Computational and Theoretical Study of Disordered Systems

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PhD Dissertation Defense

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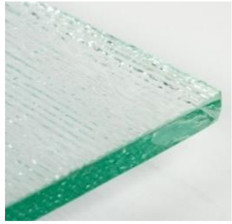
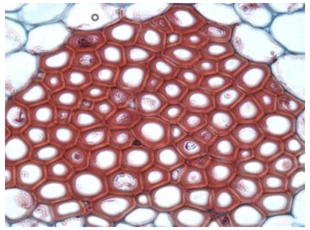
Outline

- Introduction of Disordered Systems
- **Jamming** in Hierarchical Networks (HNs)
- **Antiferromagnetic Ising model** in HNs
- Aging in **Random Field Ising Model**
- Summary

Introduction

- Disordered material is the majority

- Numerous categories:
  - Glass, polymer, granular materials, biological tissues, etc.

- More unclear questions
- Focus on theoretical models
  - Lattice glass model
  - Antiferromagnetic Ising model
  - Random Field Ising model

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- Introduction of Disordered Systems
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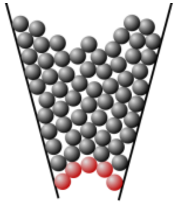
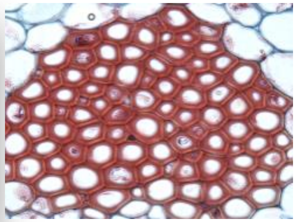
Jamming transition

- Jammed states are common.



- Characteristics
  - High packing density *(not highest)*
  - Out of equilibrium
  - Extremely slow relaxation

- A challenge to understand
  - What causes the extremely slow relaxation?
  - Equilibrium state?
  - Equilibrium phase transition?

Zhang, .et al and Liu, Nature 459, 230 (2009)

Model: lattice glass model

- Biroli-Mezard Model (BM)

  Structural disorder → *Complex Dynamics*

Biroli and Mezard, *PRL* **88**, 2 (2002); Krzakala, Tarzia, and Zdeborova, *PRL* **101**, 165702 (2008)

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  <u>*Structural disorder*</u> $\rightarrow$ <u>*Complex Dynamics*</u>

  - Each lattice site has $n_i = 0, 1$ particle with μ
  - Constraint: an occupied site can have at most l neighbors $(l = 0,1,2 \ldots)$

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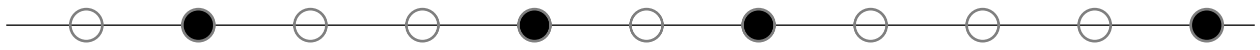
  Example: $l = 0$



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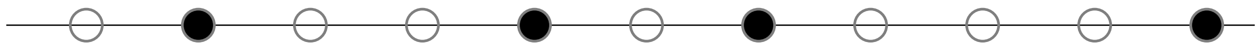

$$\Xi = \sum_{n=0}^{n_{\max}} g_n \exp(n\beta\mu)$$

- where $n_{\max}$ is the largest number of particles within constraint
- g_n is the density of state with n particles

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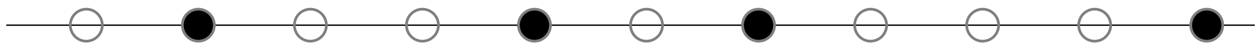

