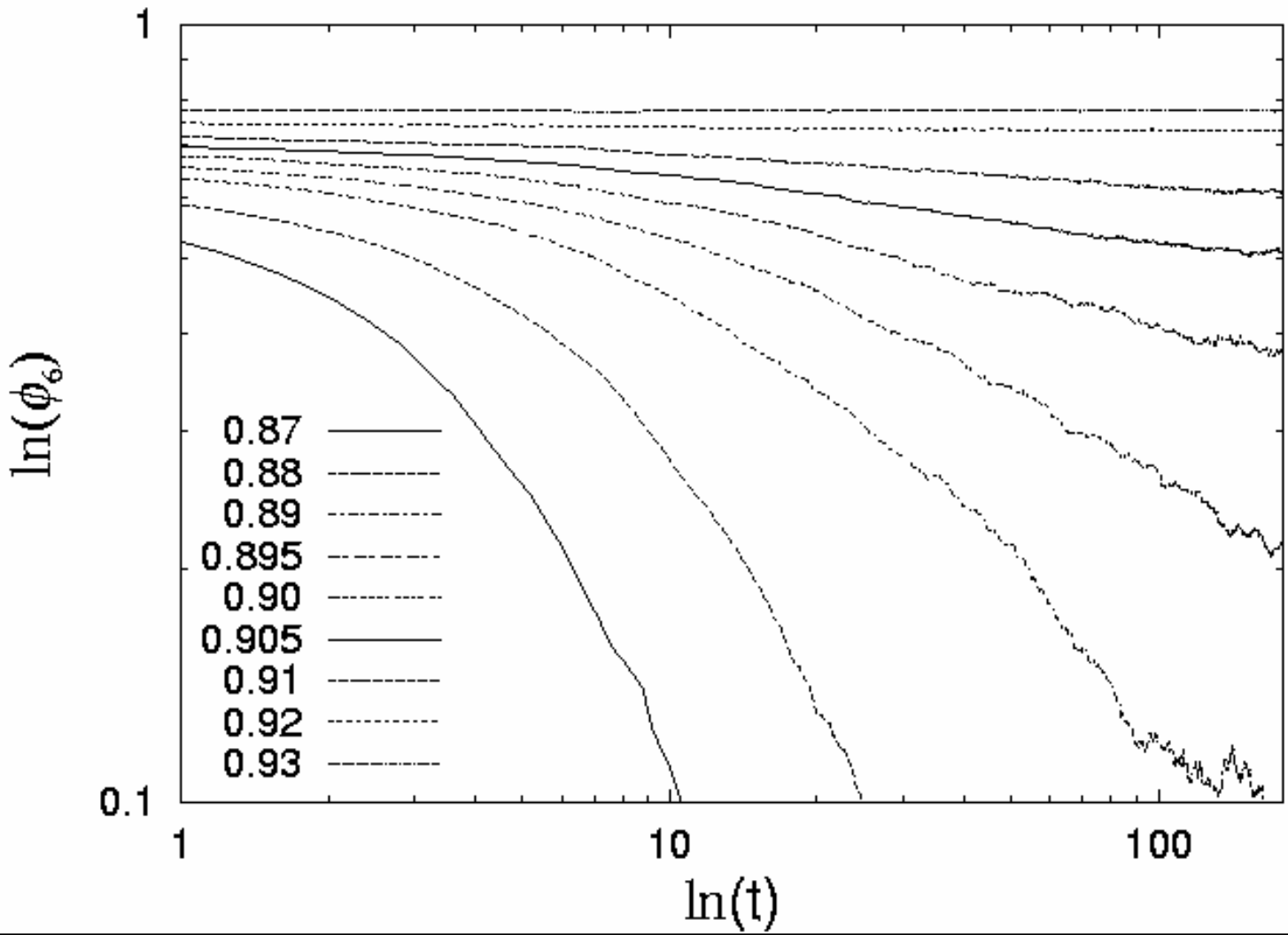
$$\phi_6 \approx \exp(-t/\tau)$$ ---------- Fluid Phase

$$\approx t^{-\lambda}$$ ---------- Hexatic Phase

$$\approx \exp(-t/\tau) + \mathrm{Const}$$ ---------- Solid Phase

Movie

Bond Orientational Order(Log-Log)



It’s hard to determine the two critical points.

Finite-time scaling

Near the critical point, the bond-orientational order can be expressed with a relaxation time as,

$$\phi_6(\varepsilon, t) = t^{-\lambda}\overline{\phi_6}(t/\tau(\varepsilon)).$$

$$\varepsilon = \left|\rho - \rho_c\right| / \rho_c$$

By renomarlization analysis, we can find the correlation length diverges as

$$\xi = g\exp(-h/\sqrt{\varepsilon}).$$

Using the dynamical scaling relations, we have

$$\tau = a\exp(-b/\sqrt{\varepsilon}).$$

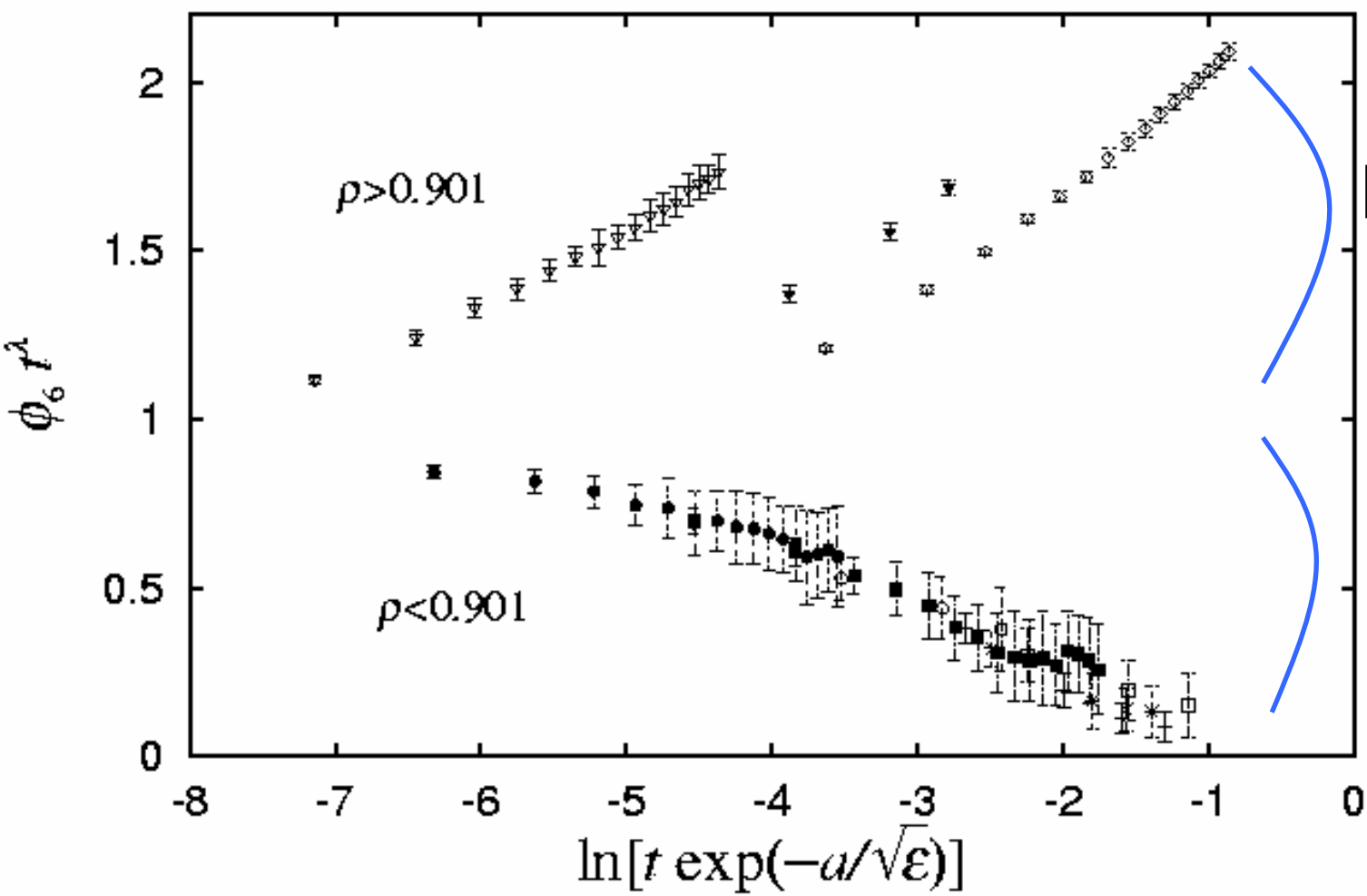
Finally, we obtained the form of the finite-time scaling function of bond-orientational order as,

$$\phi_6 = t^{-\lambda}\overline{\phi_6}(t\exp(-a/\sqrt{\varepsilon}))$$

Point!

We can scale only under the critical point.

