Hard Core Exclusion Models on Lattices: Rods, Rectangles and Discs

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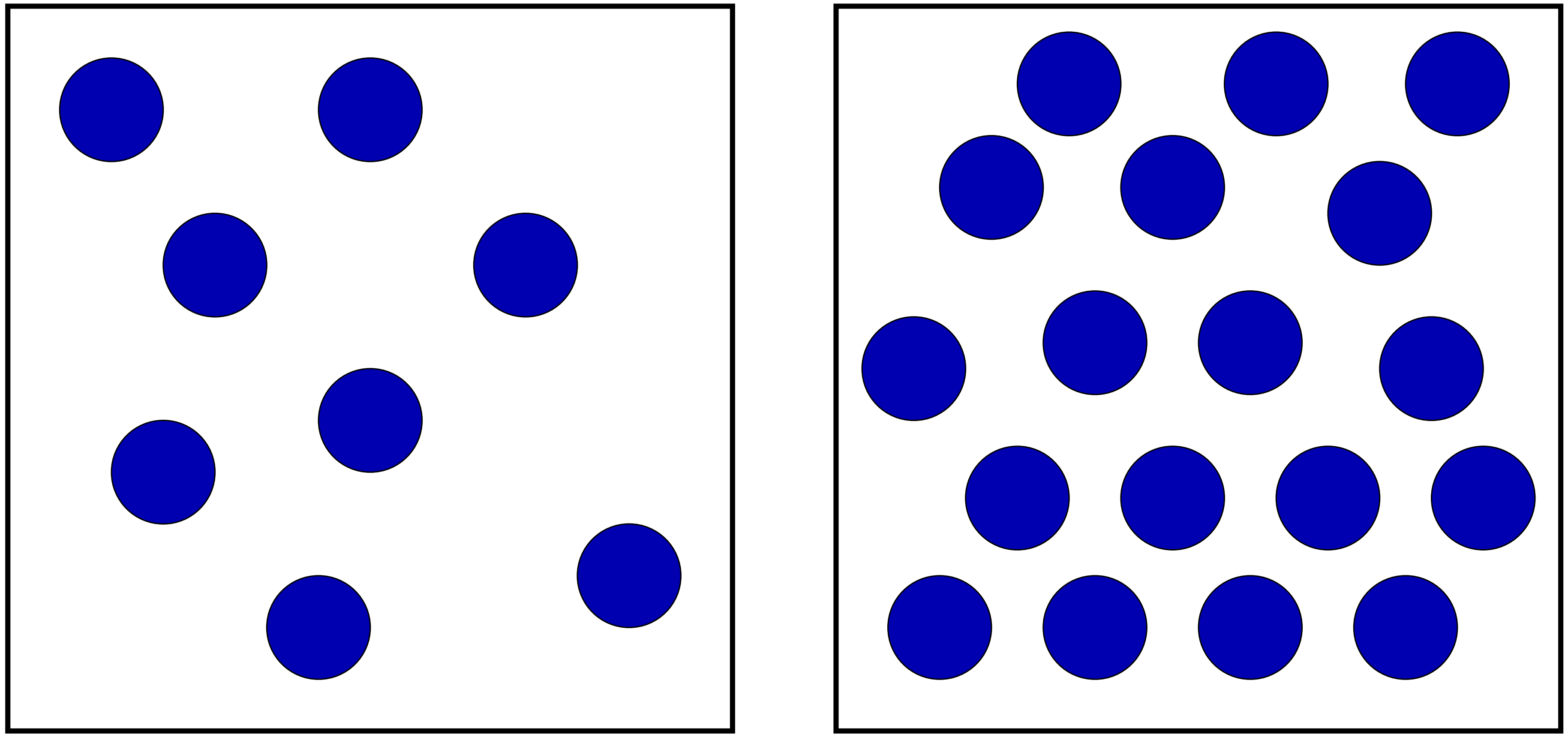
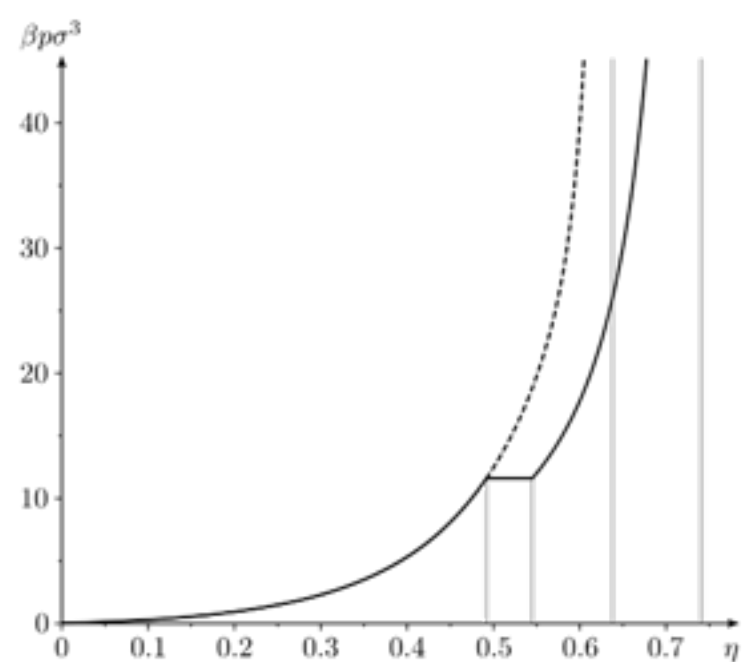
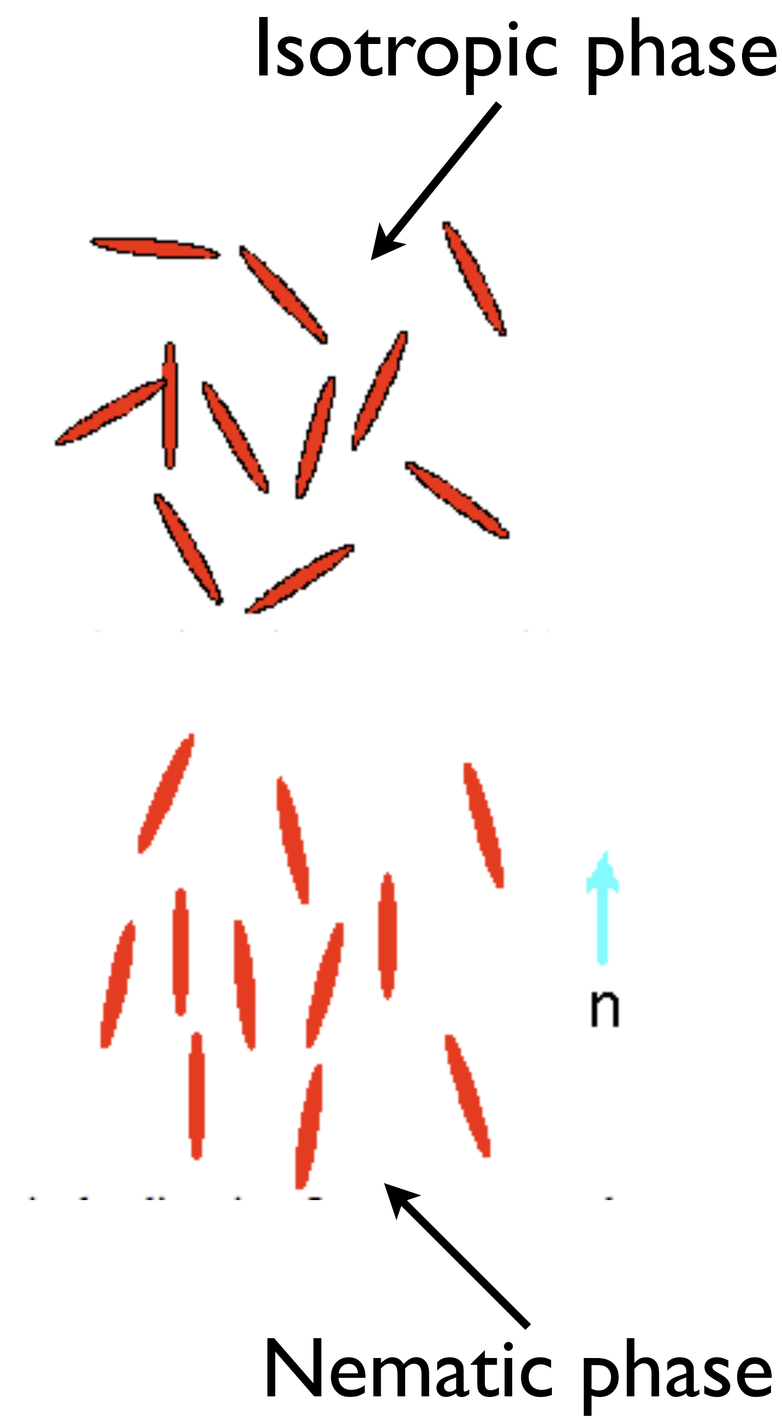
Hard Core Systems: Spheres





Hard Core Systems: Long Rods

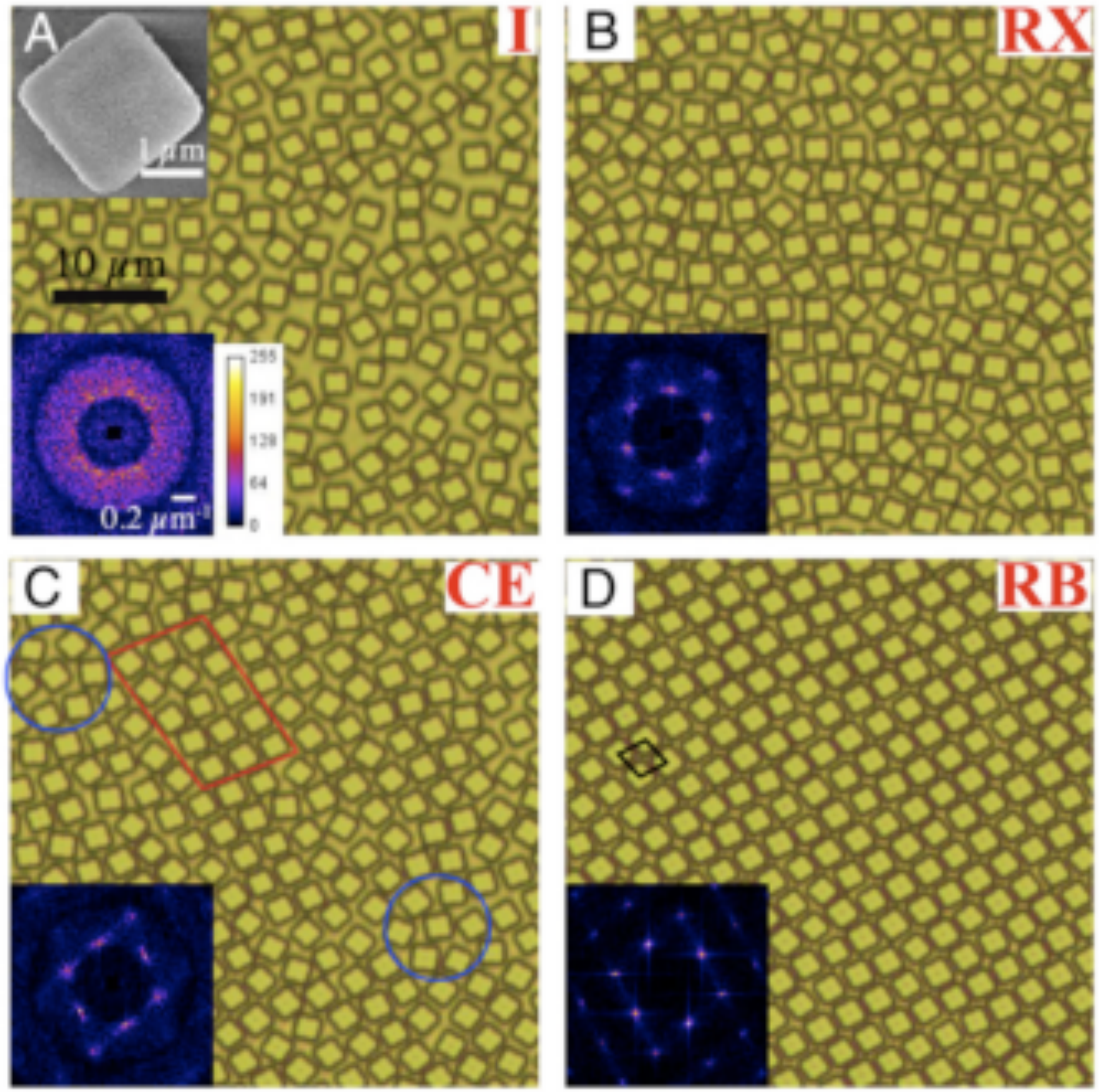
- Long rods in three dimensions interacting through excluded volume interaction
  - ⋆ Onsager, Flory, Zwanzig
- Virial expansion for free energy
- Exact for infinite aspect ratio
- Liquid crystals

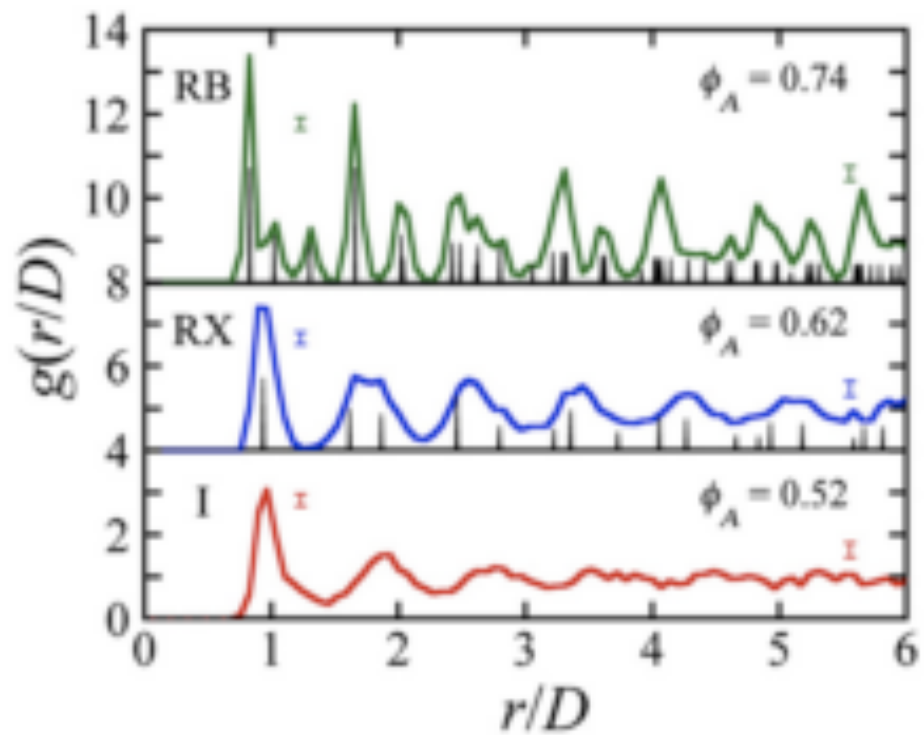


Two dimensions

- Mermin Wagner theorem
- Phases with quasi long range order
- Two step freezing of hard discs
  - liquid-hexatic transition
  - hexatic-solid transition
- Hard rods: long range correlations

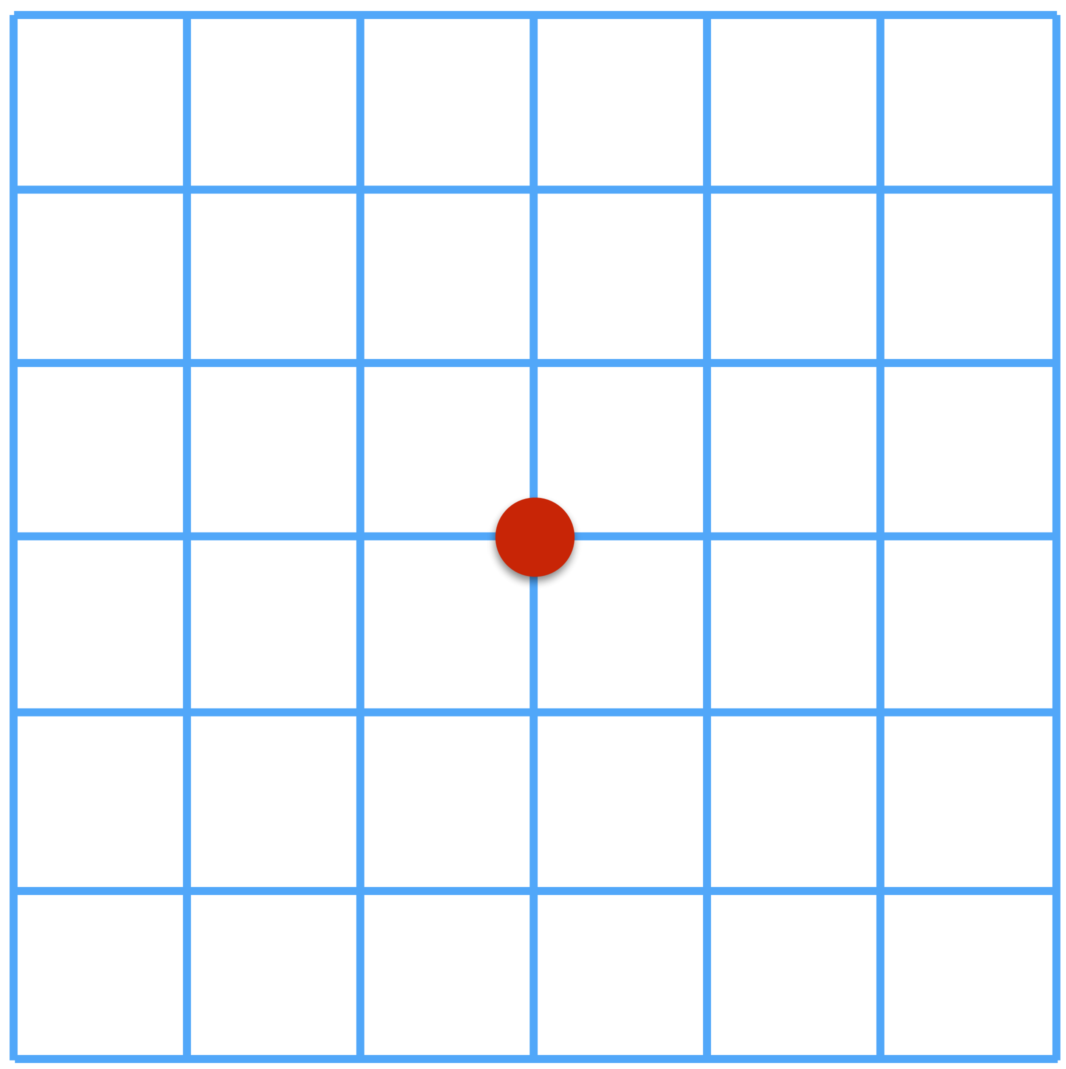
Gas of squares (example)



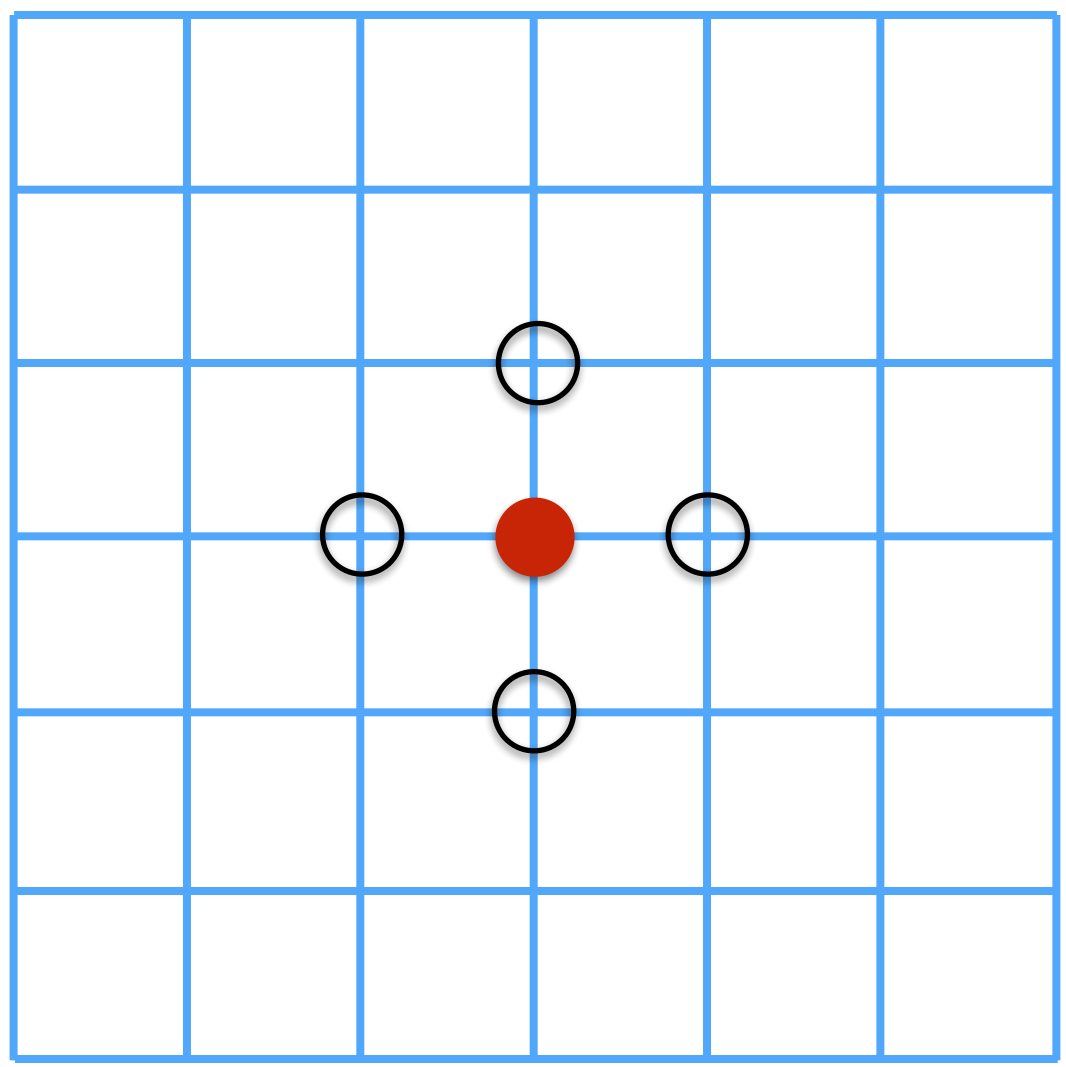


Zhao et. al., PNAS, 2011

Hard Core Lattice Gas Models

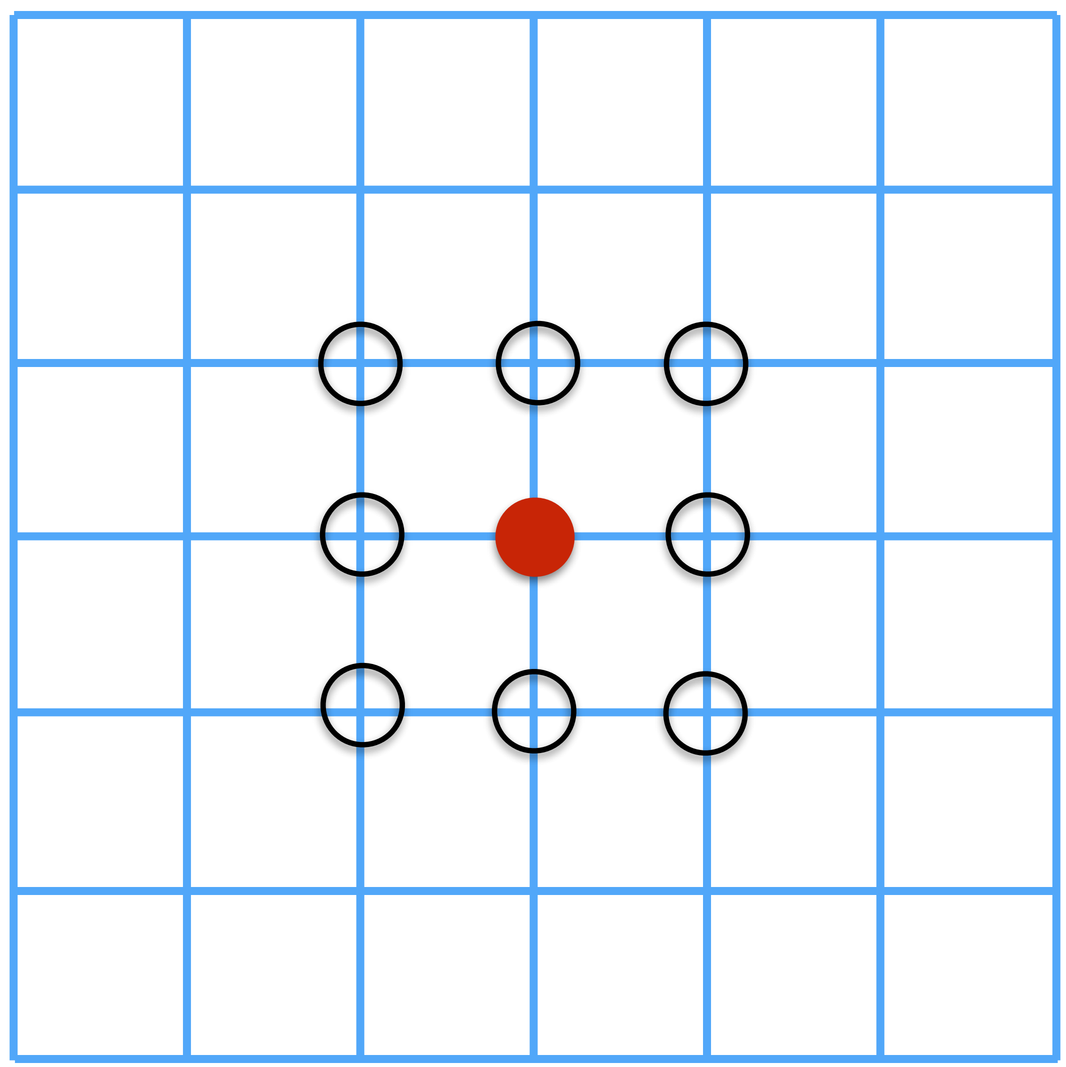


Hard Core Lattice Gas Models



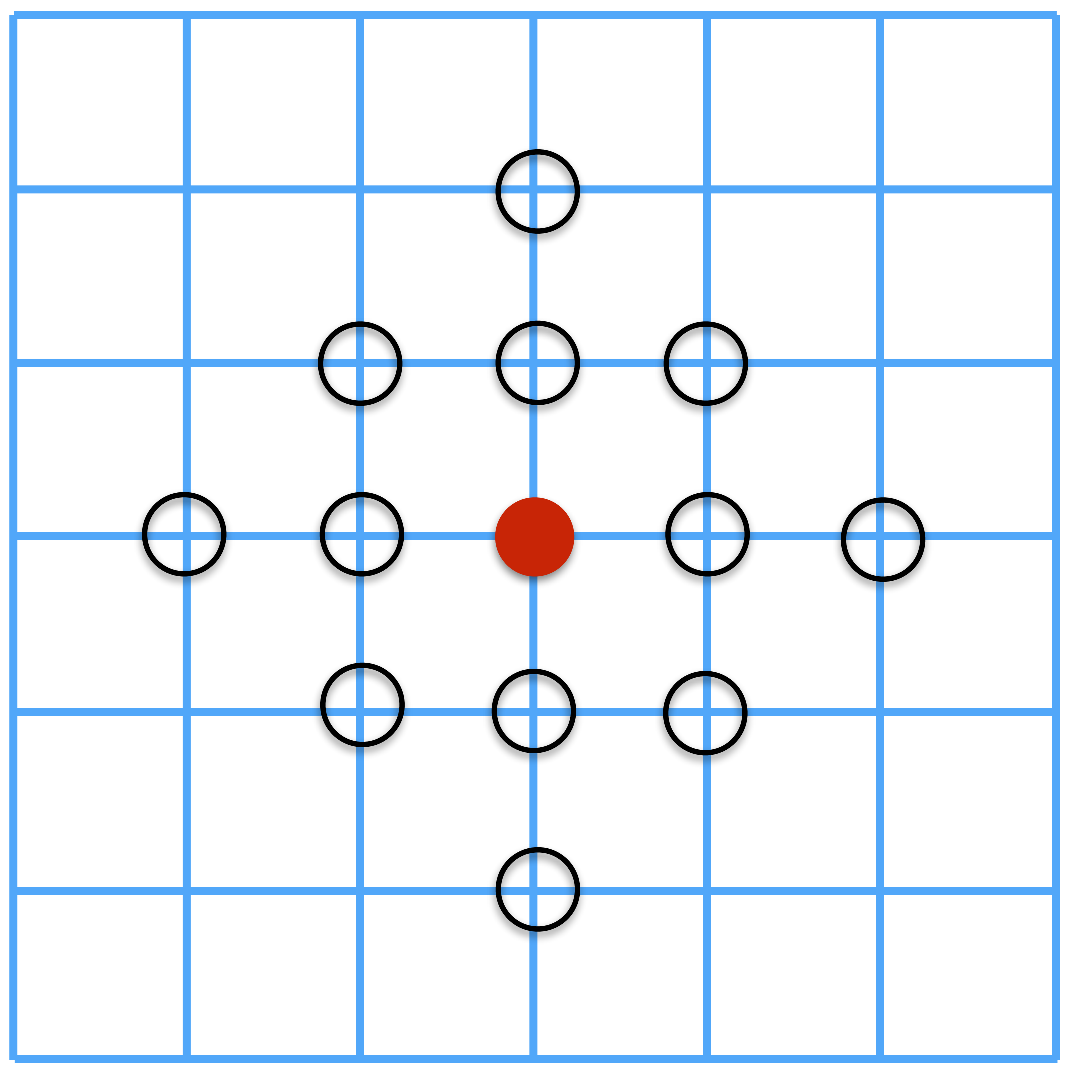
1-NN

Hard Core Lattice Gas Models



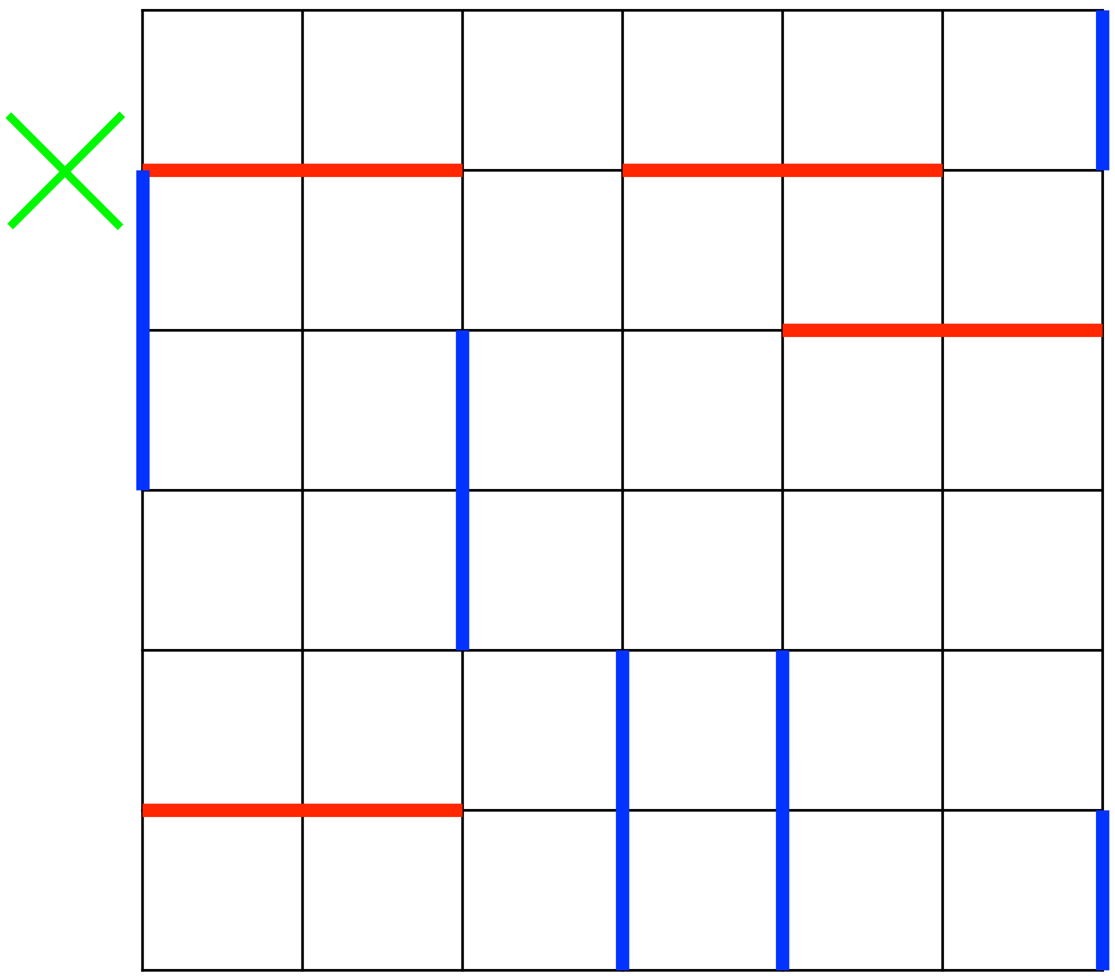
2-NN

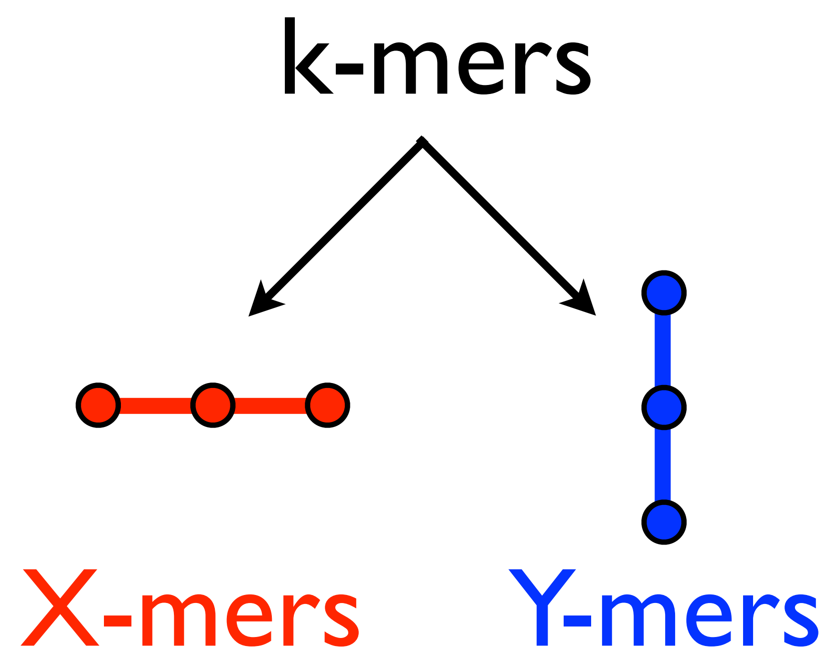
Hard Core Lattice Gas Models



3-NN

Hard rods on a lattice





Hard core exclusion

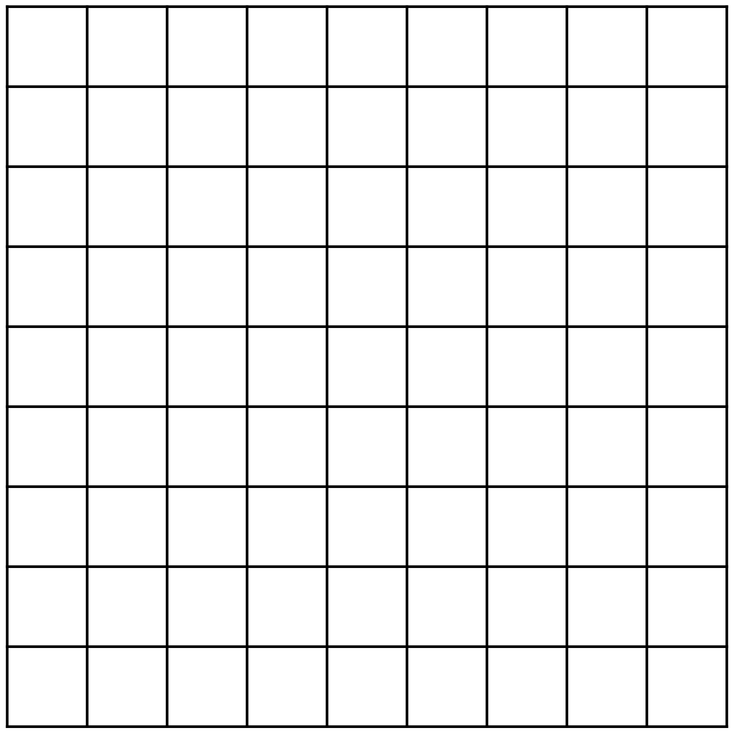
As ρ is increased from 0 to 1, what are the different phases possible? What is the nature of the phase transitions?

