Thermodynamic transition associated with irregularly ordered ground states in a lattice gas model

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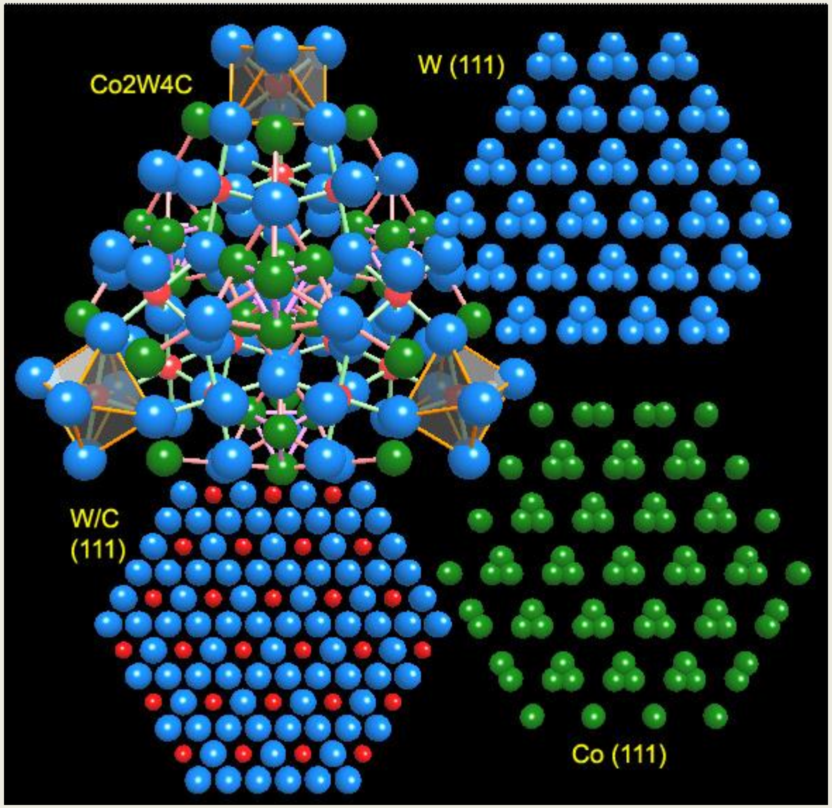
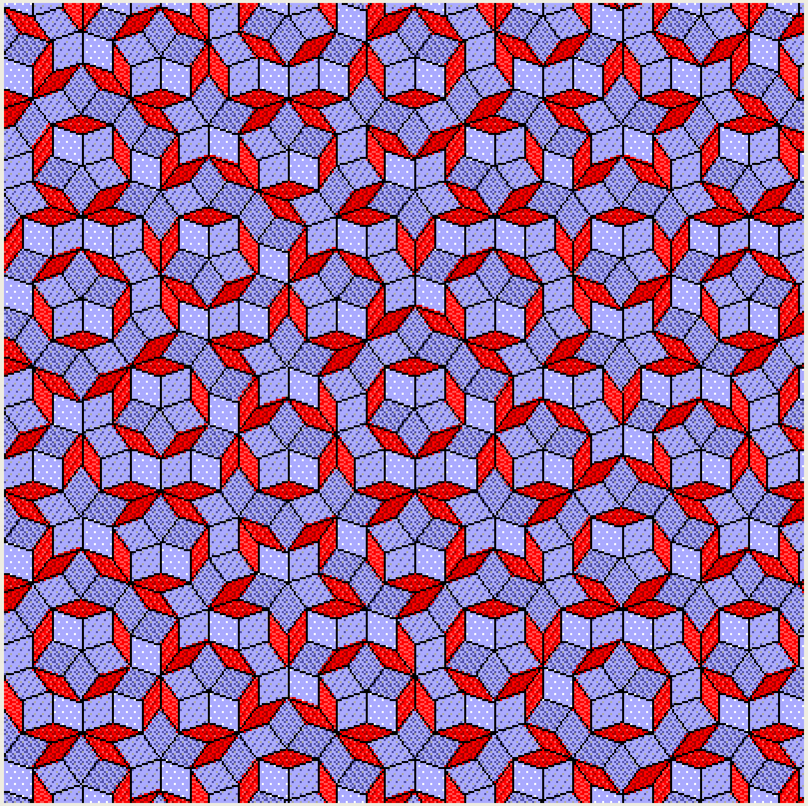
Ordered ground states

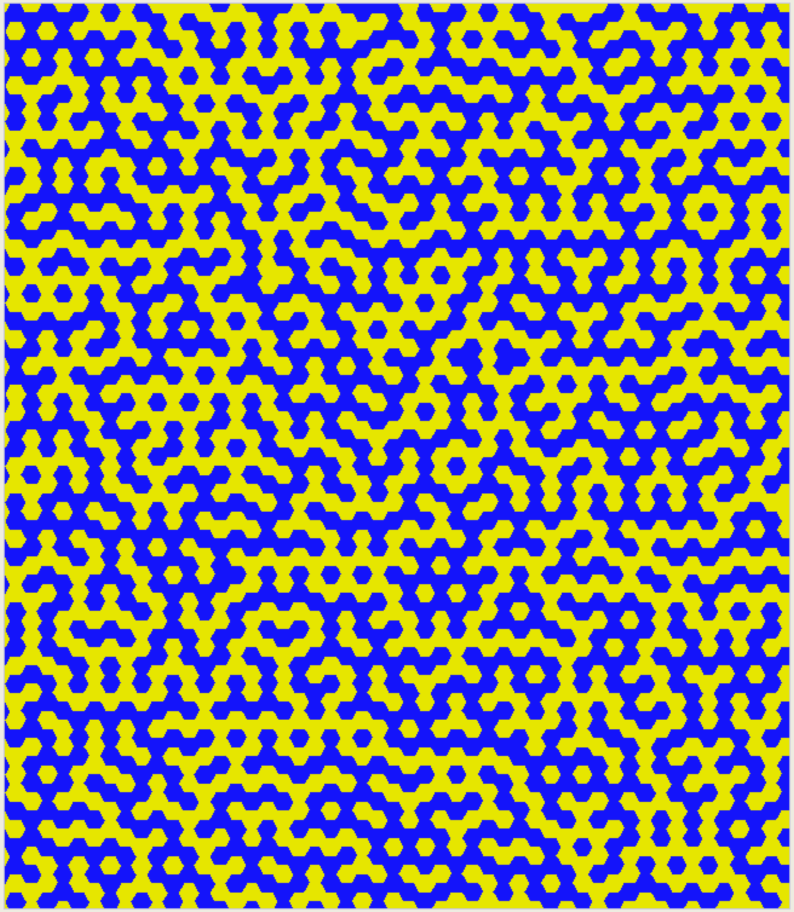




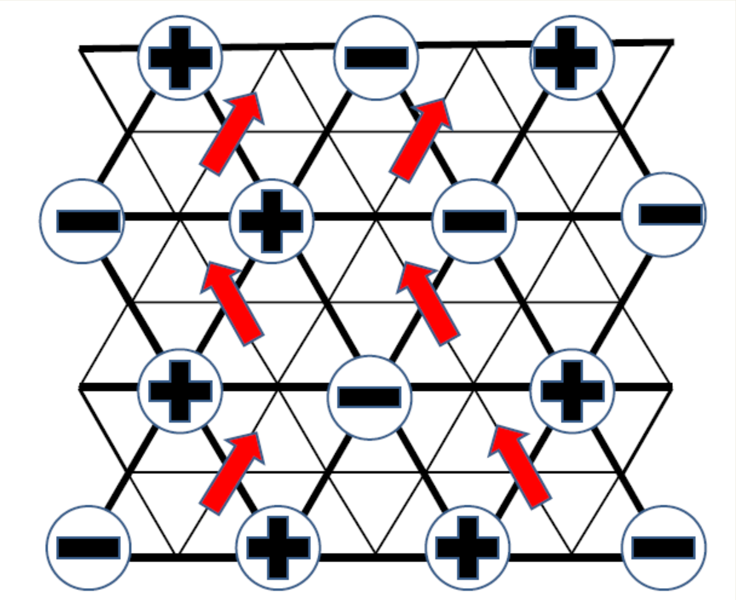
Periodic order

Quasi-periodic order

Disordered ground states



AF-Ising on TL



S=0.3383

(Wannier,1950)

Now, I ask .....