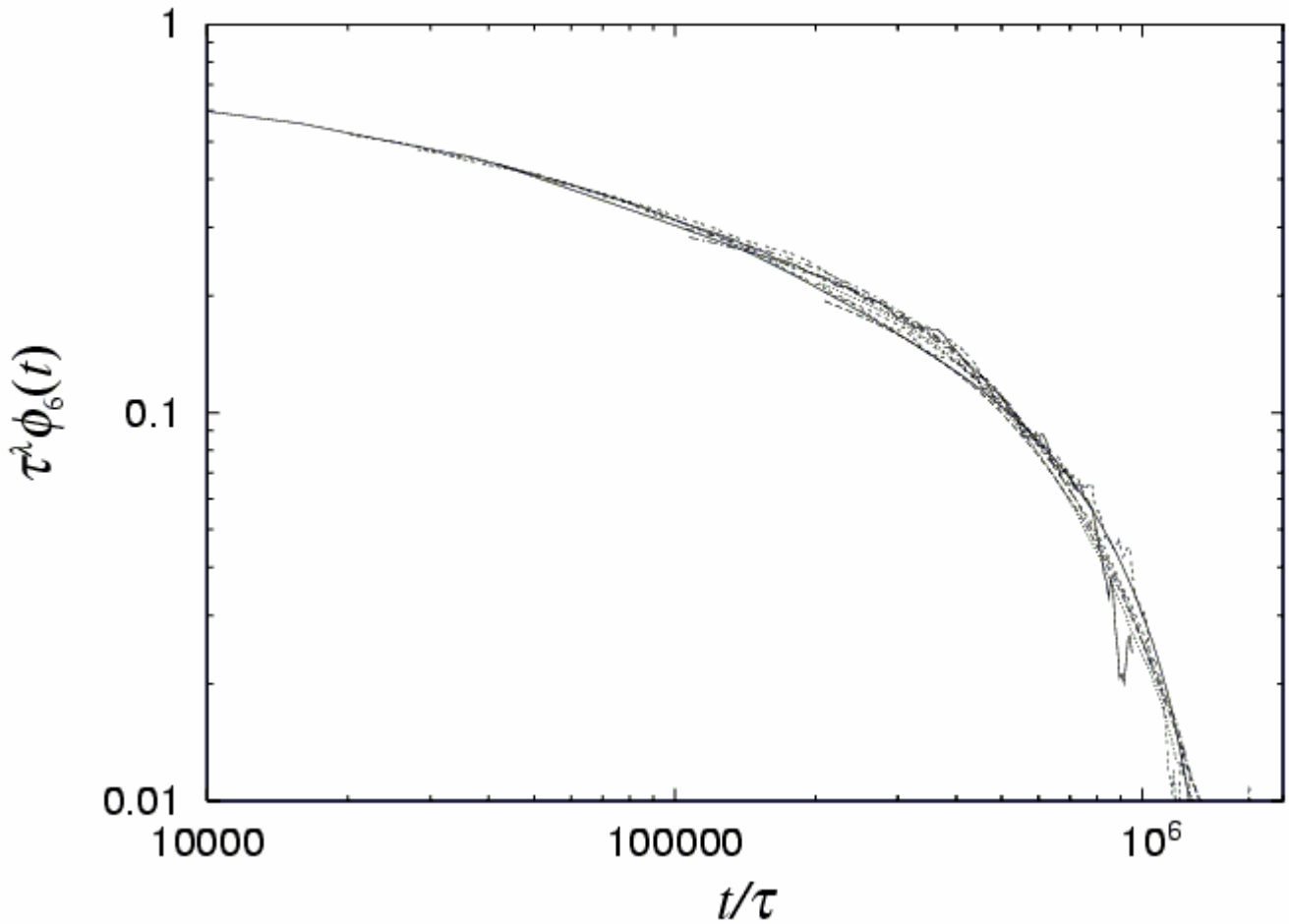
Scaling results(Hexatic-Liquid)