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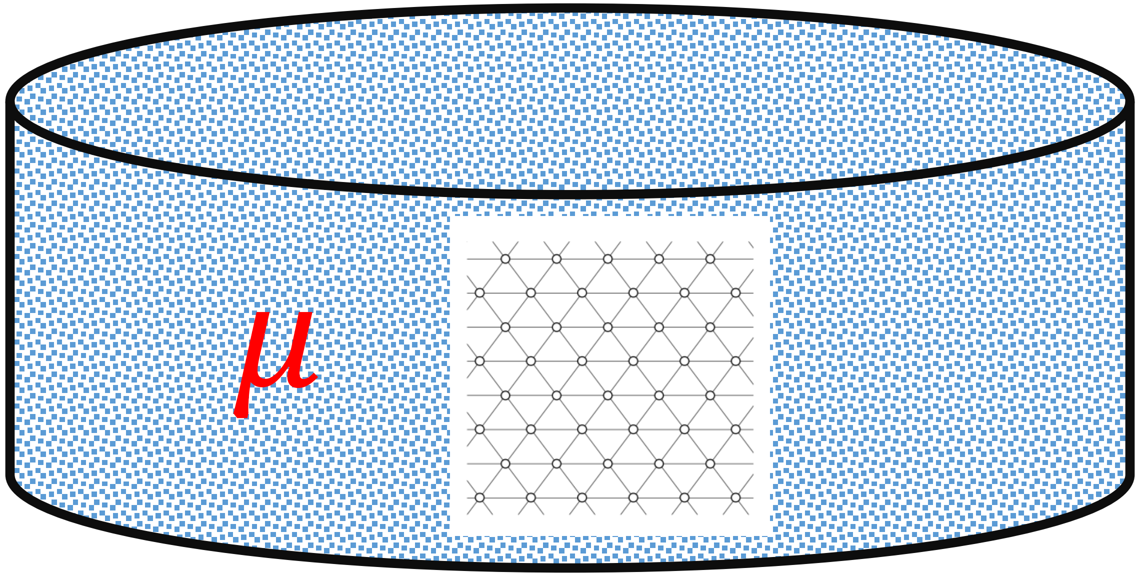
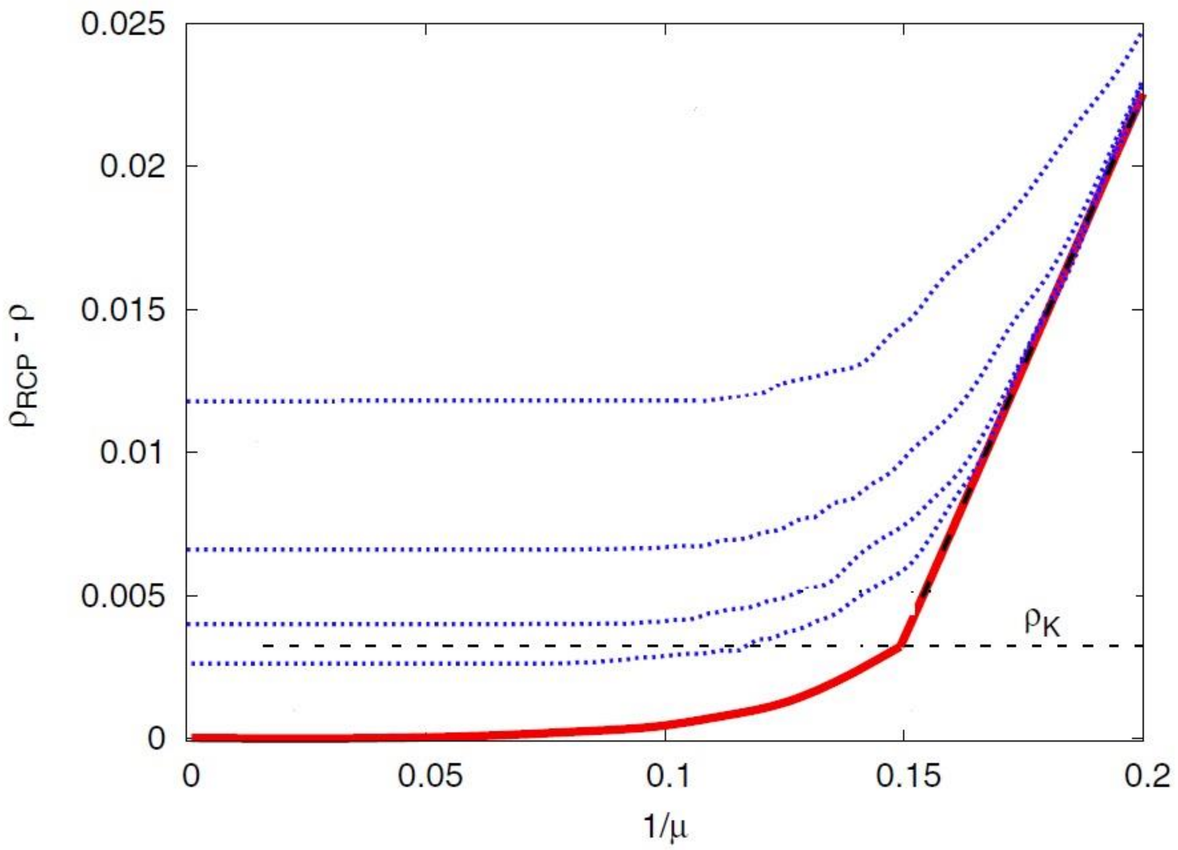
Jamming in lattice glass model