No periodic order

No quasi-Periodic order

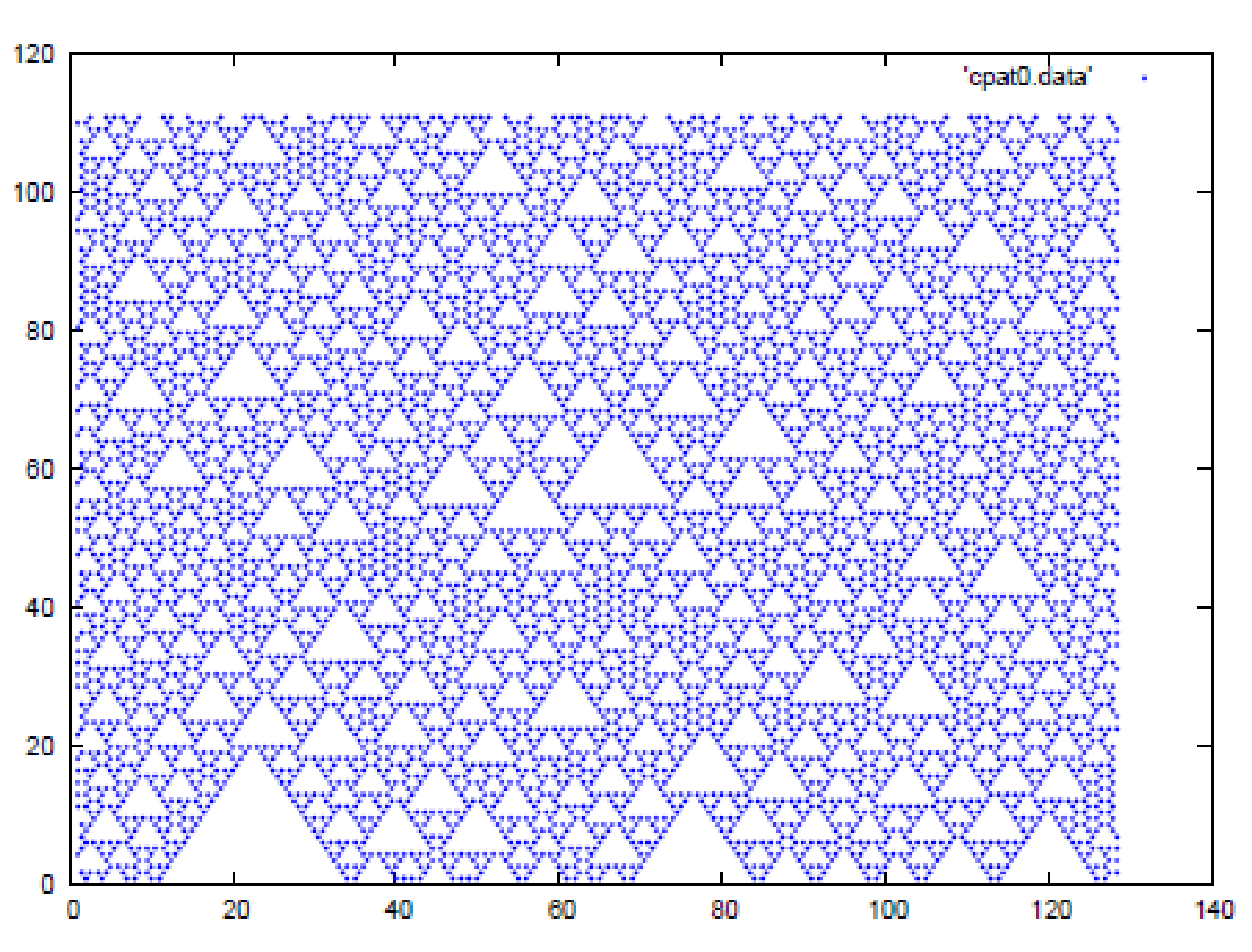
} (irregular)

Zero entropy density (ordered)