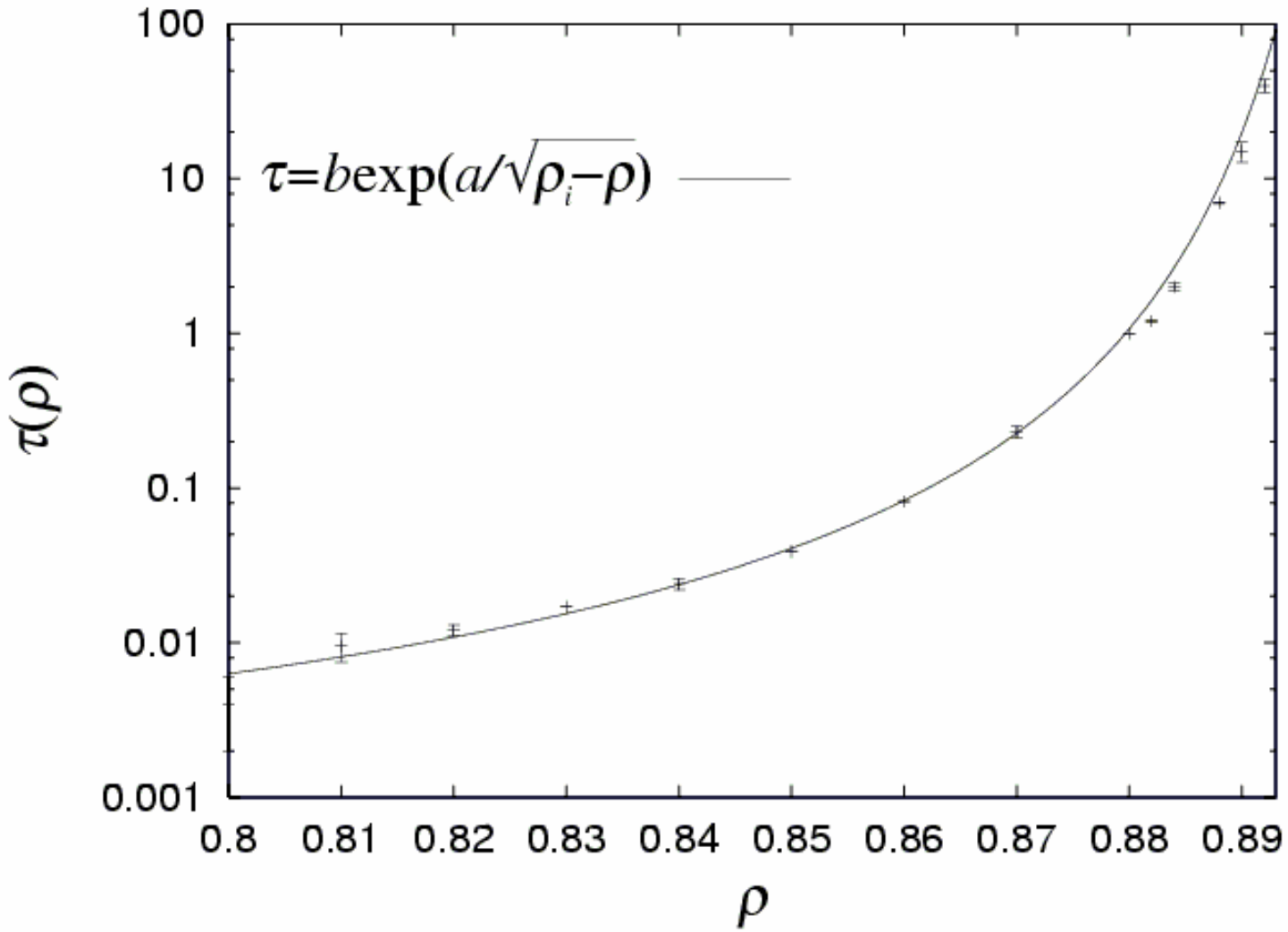
Hexatic

Liquid

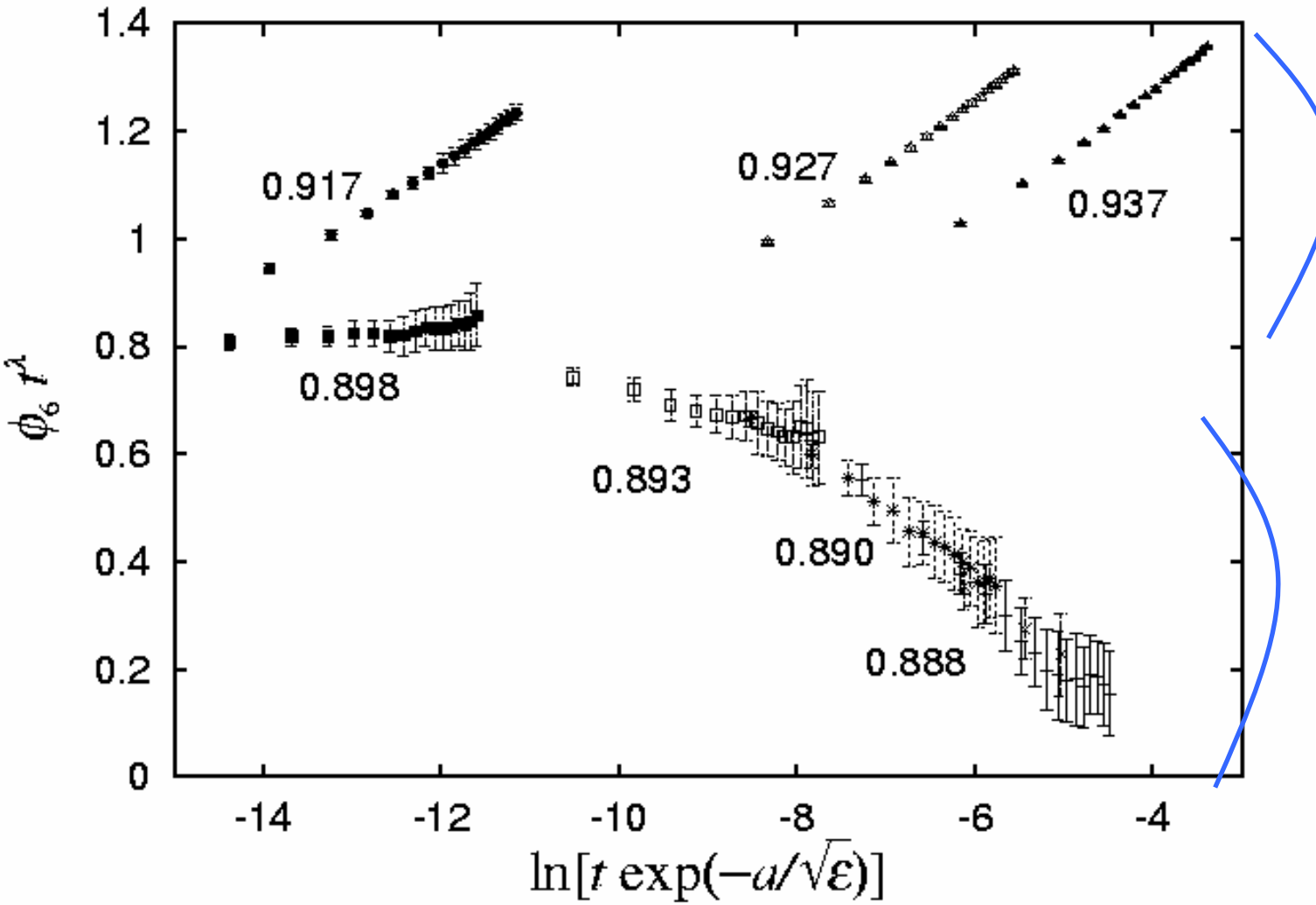
Scaling results(Hexatic-Liquid)



Correlation Time



Scaling results(Hexatic-Solid)



Solid

Hexatic

Fitting Results

Three fitting parameter λ, a , the critical point
We can determine λ and the critical point by analyzing relaxation time.

Purpose

1) Determine the two transition points
2) Confirm the KT-transition behavior

Results

- Liquid-Hexatic ・・・ 0.901(2)
- Hexatic-Solid ・・・ 0.910(2)

Jaster estimated as 0.899(1) and 0.91.
Our results are consistent with his result.

Point! Asymmetric scaling behavior ⟶ KT transition!

NER of Fluctuation

$$F(\varepsilon, h, L, t) = L^{-d}\,\overline{F}(\varepsilon L^{y_T}, hL^{y_H}, tL^{-z})$$

Asymptotic behavior of the order parameter

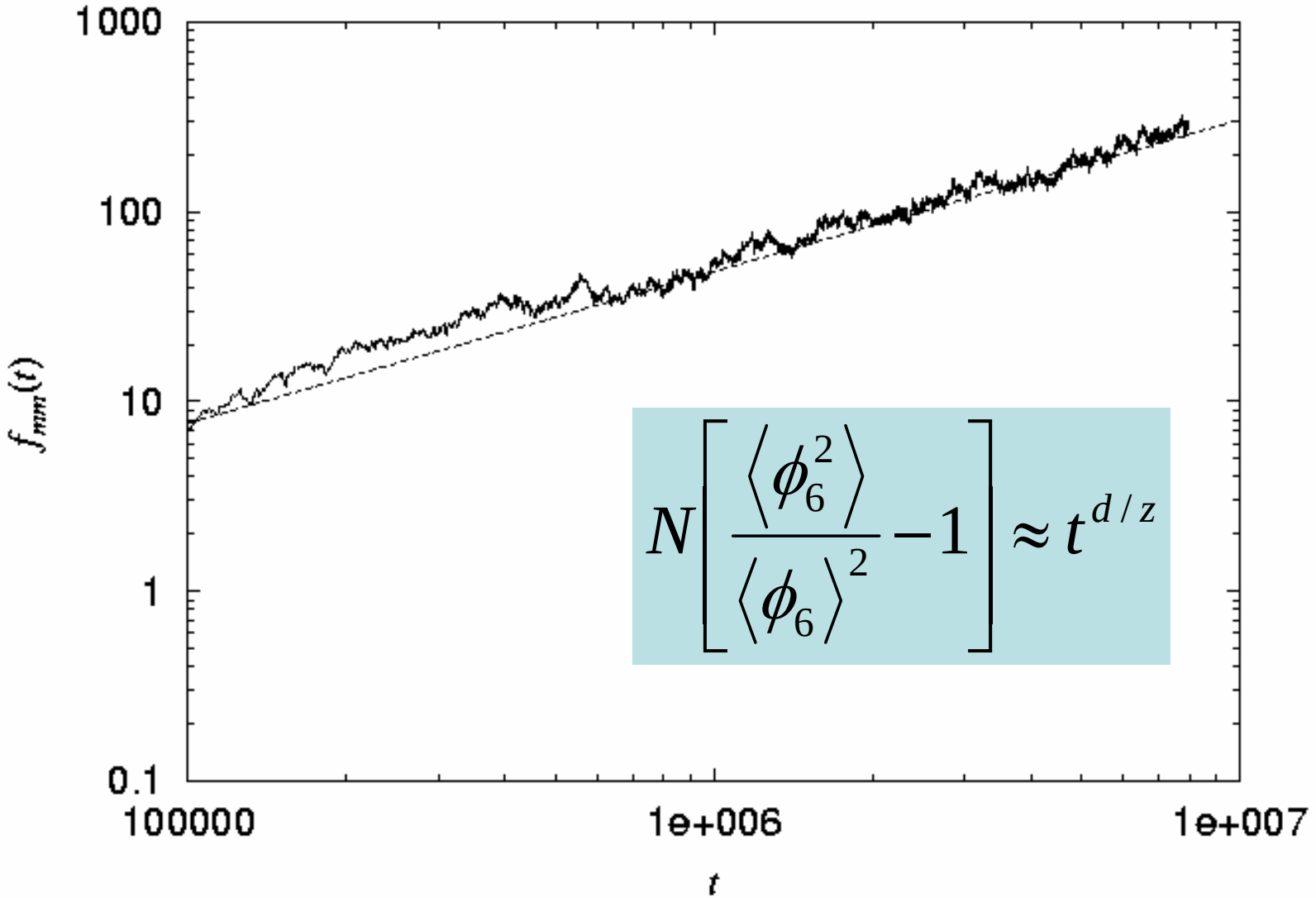
$$\left\langle \phi_6(t) \right\rangle \approx t^{-\eta/2z}$$

Fluctuation of the order parameter

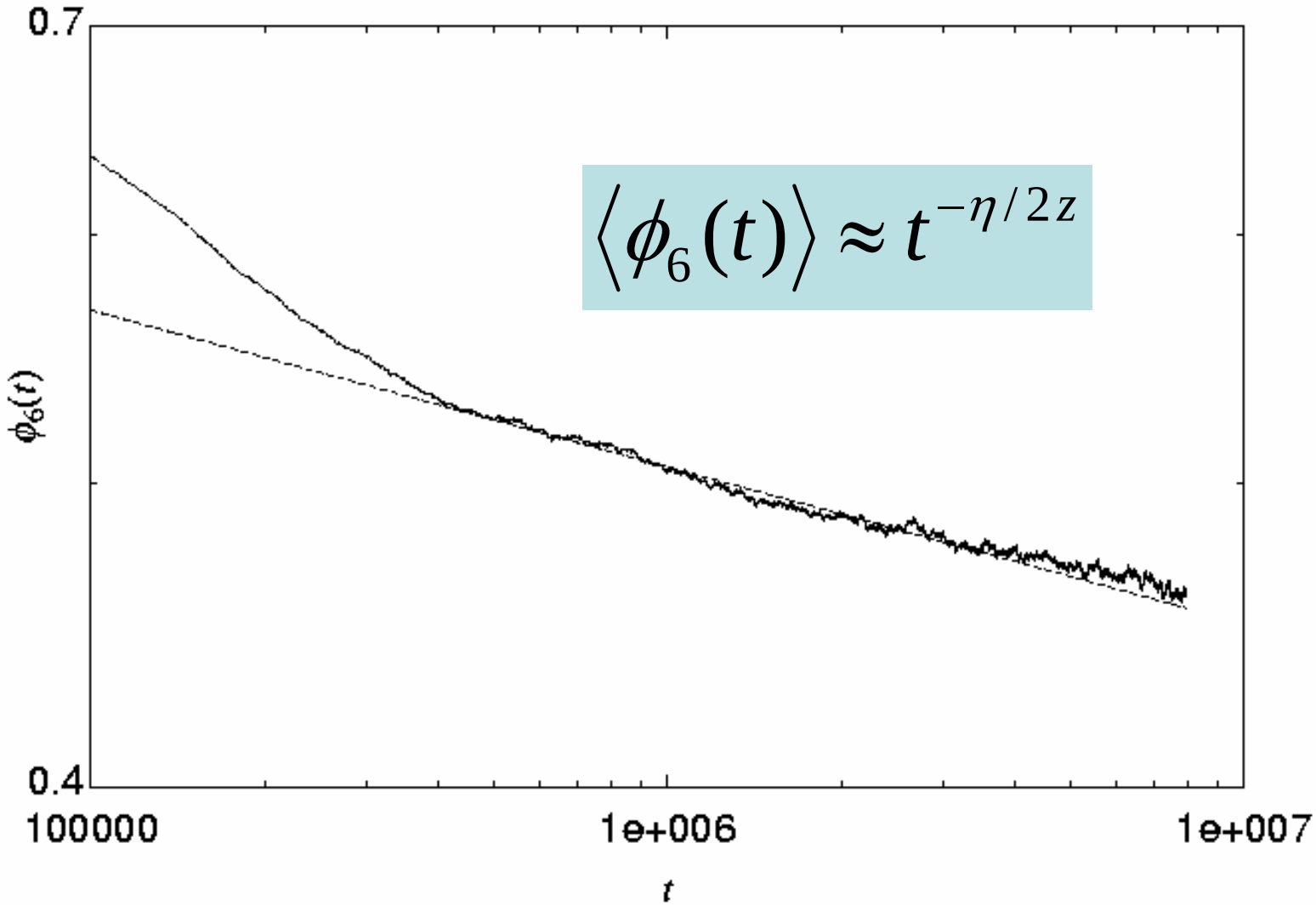
$$N\left[\frac{\left\langle \phi_6^2 \right\rangle}{\left\langle \phi_6 \right\rangle^2} - 1\right] \approx t^{d/z}$$