- Bigger μ → higher packing fraction ρ
- μ is big enough → non-equilibrium state: **Jamming state**
- Mean filed theory → phase transition underlying jamming transition

Biroli and Mezard, *PRL* **88**, 2 (2002); Krzakala, Tarzia, and Zdeborova, *PRL* **101**, 165702 (2008)

Equilibrium phase transition $\Longleftrightarrow$ Jamming Transition?



- **Mean-field model**
- **Phase transition** found underlying **jamming transition**

True in non-mean-filed model?

Krzakala, Tarzia, and Zdeborova, *PRL* **101**, 165702 (2008)

Model: Hierarchical Networks

- Hanoi networks *(small world network)*:
  fixed structure; **analytically solvable**
- Hanoi Network with degree of 3 (**HN3**)
  - Backbone: 1-D: $0 - 1 - 2 - \cdots - N$
  - Long-range links:

S. Boettcher, B. Goncalves, and H. Guclu, *J. Phys. A* **41**, 252001 (2008)

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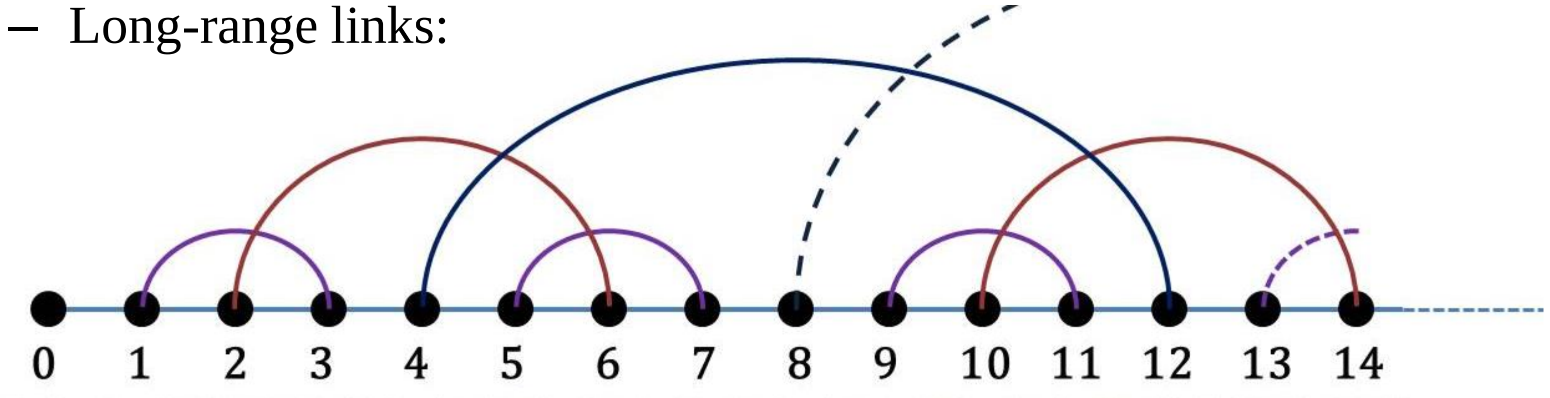

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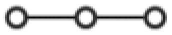
$N = 2^{1} + 1$ 