⇨ Irregularly ordered ground state

⇨ Thermodynamic phase

Irregularly ordered ground state



Outline of my talk

1. Introduction

2. Model and Main claim

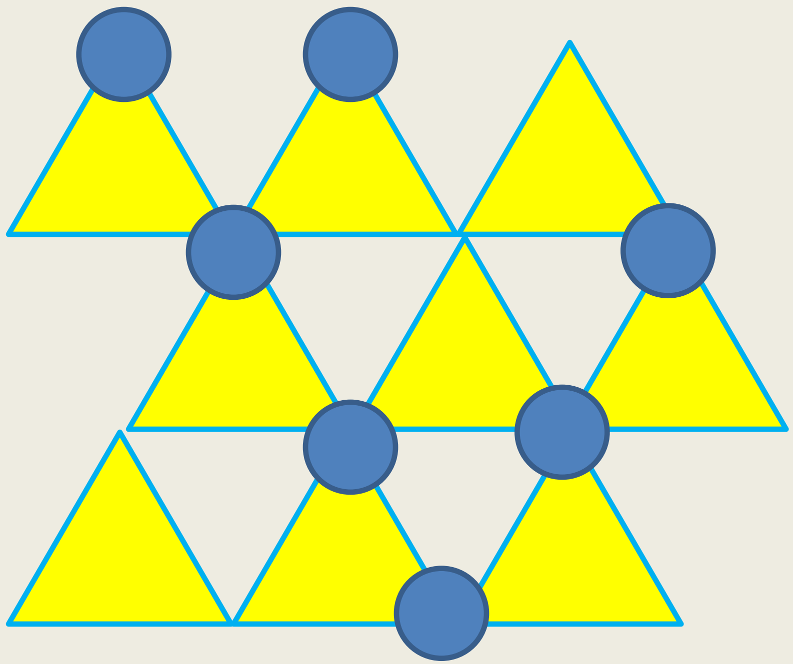
3. Ground states

4. Statistical mechanics

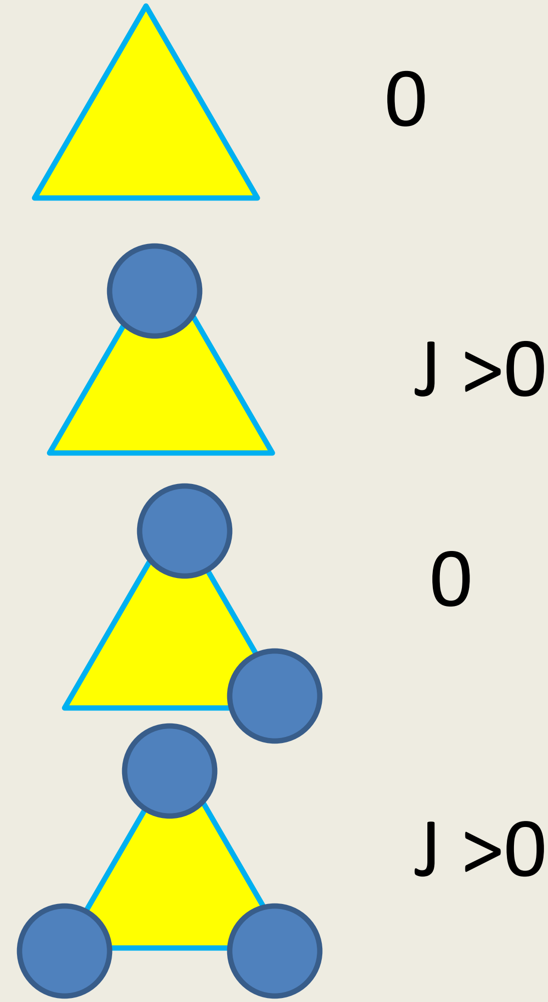
5. Thermodynamic transition

6. Summary

Model



Configuration



Local energy

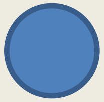
Expression of the local energy

Λ : triangular lattice of N sites

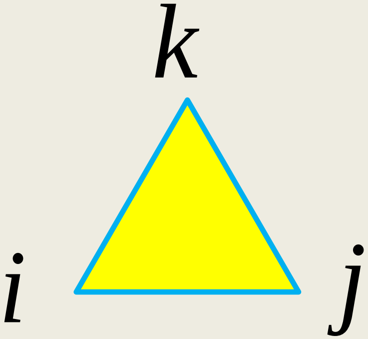
$\sigma_i, \; i \in \Lambda$

$\sigma = (\sigma_i)_{i \in \Lambda}$

$\sigma_i = 1$

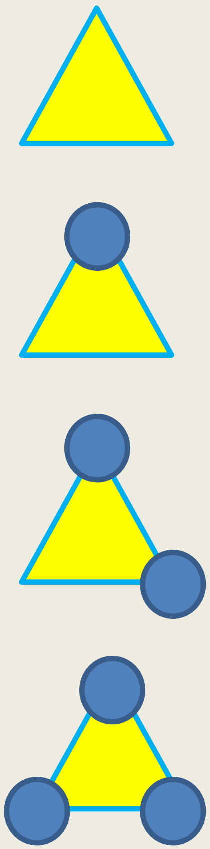


$\sigma_i = 0$



$$V = \frac{J}{2}[(2\sigma_i - 1)(2\sigma_j - 1)(2\sigma_k - 1) + 1]$$

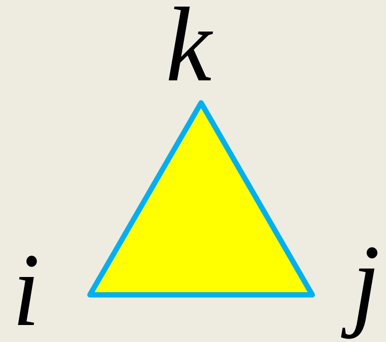
$$V = J[\sigma_i + \sigma_j + \sigma_k \;\; (\mathrm{mod})\; 2]$$



Statistical mechanics - free energy

$$H(\sigma) = \frac{J}{2} \sum_{i<j<k} \Delta_{ijk} [(2\sigma_i - 1)(2\sigma_j - 1)(2\sigma_k - 1) + 1]$$

$$\Delta_{ijk} = 1$$



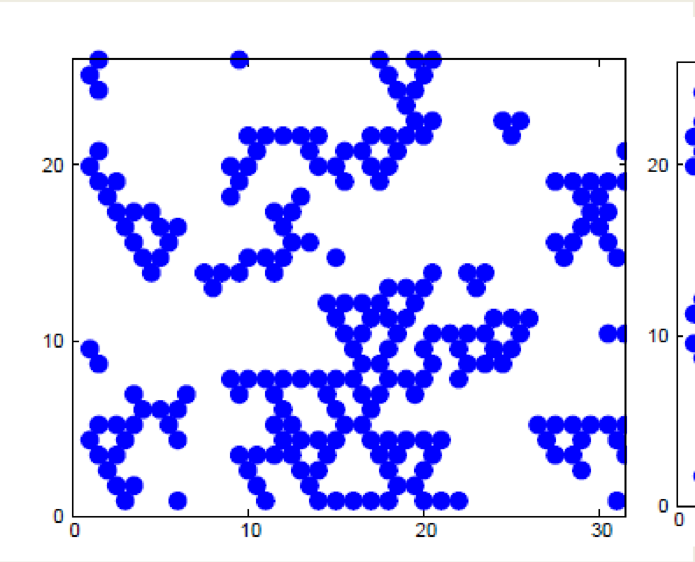
otherwise

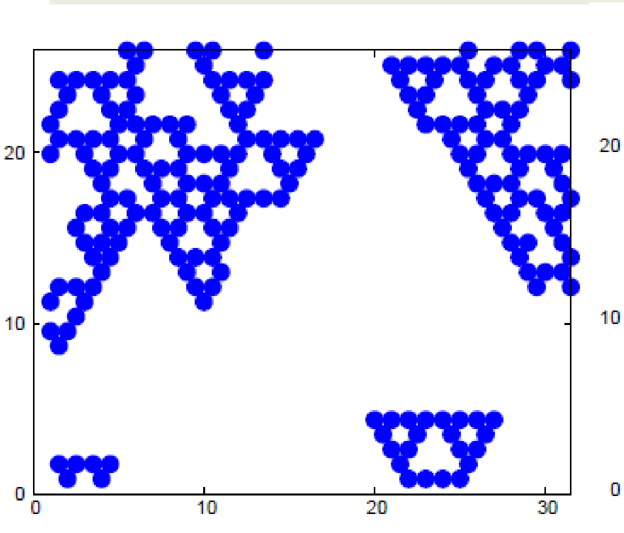
$$\Delta_{ijk} = 0$$

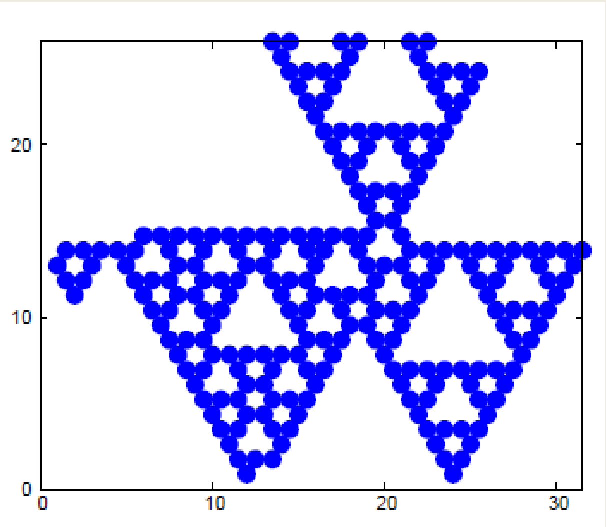
$$Z(T,\rho) = \sum_{\sigma} \exp(-\beta H(\sigma)) \delta(\rho N, \sum_{i=1}^{N} \sigma_i) \qquad \beta = 1/T$$