NOTE: $\left\langle \cdot \right\rangle$ implies sample averaging.

Fluctuation of the Order Parameter



Relaxation of the Order Parameter



The critical exponents

From relaxation of the order parameter, we obtain

$$\frac{\eta}{2z} = 0.05(1)$$

From fluctuation of the order parameter, we obtain

$$\frac{d}{z} = 0.8(1)$$

Finally,

$$z = 2.5(2)$$

$$\eta = 0.25(3)$$

Summary

1) We have studied the non-equilibrium relaxation behavior of the bond-orientational order to confirm the KTHNY theory.

2) We confirmed the existence of the hexatic phase.

3) Using finite-time scaling, the two transition points are determined as 0.901(2) and 0.910(2), and we find the two transitions are of the KT transition.

4) By NER of fluctuation, two critical exponents η and z are determined as 0.25(3) and 2.5(2).

References

1) Non-equilibrium Relaxation Analysis on Two-dimensional Melting
H. Watanabe, S. Yukawa, Y. Ozeki, N. Ito
Phys. Rev. E 66, (2002) 041110

2) Critical exponents of isotropic-hexatic phase transition in the hard-disk system
H. Watanabe, S. Yukawa, Y. Ozeki and N. Ito
Phys. Rev. E 69, (2004) 045103

3) Phase Diagram of Hard-disk Systems with Size-dispersity
H. Watanabe, S. Yukawa and N. Ito
Submitted to Phys. Rev. Lett.

備考

・１次転移　→　相関長が有限
　連続転移　→　相関長が無限(臨界点で)

(相関長ー界面の大きさ)

・潜熱の小さい一次転移と二次転移の区別は難しい
(cf. q-state Potts Model)
→相関長が系のサイズに達した時、無限か有限かは原理的にわからない