$\rho \rightarrow 0$

Rods are far from each other
randomly oriented

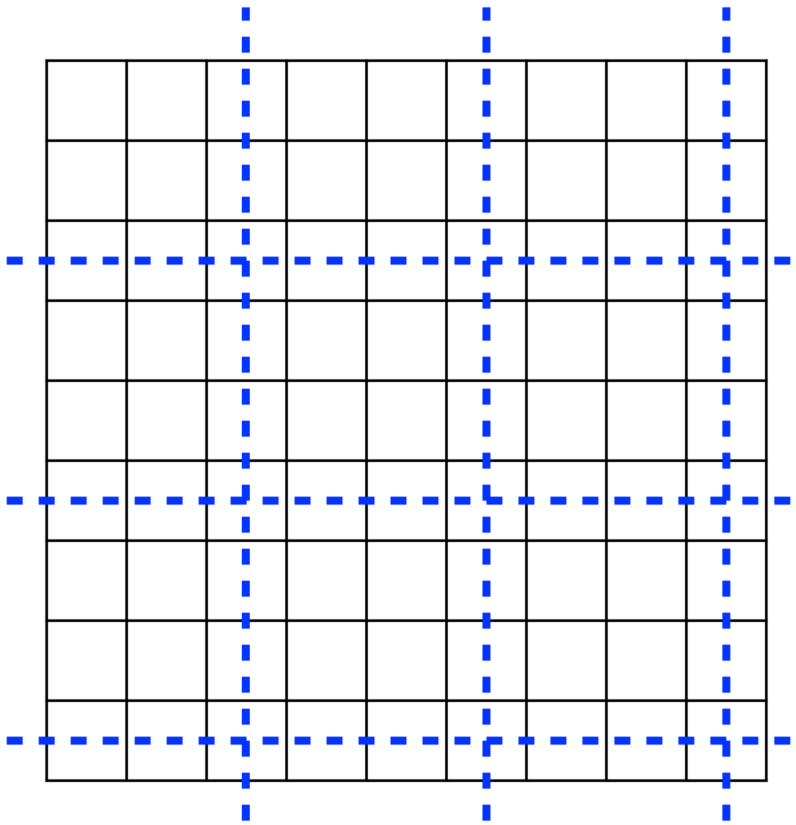
Isotropic phase: $\langle|\rho_x - \rho_y|\rangle = 0$

ρ = 1 (fully packed)



Disordered

ρ = 1 (fully packed)



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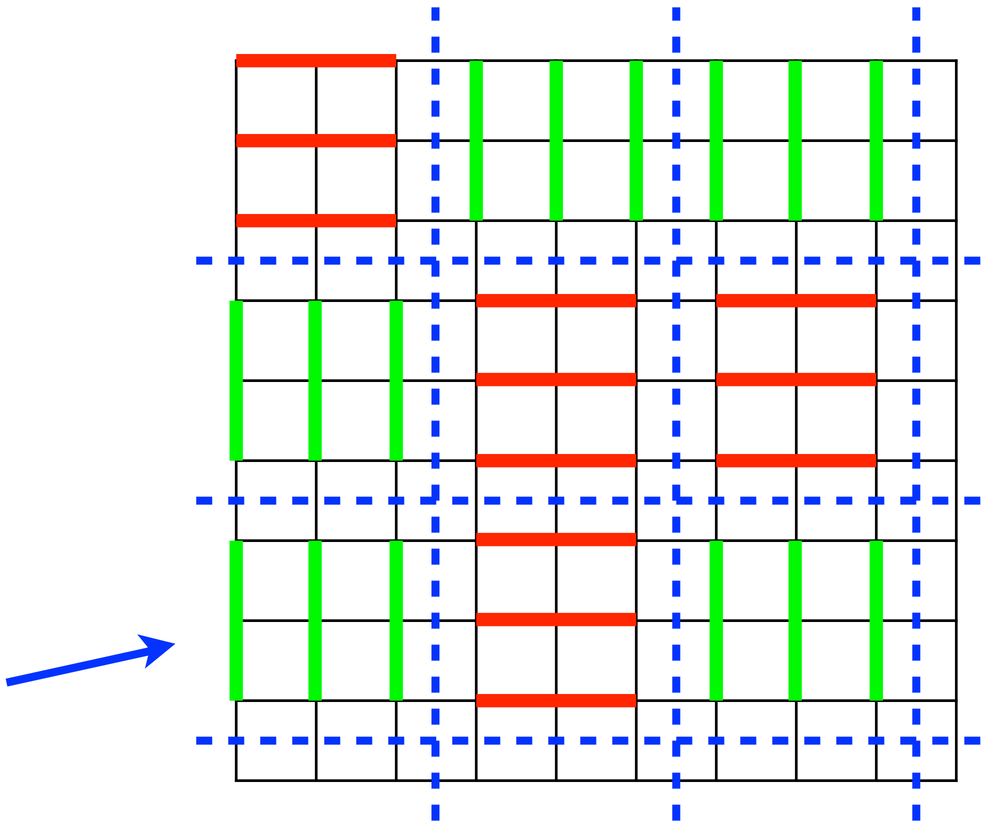

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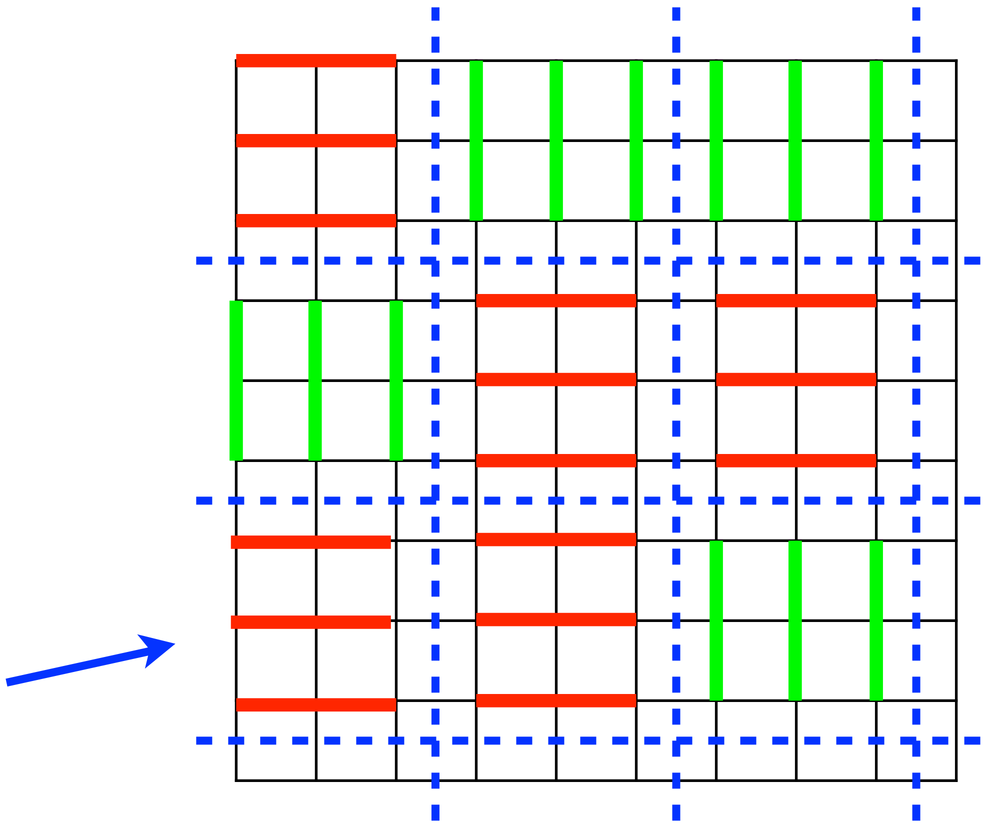

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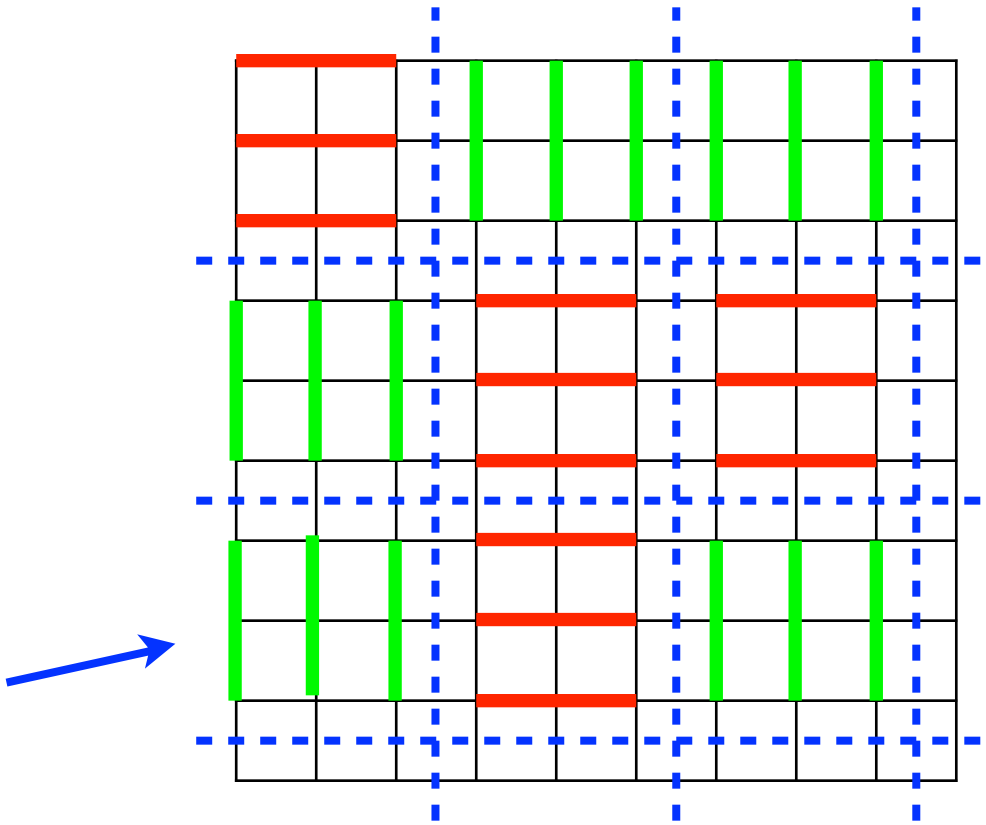

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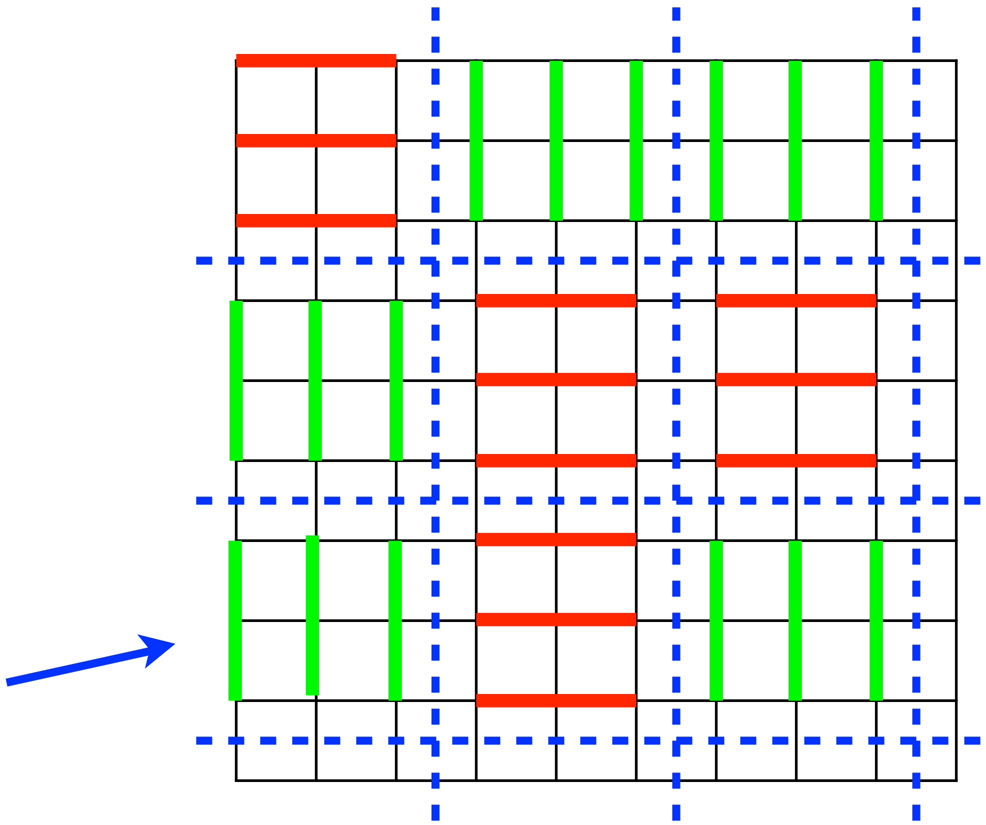
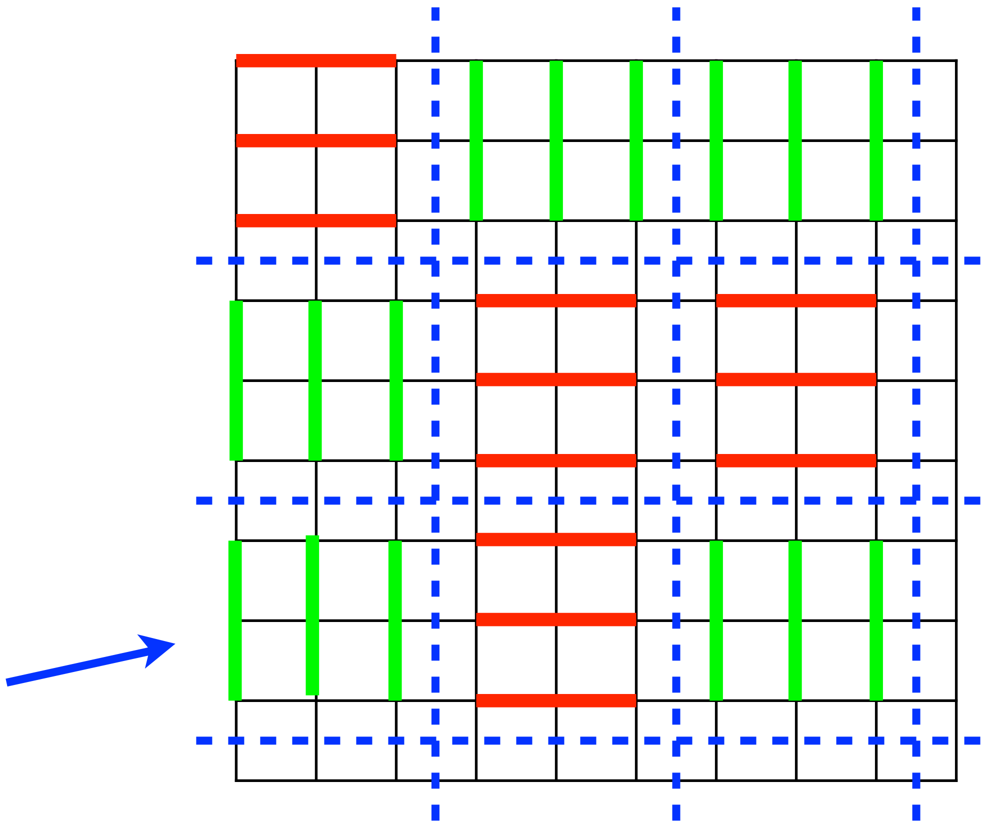


Disordered

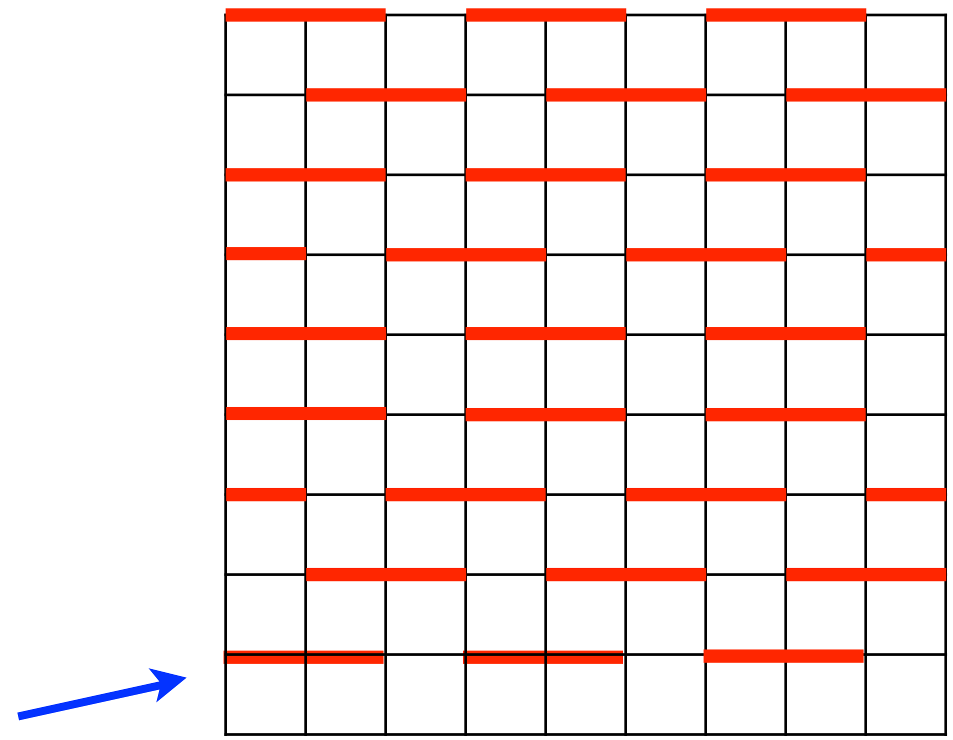
$$\Omega \geq 2^{(L/k)^2}$$

$$\frac{S}{L^2} \geq \frac{\ln(2)}{k^2} > 0$$

ρ = 1 (fully packed)



Disordered

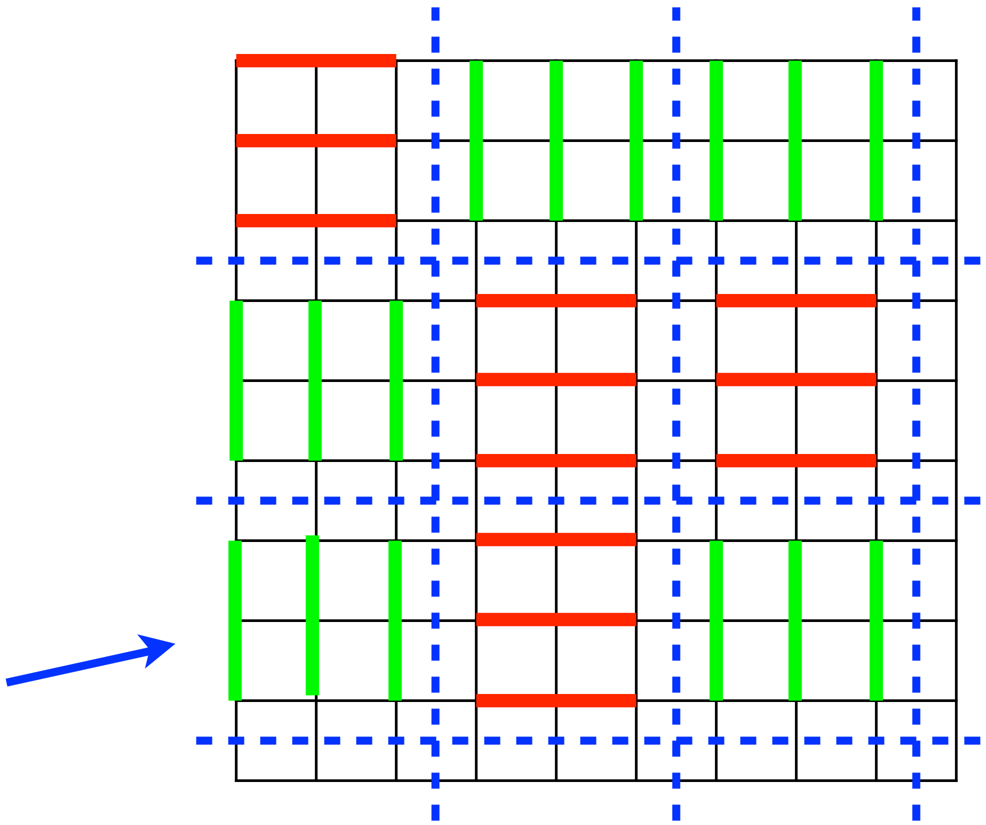


Nematic

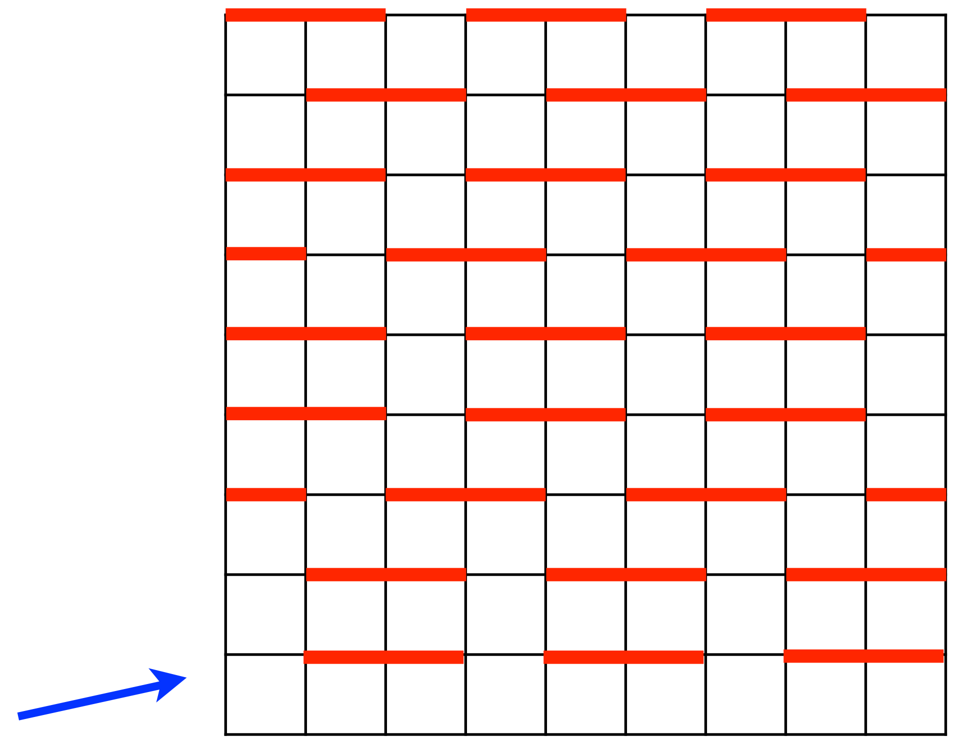
$$\Omega \geq 2^{(L/k)^2}$$

$$\frac{S}{L^2} \geq \frac{\ln(2)}{k^2} > 0$$

ρ = 1 (fully packed)



Disordered



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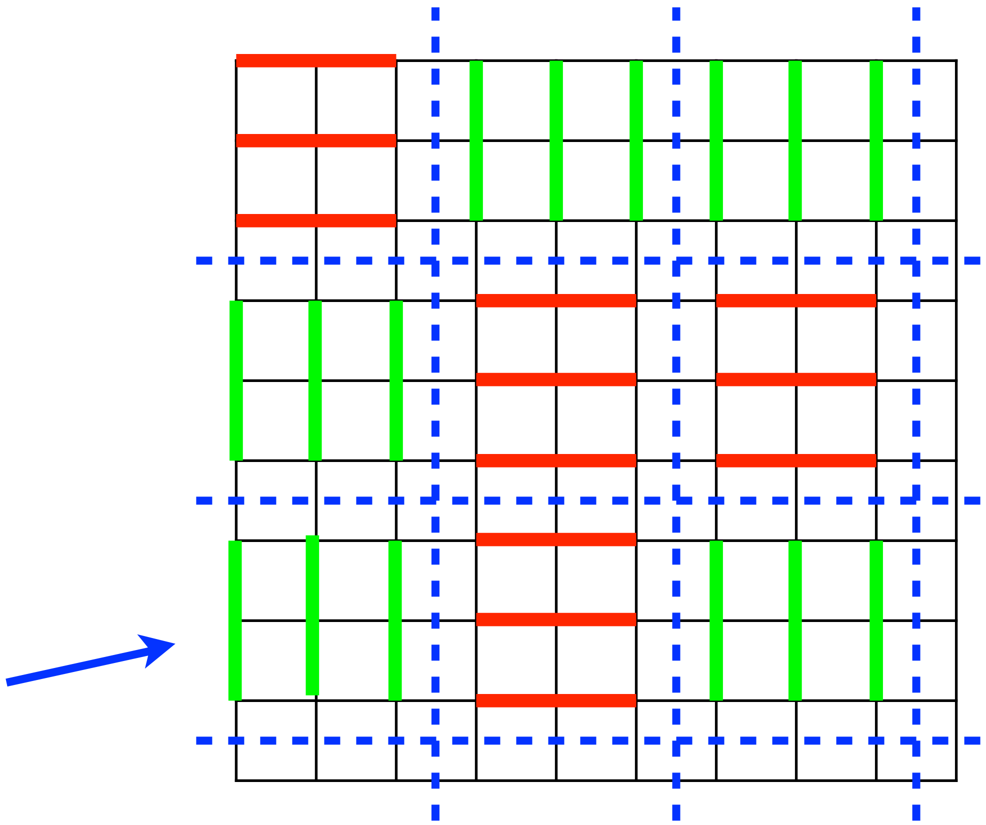

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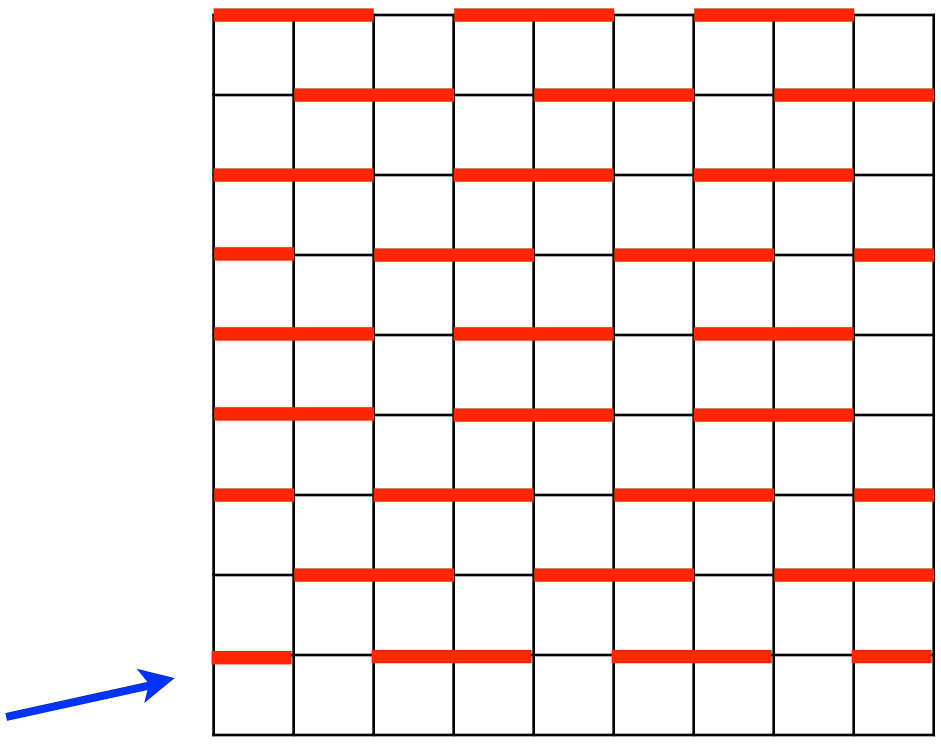

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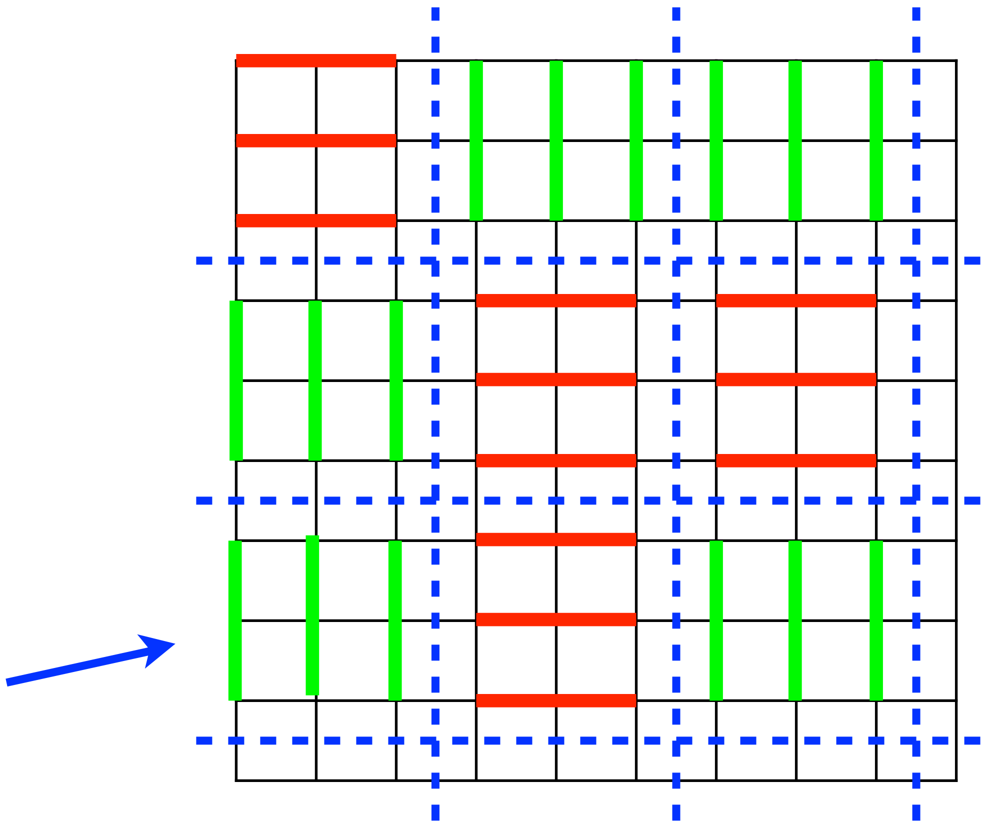
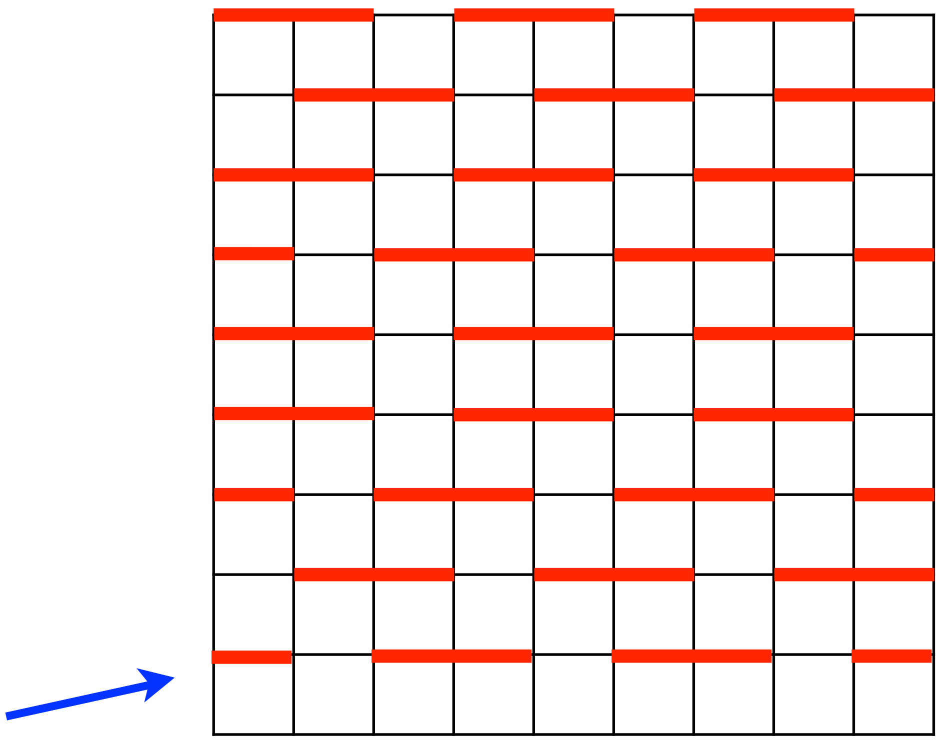




<u>Disordered</u>

$$\Omega \geq 2^{(L/k)^2}$$

$$\frac{S}{L^2} \geq \frac{\ln(2)}{k^2} > 0$$

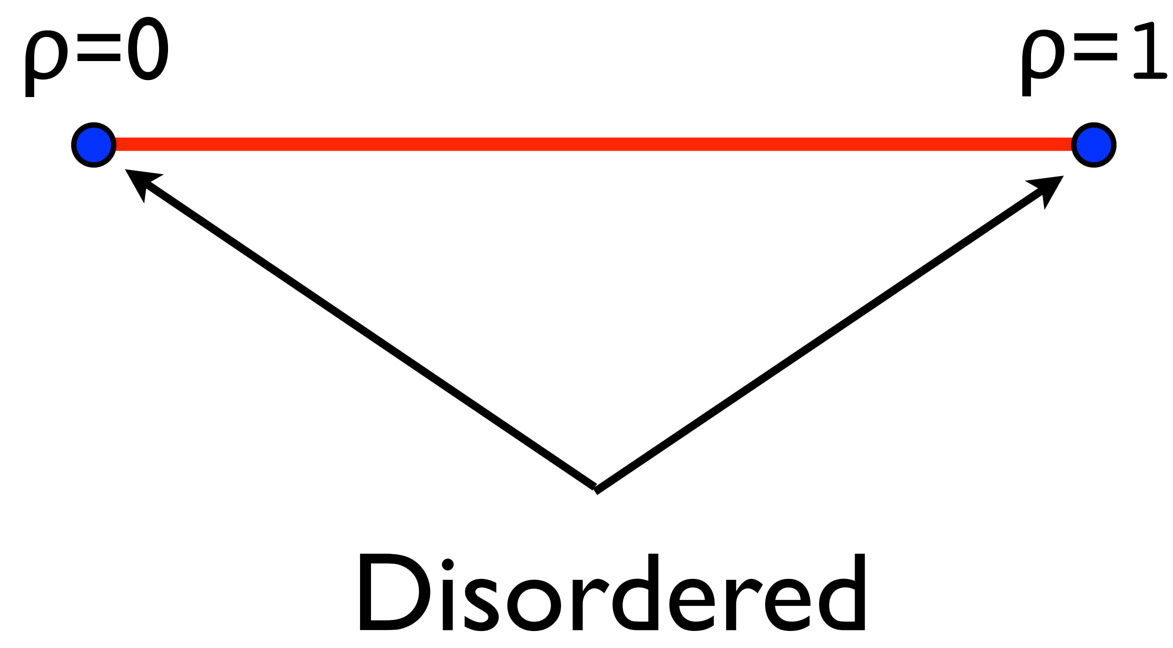
<u>Nematic</u>

$$\Omega = 2k^L$$

$$\frac{S}{L^2} = \frac{\ln(k)}{L} \to 0$$

Disordered phase: $\langle|\rho_x - \rho_y|\rangle = 0$

Low and high densities

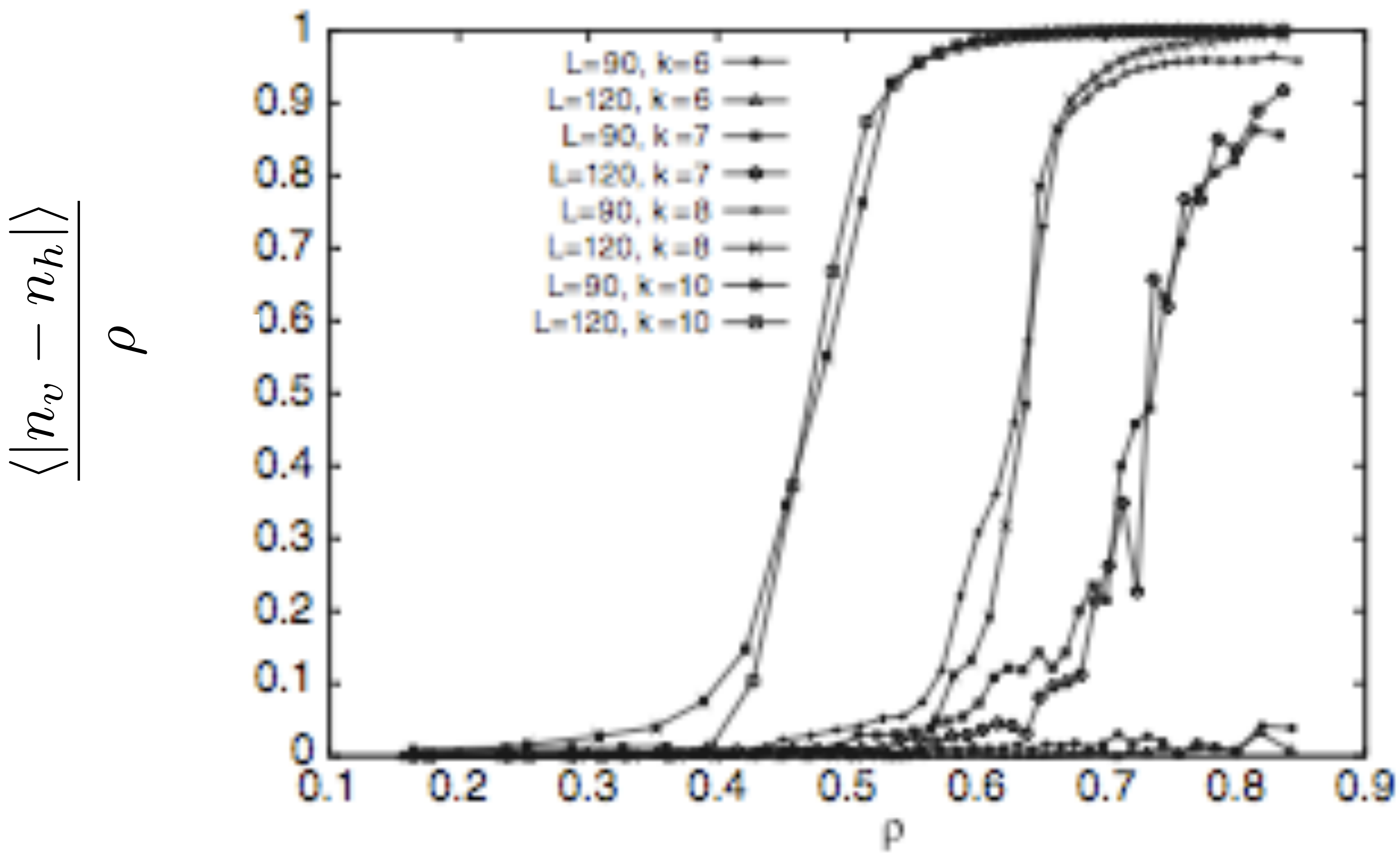


What happens at intermediate densities?