S. Boettcher,

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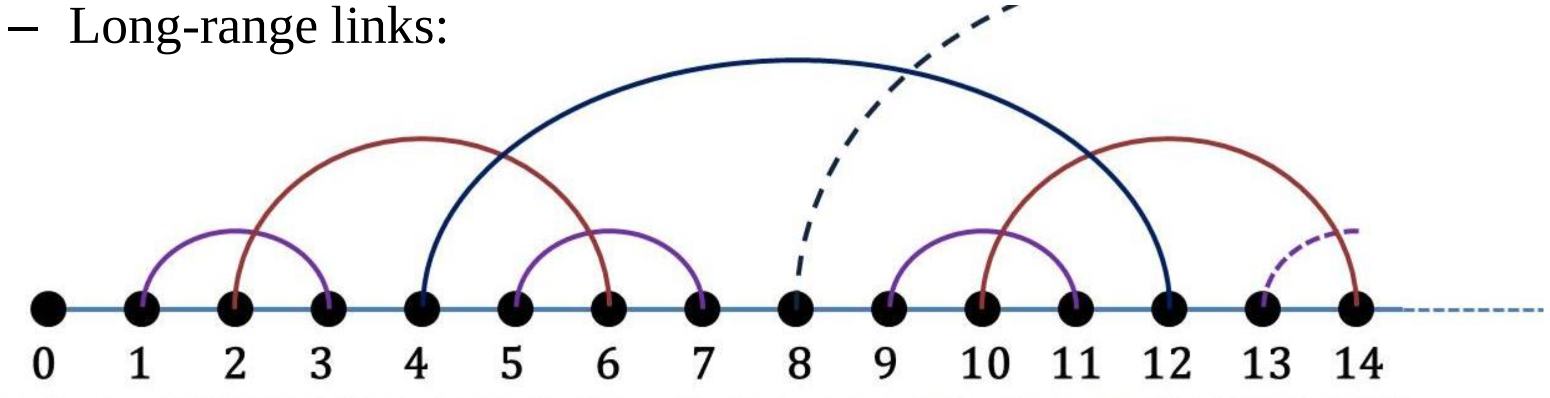


- HN5: average degree of 5
- HNNP: average degree of 4
- HN6: average degree of 6

S. Boettcher, B. Goncalves, and H. Guclu, *J. Phys. A* **41**, 252001 (2008)

Why Hierarchical Networks (HNs)?

- Exactly solvable by Renormalization Group (RG)
- Lattice-like structure
  - Mean-Field ⇨ HNs ⇨ Regular lattice
- Different structures

Network	Degree	Planarity	Diameter
HN3	3	Planar	$\sqrt{N}$
HN5	5	Planar	$\ln N$
HNNP	4	Nonplanar	$\ln N$
HN6	6	Nonplanar	$\ln N$

Methods

- Monte Carlo Methods:
  - **Simulated Annealing** $\rightarrow$ Experiment
    randomly add or remove particle with $P(\mu)$;
    μ is increased by $d\mu$ per MC sweep;