$$f(T,\rho) = -T \lim_{N\to\infty} \frac{1}{N} \log Z(T,\rho)$$

Configurations



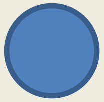




$\beta = 1.5$ $\beta = 3.0$ $\beta = 4.5$

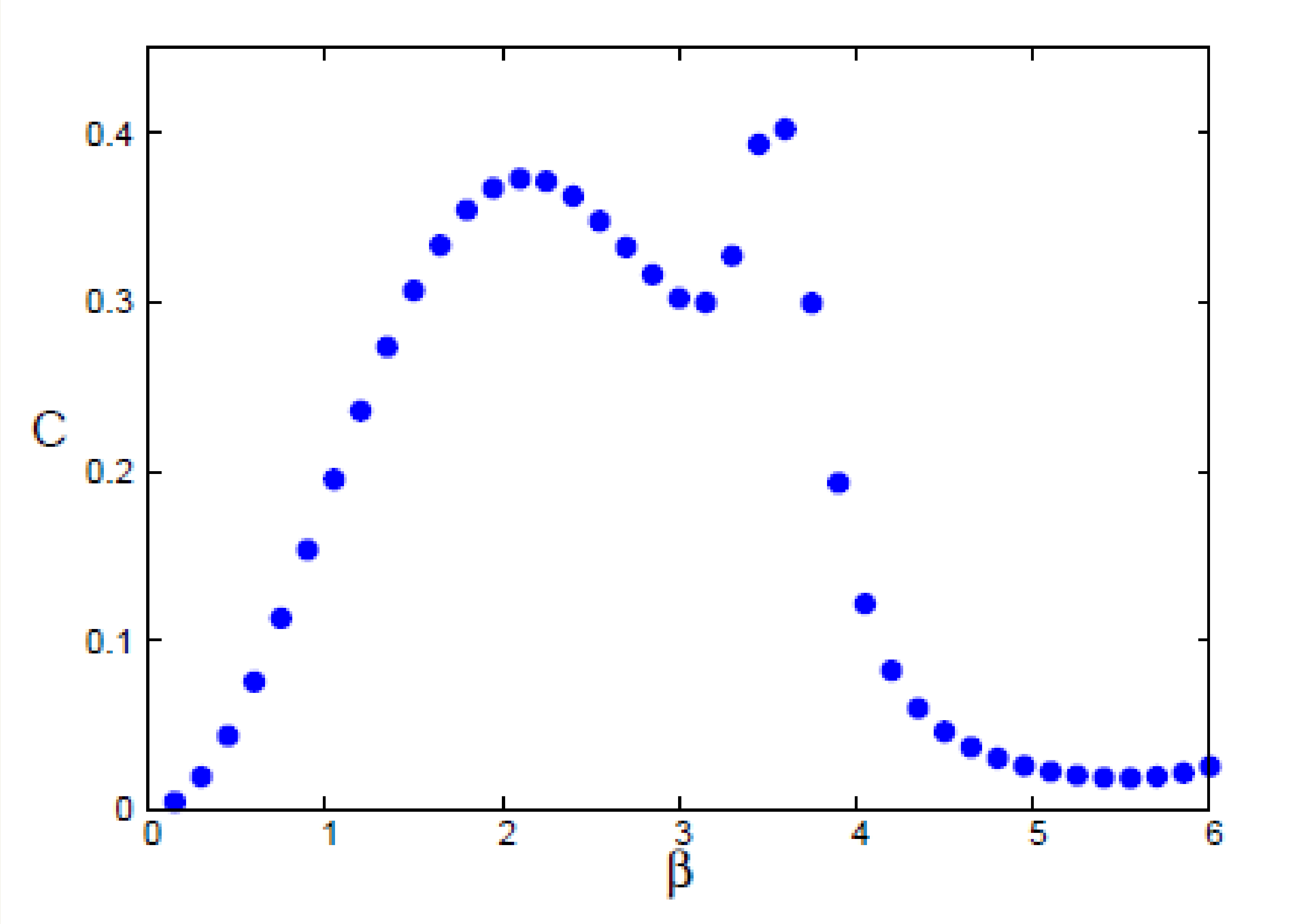
$J = 1.0, \ \rho = 0.25$

$N = 1024$

$\sigma_i = 1$ 

$\sigma_i = 0$

Preliminary result



Main claim

This is a thermodynamic transition associated with irregularly ordered ground states

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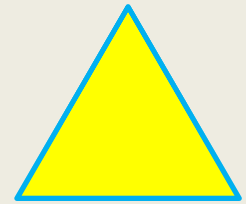
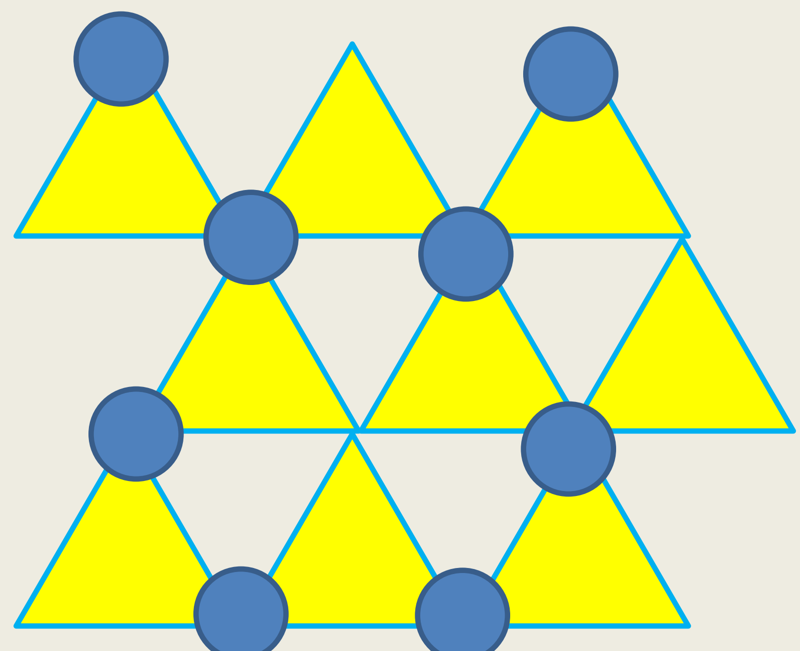
Ground states

configurations $V = 0$ for all 

$\longrightarrow$ grand state for a given ρ

Trivial case I :

$\sigma_i = 0$ for all i $\longrightarrow$ $\rho = 0$

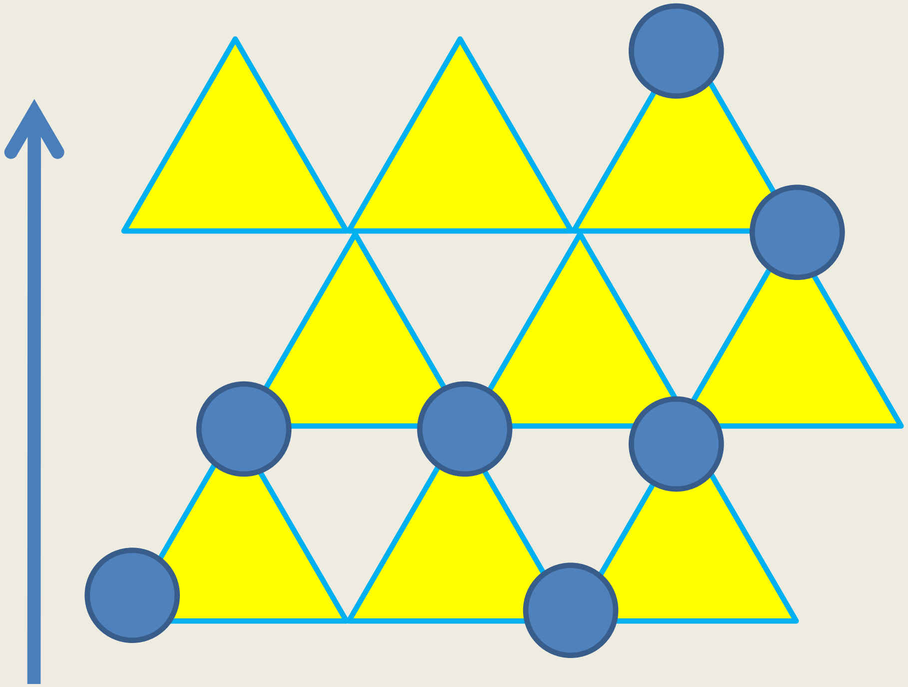


Trivial case II :

Crystal configuration $\rho = 2/3$

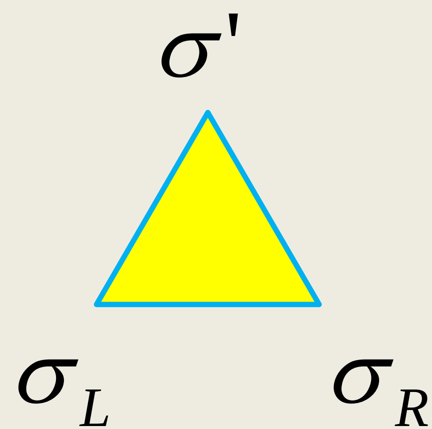
(maximally packed ground state)

Non-trivial ground states

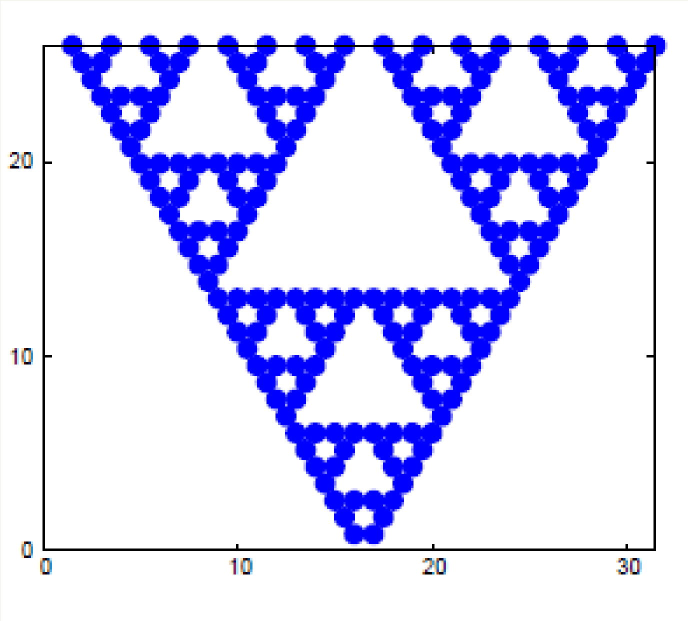


Cellular Automaton

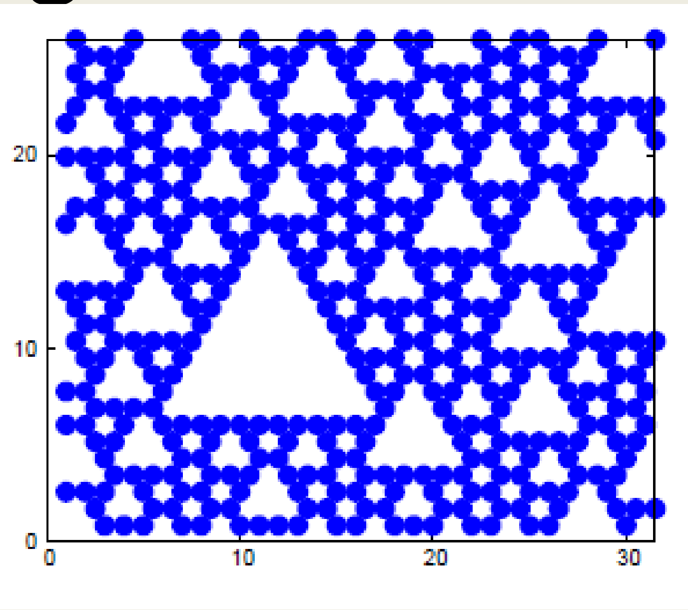
$$\sigma' = \sigma_L + \sigma_R \bmod 2$$