Dimers (k=2)

- Fully packed — Kastelyn, 1961
- Isotropic at all densities — Heilmann, Lieb, 1970; Kunz, 1970
- Power law correlations when fully packed
- What about k>2?

Monte Carlo simulation



Nematic phase exists for k≥7 Ghosh, Dhar, EPL, 2007

Nematic phase exists for k≫1

Disertori, Giuliani, Commun. Math. Phys. 2013

ρ = 1-ε

Entropy for nematic phase

Each row has $L\epsilon$ holes and $\frac{L(1-\epsilon)}{k}$ rods

A simple combinatorial problem

$$\frac{S_{nem}}{L^2} = -\epsilon \ln(k\epsilon) + \epsilon + \ldots$$

ρ = 1-ε

Entropy for disordered phase

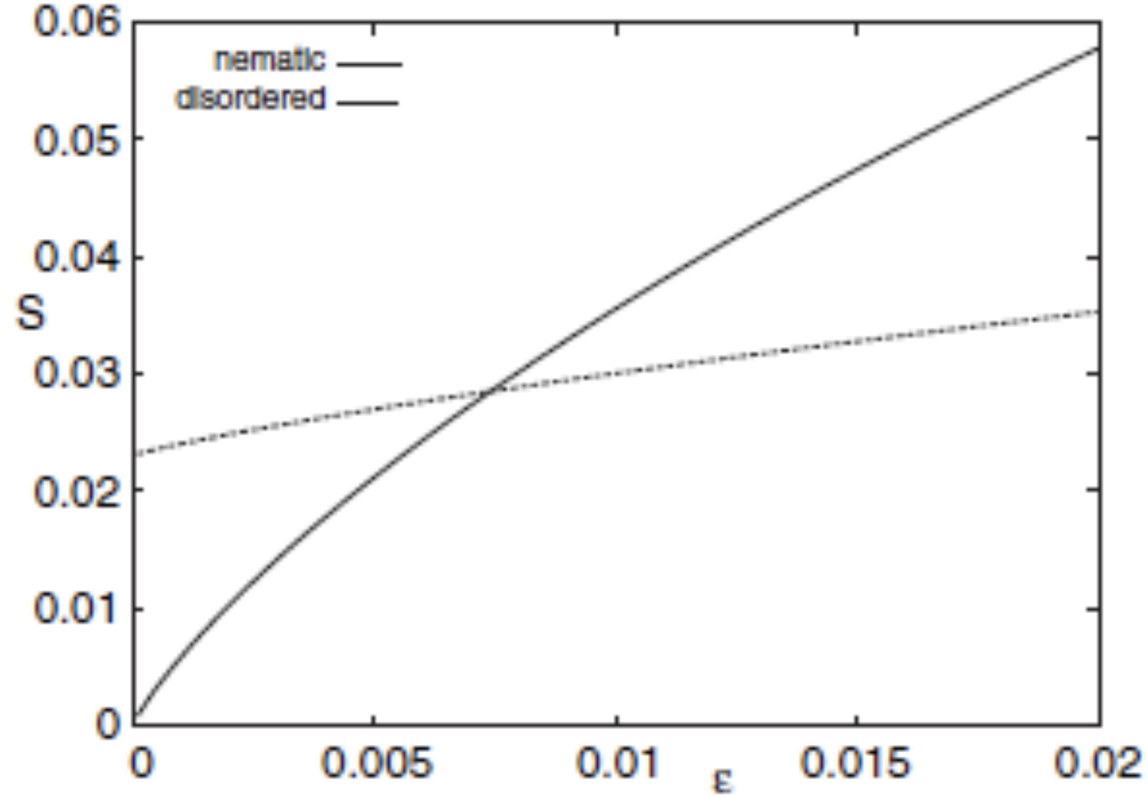
Number of holes $= L^2\epsilon$

Number of rods to be removed $= \frac{L^2\epsilon}{k}$

Remove randomly

$$\frac{S_{dis}}{L^2} = \frac{\ln(k)}{k^2} + \frac{1}{k}\left[-\epsilon\ln(\epsilon) - (1-\epsilon)\ln(1-\epsilon)\right]$$

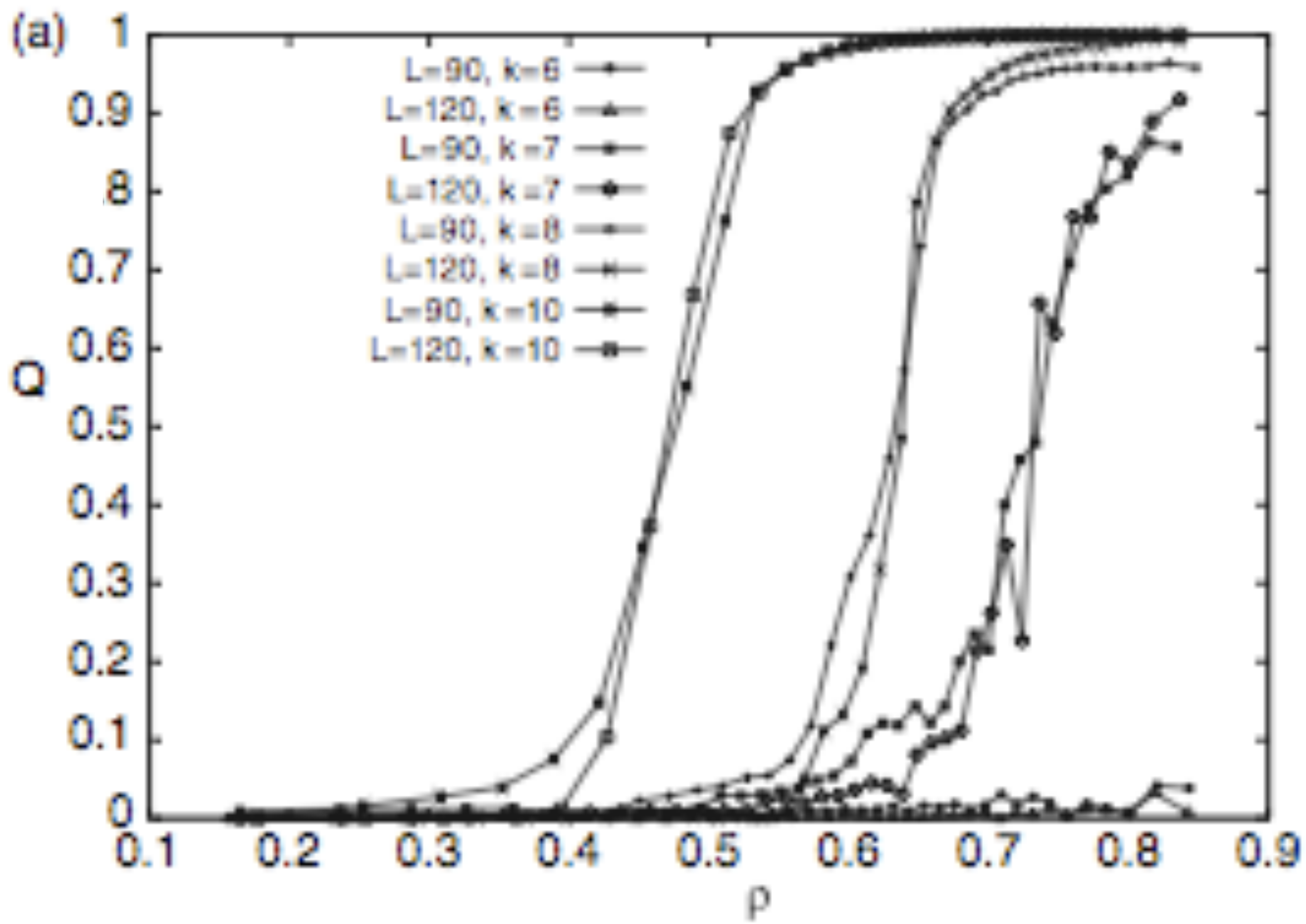
ρ = 1-ε



$$\epsilon_c \approx \frac{a}{k^2}$$

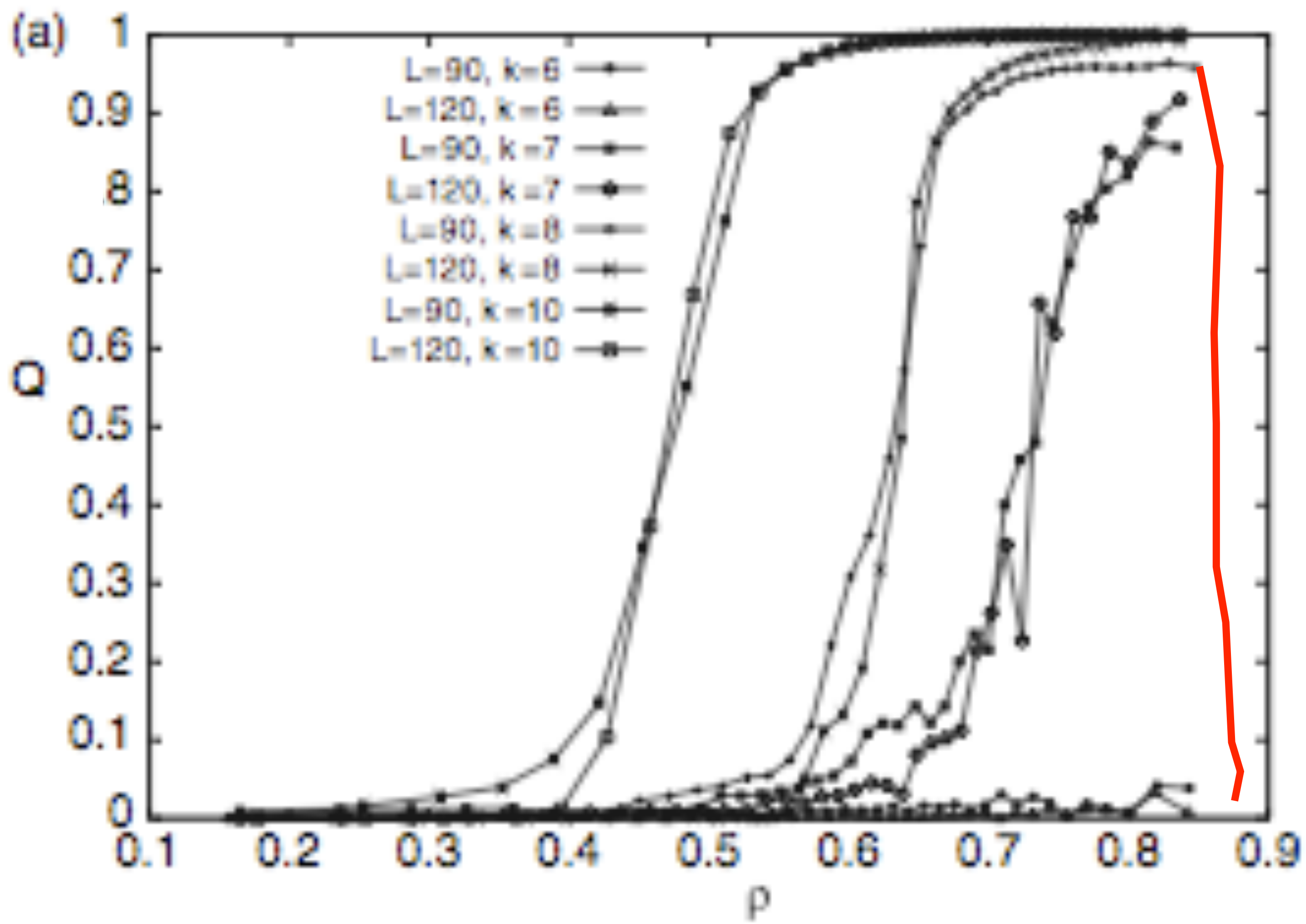
First transition ⇒ second transition

$$\frac{\langle |n_v - n_h| \rangle}{\rho}$$



First transition ⇒ second transition

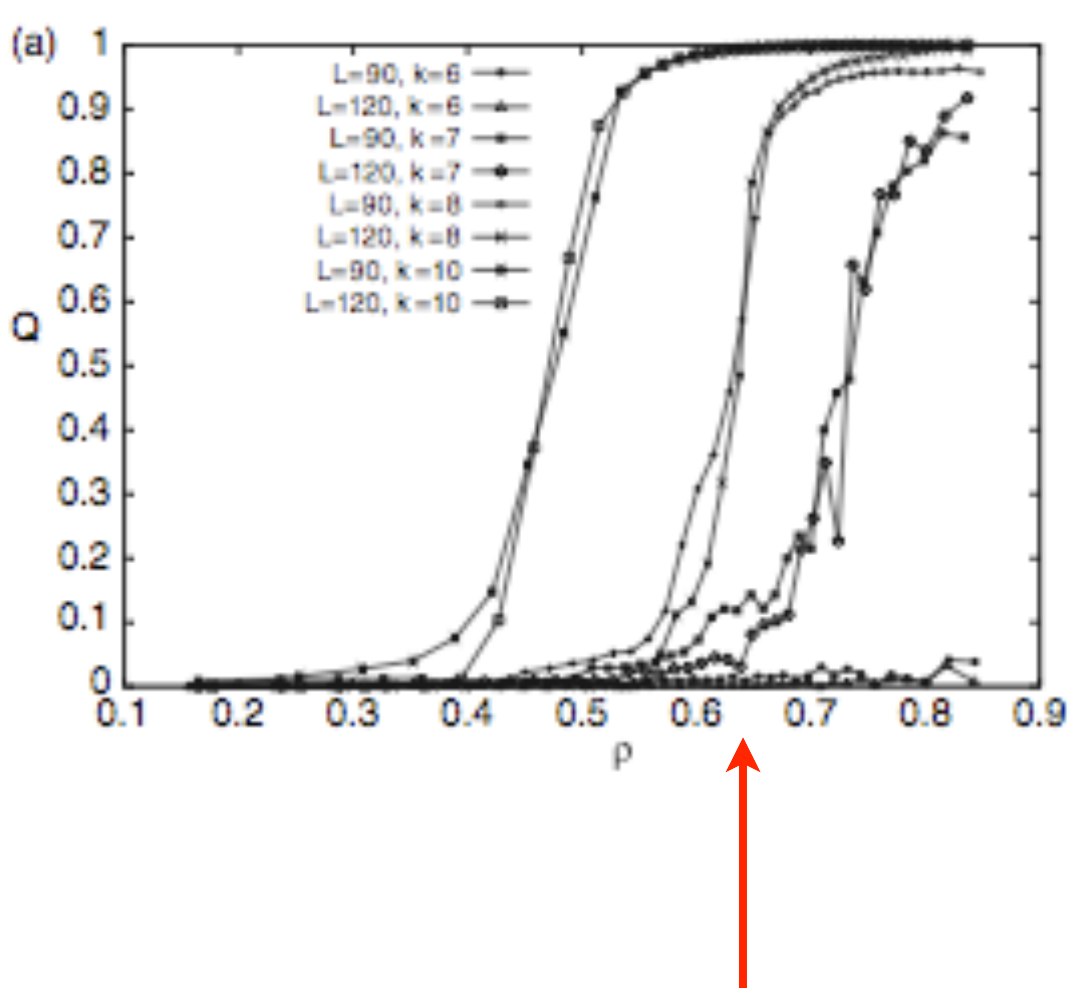
$$\frac{\langle |n_v - n_h| \rangle}{\rho}$$



Questions

- What is the nature of the first transition?
- Does the second transition exist?
- If it exists, what is the nature of the second transition, high density phase?
- Is it possible to find an exact solution to the problem?
- What is the phase diagram for rectangles?

Nature of first transition



- Low density: isotropic
- Intermediate density: nematic phase
  - ⋆ vertical
  - ⋆ horizontal
- Universality class?

Critical Phenomena

- Diverging correlation length ξ
- Order parameter m
- Characterised by critical exponents

$$\xi \sim \epsilon^{-\nu}$$

$$m \sim \epsilon^{\beta}$$

$$\chi \sim \epsilon^{-\gamma}$$

Isotropic-Nematic transition

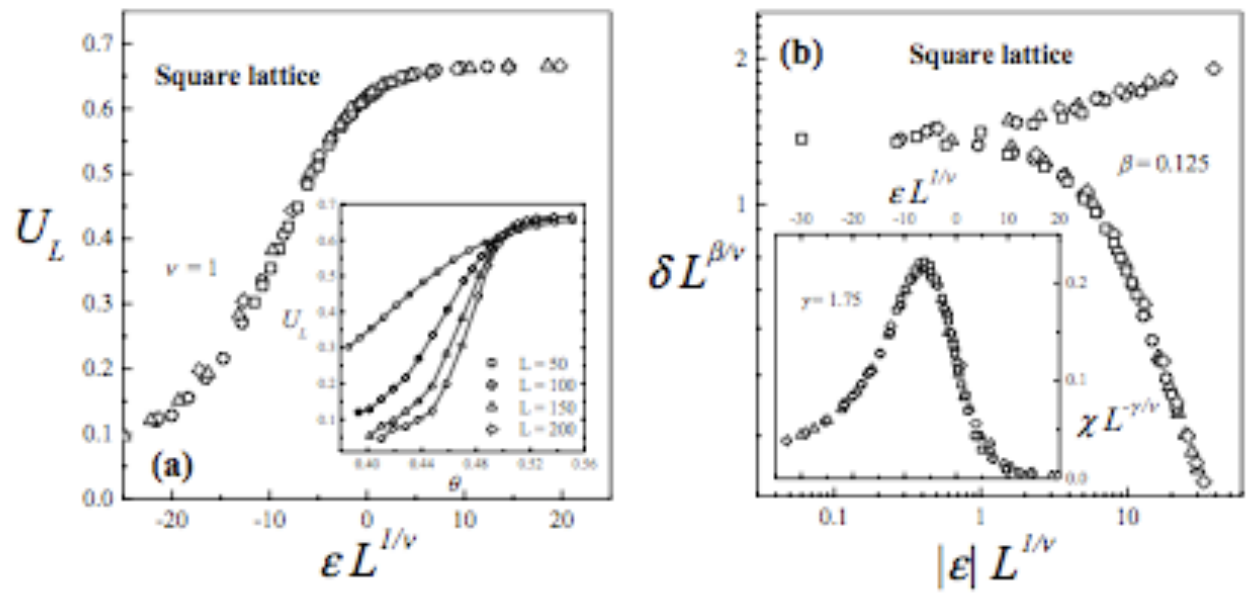


Fig. 3: (a) Data collapsing, U_L vs. $\epsilon L^{1/\nu}$, for the cumulants in fig. 2. In the inset, the data in fig. 2 are plotted over a wide range of coverage. (b) Data collapsing of the order parameter, $\delta L^{\beta/\nu}$ vs. $|\epsilon|L^{1/\nu}$, and of the susceptibility, $\chi L^{-\gamma/\nu}$ vs. $\epsilon L^{1/\nu}$ (inset). The plots were made using $\theta_c = 0.502$ and the exact 2D Ising exponents $\nu = 1$, $\beta = 0.125$ and $\gamma = 1.75$.

Ising

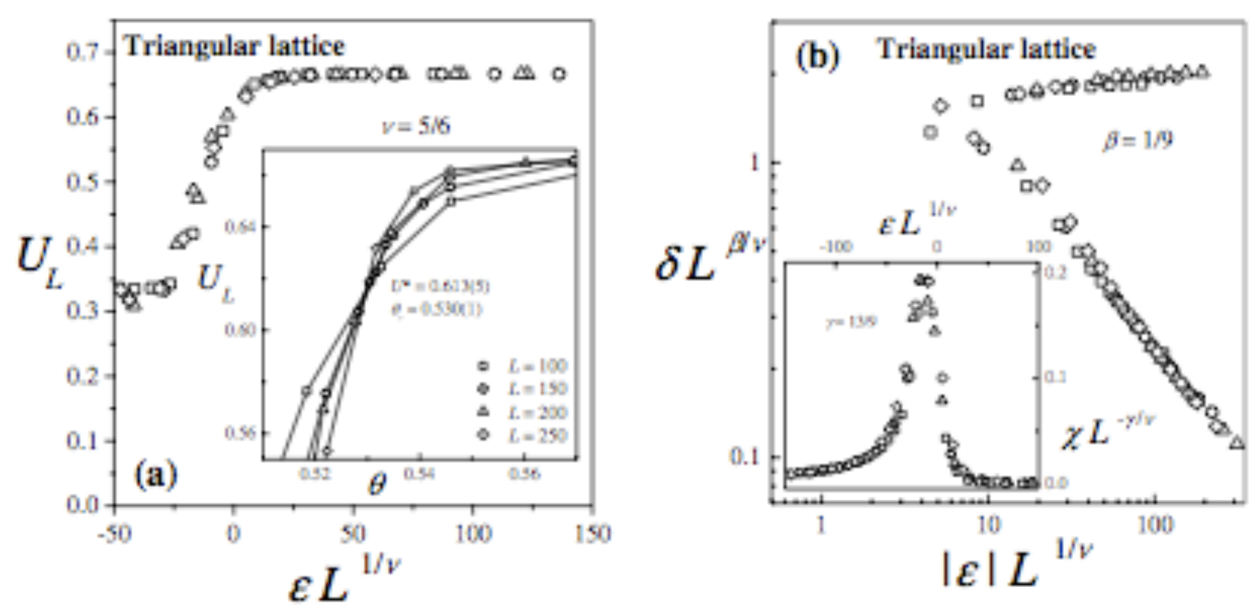


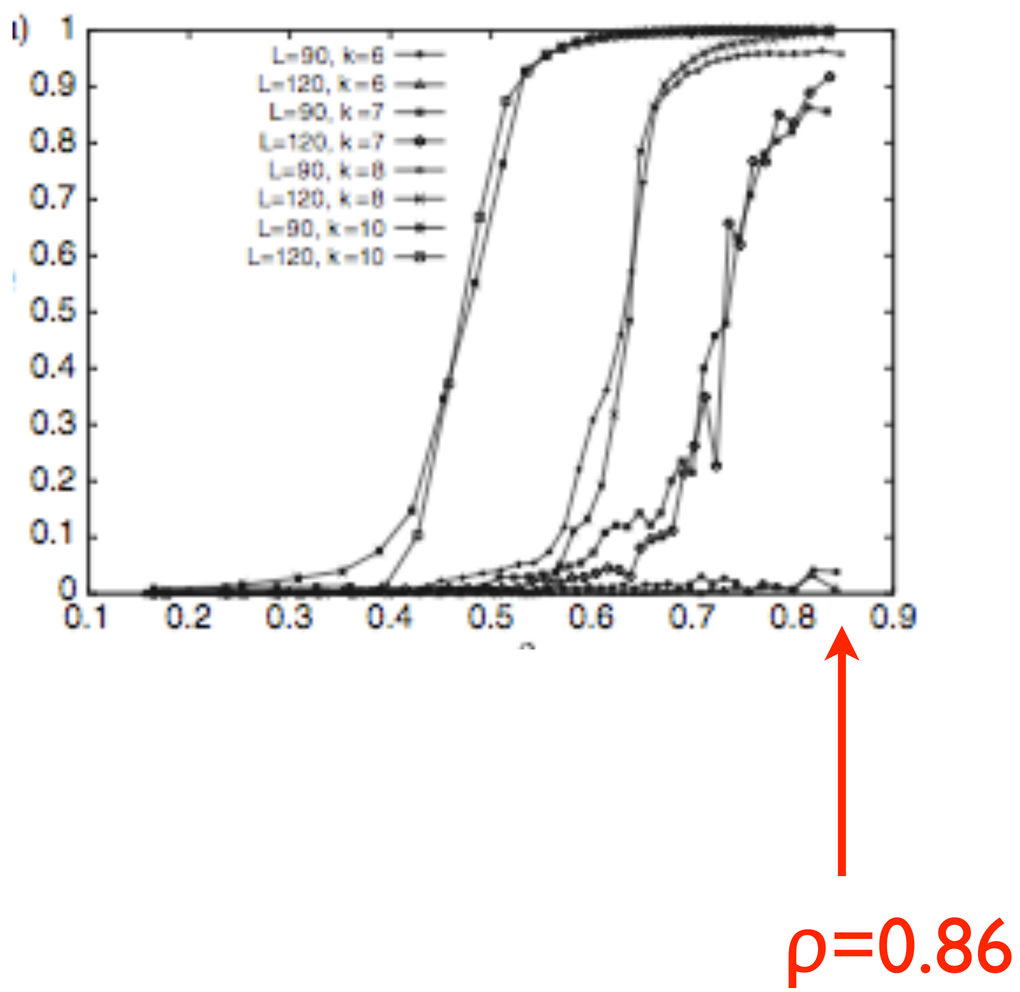
Fig. 4: (a) Data collapsing of the cumulants for triangular lattices. The corresponding curves of $U_L(\theta)$ vs. θ are shown in the inset. (b) Same as fig. 3(b) for triangular lattices. The plots were made using $\theta_c = 0.530$ and the exact three-state Potts model exponents $\nu = 5/6$, $\beta = 1/9$ and $\gamma = 13/9$.

3 state Potts

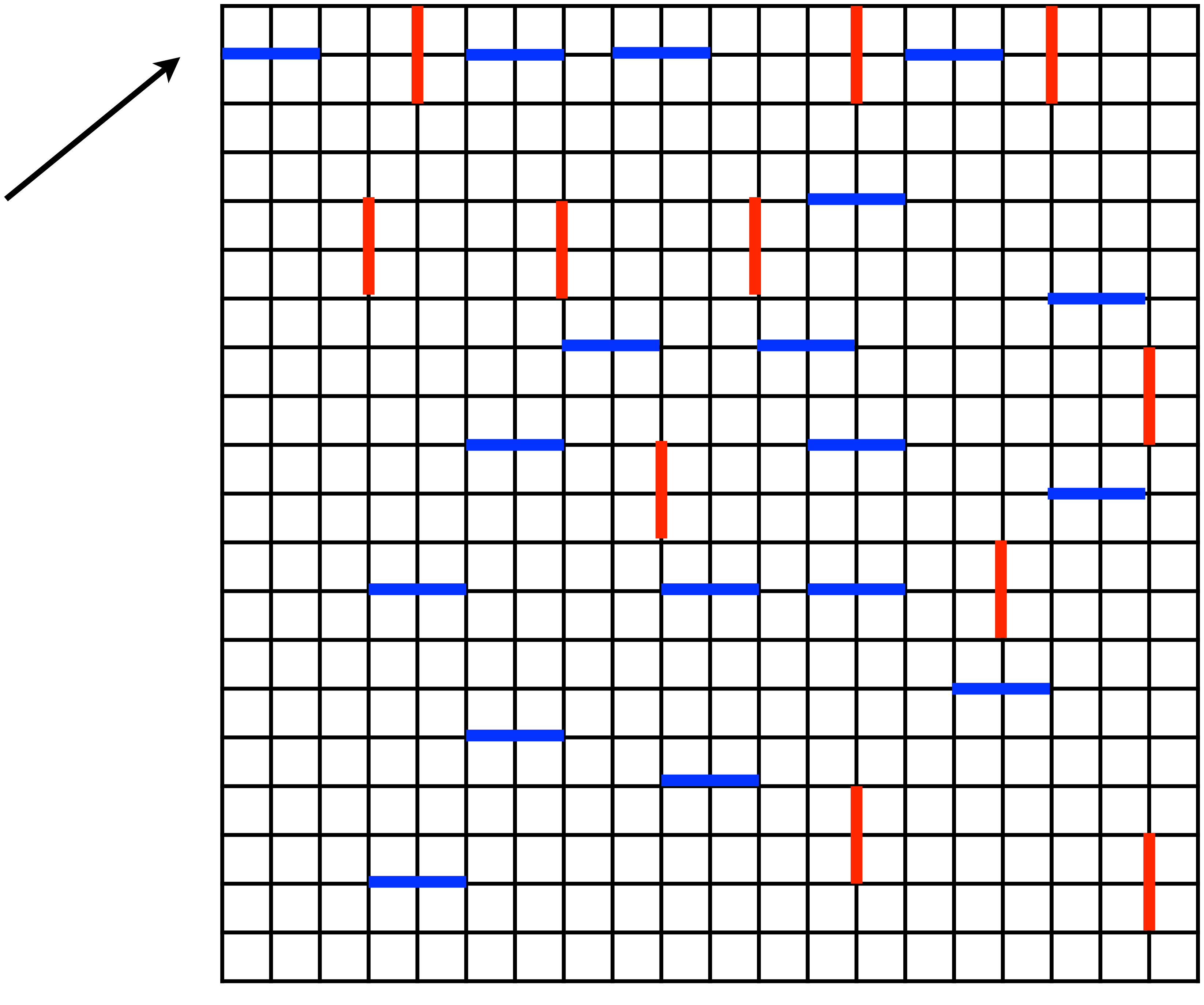
D M.-Fernandez et.al., EPL, 2008

Second transition?

- Occurs at high densities (≈ 0.92 for k=7)
- Evaporation, deposition Monte Carlo gets jammed
- Is there an efficient algorithm?