  - Wang-Landau Sampling $\rightarrow$ Density of States $\boldsymbol{g_n}$

$$\Xi = \sum_{n=0}^{n_{\max}} \boldsymbol{g_n} \exp(\boldsymbol{n}\mu)$$

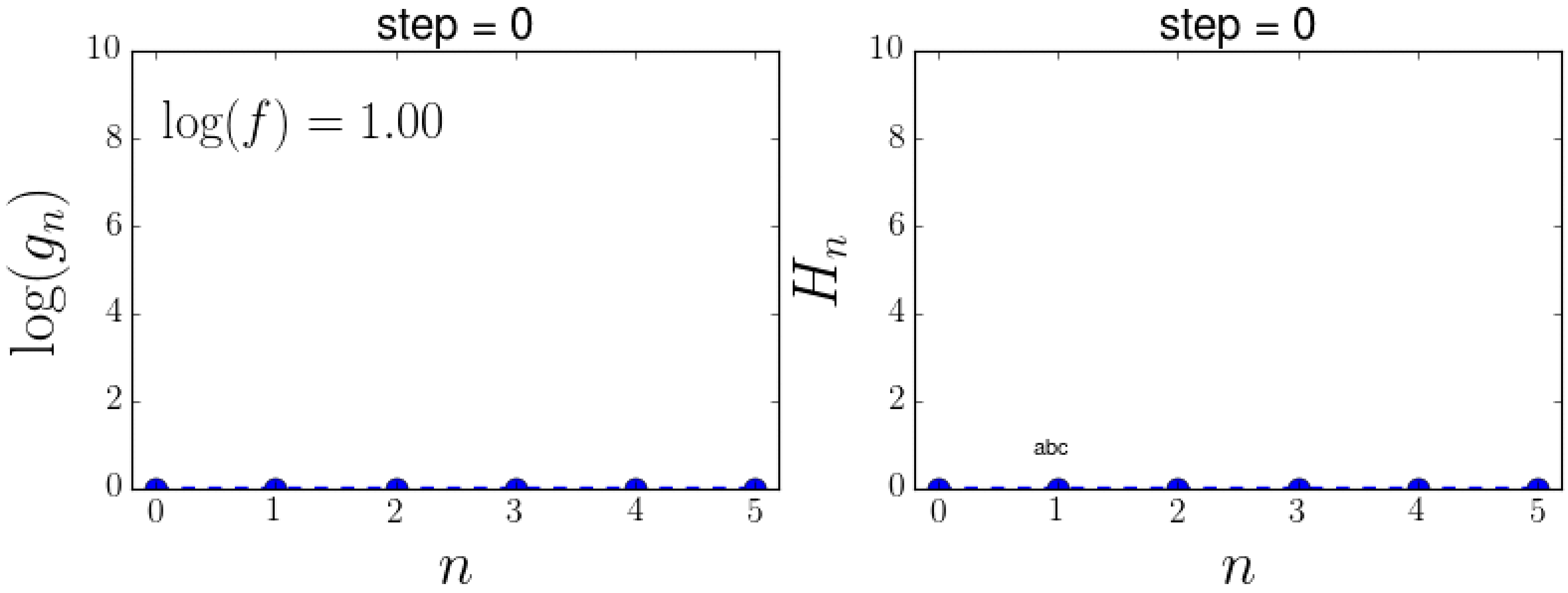
- Analytical Method:
  - Renormalization Group (HN3, HN5, 0 allowed neighbors)

Wang-Landau sampling

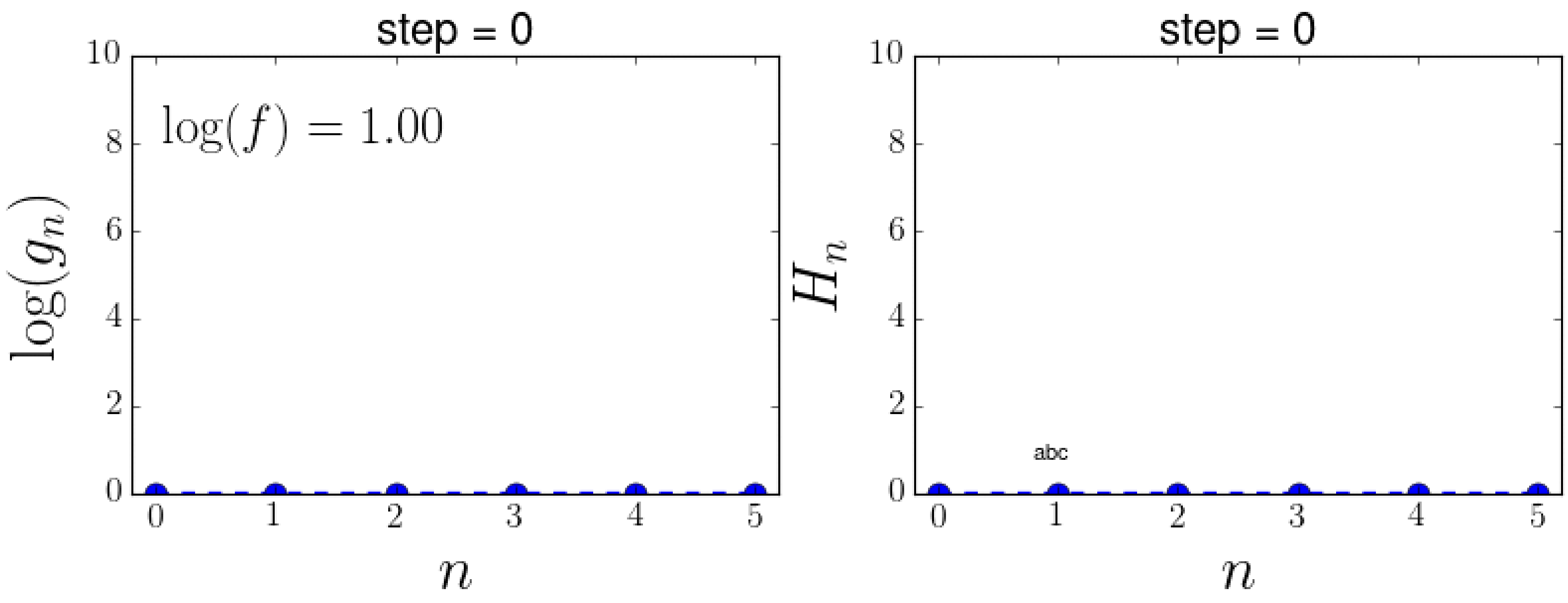
- Histogram method
  - Sampling with probability $\hat{P} \propto 1/P$ → **flat histogram**
  - Non-thermodynamic, Non-Markov-Chain Monte Carlo