Space-time configuration of CA



Sierpinski gasket



Superposition of Sierpinski gasket

Ground state configurations under zero energy boundary conditions

$$\text{the number of the configurations} : 2^{\mathrm{L}} \qquad N = L^2$$

Entropy density of the ground states is less than $\frac{1}{N}\log 2^{L} = \frac{1}{\sqrt{N}} \to 0$

Remarks

To determine ground state configurations for a given density under general boundary conditions is quite difficult

Zero energy configurations under periodic boundary conditions are determined by an algebraic method (Martin et al, CMP, 1984)

The number of the configurations depends on the system size in a quite complicate manner which comes from its arithmetic nature

In some cases, there is no zero-energy configuration for a given density. The ground state configurations involve "defects" whose best positions are determined in an irregular manner of the density and the system size

Summary of the ground states

“ordered ground state”

The entropy density of the ground state is zero, because the ground state configurations are determined by a deterministic rule of L-elements.

“irregular ground state”

They are non-periodic, non-quasi periodic, and basically near superposition of Sierpinski gaskets.

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Statistical mechanics – pressure

$$\Xi(\beta,\mu)=\sum_{\sigma}\exp(-\beta[H(\sigma)-\mu\sum_{i=1}^{N}\sigma_i])$$

$$p(T,\mu)=T\lim_{N\to\infty}\frac{1}{N}\log\Xi(T,\mu)$$

$$\Rightarrow\quad f(T,\rho)=\sup_{\mu}[\mu\rho-p(T,\mu)]$$

Statistical mechanics – spin model

$$K_1 = \frac{\beta J}{2} \qquad K_2 = -\frac{\beta\mu}{2}$$

$$\Xi(\beta,\mu) = e^{-(K_1+K_2)N} Y(K_1, K_2)$$

$$s_i = 2\sigma_i - 1 \qquad s_i = \pm 1$$

$$Y(K_1, K_2) = \sum_s \exp(-K_1 \sum_{i<j<k} \Delta_{ijk} s_i s_j s_k - K_2 \sum_{i=1}^{N} s_i)$$

$$K_2 = 0$$

Newman, Moore, 1999, Phys. Rev. E

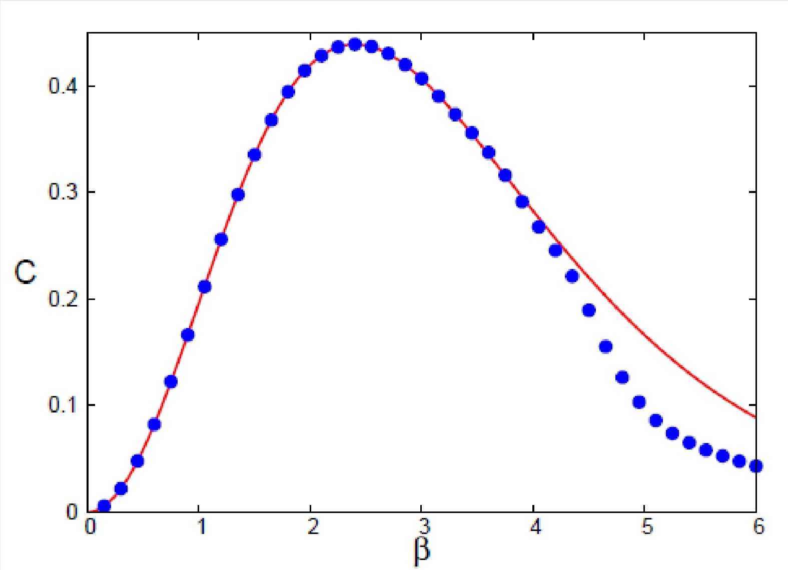
Garrahan, Newman, 2000, Phys. Rev. E

Jack, Garrahan, 2005, J. Chem. Phys.

$$K_2 = 0$$

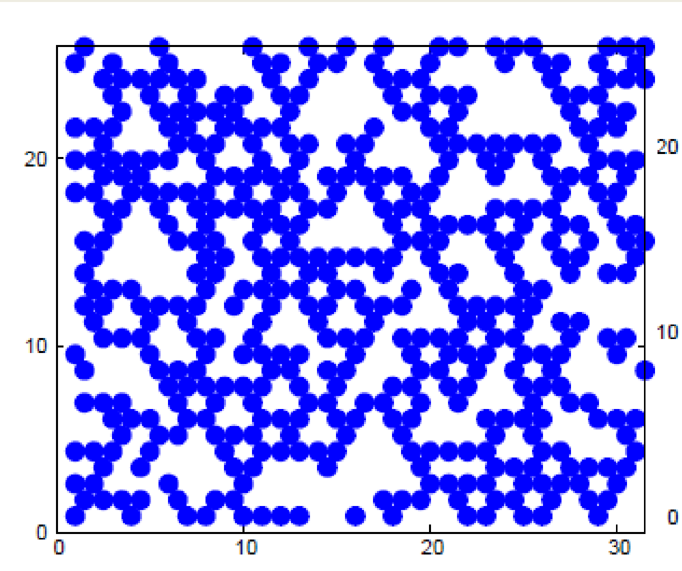
$$p(T,0) = -\frac{J}{2} + T\left[\log\left(2\cosh\frac{J}{2T}\right)\right]$$

$$\rho = 0.5$$

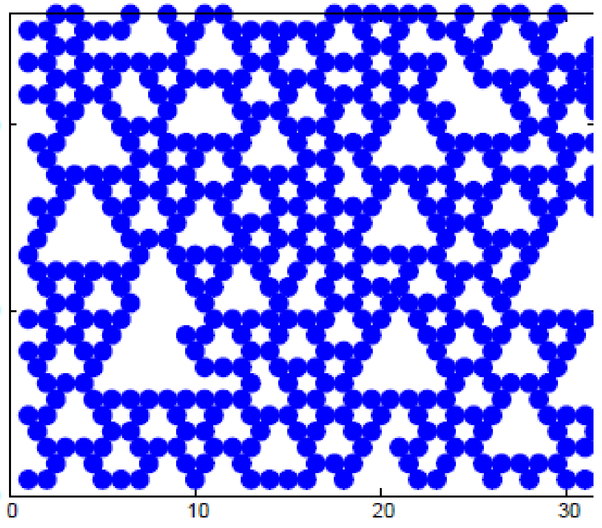


$$f(T,\rho = 0.5) = \frac{J}{2} - T\left[\log\left(2\cosh\frac{J}{2T}\right)\right]$$