An efficient algorithm



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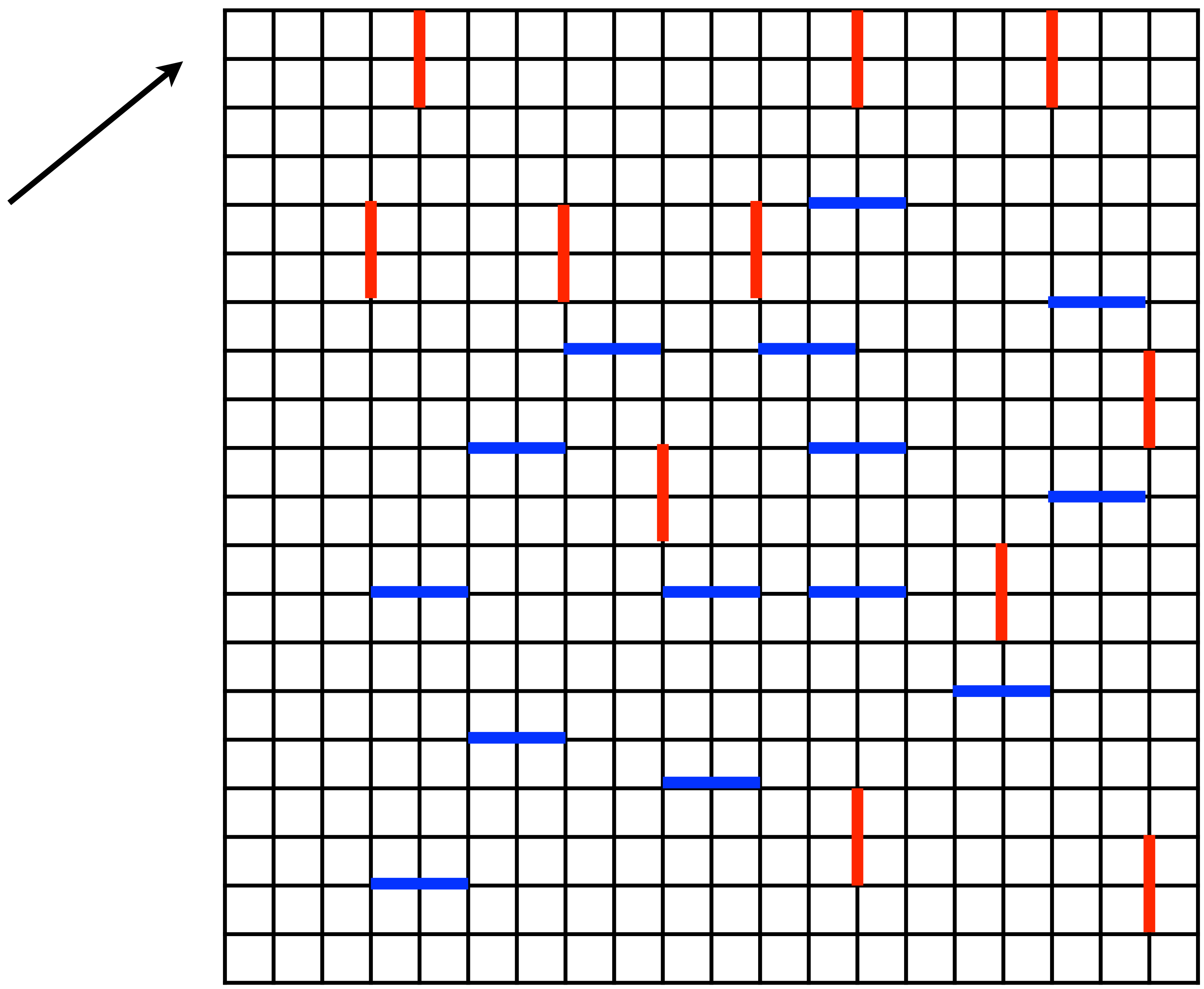

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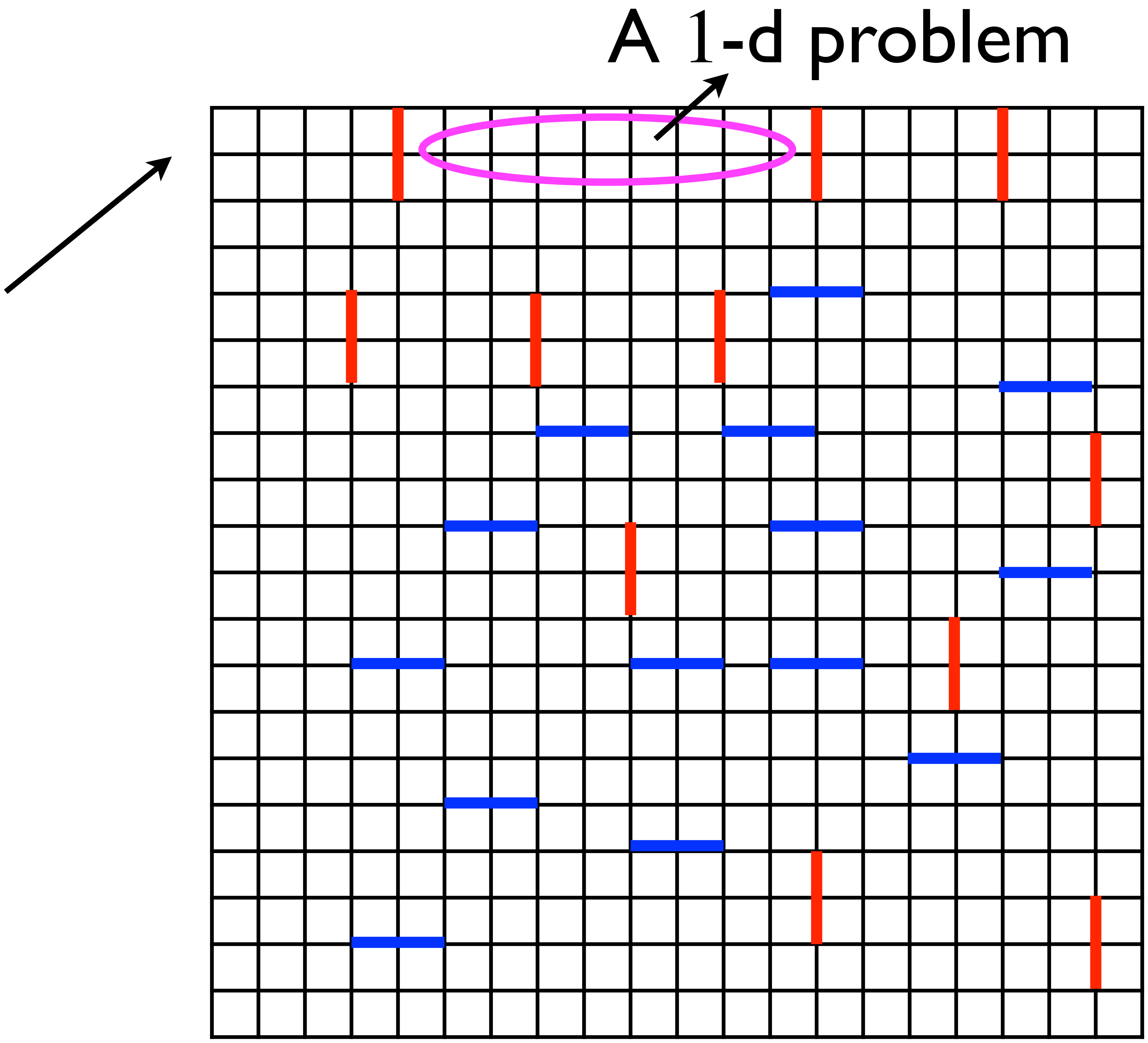
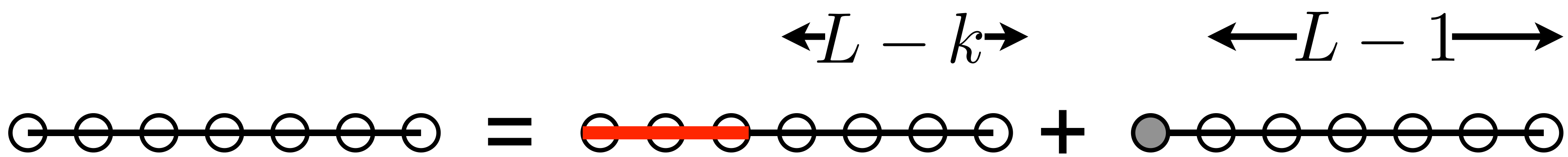


An efficient algorithm

1-d problem



$$Z(L) = zZ(L-k) + Z(L-1)$$

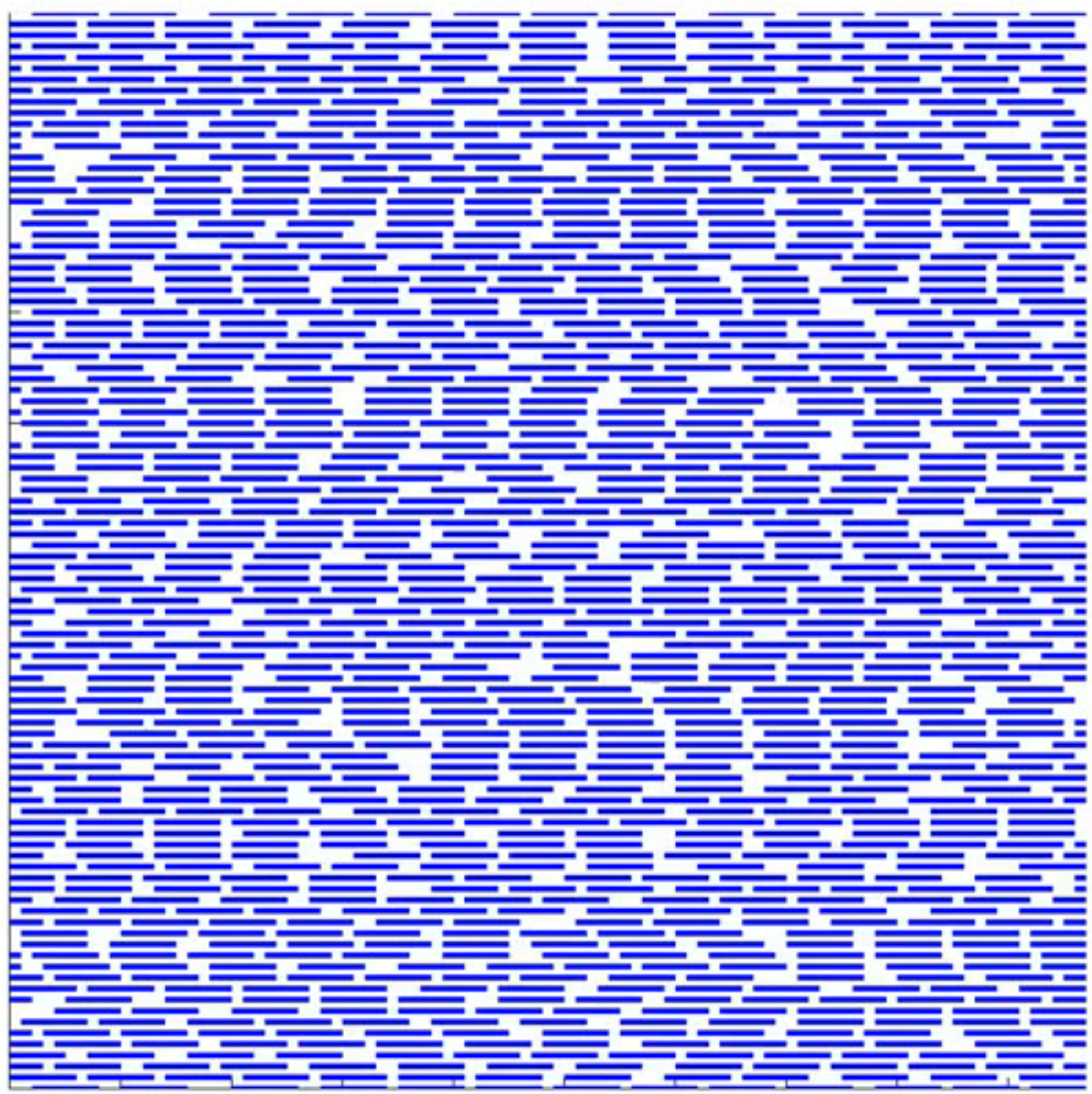
$$\mathrm{Prob} = \frac{zZ(L-k)}{Z(L)}$$

Equilibrates

Efficient

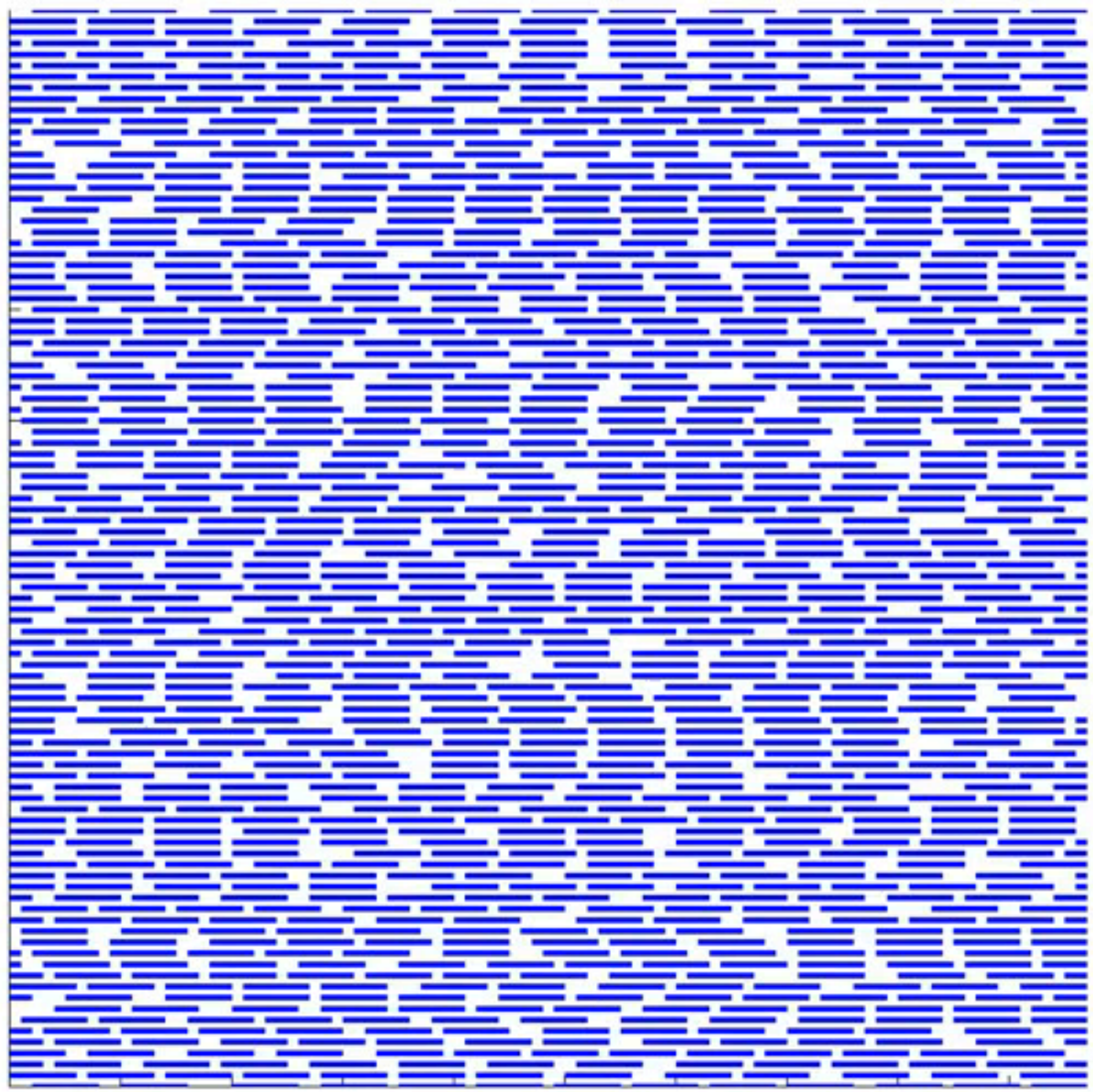
Parallelizable

Equilibration



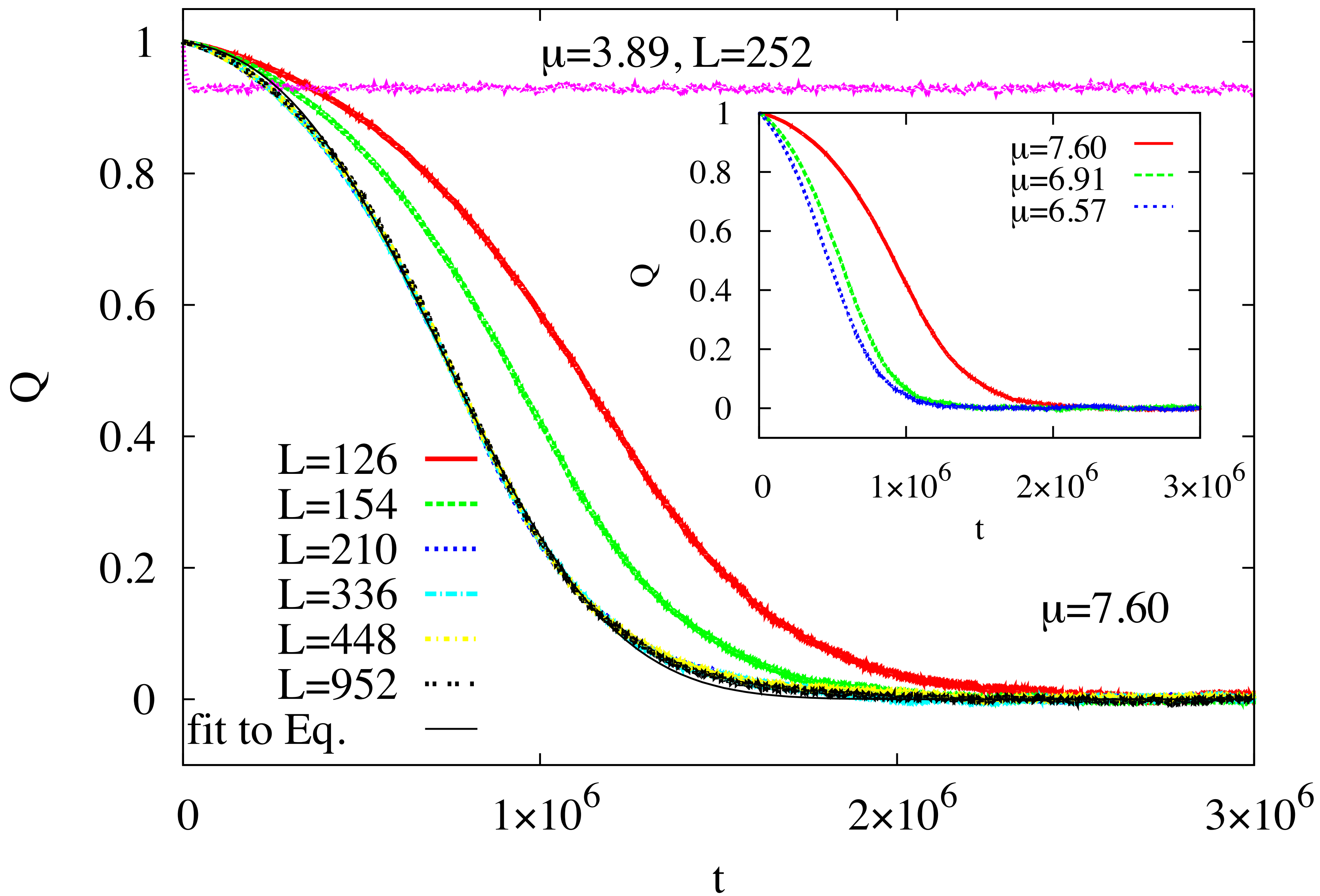
$\rho \approx 0.96$

Equilibration



$\rho \approx 0.96$

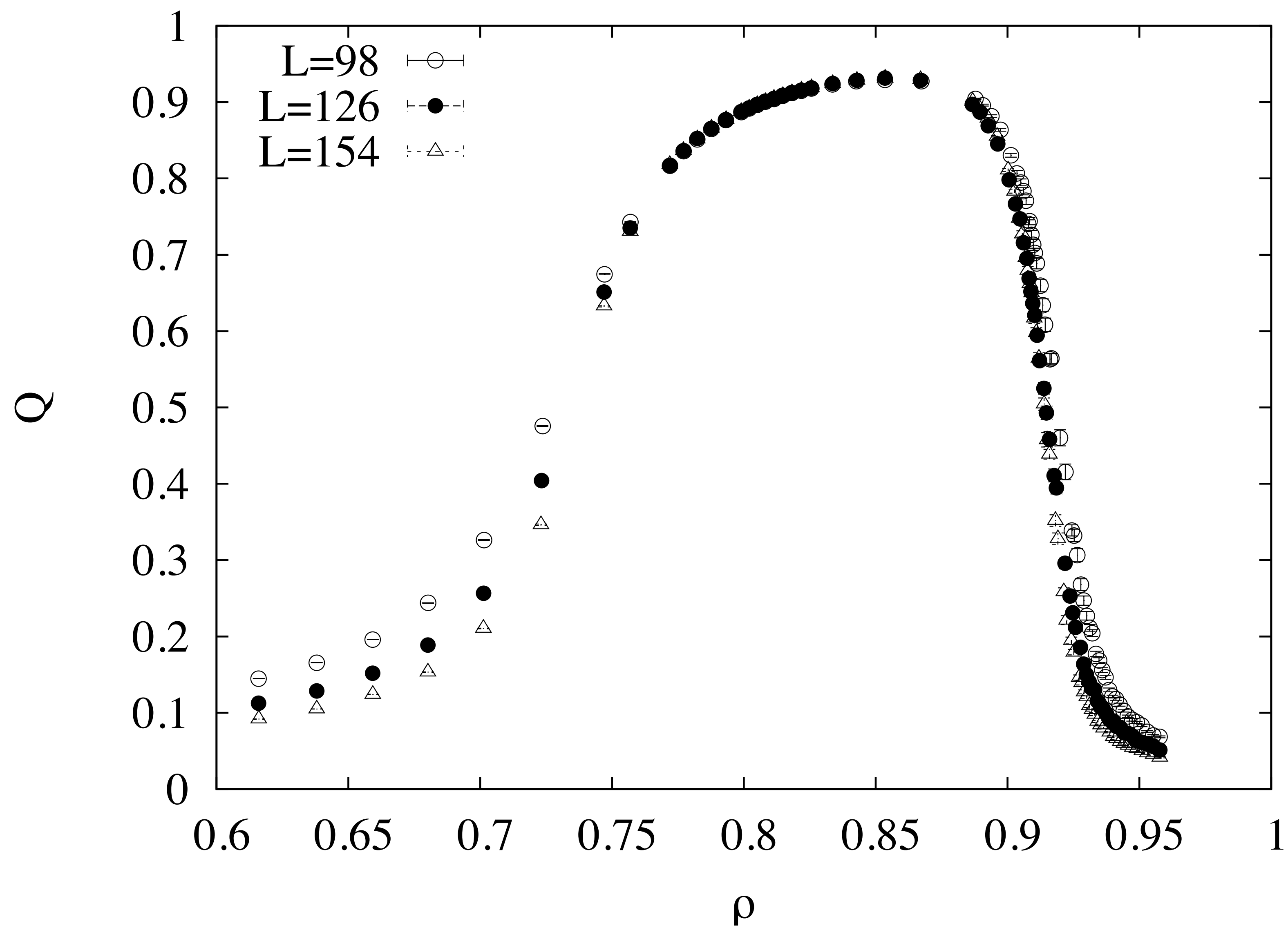
Existence of high density disordered phase



$$Q(t) = \exp\left[-\frac{\pi}{3}\epsilon v^2 t^3\right]$$

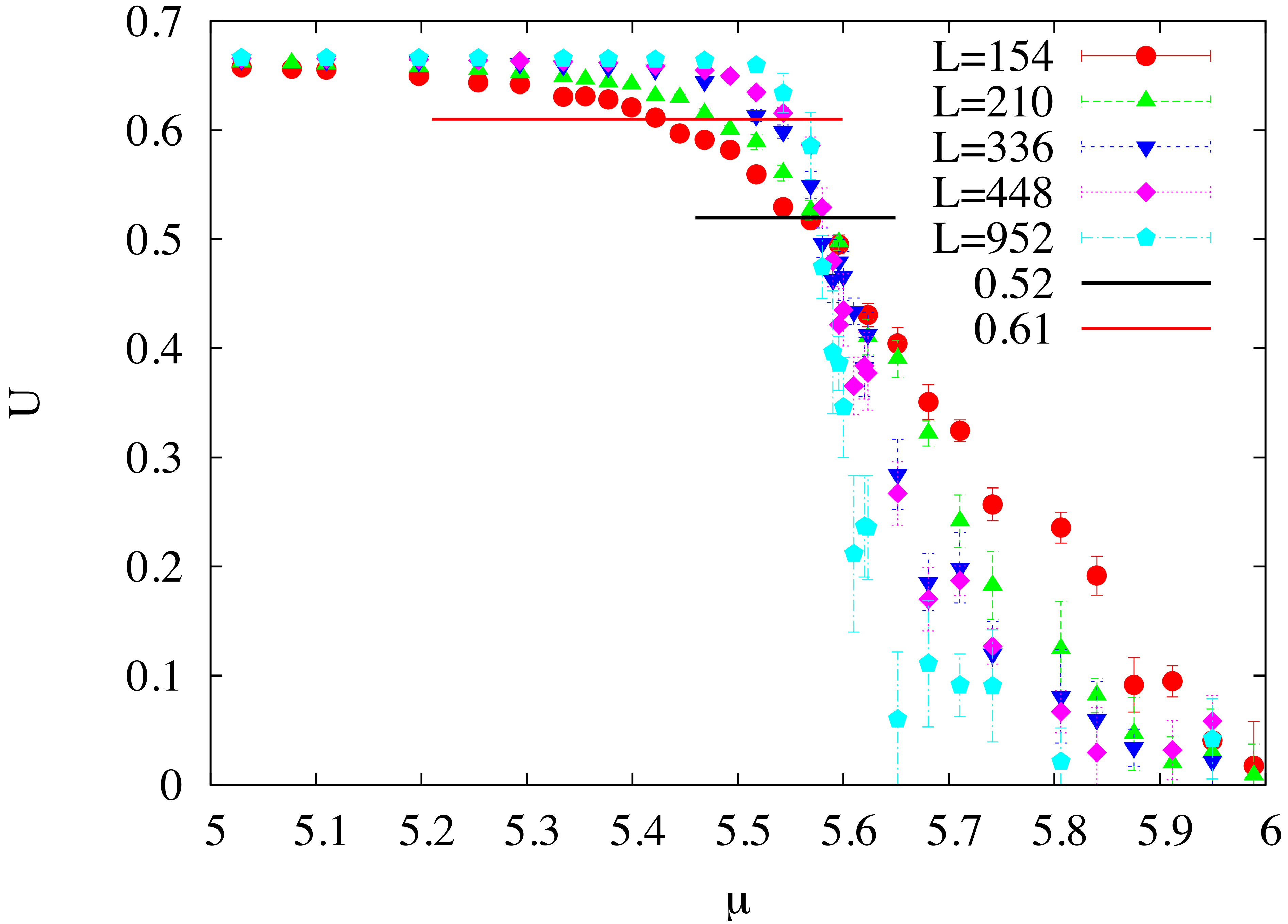
Continuous transition?

$$Q = \frac{|n_v - n_h|}{\langle n_v + n_h \rangle}$$



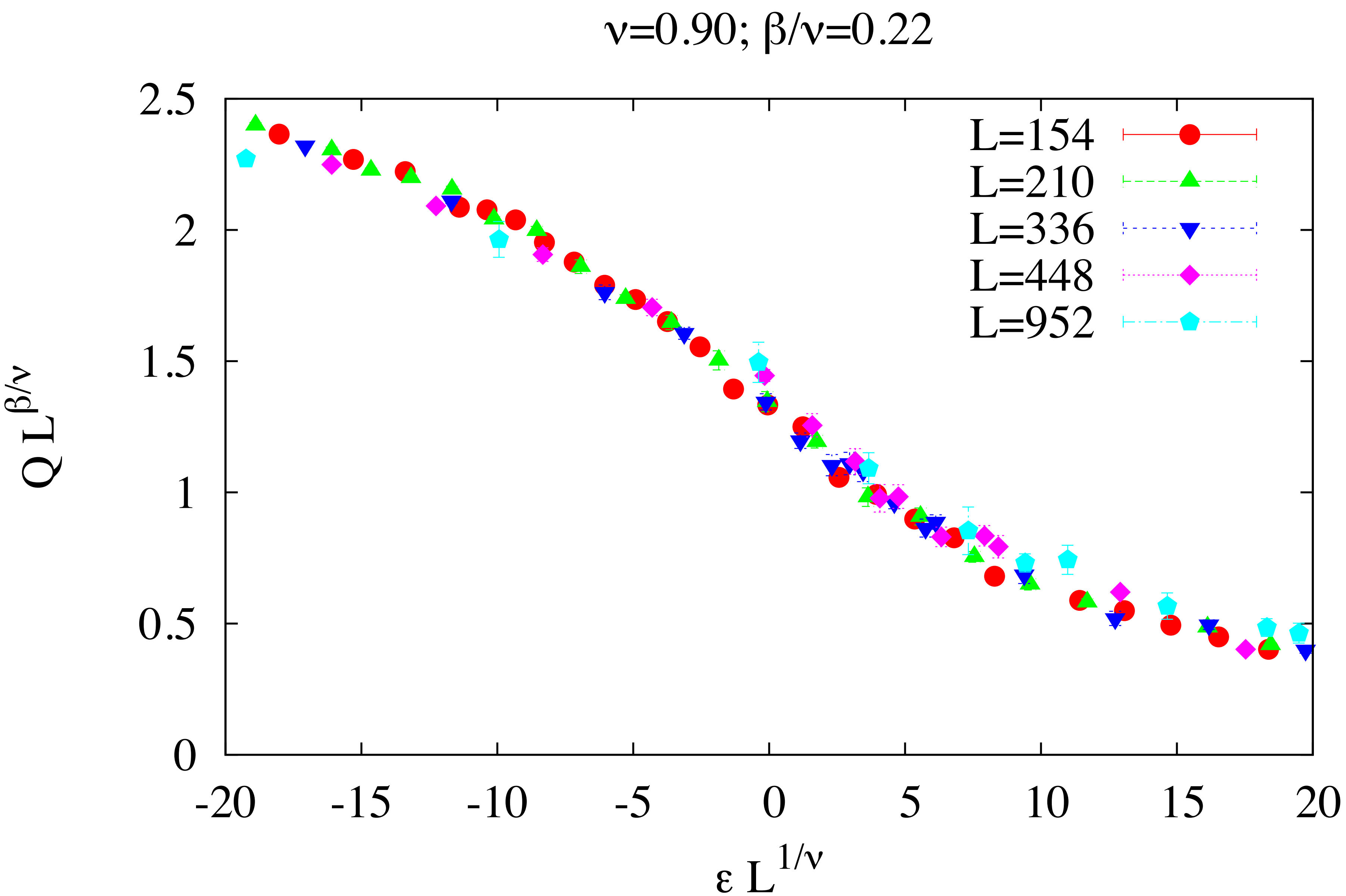
Binder Cumulant U

$$U = 1 - \frac{\langle Q^4 \rangle}{3\langle Q^2 \rangle^2}.$$



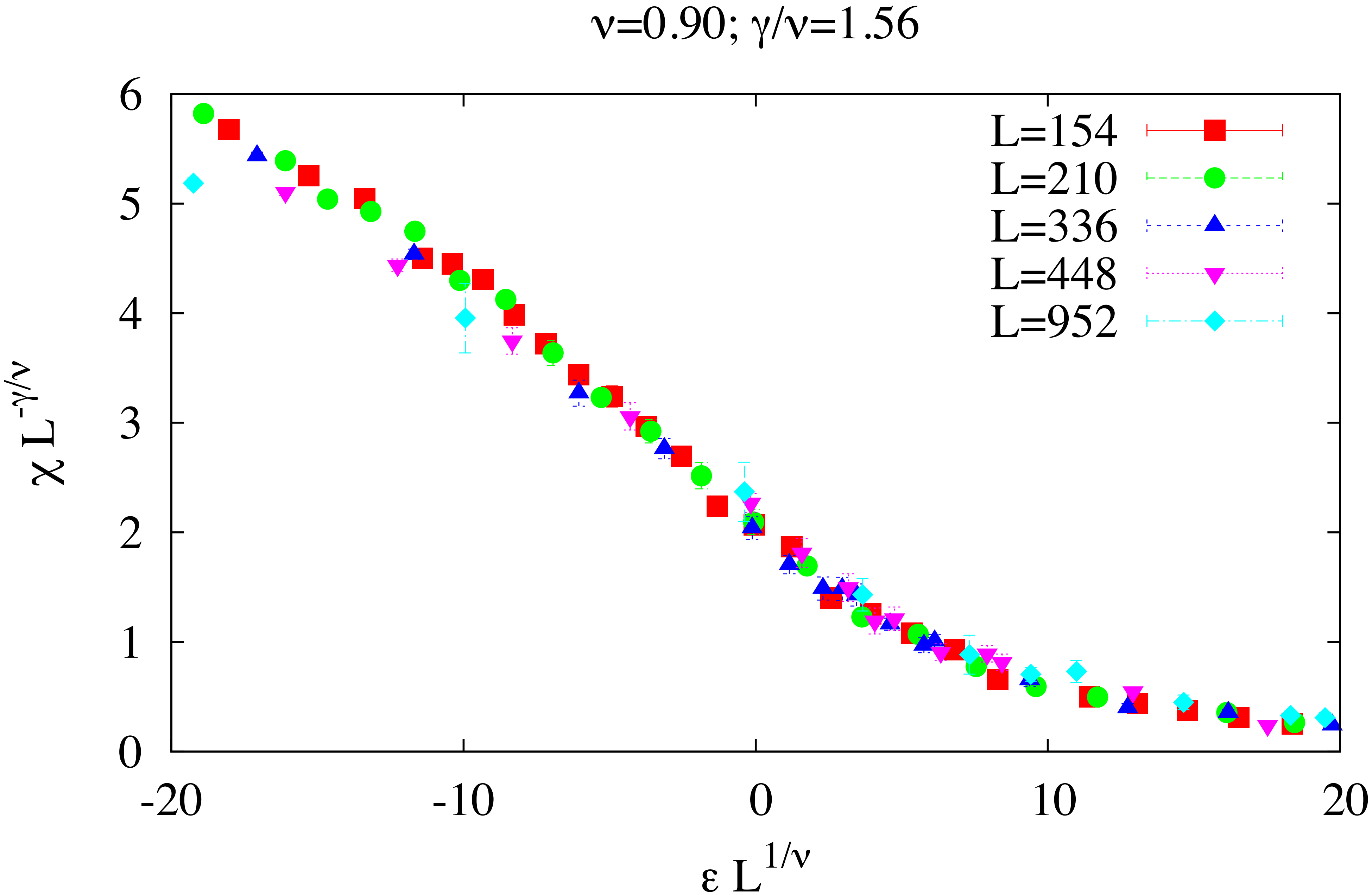
Order parameter

$$Q \simeq L^{-\beta/\nu} f_q(\epsilon L^{1/\nu})$$



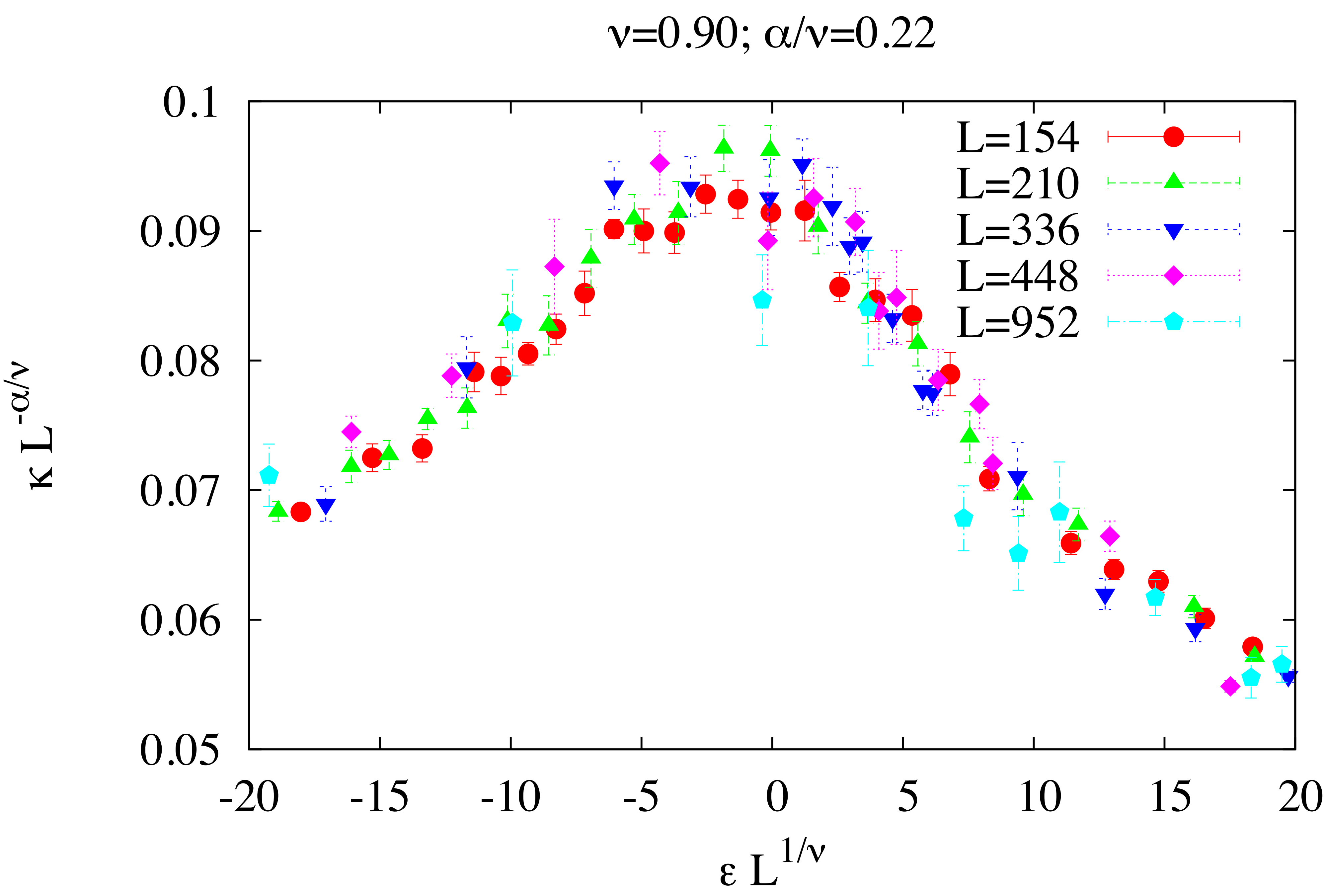
Susceptibility

$$\chi \simeq L^{\gamma/\nu} f_\chi(\epsilon L^{1/\nu})$$



Compressibility

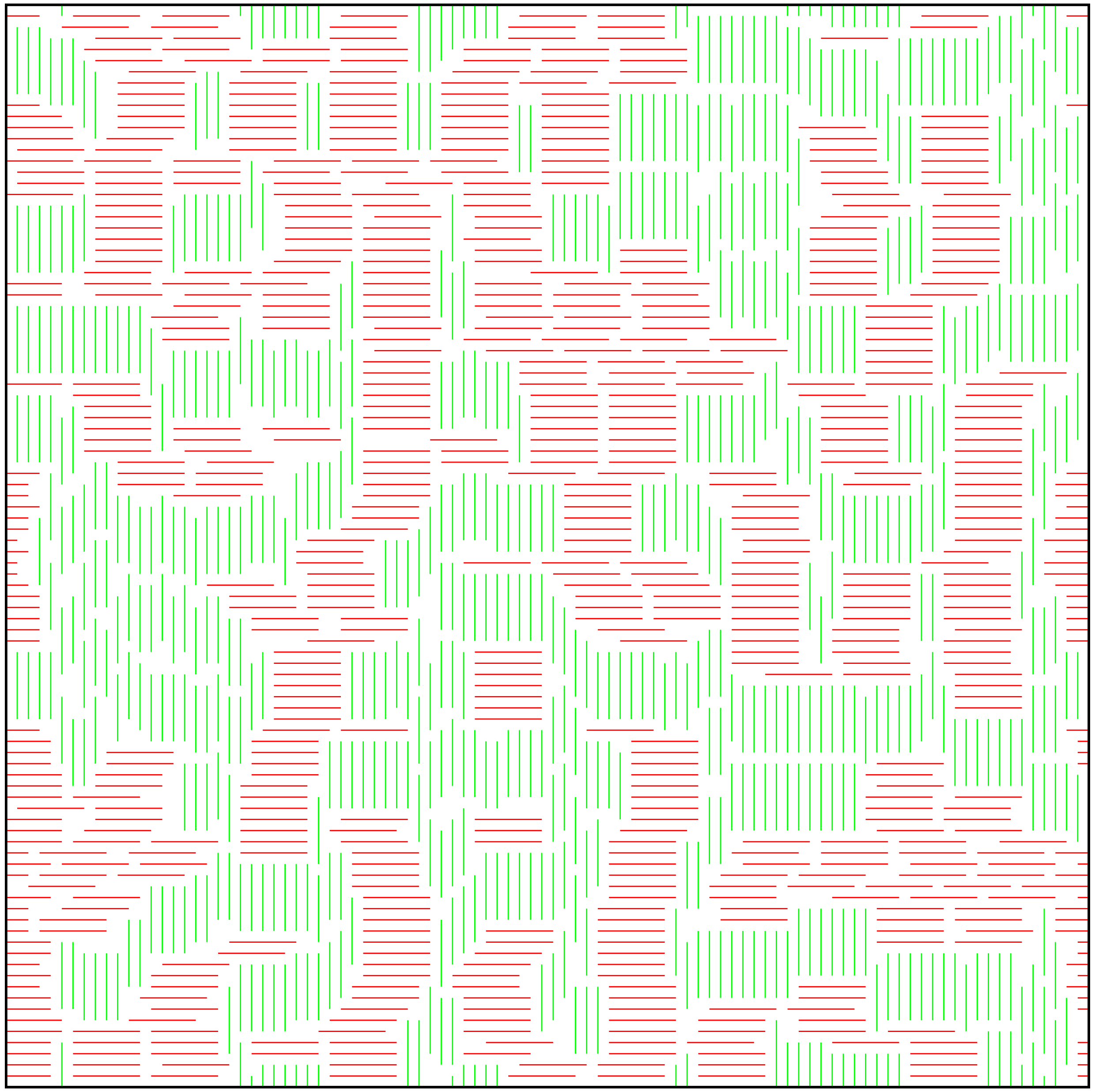
$$\kappa \simeq L^{\alpha/\nu} f_\kappa(\epsilon L^{1/\nu})$$



Ising?