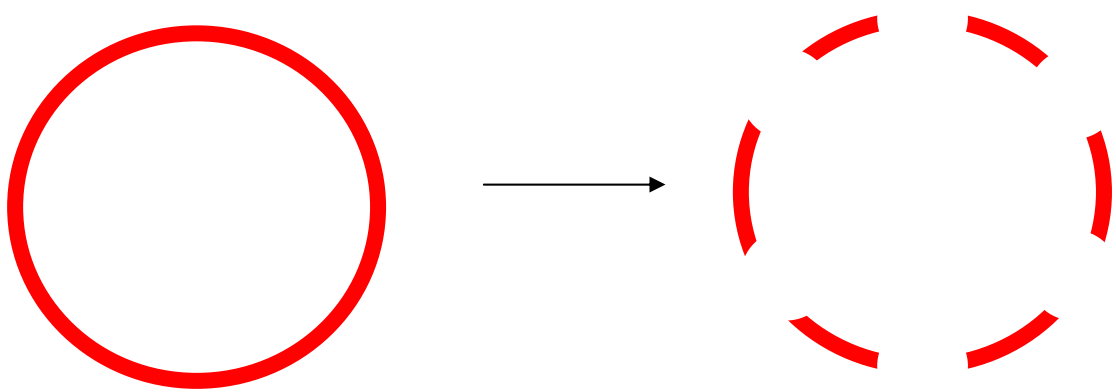
Experiments

Materials

1) Absorbed gas on graphite.
2) Smectic phase of liquid crystals

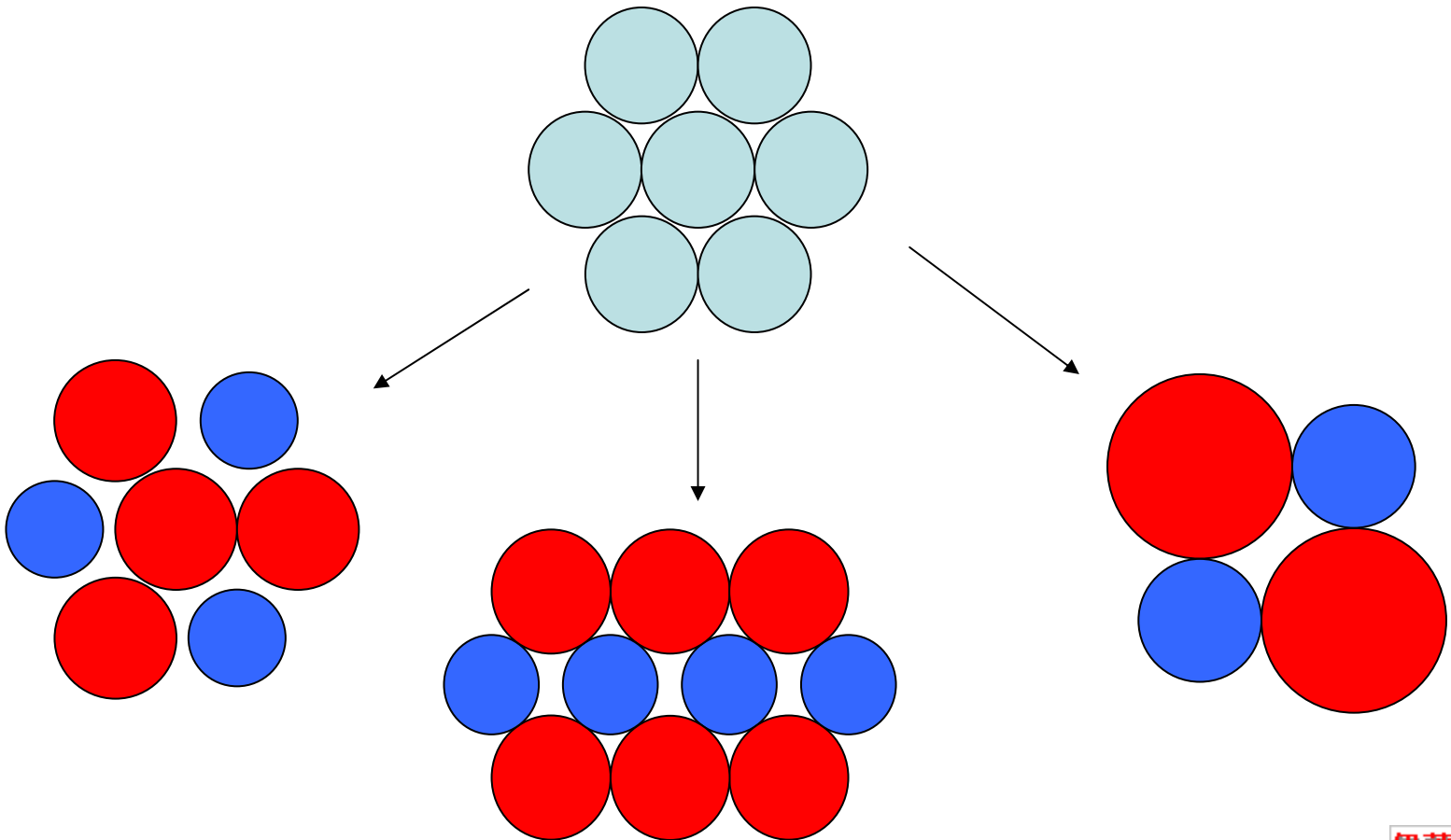
Observable

1) Frank elasticity
2) X ray diffraction ⟷ Bond-orientational order



Ito Group, Univ. of Tokyo

Dispersity effect on the two-dimensional melting



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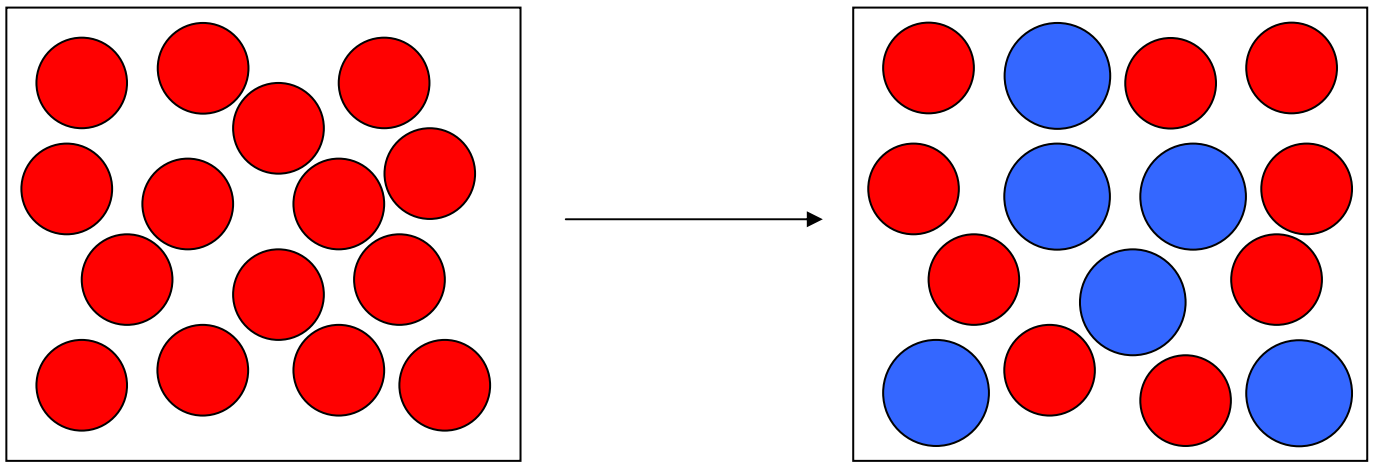
Motivation

Study complexity from a simple model

cf.) Granular Media

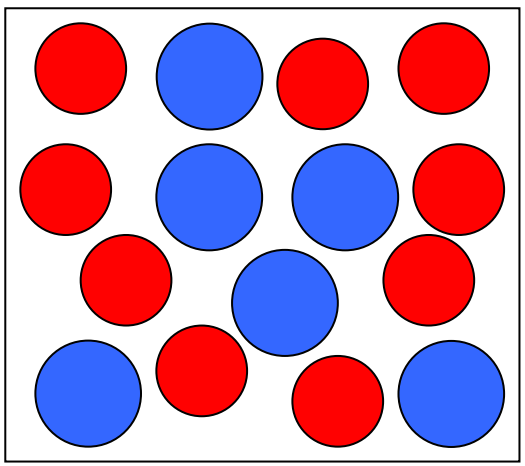


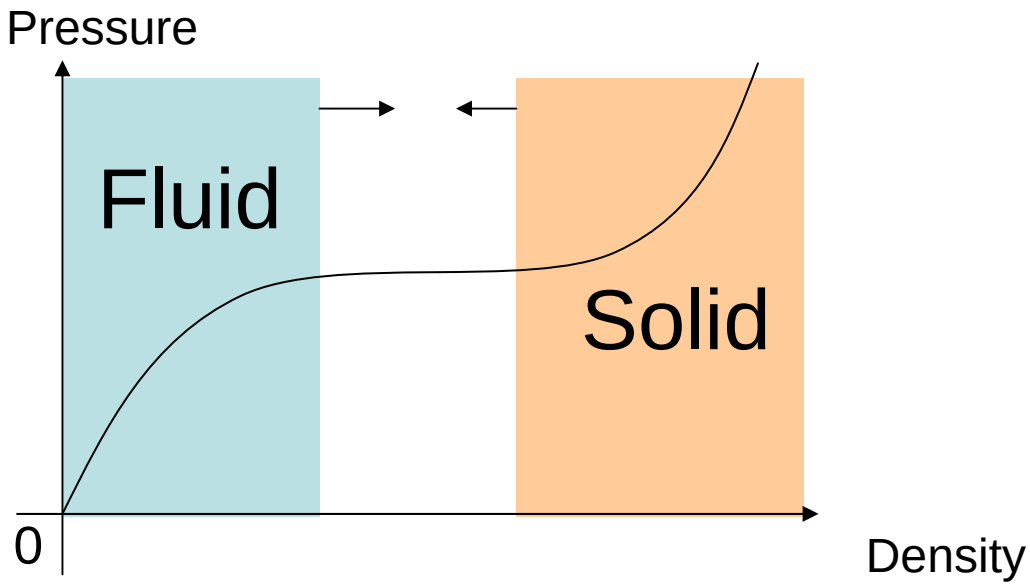
Quantitative approach

Critical points
Critical exponents

Introduction

Dispersity effect on two-dimensional melting





E. Dickinson and R. Parker, Chem. Phys. Lett. 79 (1981) 578.

W. Vermohlen and N. Ito PRE 51 (1995)4325

We study the structure's behavior by observing the bond-orientational order.

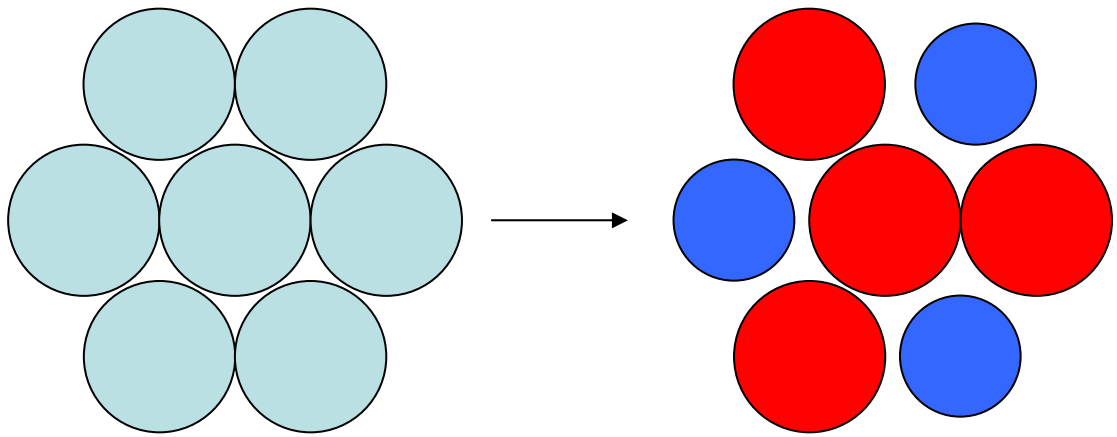
Closest Packing (Hexatic)

Dispersity (binary disperse system)

$$\sigma = \frac{r_a - r_b}{r_a + r_b} \qquad (r_a > r_b)$$

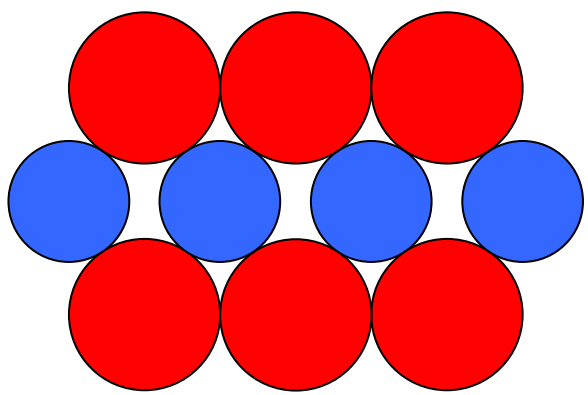
$$\rho = \frac{2}{\sqrt{3}} \frac{\sigma^2 + 1}{(\sigma + 1)^2}$$

Decreasing Function



$$\rho = \frac{2(\theta + \varphi)(r_a^2 + r_b^2)}{\pi r_a \sqrt{r_a^2 + 2 r_a r_b}}$$

$$\cos\theta = \frac{r_a}{r_a + r_b} \qquad \sin\varphi = \frac{r_a}{r_a + r_b}$$

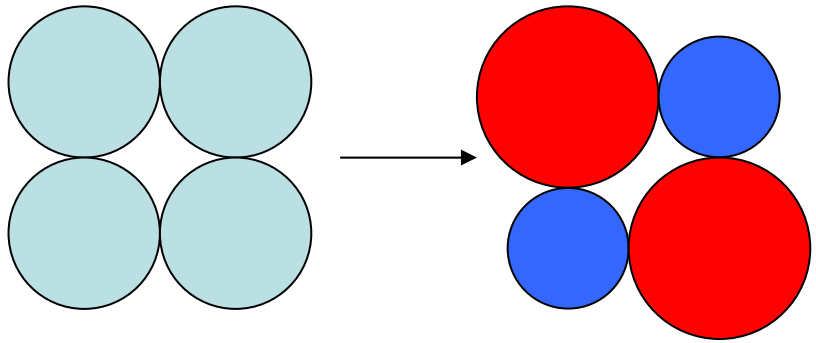


Closest Packing (Quadratic)