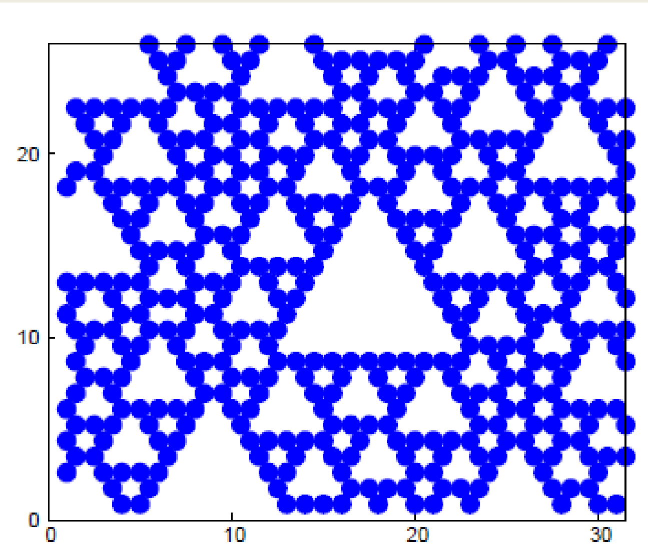
configurations



$\beta = 1.5$



$\beta = 3.0$



$\beta = 6.0$

$N = 1024$

$\sigma_i = 1$

$\sigma_i = 0$

Meta-stable state

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Duality relation

$$\sinh(2K_1)^{-N/2} Y(K_1, K_2) = \sinh(2K_1^{\ *})^{-N/2} Y(K_1^{\ *}, K_2^{\ *})$$

$$K_1^{\ *} = \frac{\beta^* g}{2}$$

$$\sinh(2K_1)\sinh(2K_2^{\ *}) = \sinh(2K_2)\sinh(2K_1^{\ *}) = 1$$

$$K_2^{\ *} = -\frac{\beta^* \mu^*}{2}$$

$$p(T,\mu) = p(T^*,\mu^*) - \frac{J}{2} + \frac{\mu}{2} + T\left[\log\left(2\cosh\frac{J}{2T}\cosh\frac{\mu}{2T}\right)\right]$$

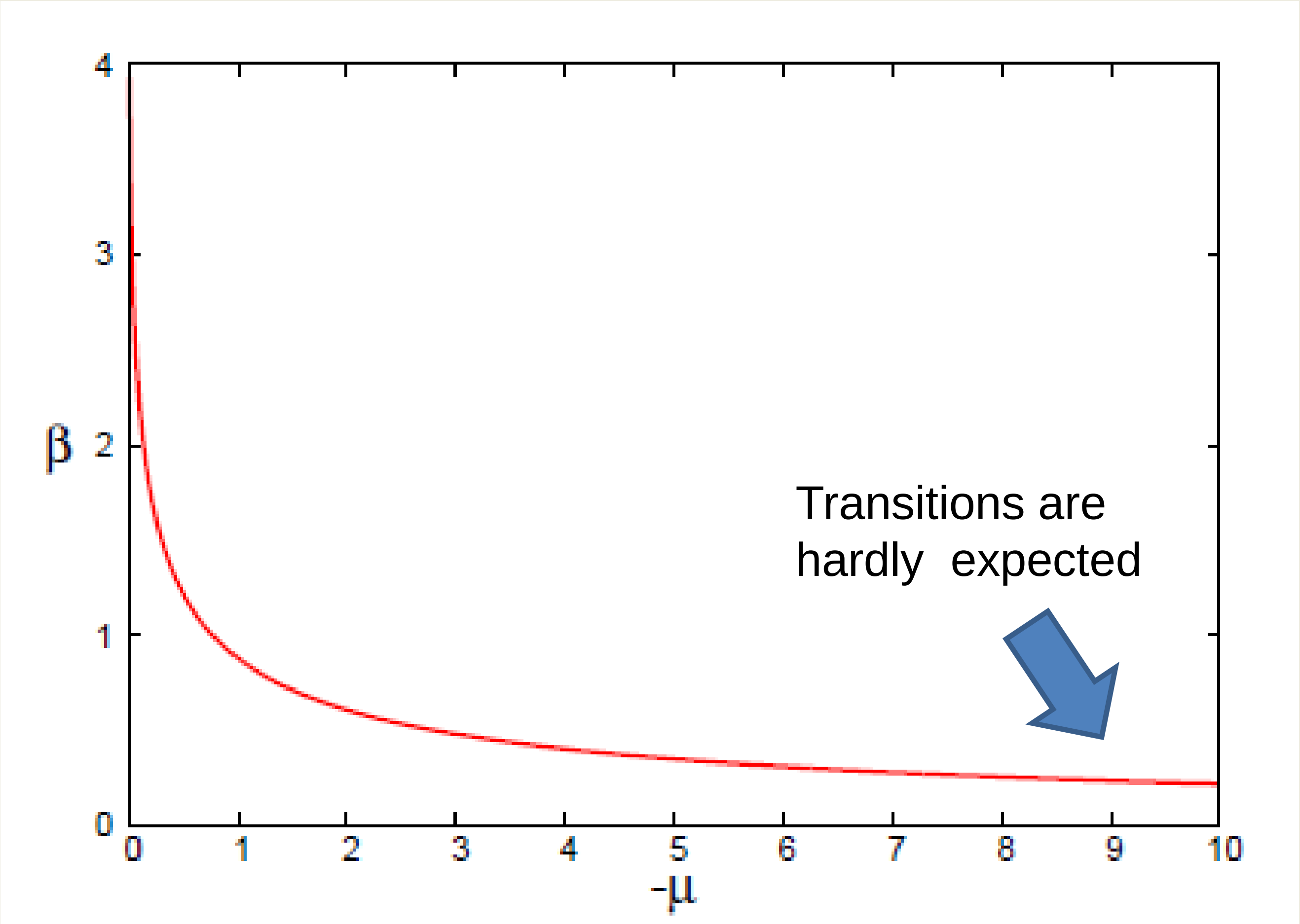
arXiv:1006.4972

$$\Rightarrow \quad \text{singular at } (\beta,\mu) \Leftrightarrow \text{singular at } (\beta^*,\mu^*)$$