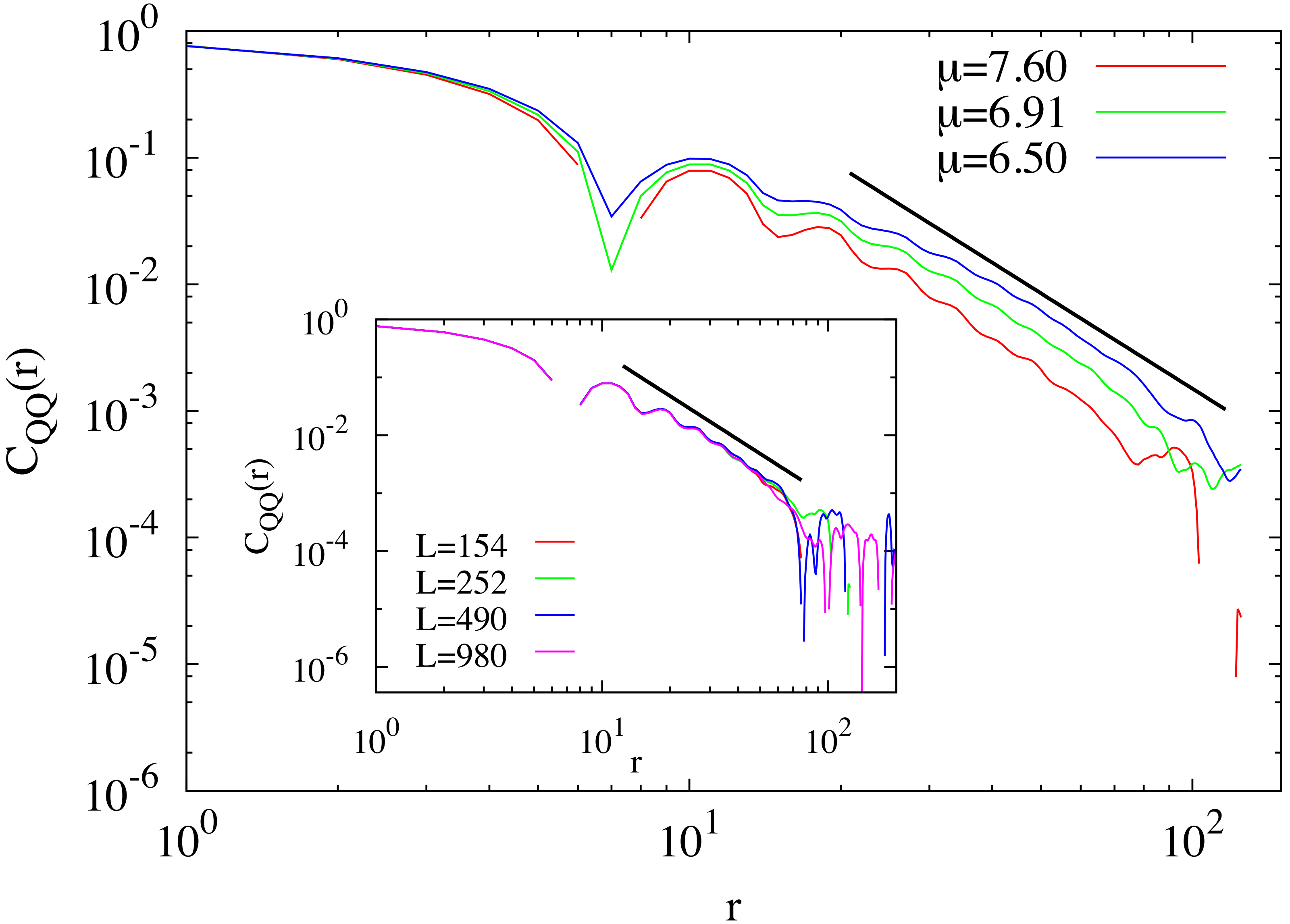
- Transition appears not to be in Ising universality
- But two symmetric ordered states
- High density disordered phase different from low density isotropic phase? An order parameter?

High density phase



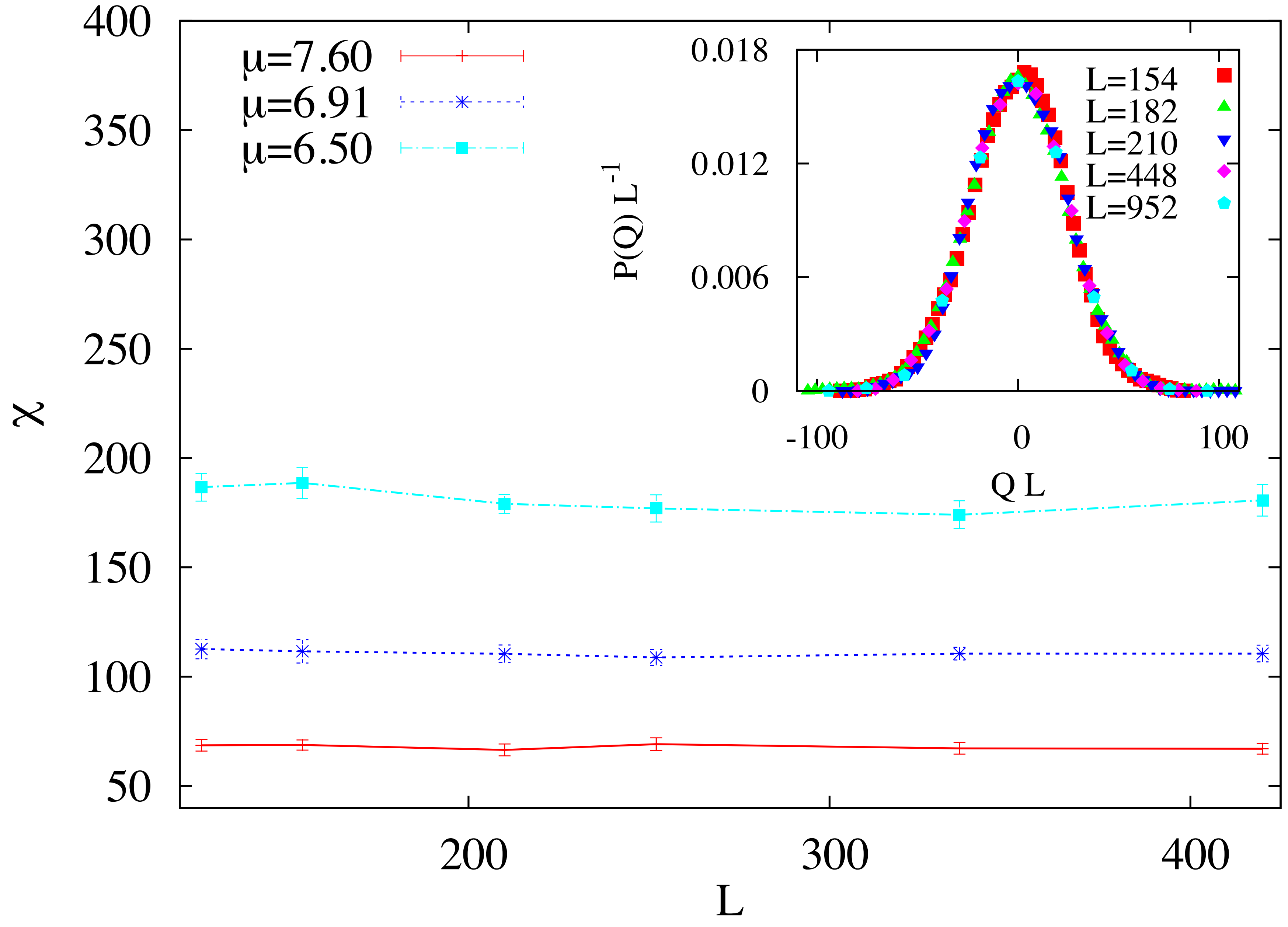
What it is not

Correlations



A power law?

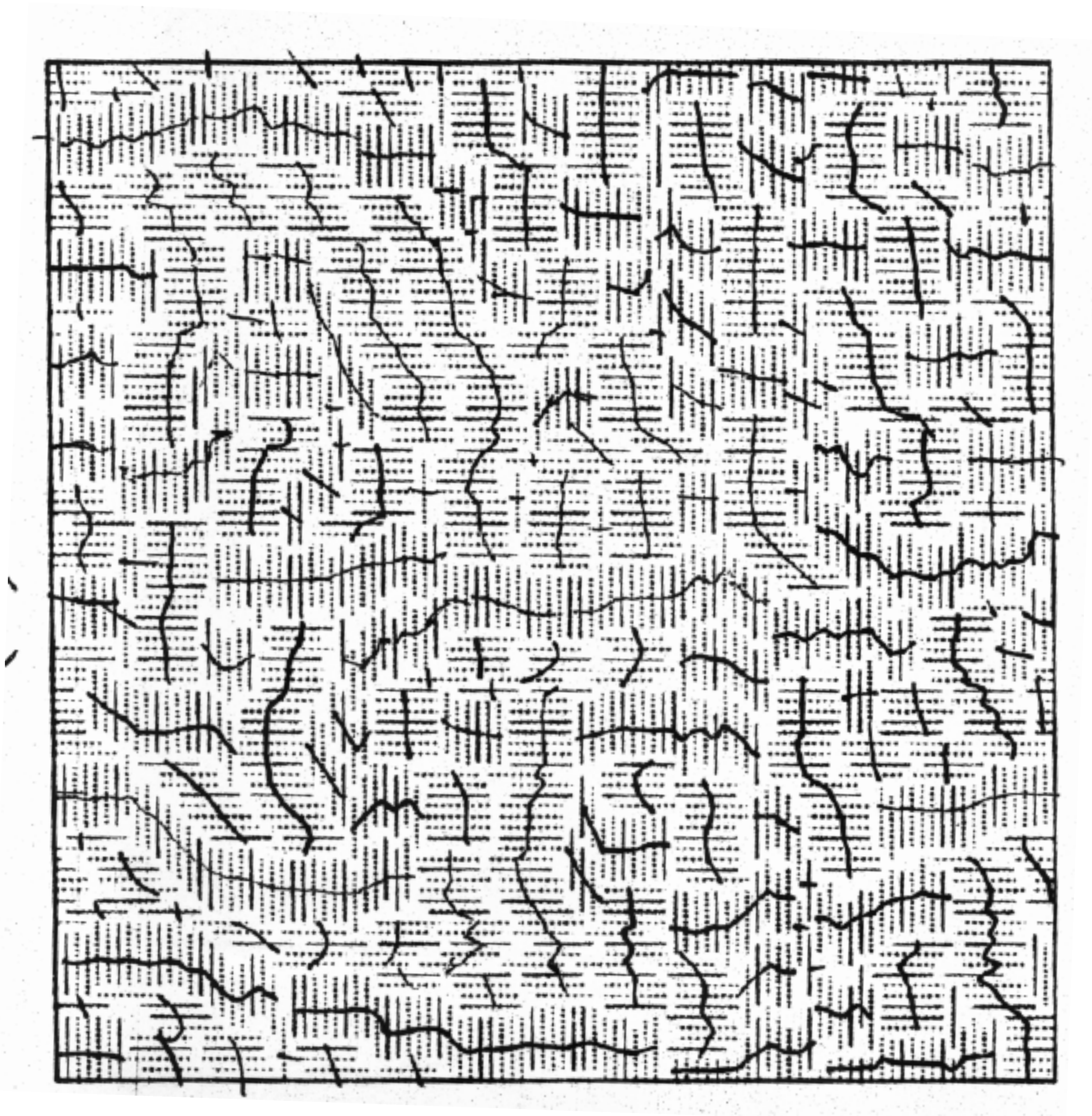
Susceptibility



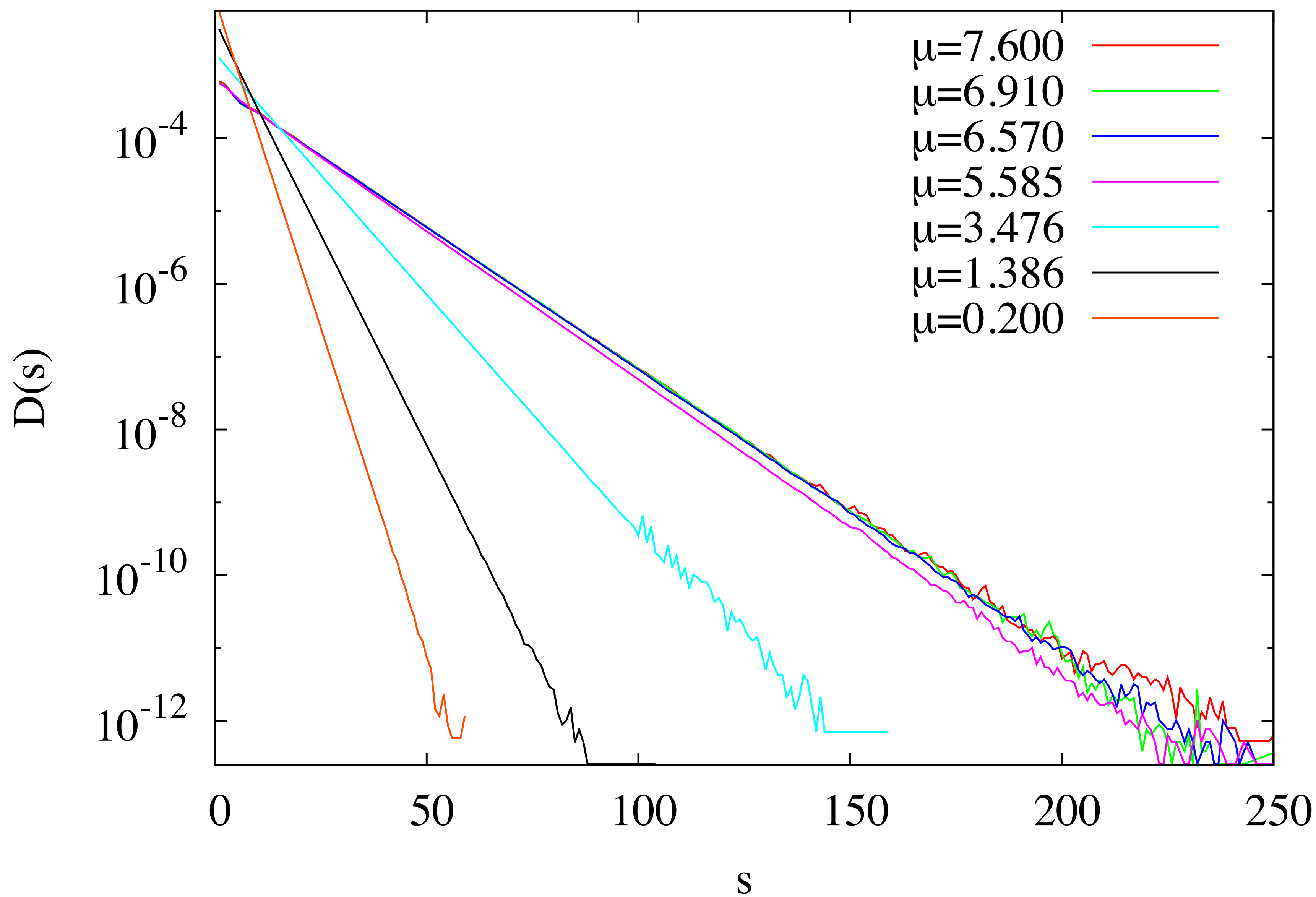
No divergence with L.

If power law, then exponent > 2

Stacks

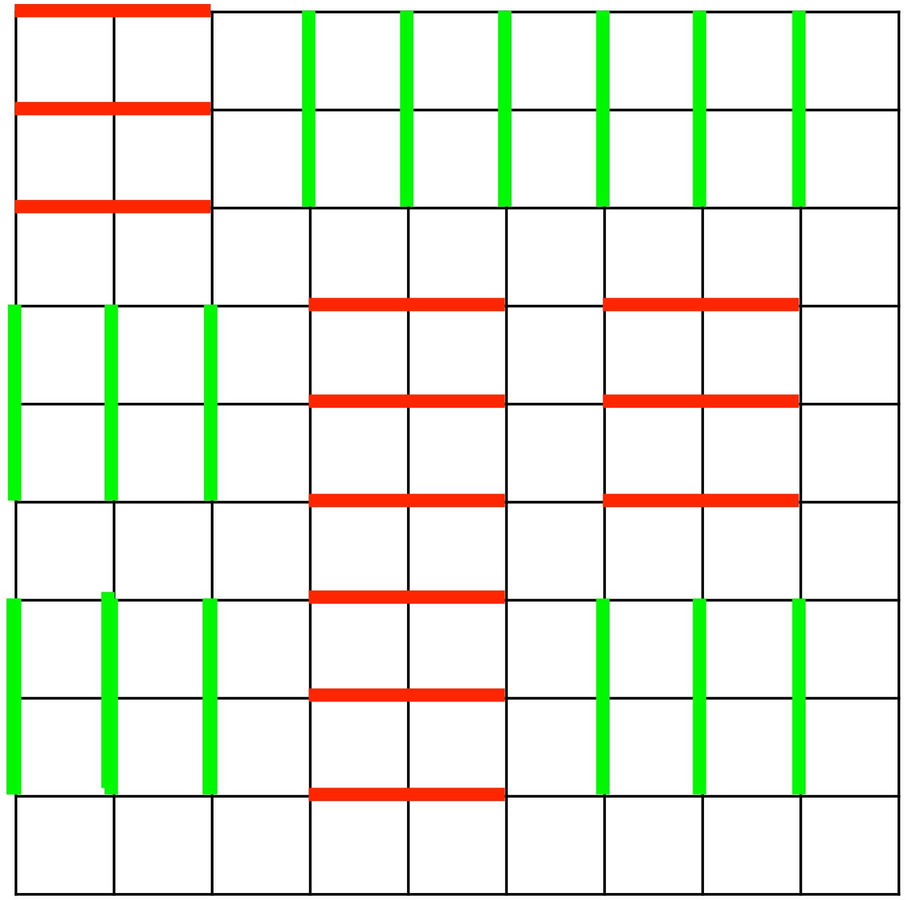


Stack distribution

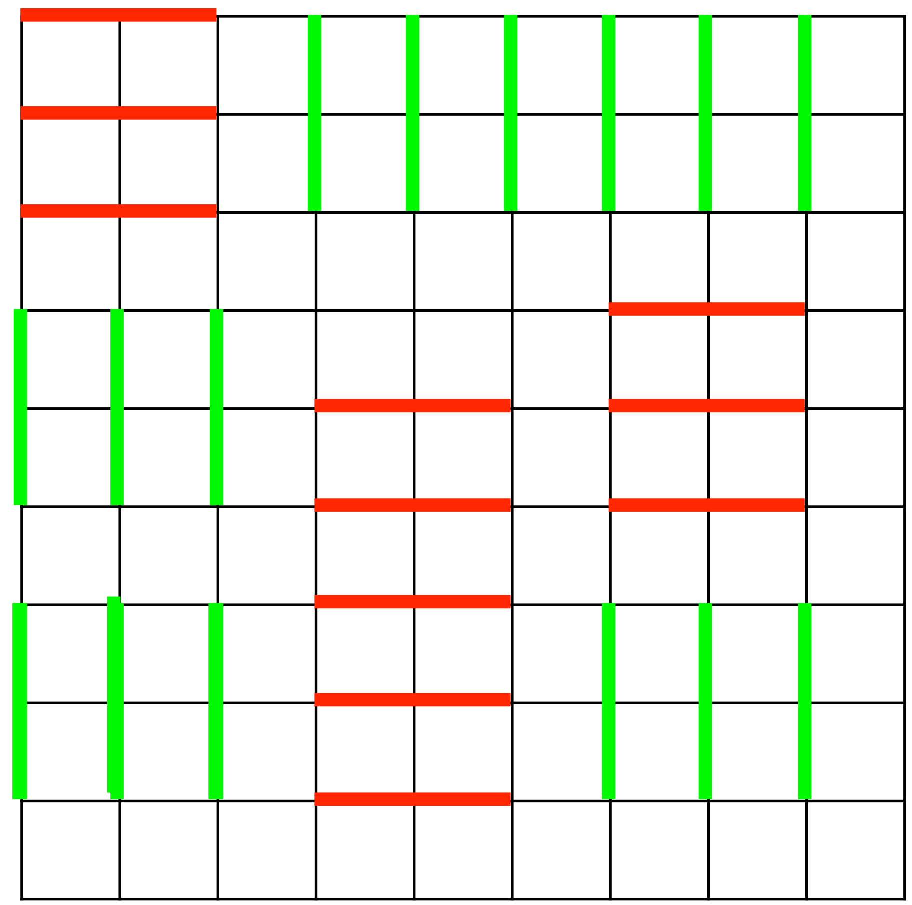


Exponential at all chemical potentials

Binding-unbinding transition?



Binding-unbinding transition?



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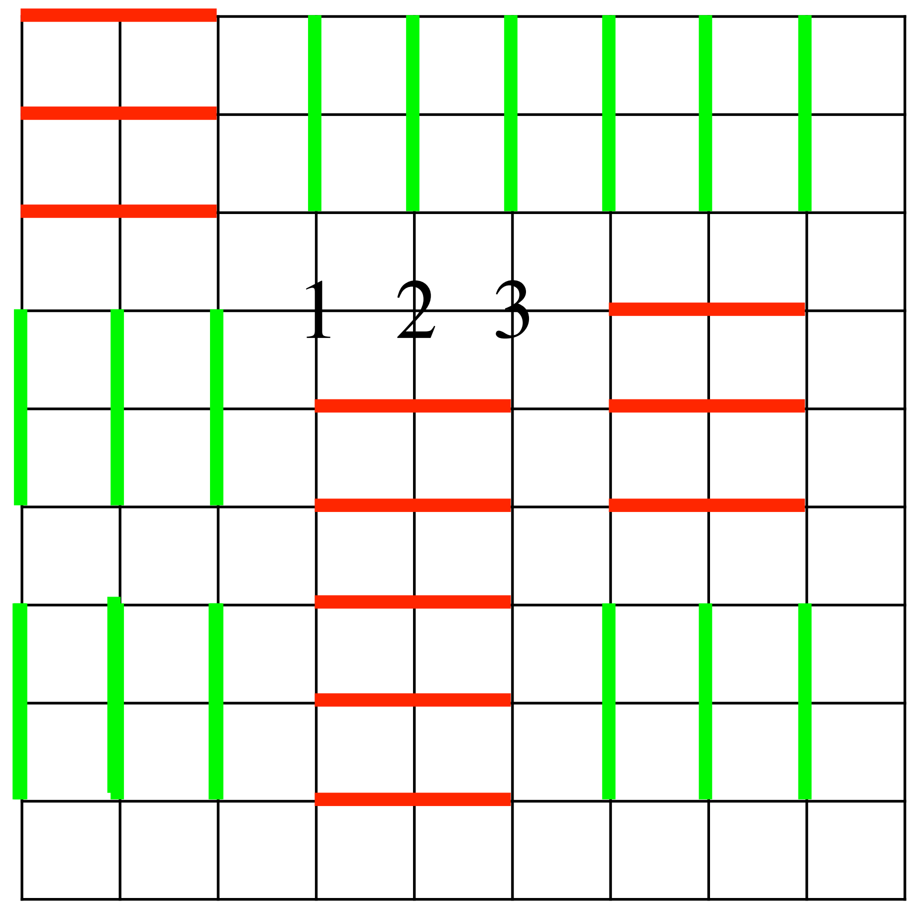

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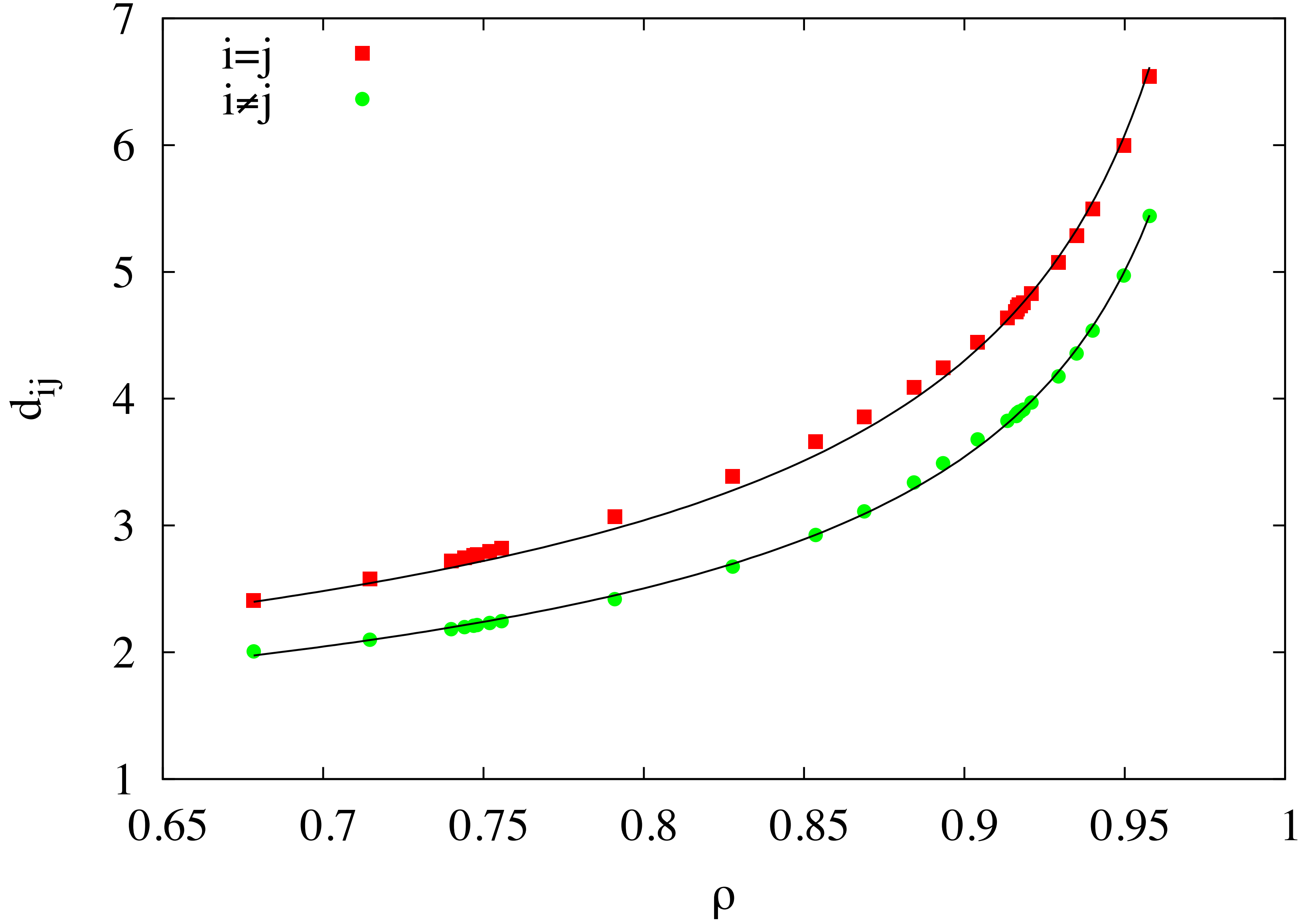
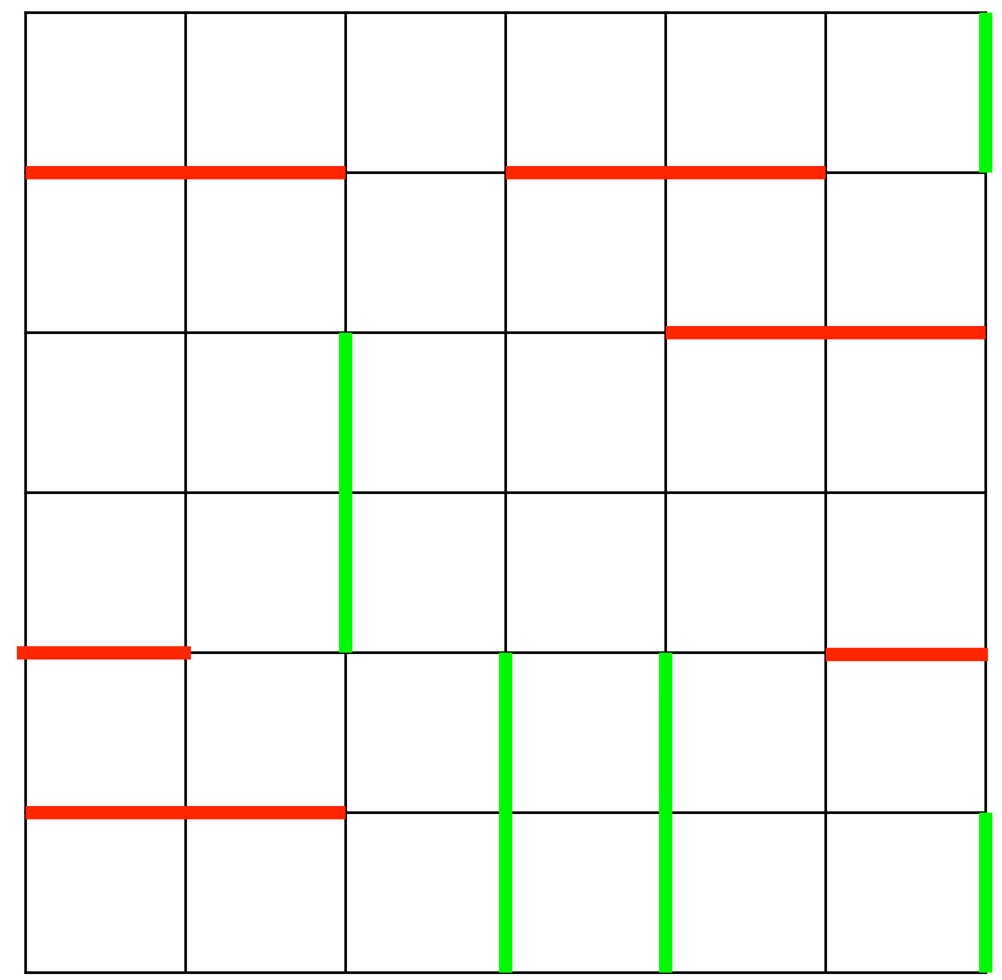