No overlap between big circles

$$\rho = \sigma^2 + 1$$

Increasing Function

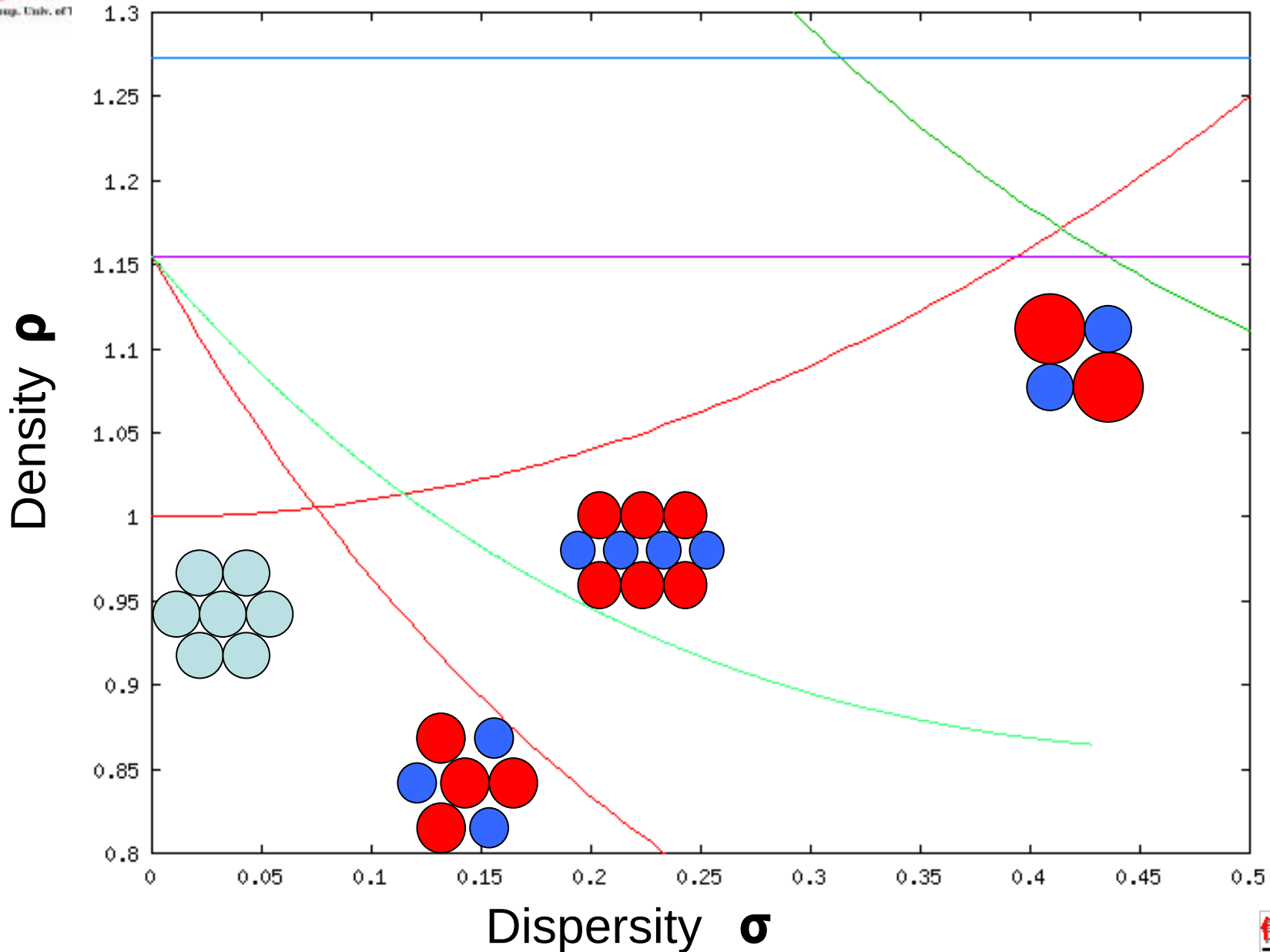


No overlap between big and small circles

$$\rho = \frac{2(\sigma^2 + 1)}{(\sigma + 1)^2}$$

Quadratic Solid at high dispersity condition

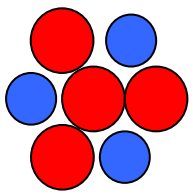
Phase diagram of binary disperse system



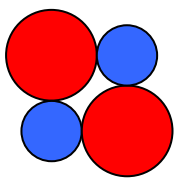
Simulation

Study stability of the configurations.

Observe relaxation behavior of bond-orientational orders.



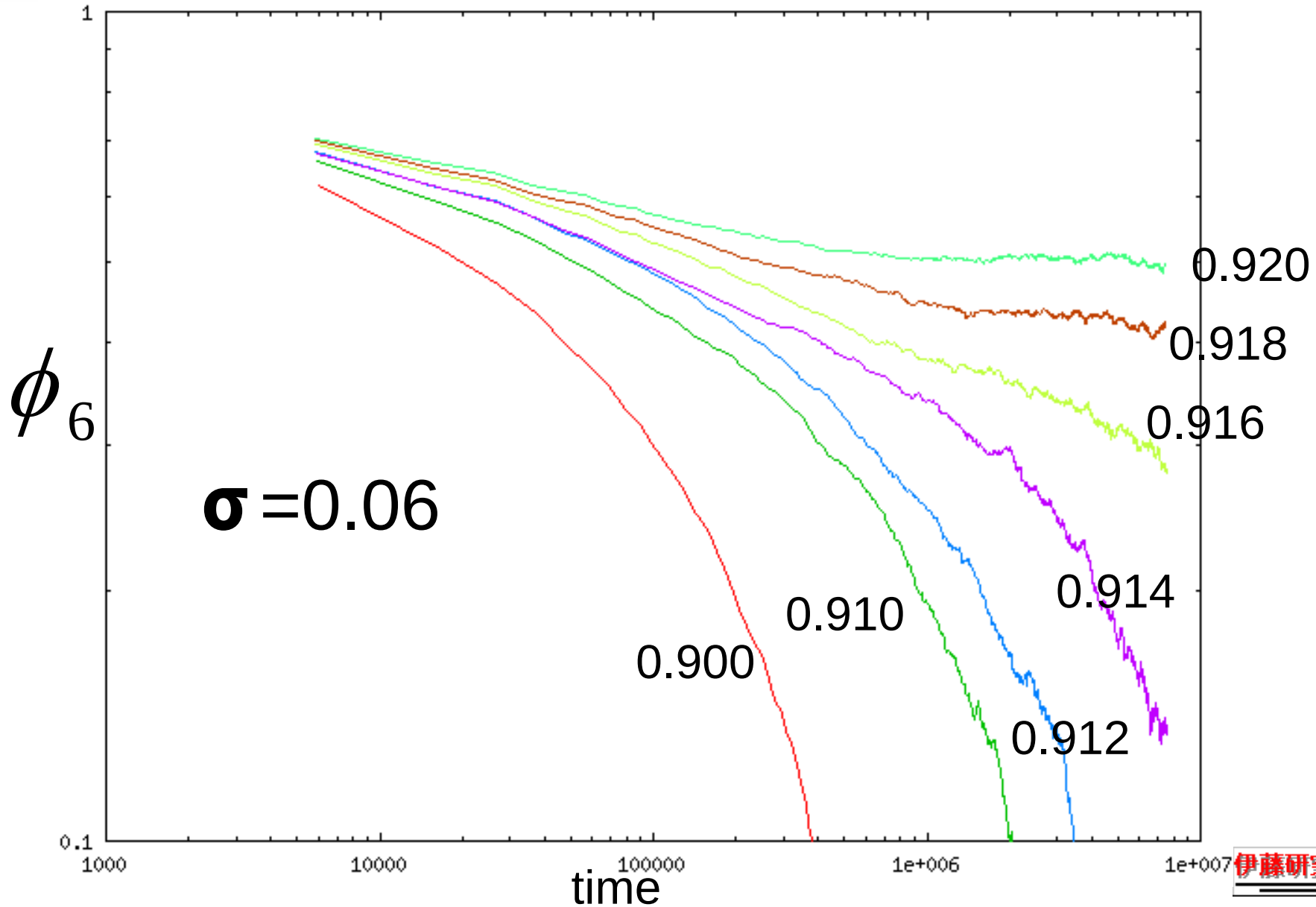
$$\phi_6 = \left| \sum_j \exp(6 i \theta_j) \right|$$