$$\Rightarrow \quad \text{self-dual points } (\beta,\mu) = (\beta^*,\mu^*)$$

are candiates of singular points

Self-dual line

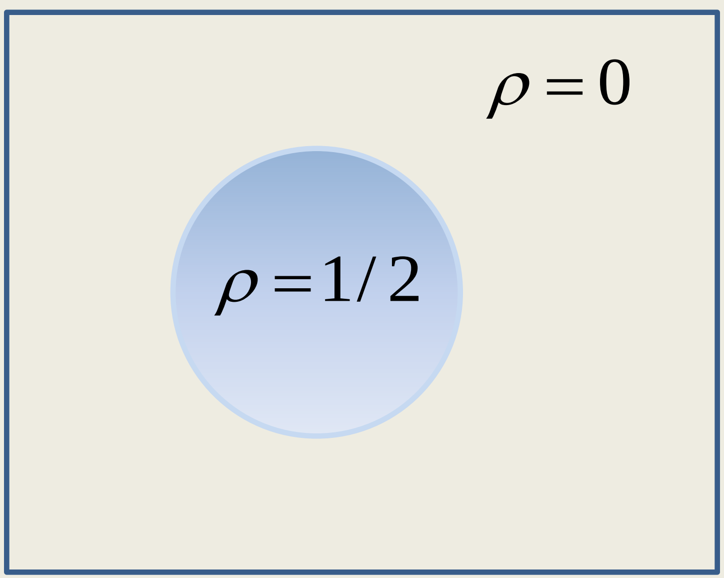


Phenomenological argument

$$0 < -\mu / T << 1 \quad \text{fixed}$$

For a sufficiently small T, $p \cong 0$ and $\rho \cong 0$

Check the instability of this state when increasing T



$$\Delta p \cong \frac{\mu}{2} + Te^{-J/T}$$

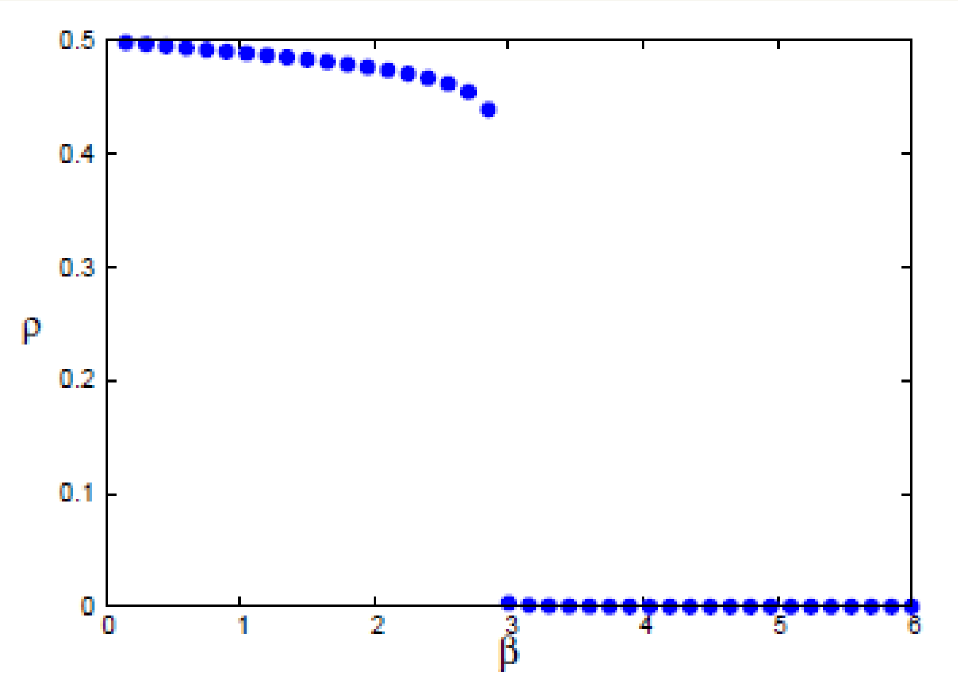
The domain grows when $\Delta p > 0$

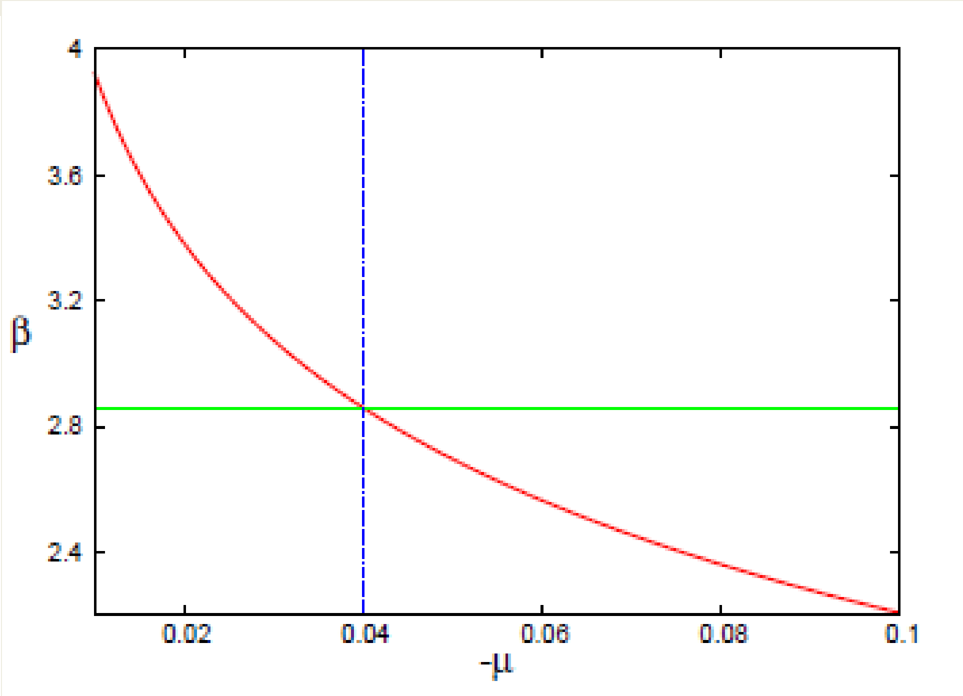
The transition point

$$\frac{\mu}{2T} e^{J/T} \cong -1$$

Leading order term of the self-dual line

Numerical result I

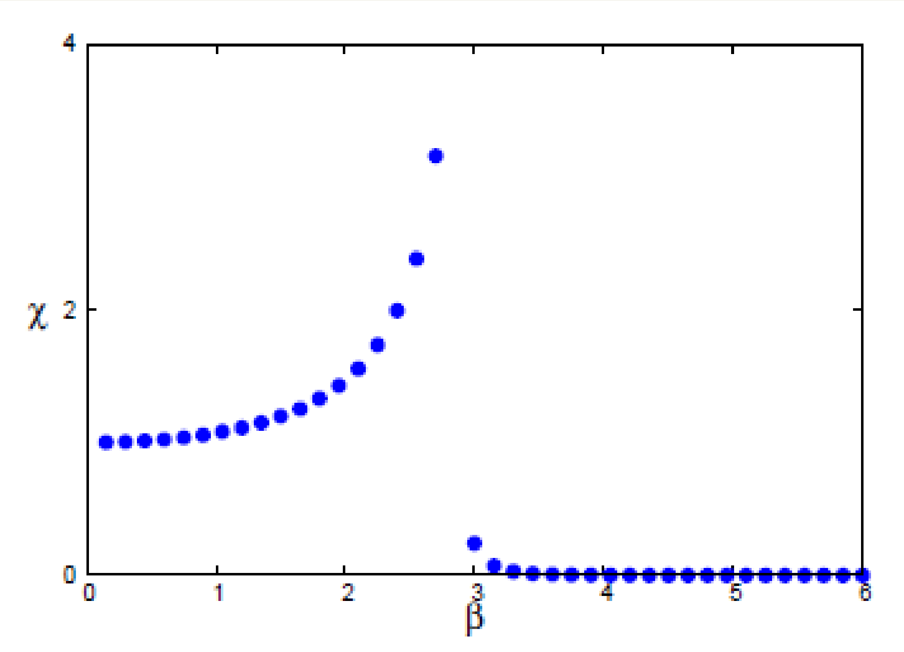


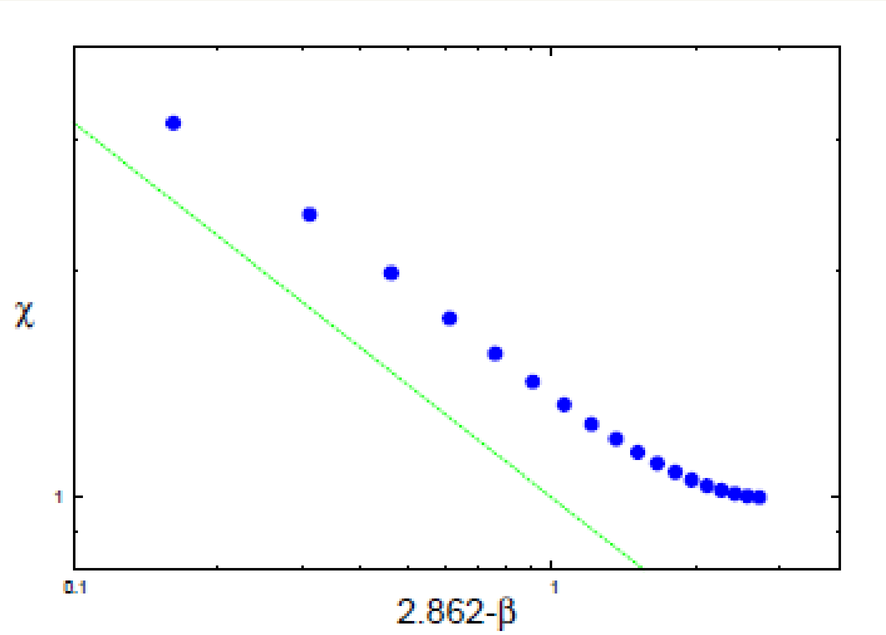


$$\mu = -0.04$$

Numerical result II

$$\chi = N\left\langle \left(\rho - \langle \rho \rangle\right)^2 \right\rangle$$