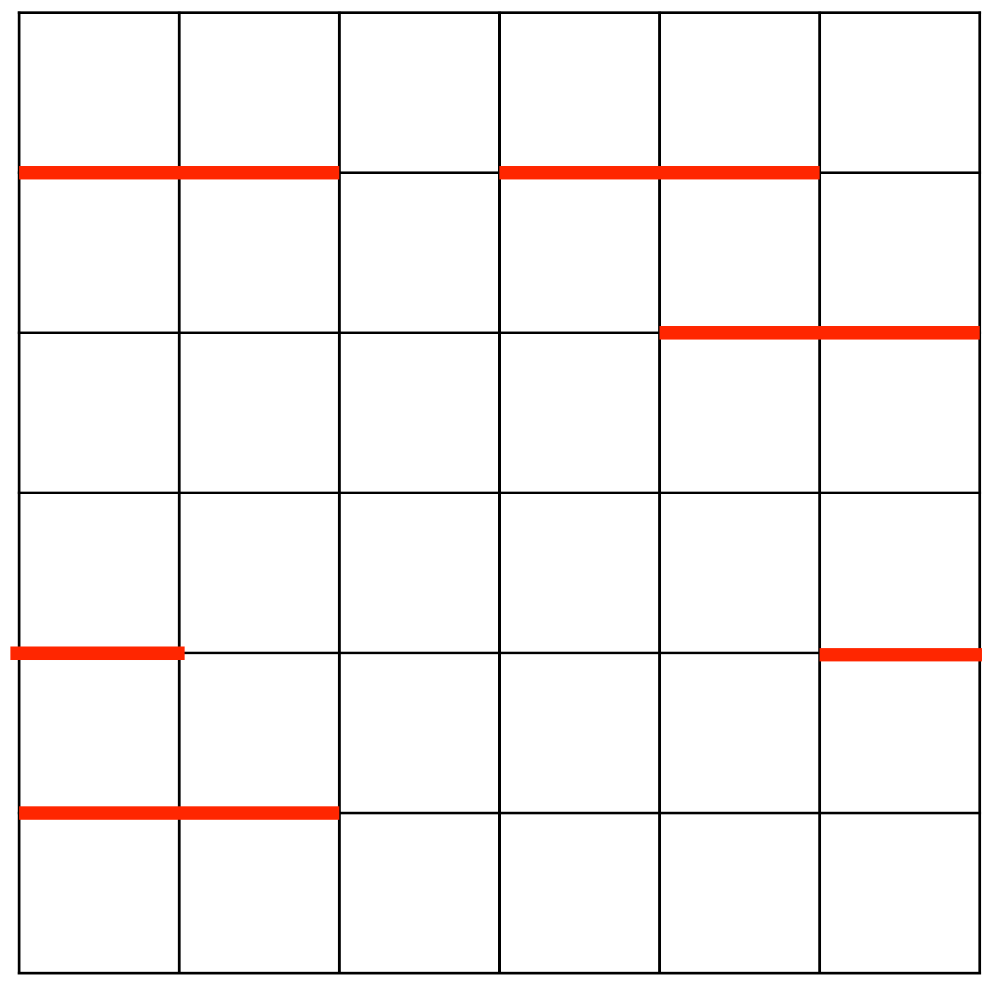
No evidence for bound state

Geometric Clusters



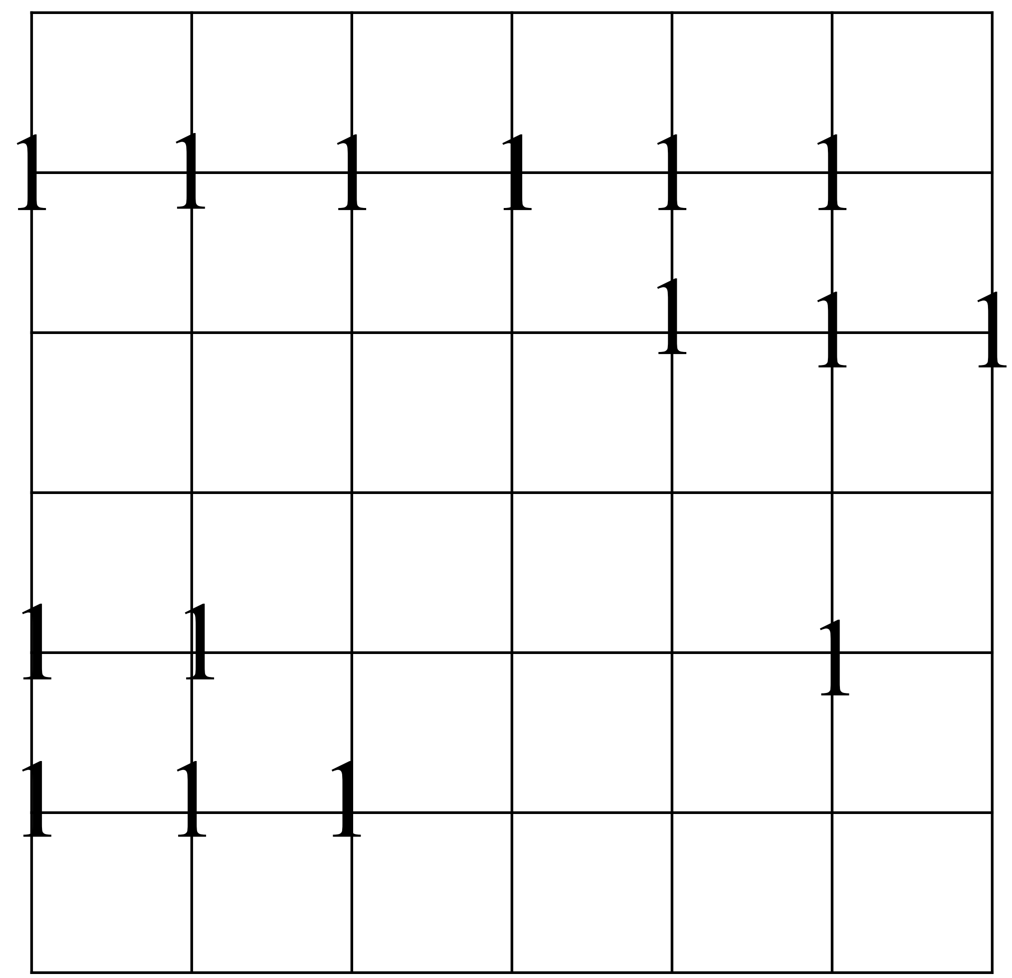
Replace x-mers by 1
Rest by 0

Geometric Clusters



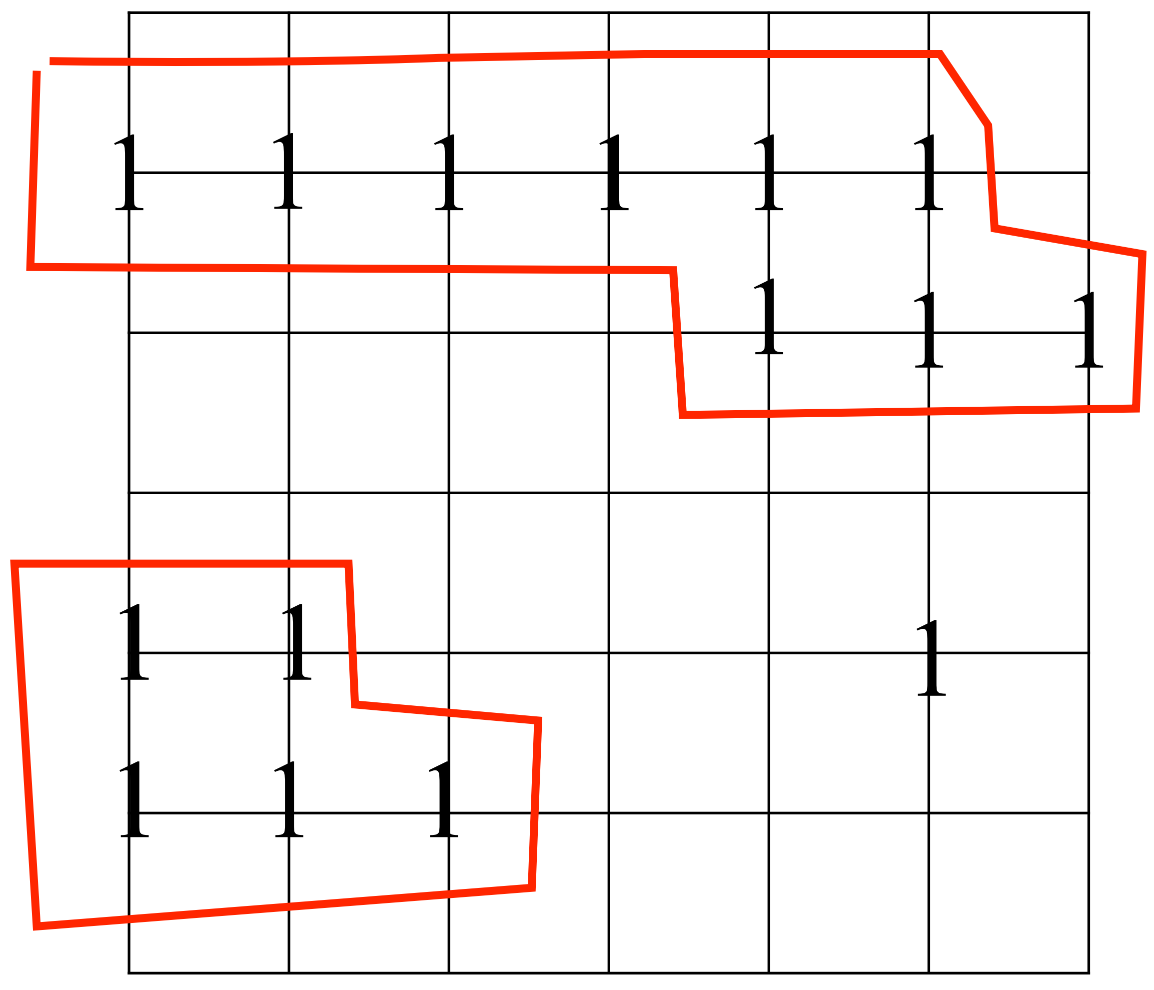
Replace x-mers by 1
Rest by 0

Geometric Clusters



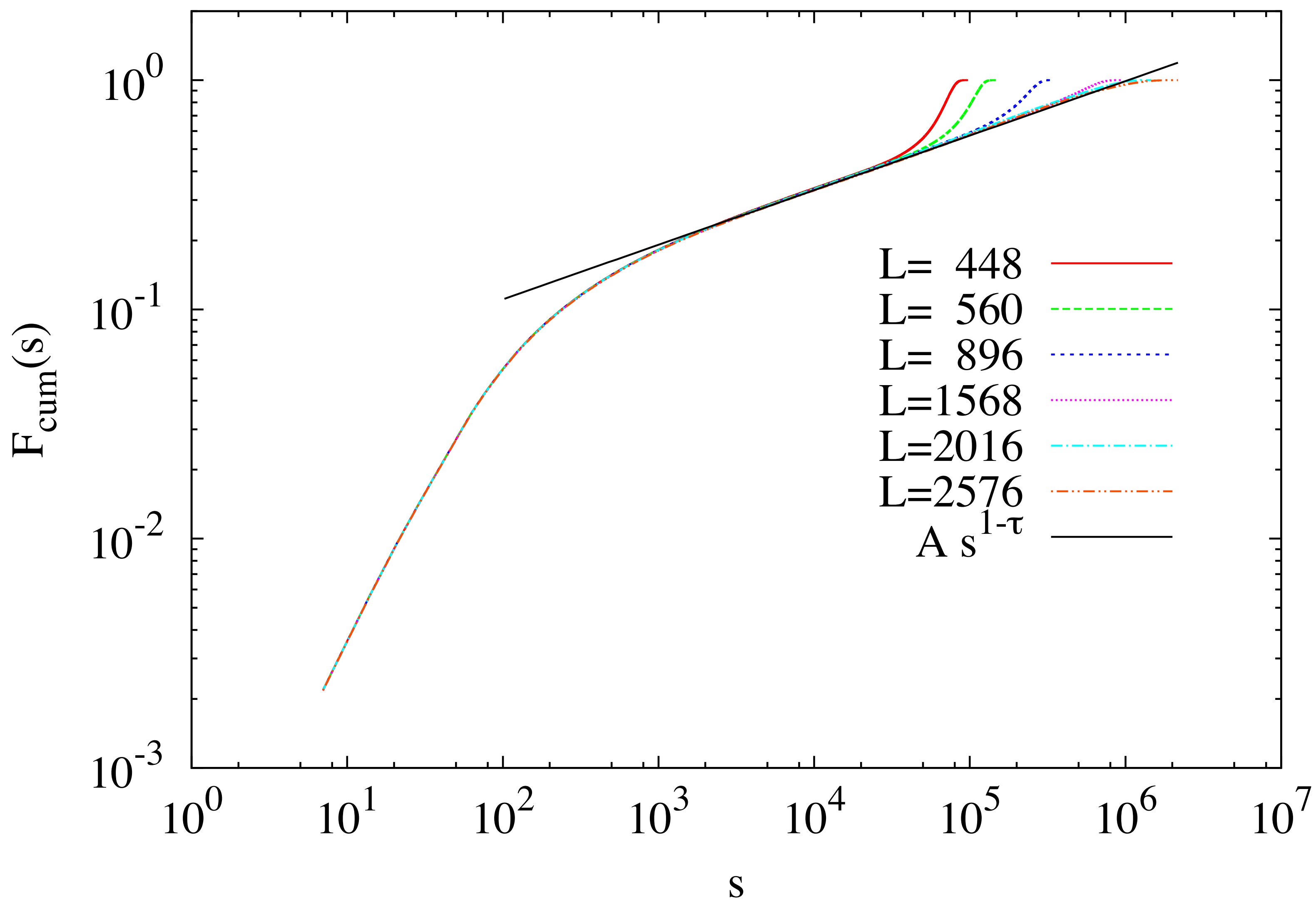
Replace x-mers by 1
Rest by 0

Geometric Clusters



Replace x-mers by 1
Rest by 0

Cluster size distribution



Cutoff ~ 10^6

A crossover length scale $\xi \approx 1500$

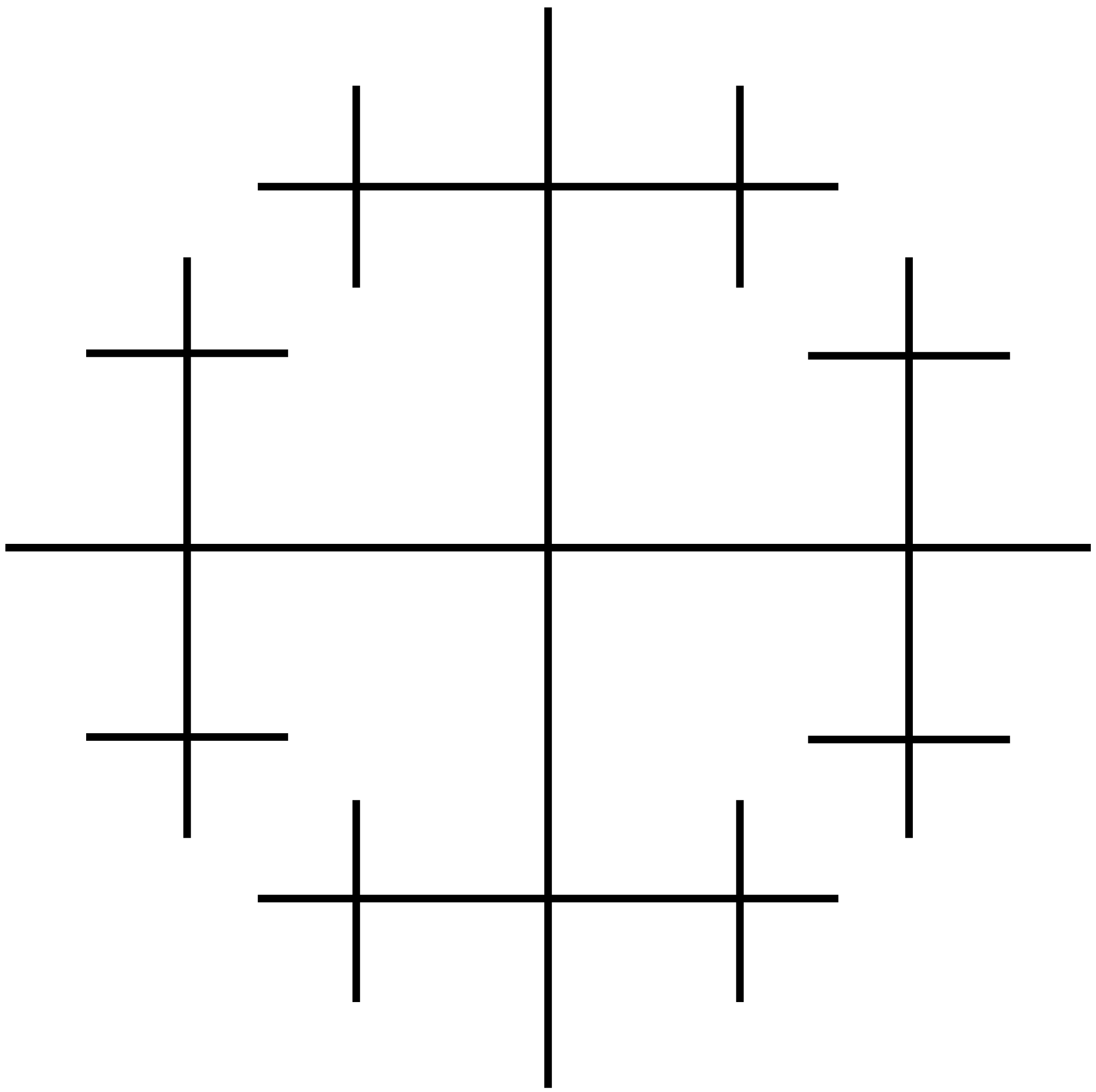
Nature of high density phase

- Circumstantial evidence for long range correlations
- A large crossover length scale
- What happens at larger length scales?

Bethe Approximation

- Beyond numerics
- Onsager solution exact for ∞ aspect ratio
- Bethe approximation treats nearest neighbour interactions exactly
- What is the Bethe approximation for finite length rods?
- Is there a second transition?

Bethe Lattice



Each site connected to q nbrs

No loops

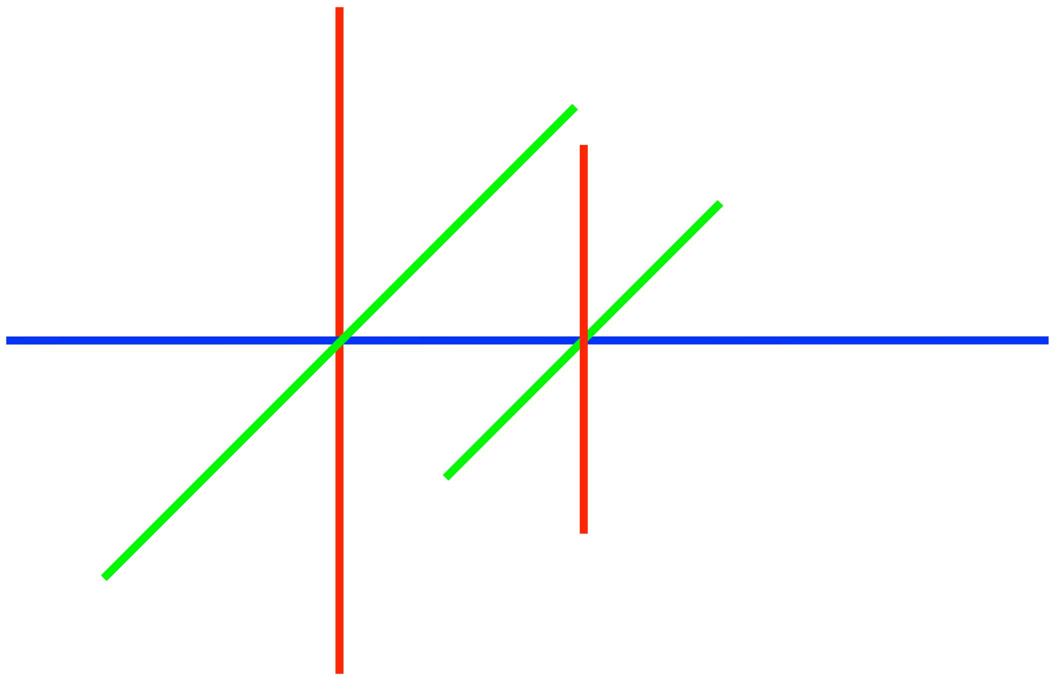
$$\frac{\text{Perimeter}}{\text{Volume}} \to \text{constant}$$

Cayley tree: dominated by perimeter

Bethe lattice: Core of the Cayley tree

Some issues with Bethe lattice

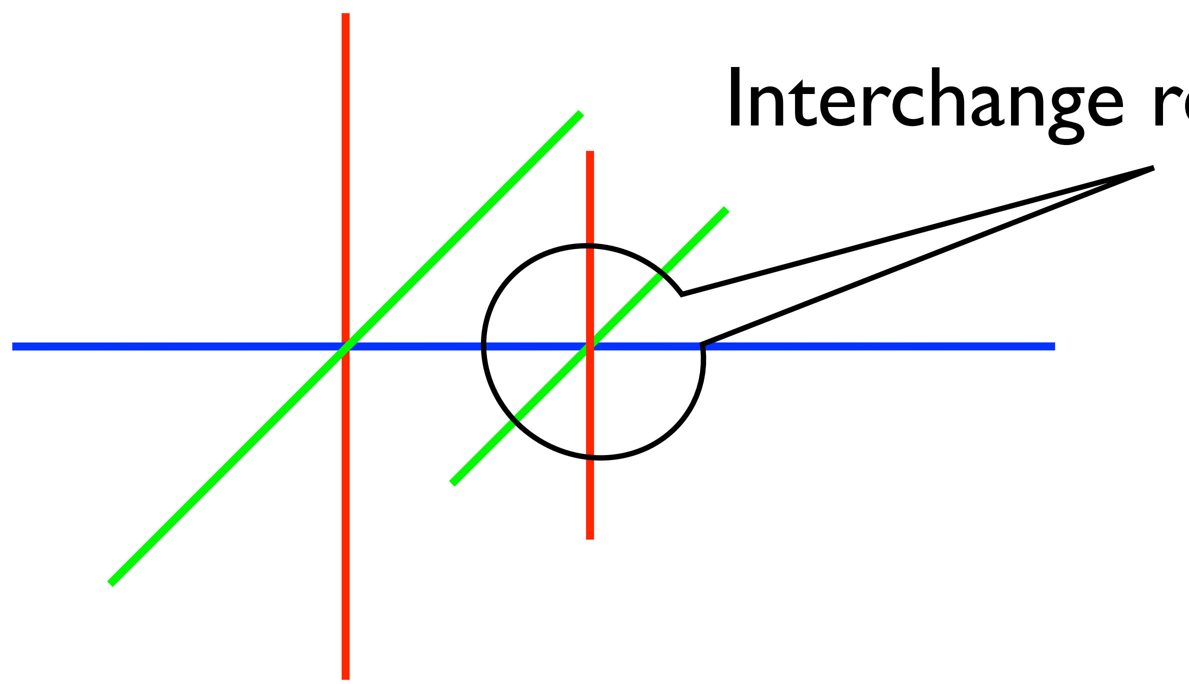
Consider coordination number 6



Suppose $\rho_{red} > \rho_{green} = \rho_{blue}$

Some issues with Bethe lattice

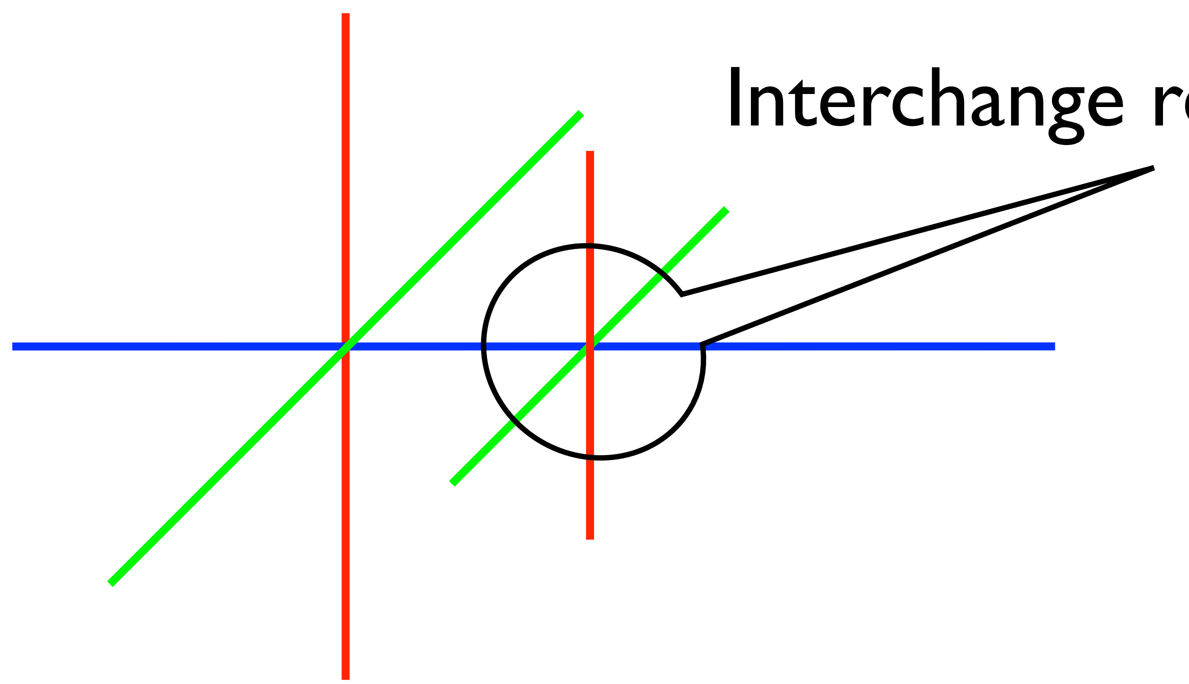
Consider coordination number 6



Suppose $\rho_{red} > \rho_{green} = \rho_{blue}$

Some issues with Bethe lattice

Consider coordination number 6

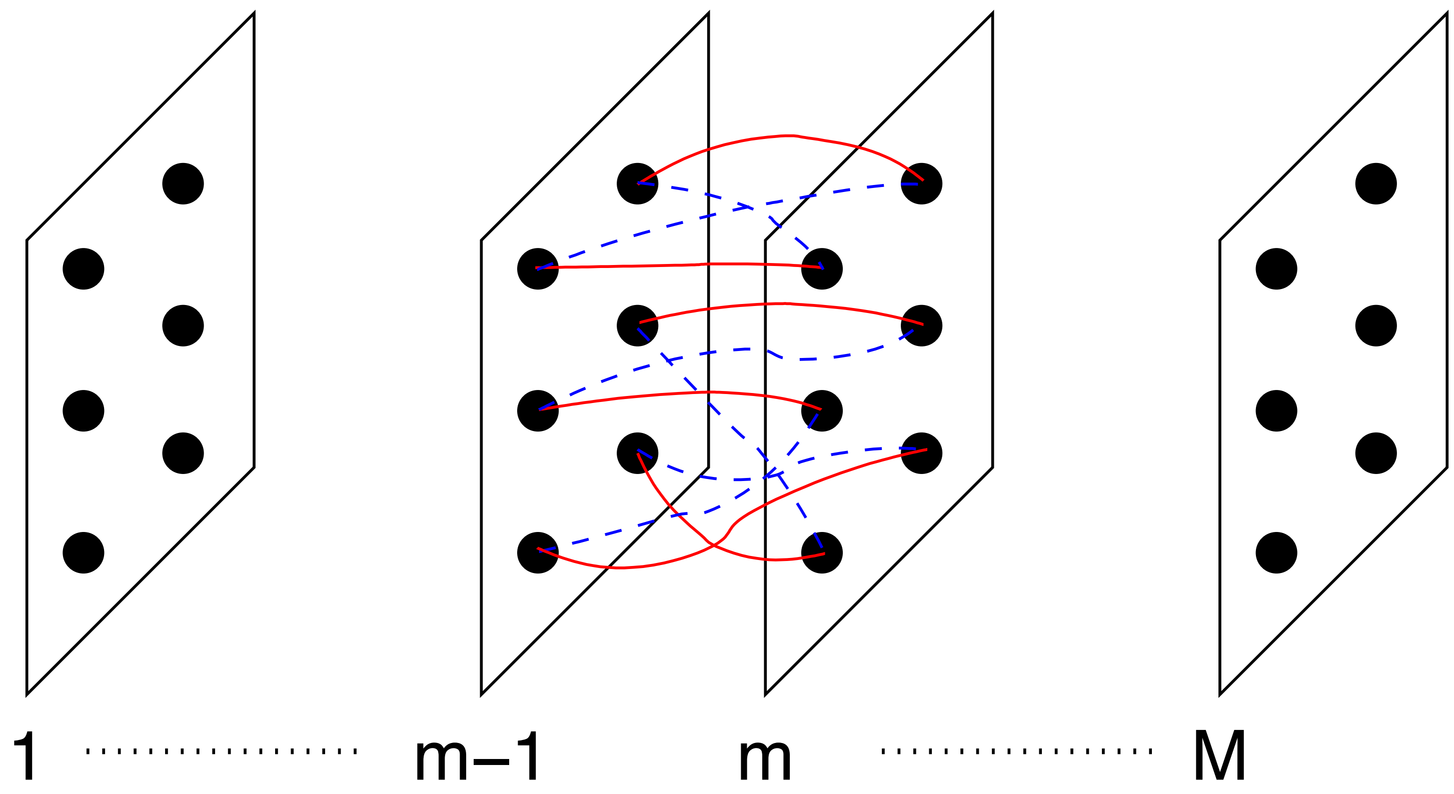


Suppose $\rho_{red} > \rho_{green} = \rho_{blue}$

Then, $\rho_{red} = \rho_{green}$

Contradiction ⇒ no nematic order possible

Random Locally Tree-like Lattice (RLTL)

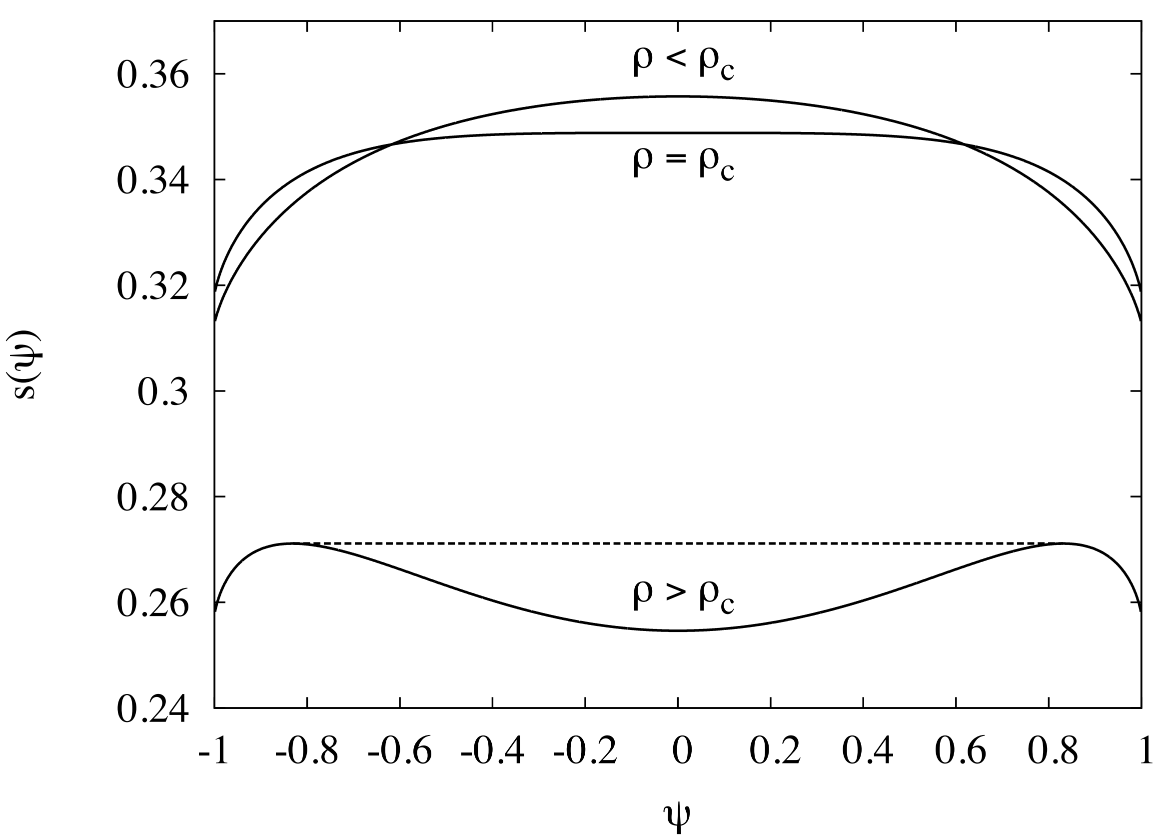


Each site connected to two
sites in next layer by a x- and y- bond

Solution

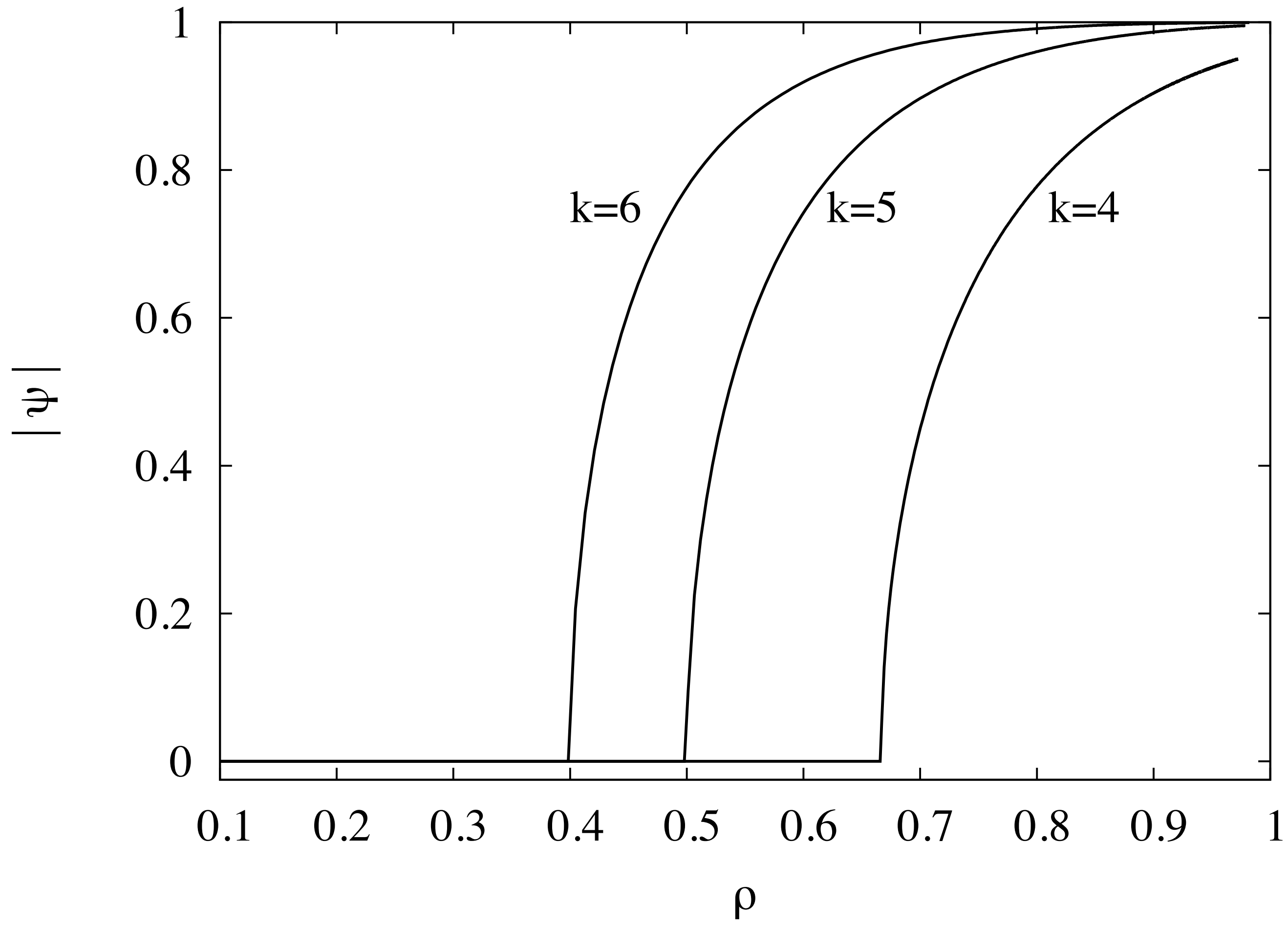
$$
\begin{aligned}
s(\rho_x,\rho_y) &= \left(1-\frac{k-1}{k}\rho_x\right)\ln\left(1-\frac{k-1}{k}\rho_x\right) \\
&+ \left(1-\frac{k-1}{k}\rho_y\right)\ln\left(1-\frac{k-1}{k}\rho_y\right) \\
&- (1-\rho)\ln(1-\rho) - \frac{\rho_x}{k}\ln\frac{\rho_x}{k} - \frac{\rho_y}{k}\ln\frac{\rho_y}{k}
\end{aligned}
$$