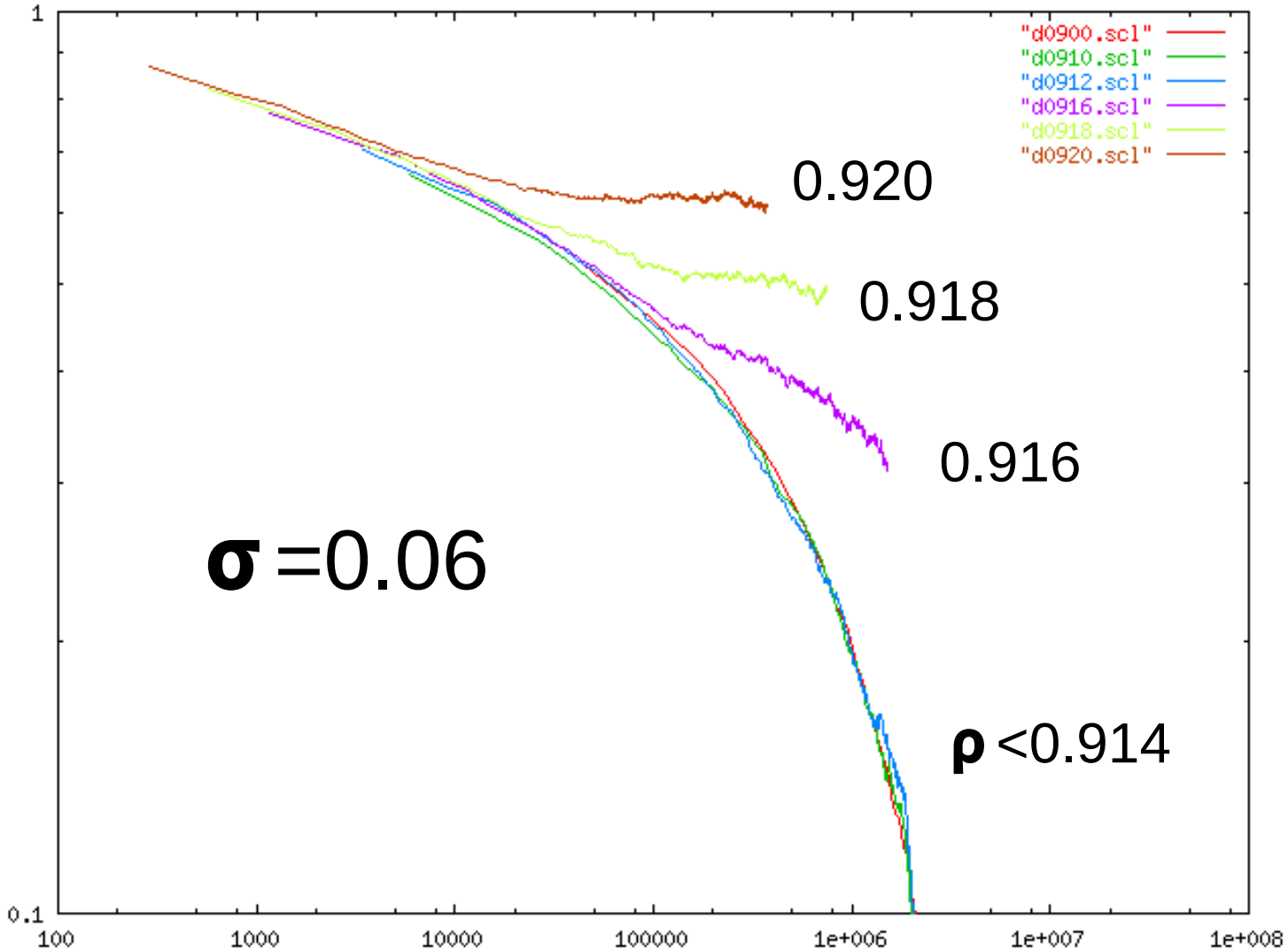
$$\phi_4 = \left| \sum_j \exp(4 i \theta_j) \right|$$

DEMO

Results (Hexatic)



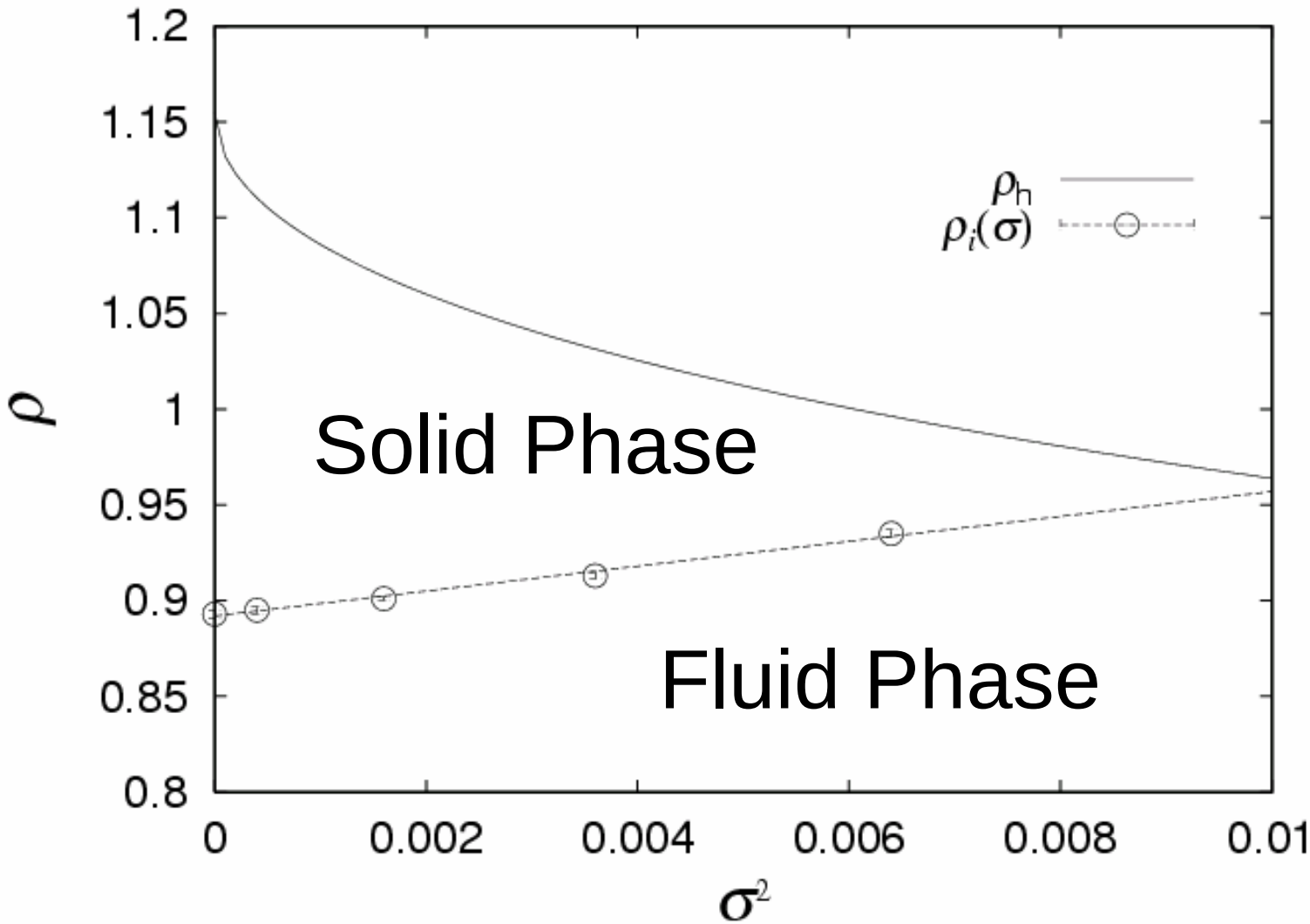
Scaled Results (Hexatic)