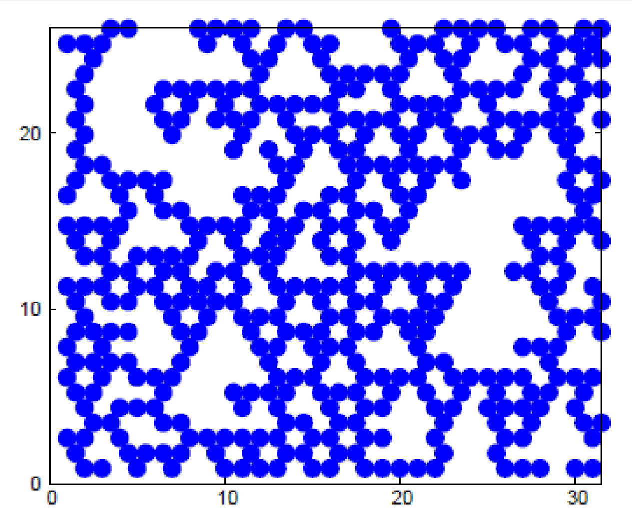




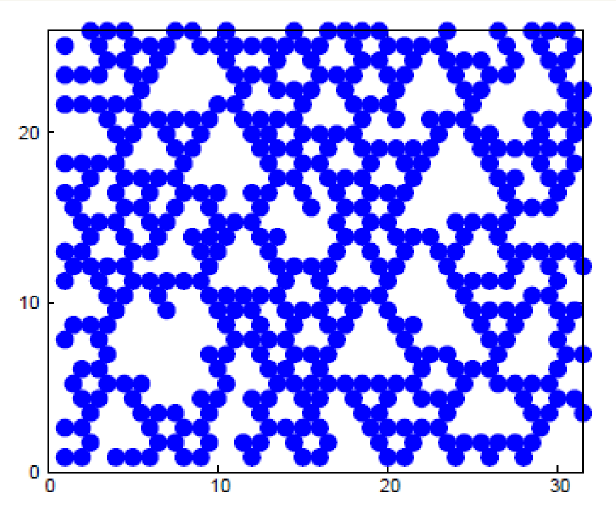
$$\mu = -0.04$$

$$\chi \approx (T - T_{\mathrm{dis}})^{-1/2}$$

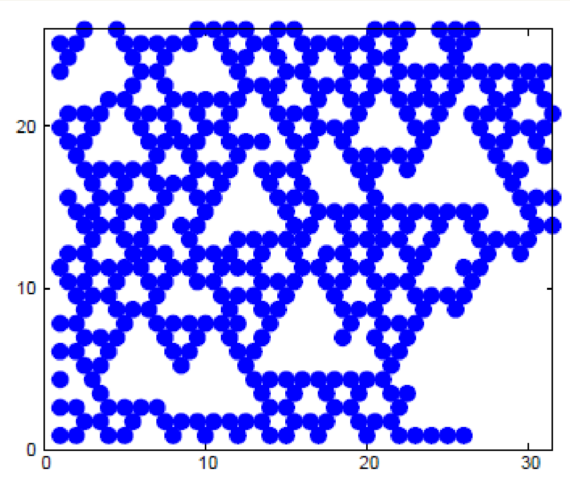
configurations



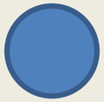
$\beta = 1.8$



$\beta = 2.25$



$\beta = 2.7$

$N = 1024$ $\sigma_i = 1$ 

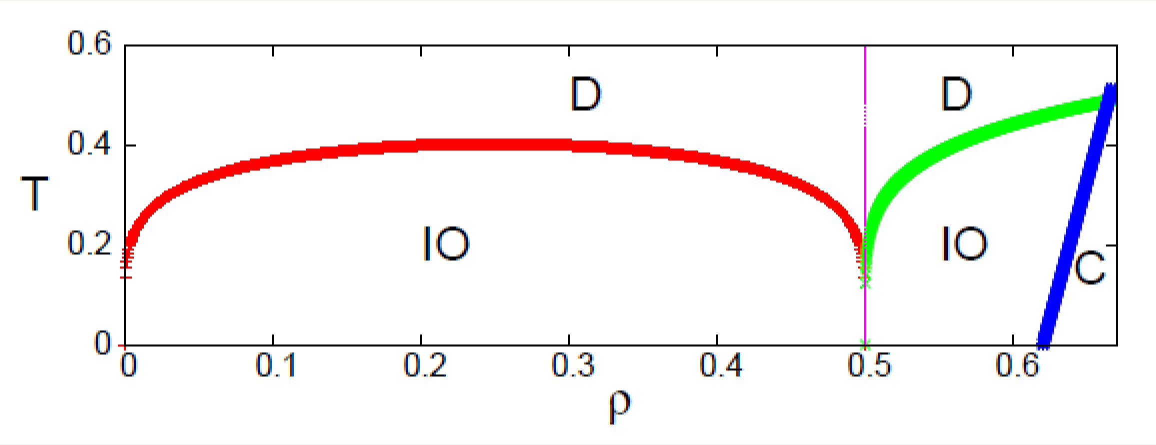
$\mu = -0.04$ $\sigma_i = 0$

Schematic phase diagram

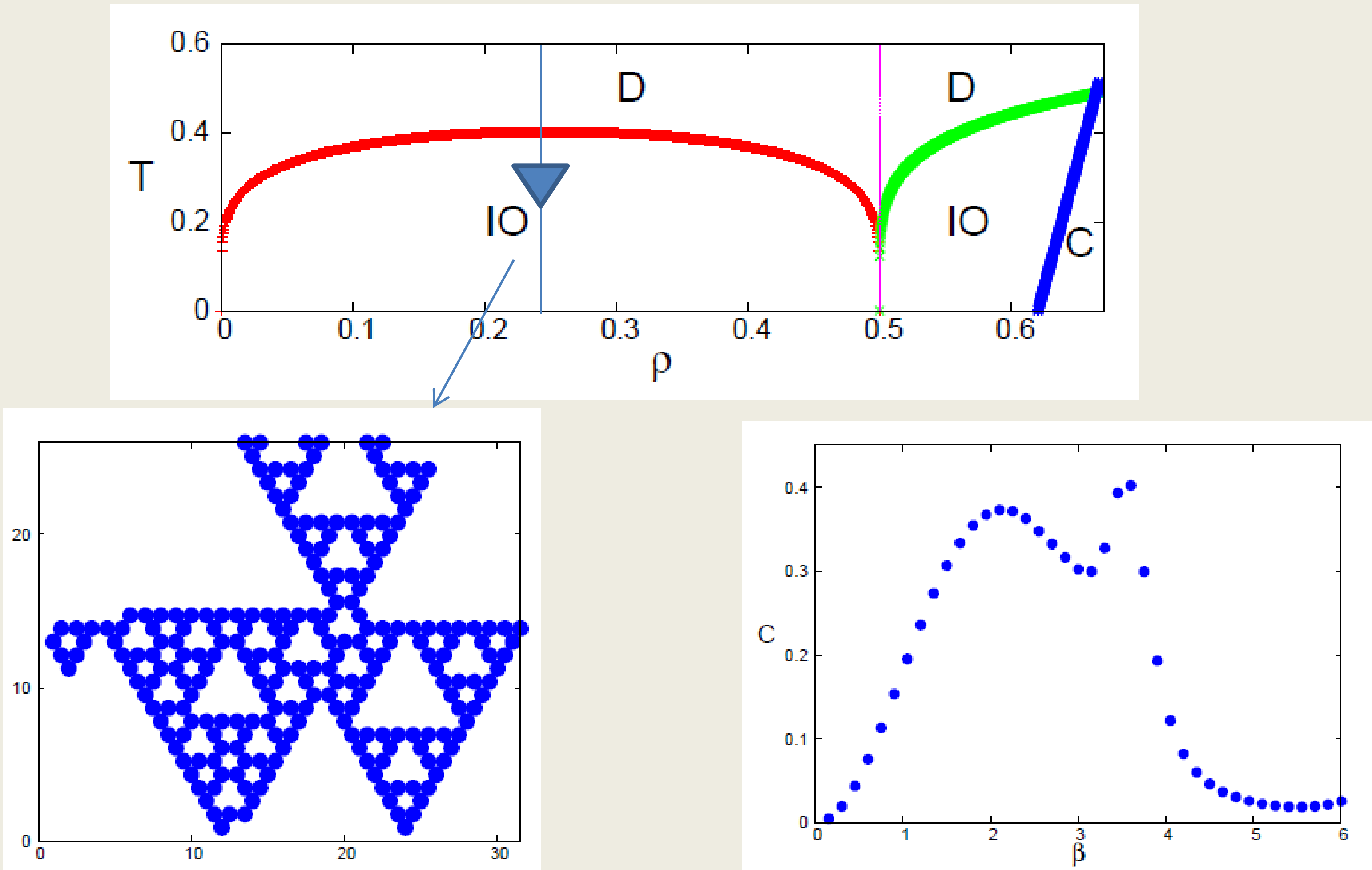
the first order transition in the (T, μ) space

the critical point

the transition to crystals



Irregularly ordered phase



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Summary and future problems

We have shown an example of thermodynamic transitions associated with irregularly ordered ground states

- Nature of "irregularly ordered phase" ?
- Relation to "thermodynamic glass phase" ?
- Non-equilibrium, dynamical behavior ?