Keep ρ fixed and maximize entropy



$$\psi = \rho_x - \rho_y$$

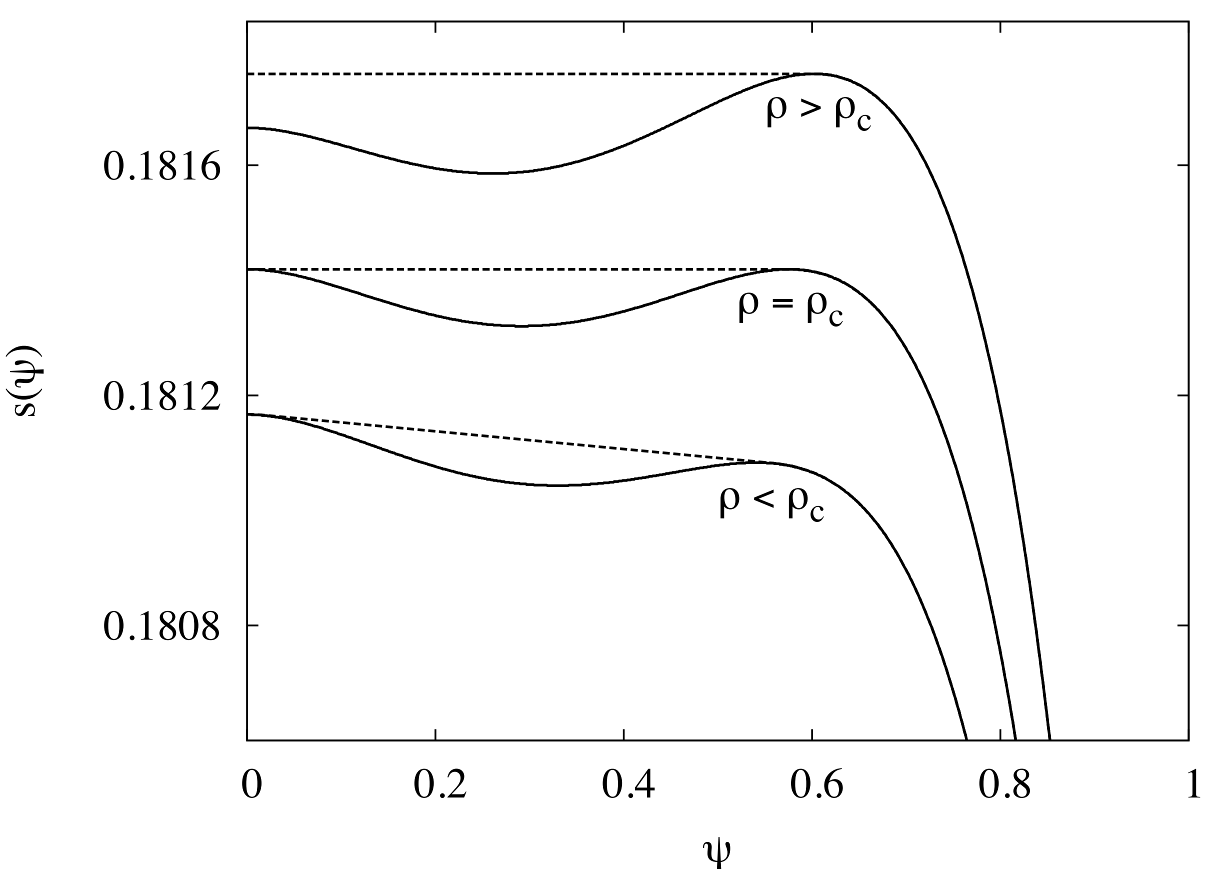
Results:order parameter

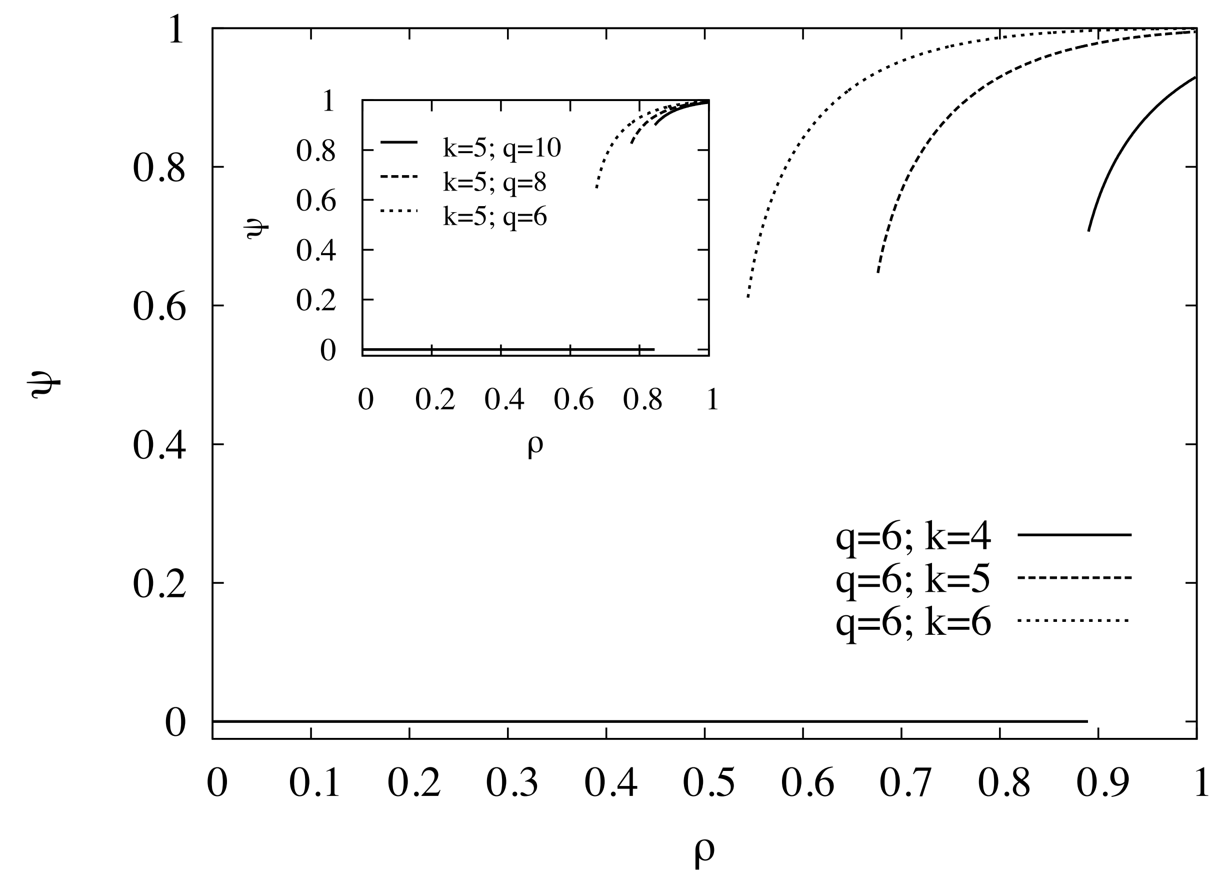


q=4

No second transition

Order parameter q>4

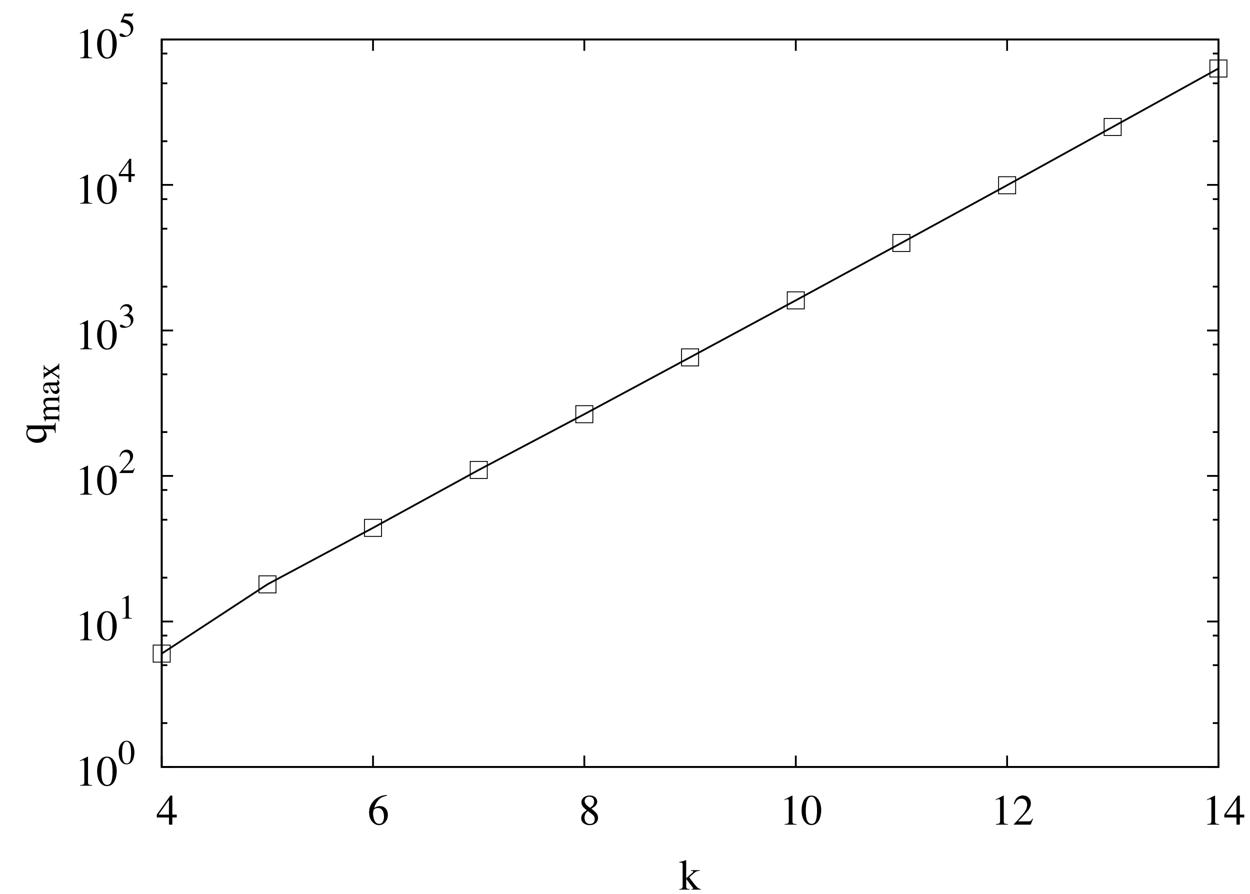




$$\psi = \rho_{||} - \rho_{\perp}$$

Results: k_{min}

k	q
4	6
5	18
6	44
7	110
8	266
9	654
10	1612
11	3994
12	9968
13	25028



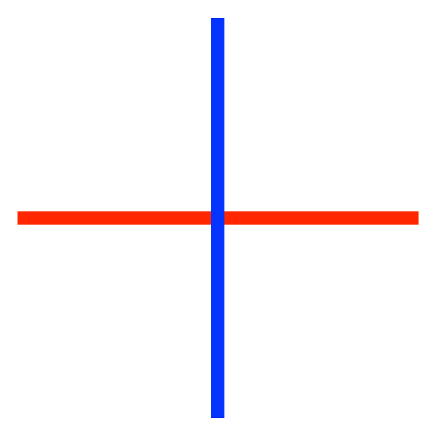
$$q_{\max} \sim \exp(k)$$
$$k_{min} \sim \ln(q)$$

Is there a second transition?

No

Interacting rods

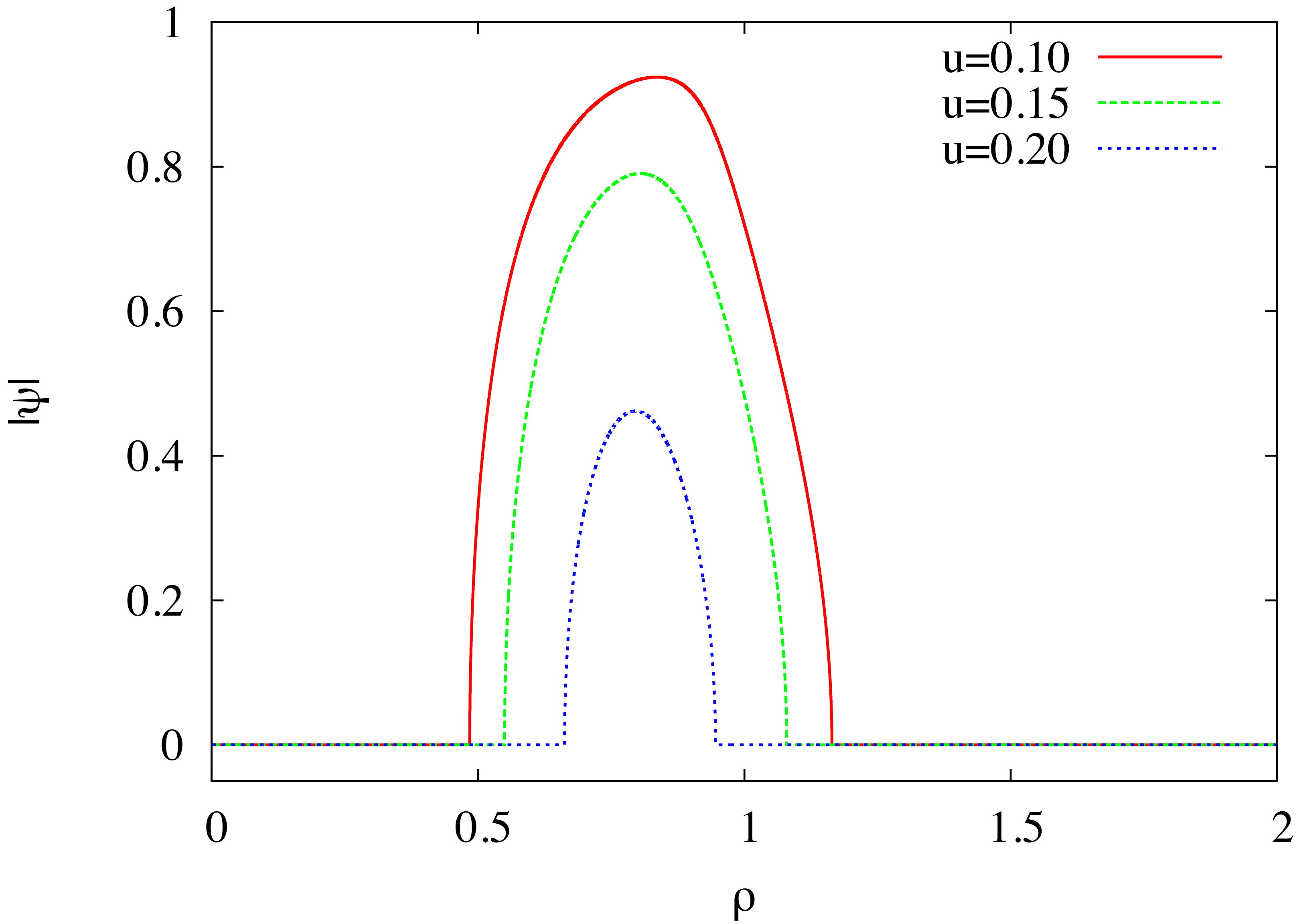
A site allowed to have two monomers,
but only perpendicular intersection allowed



Weight = u

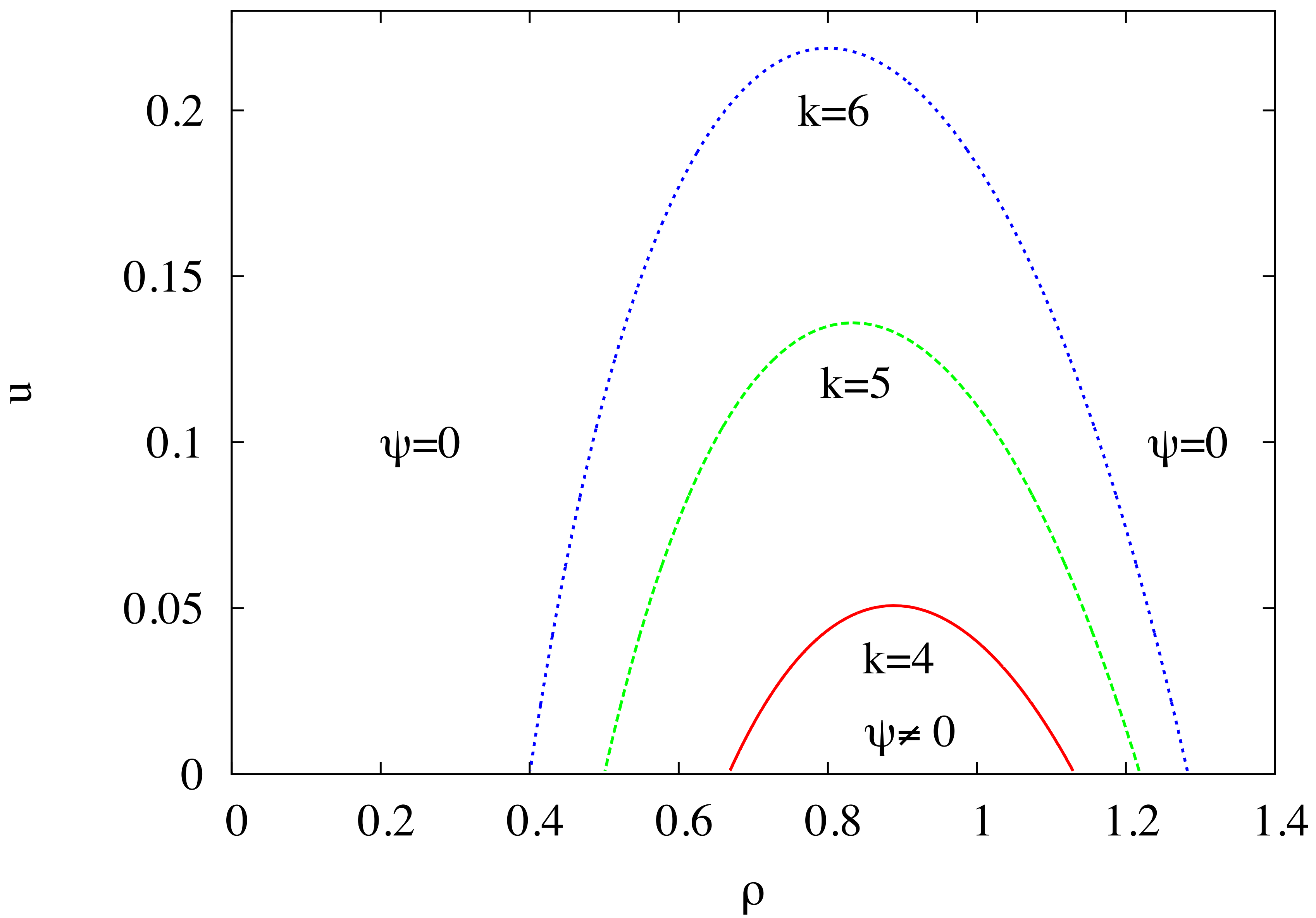
$$u = 0: \text{ hard rods}$$
$$u \neq 0: \text{ promotes disorder}$$