- Procedure
  - Initial guess: flat g_n $\{1, 1, 1, 1, \cdots\}$ and flat H_n $\{0, 0, 0, 0, \cdots\}$
  - Randomly pick a site i
  - Add (remove) a particle with $P = \min[1, \frac{g_n}{g_{n+1}}]$ ($\min[1, \frac{g_n}{g_{n-1}}]$)
  - Update g_n and H_n of the current state, i.e. $H_n = H_n + 1$; $g_n = g_n \times \boldsymbol{f}$
  - Random walk until flat histogram H_n
  - Reset $\{ H_n = 0 \}$ and $f = \sqrt{f}$ (from e to $< 1 + 10^{-8}$)

Wang-Landau sampling



Wang-Landau sampling

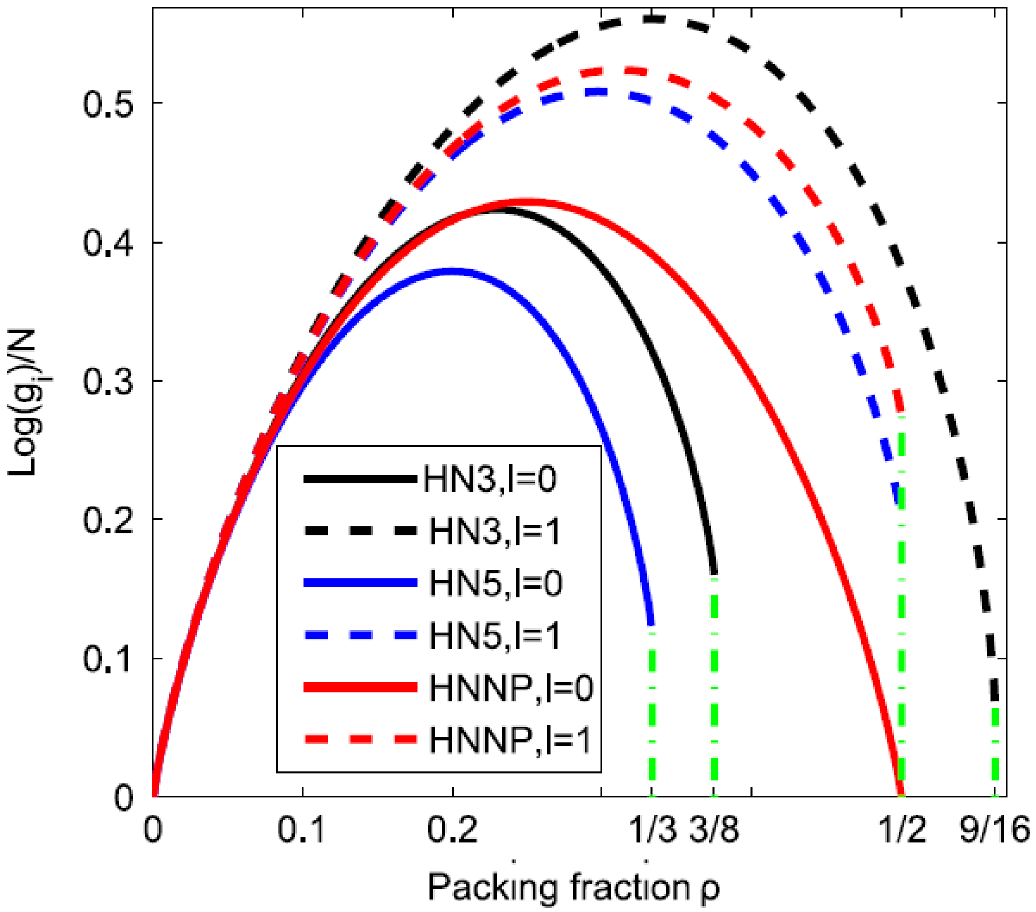


Extremely slow for large system size

Wang-Landau sampling

- Histogram method
  - Sampling with probability $\hat{P} \propto 1/P$ → **flat histogram**
  - Non-thermodynamic, Non-Markov-Chain Monte Carlo
- Procedure
  - Initial guess: flat g_n $\{1, 1, 1, 1, \cdots\}$ and flat H_n $\{0, 0, 0, 0, \cdots\}$
  - Randomly pick a site i
  - Add (remove) a particle with $P = \min[1, \frac{g_n}{g_{n+1}}]$ $(\min[1, \frac{g_n}{g_{n-1}}])$
  - **Exchange particle with an empty site**
  - Update g_n and H_n of the current state, i.e. $H_n = H_n + 1;\ g_n = g_n \times \boldsymbol{f}$
  - Random walk until flat histogram H_n
  - Reset $\{\, H_n = 0 \,\}$ and $f = \sqrt{f}$ (from e to $< 1 + 10^{-8}$)

Results of Wang-Landau sampling



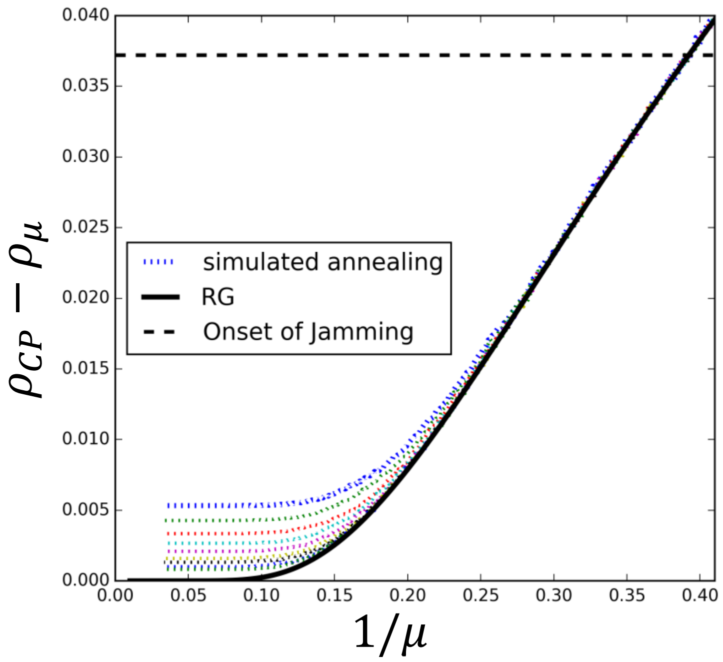
- N=512
- Does NOT converge for larger system size