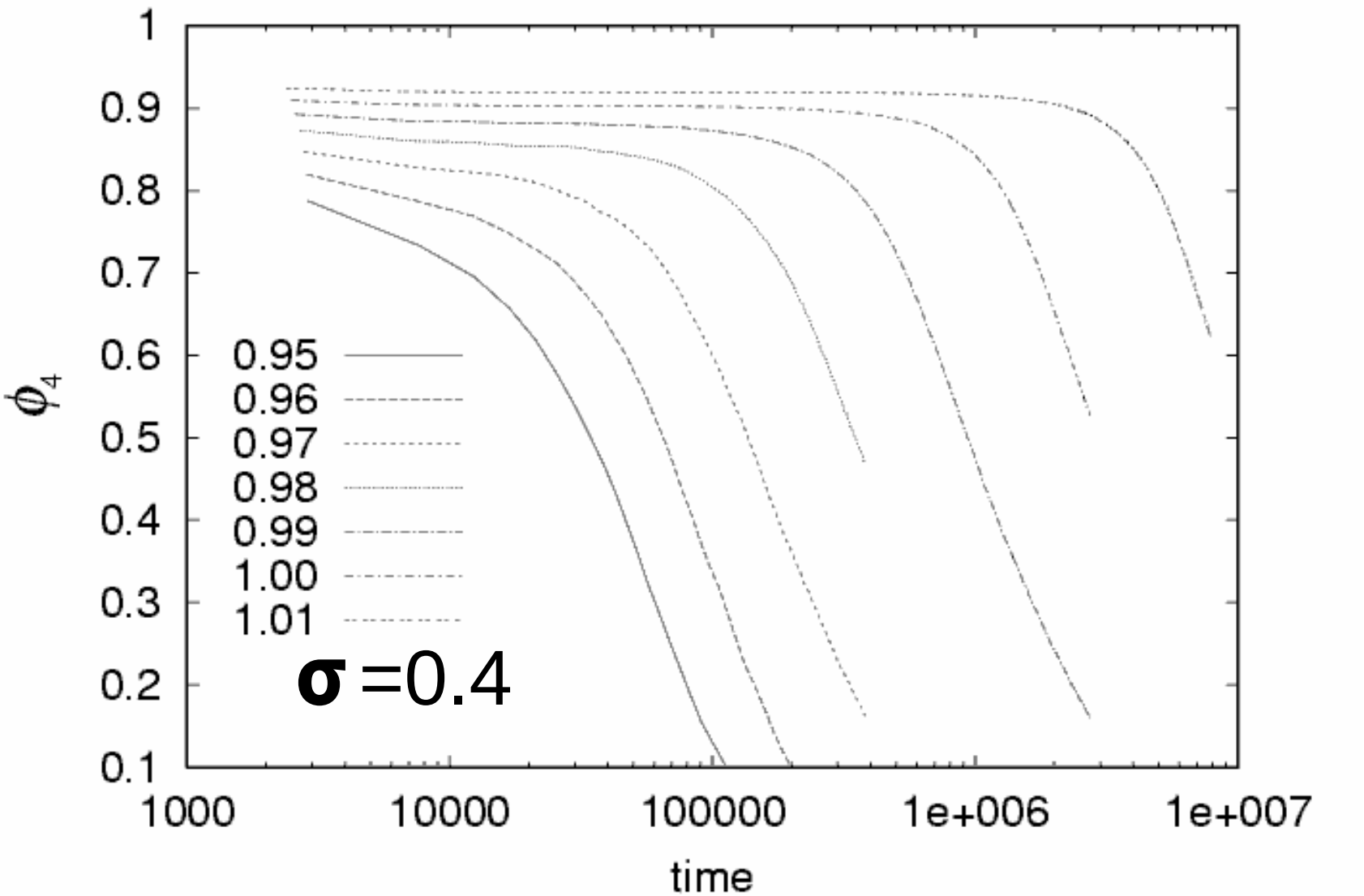
ϕ_6

time

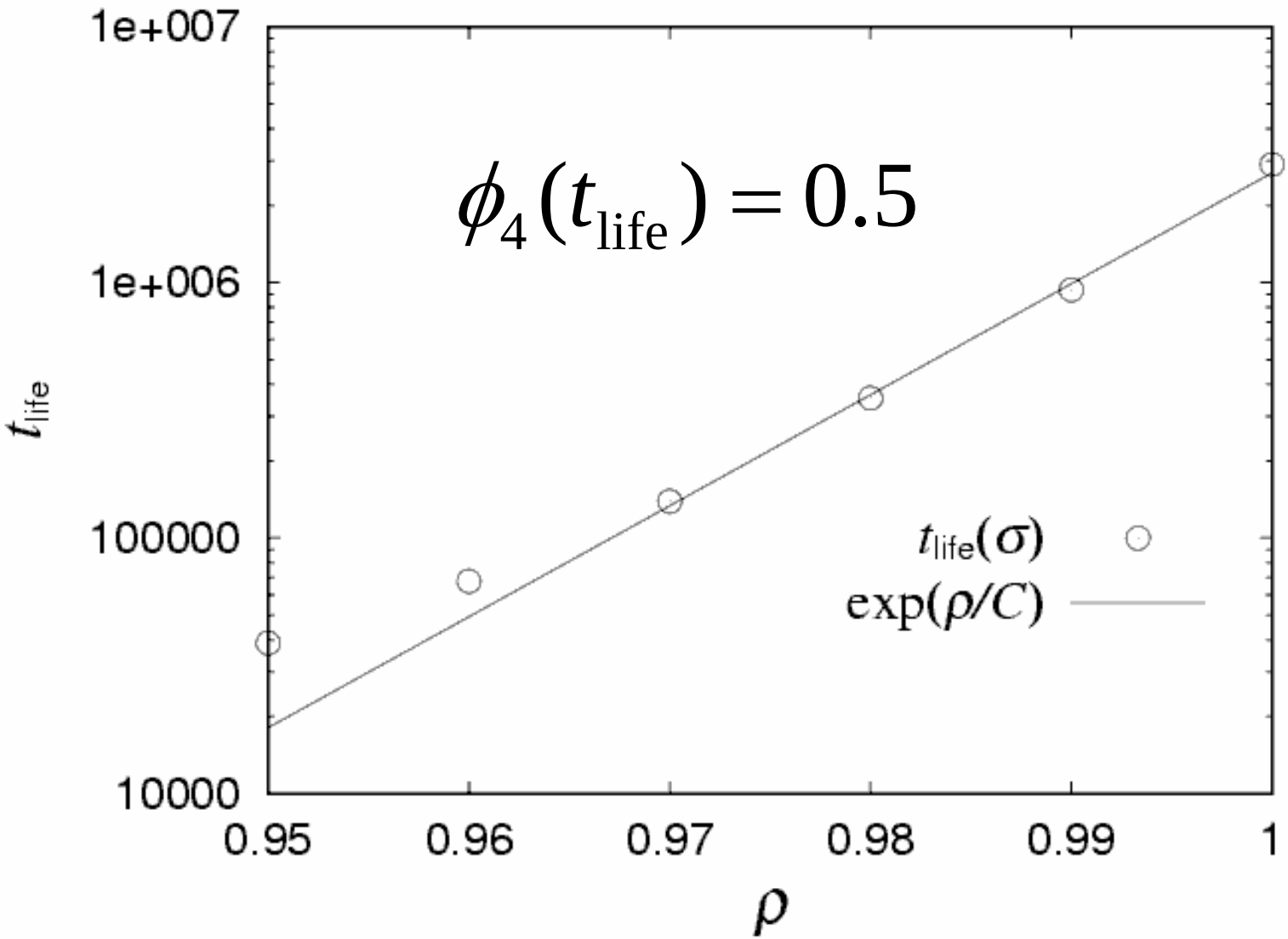
Shift of Critical Point



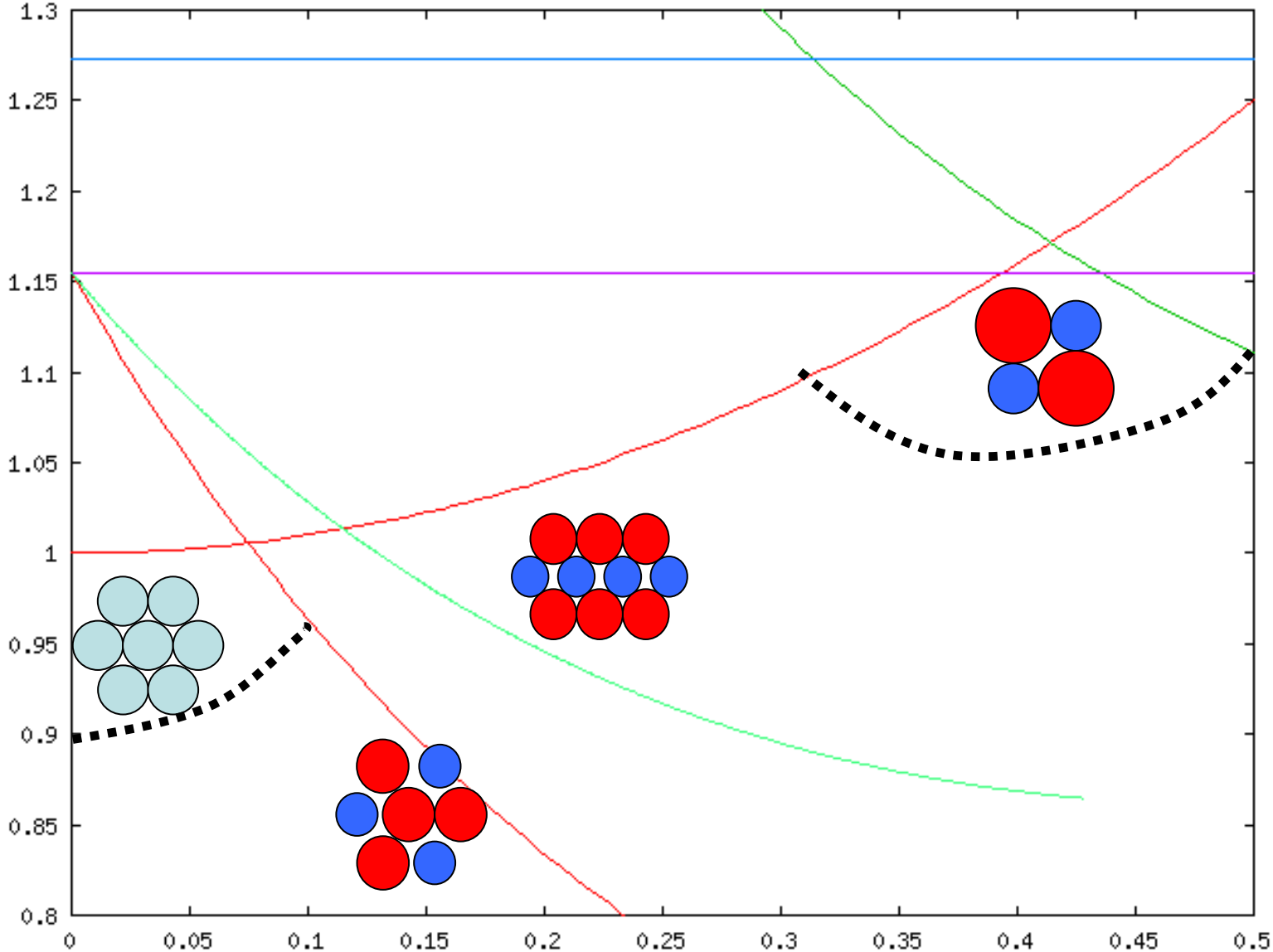
Quadratic Packing Configuration



Lifetime of the Quadratic Structure



Phase diagram of bi-disperse system



Summary and Discussion

1) We study a phase diagram of the binary disperse systems.
2) The phase boundary of hexagonal solid is determined.
3) The stability of Quadratic solid is investigated.
   However, transition behavior is not observed.