Results: order parameter



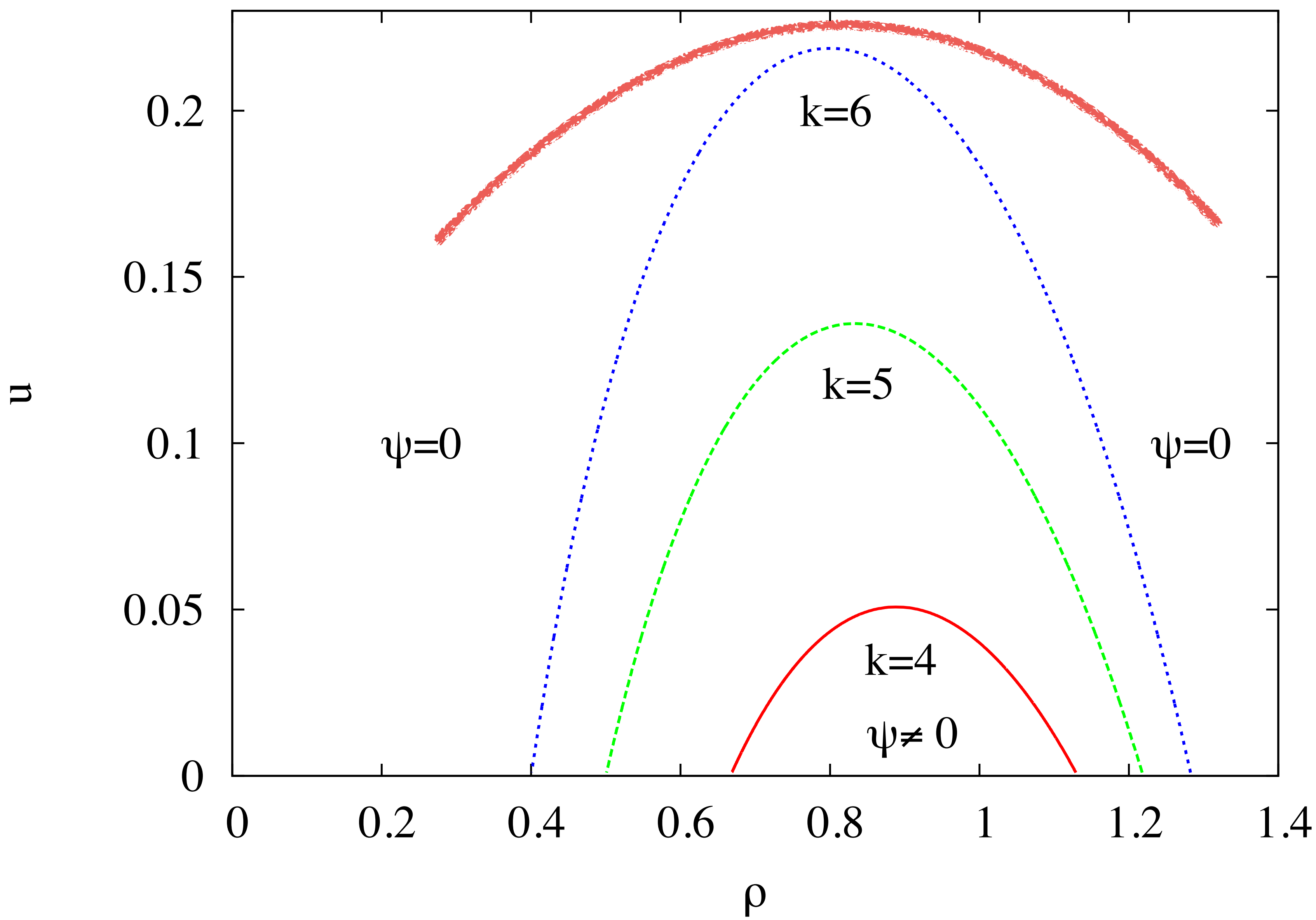
q=4; k=4

Results: phase diagram



q=4

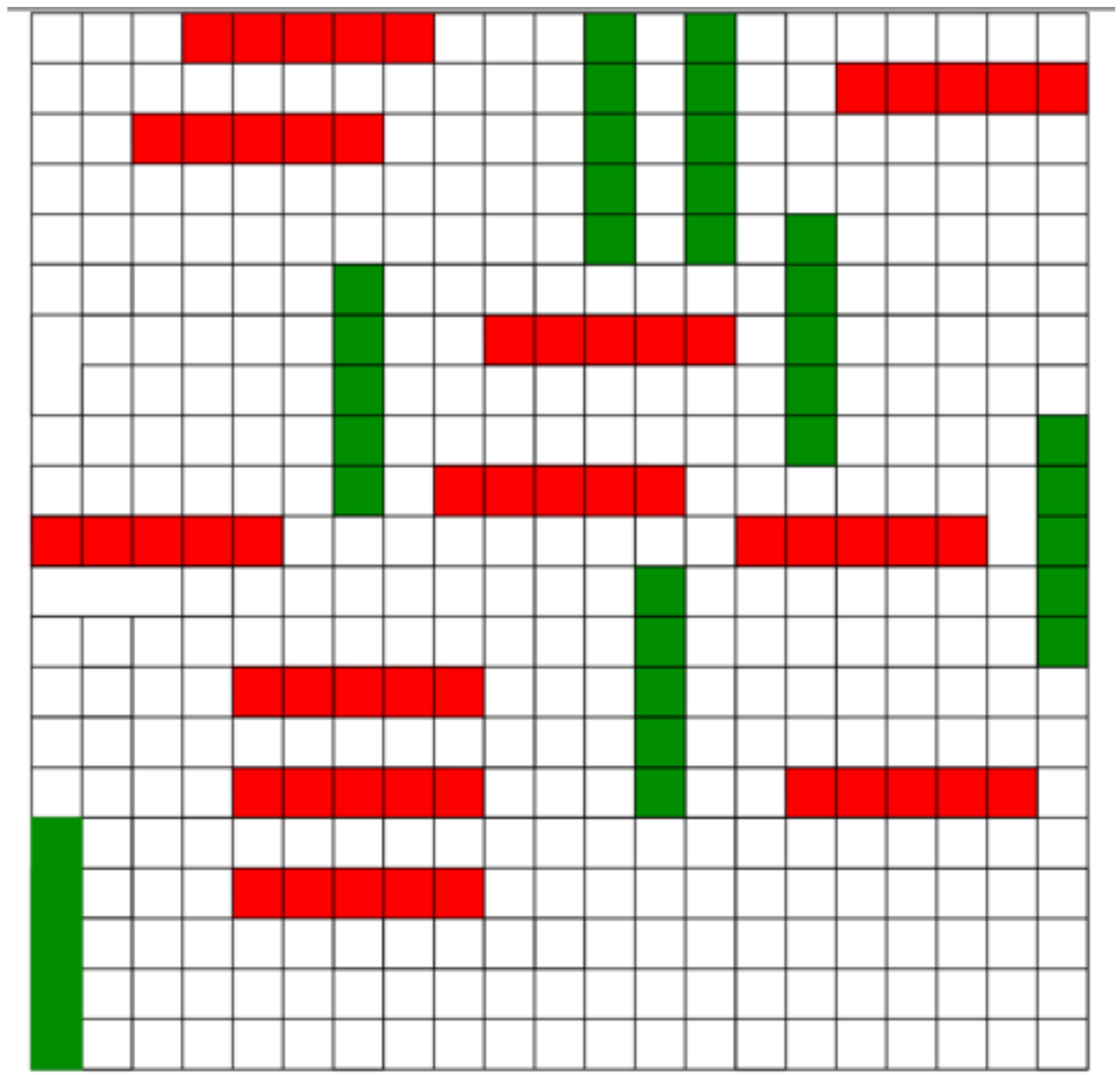
Results: phase diagram



q=4

LDD=HDD

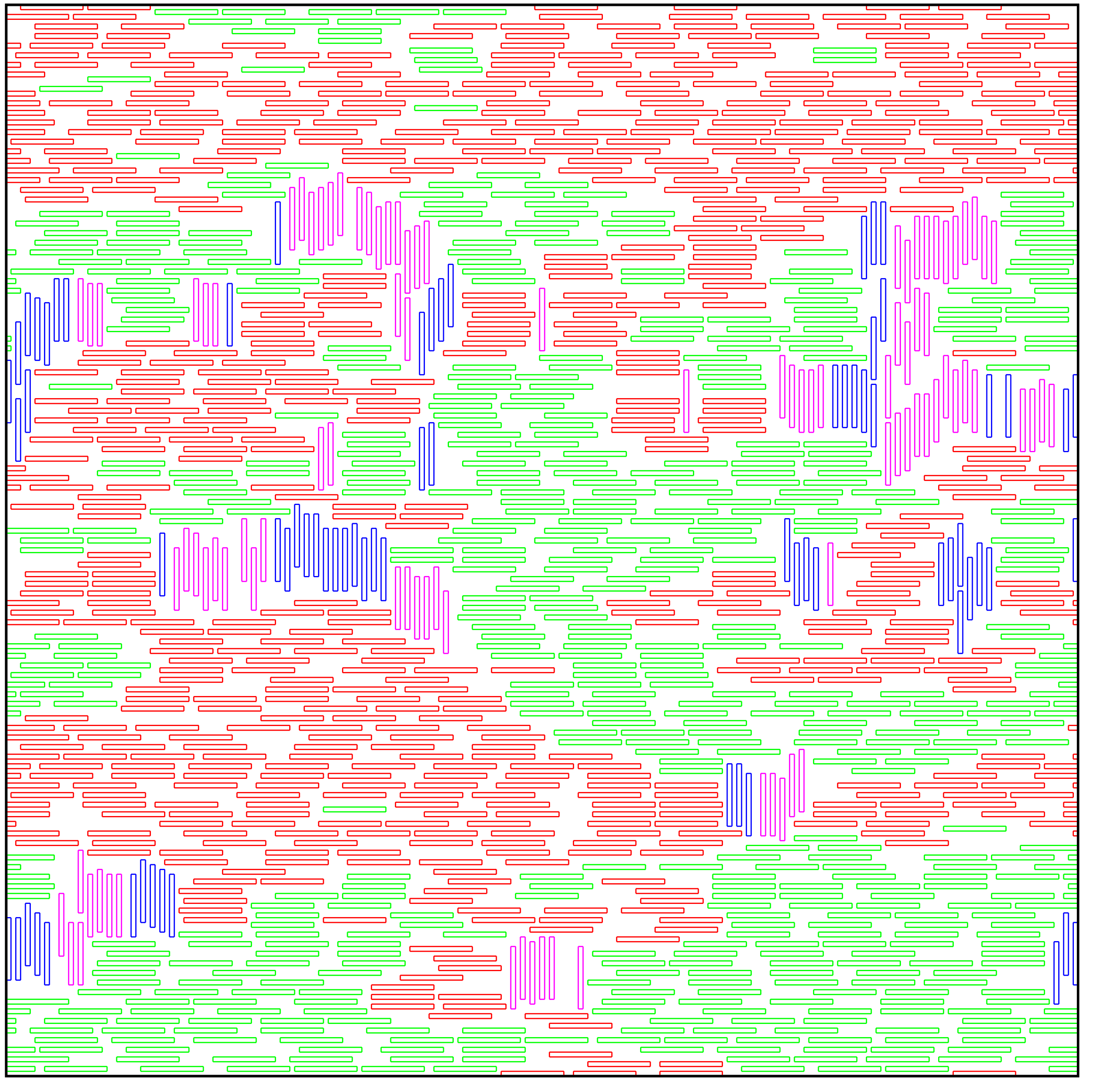
Hard Rectangles



$$m \times mk$$

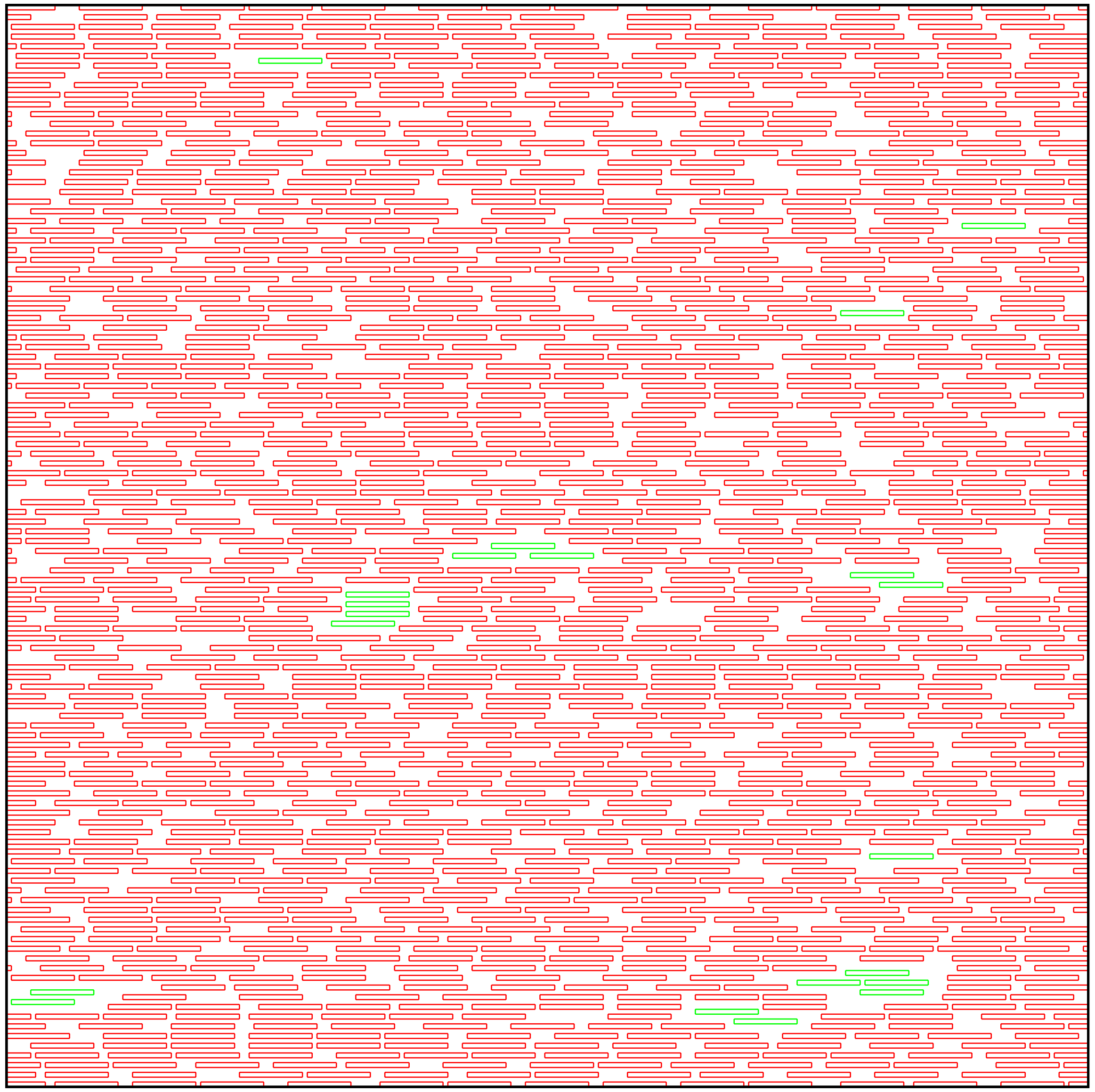
$$k \to \text{aspect ratio}$$

Rectangles 2x14



Nematic

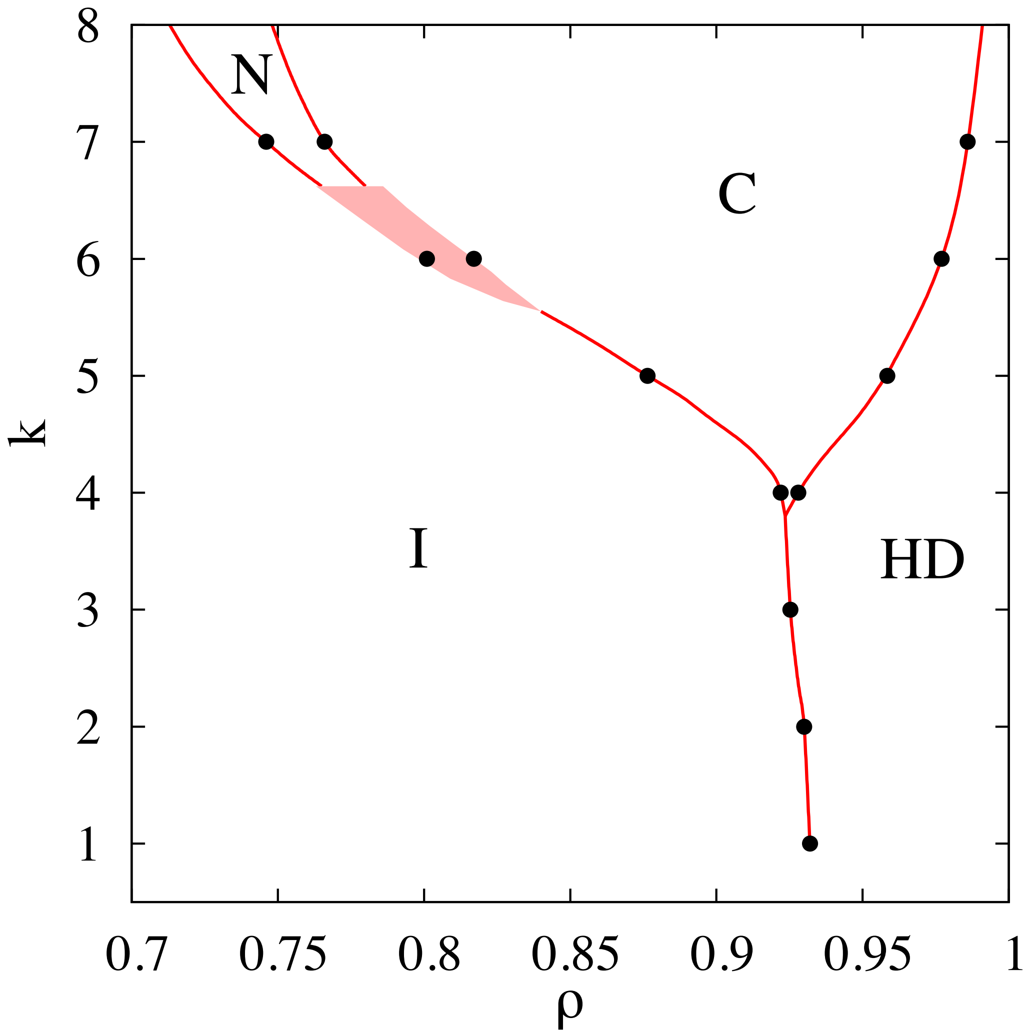
Rectangles 2x14



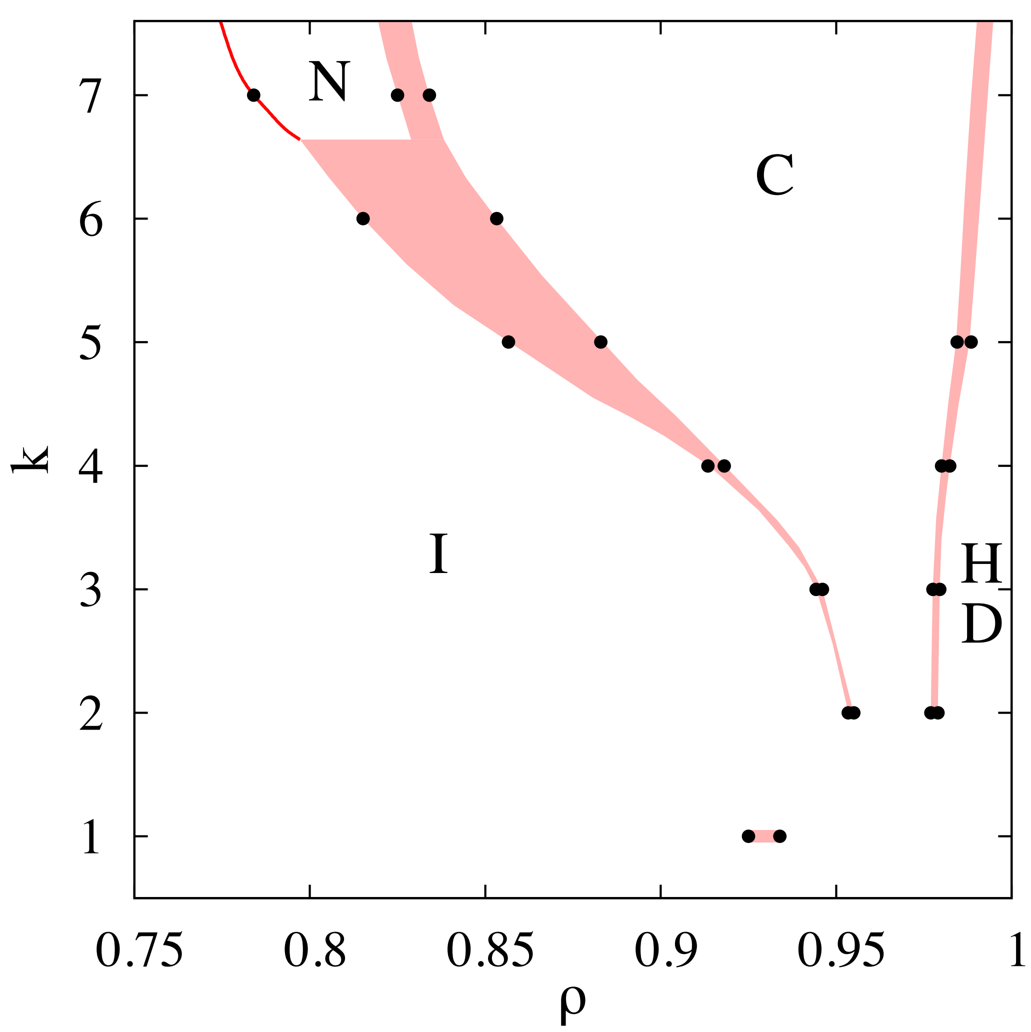
Columnar

Phase Diagram for Rectangles

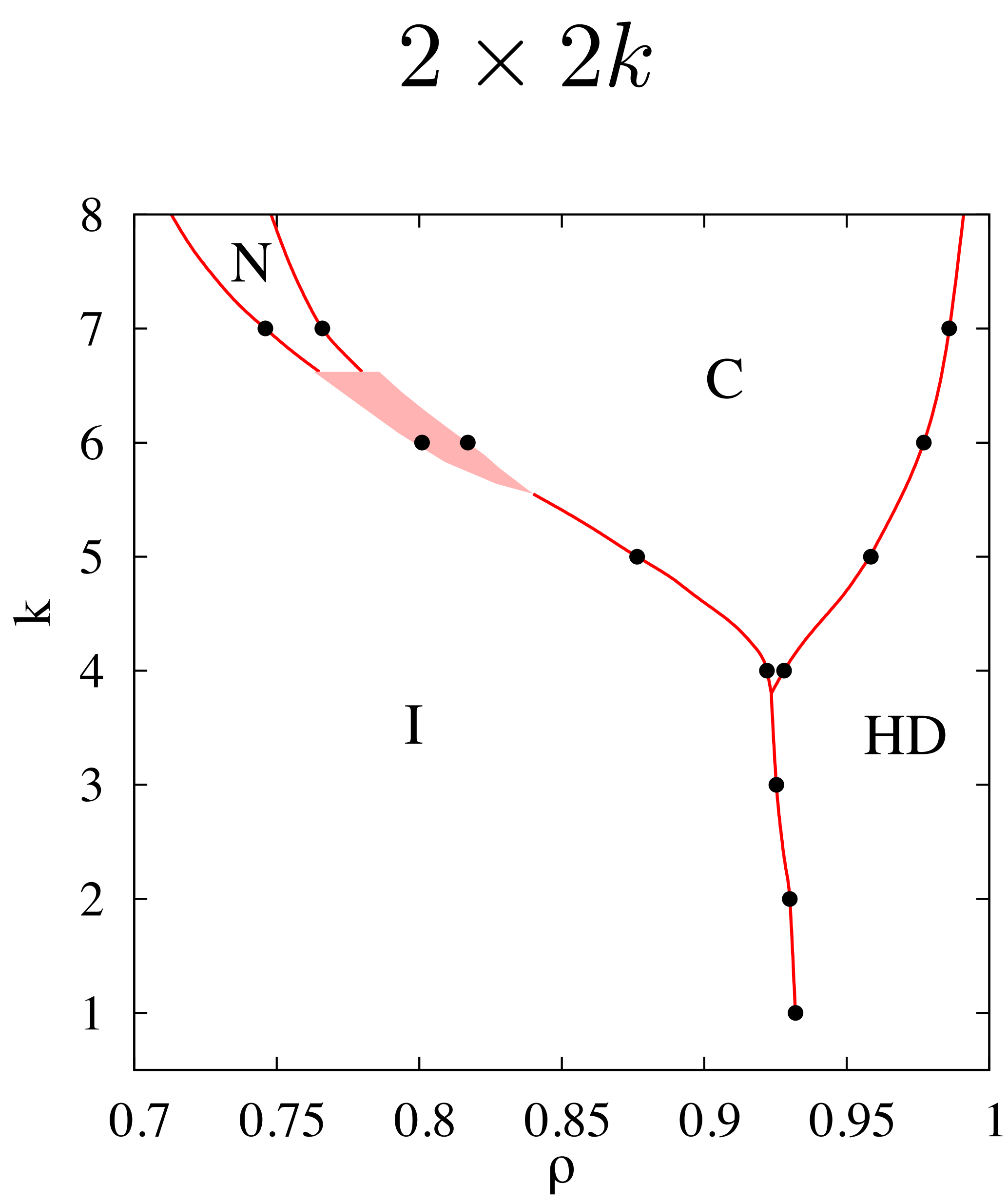
$2 \times 2k$

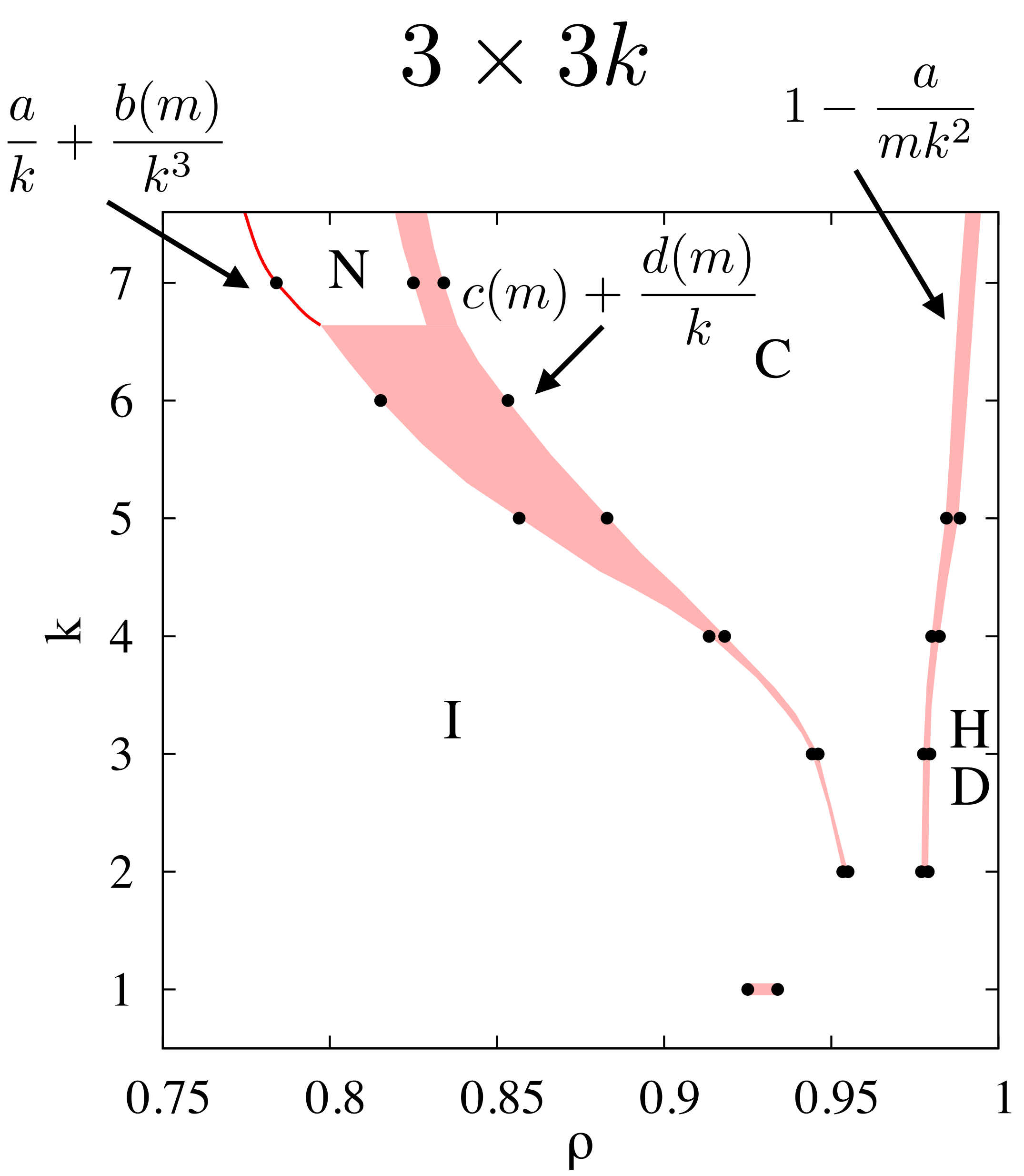


$3 \times 3k$



Phase Diagram for Rectangles





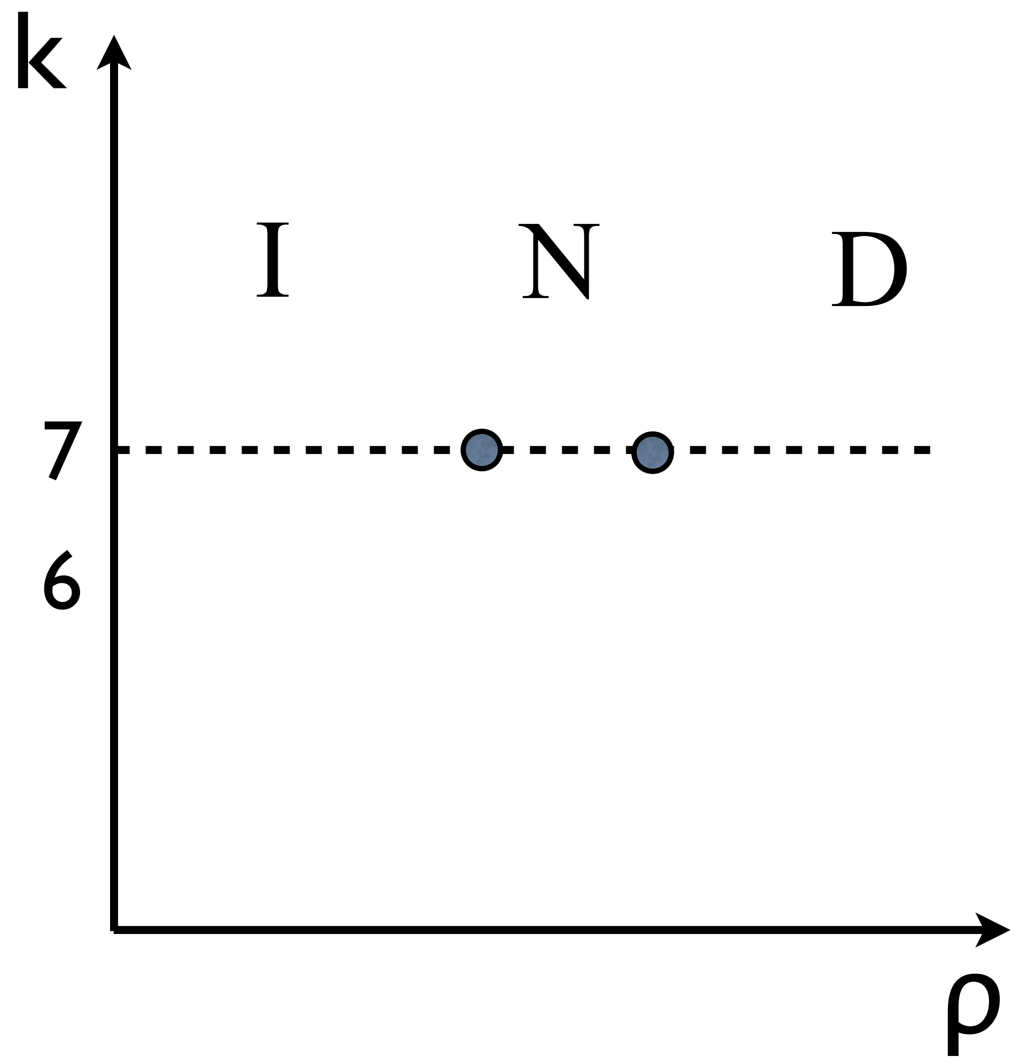
Summary

- Introduced a Monte Carlo algorithm
  - ⋆ Overcame jamming
  - ⋆ Efficient and easily parallelised
  - ⋆ Works for all shapes
- A continuous second transition
- Square: $\alpha/\nu \approx 0.22$; $\beta/\nu \approx 0.22$; $\gamma/\nu \approx 1.55$; $\nu \approx 0.90$
- Triangle: indistinguishable from q=3 Potts model
- High density phase indistinguishable from low density phase

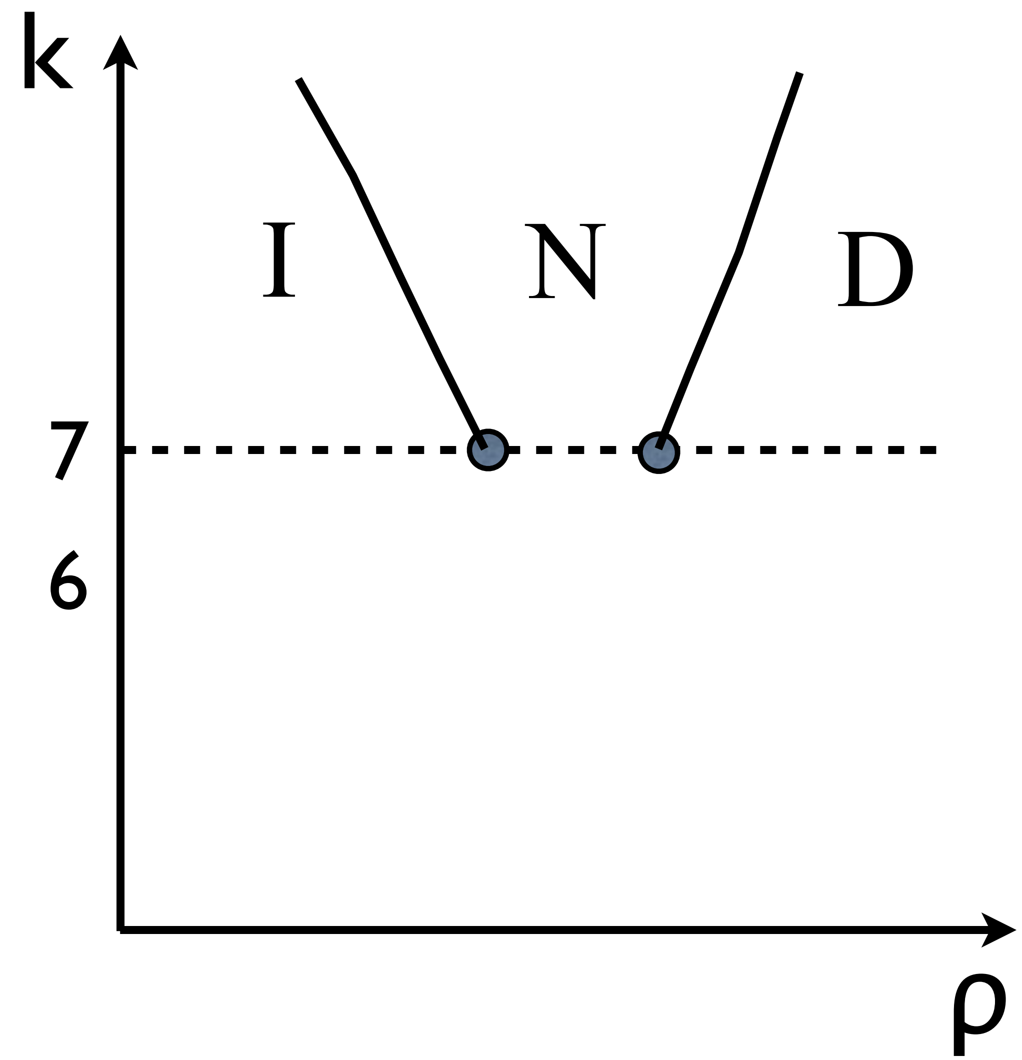
Summary

- Bethe lattice not useful for studying systems with orientational order
- Introduced a new lattice: RLTL
  - ⋆ existence of a nematic phase
  - ⋆ k_{min} is a function of coordination number
- Introduction of finite repulsive interaction results in two transitions; HDD=LDD

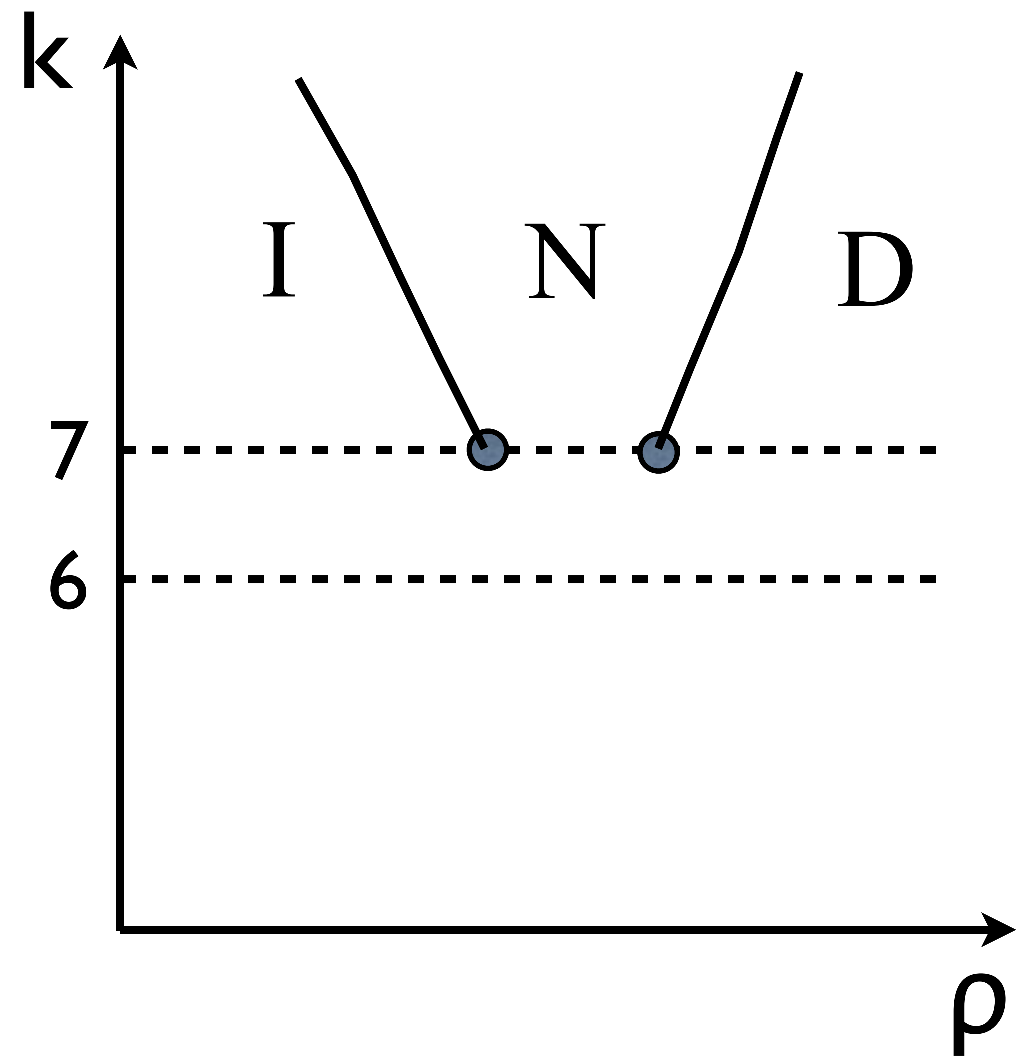
Outlook



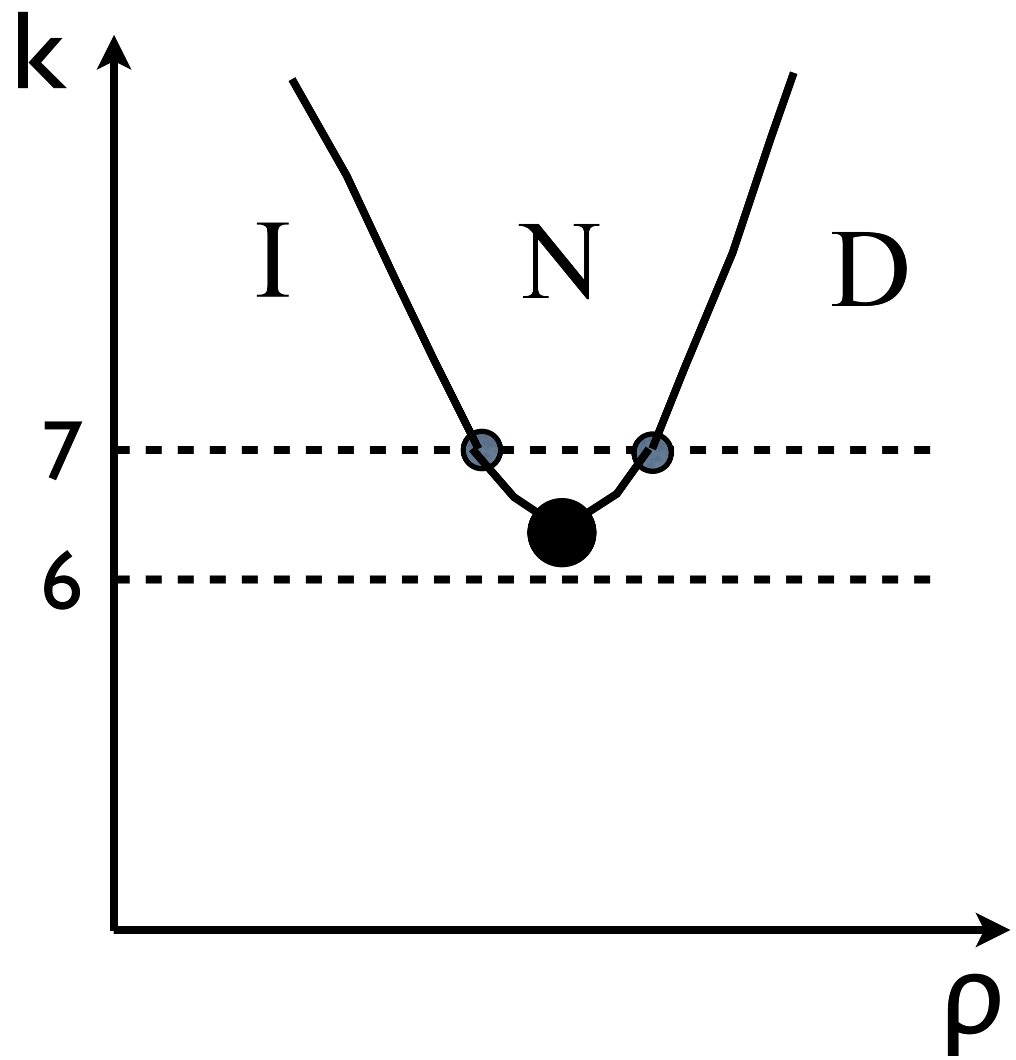
Outlook



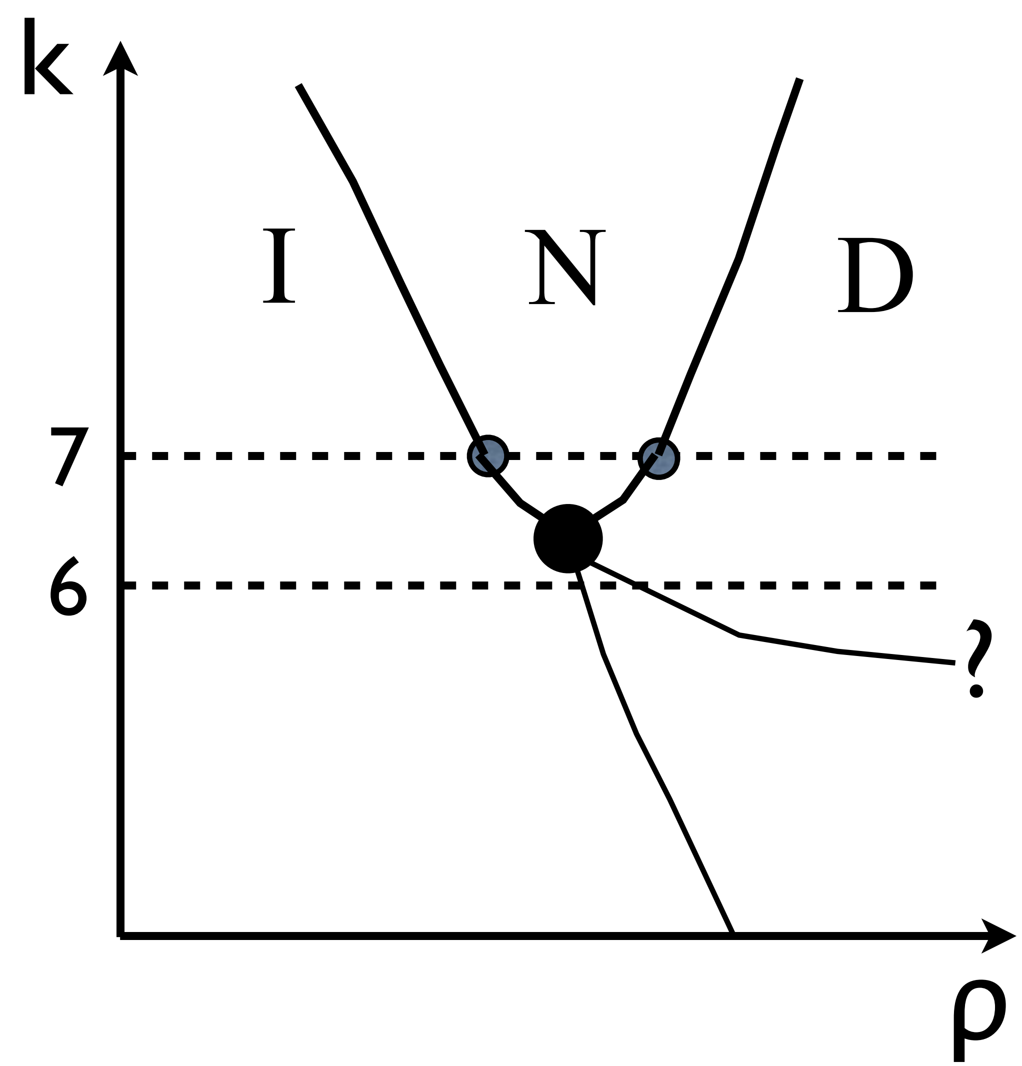
Outlook



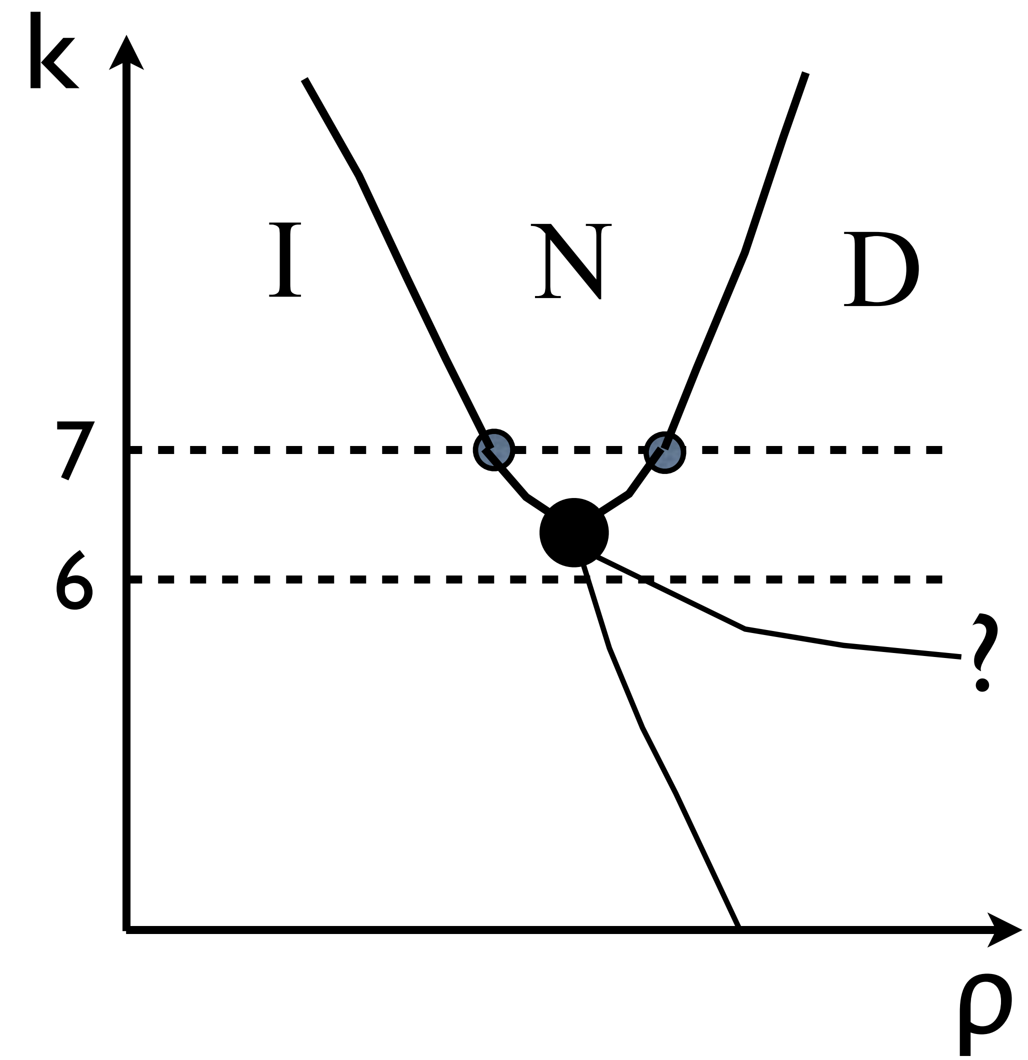
Outlook



Outlook



Outlook



Continuum model but with oriented rectangles

Zeroes of partition function

Outlook

- Rectangles with non-integer aspect ratio
- Fully packed problem
- Three dimensions
- Poly-dispersed systems