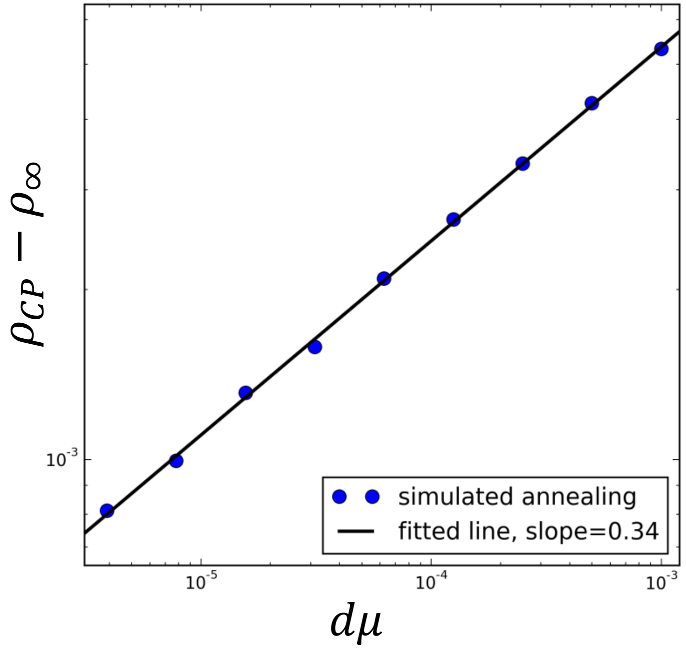
Results of $l = 0$ for HN3

- Simulated annealing vs RG

- Power-law relaxation

- **Jamming transition exists**;
- **No Phase Transition**

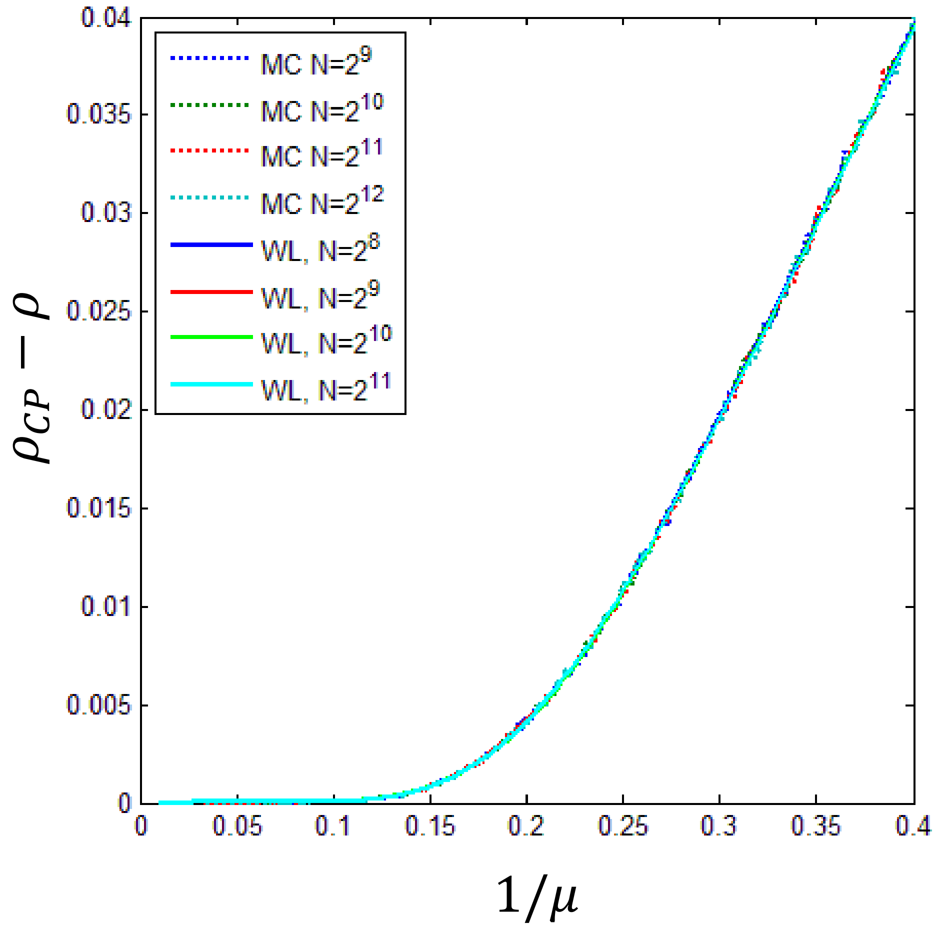




Results of $l = 1$ for HN5

- Simulation agrees well with Wang-Landau;
- Converge faster for large system sizes;

- Jamming state DOES NOT exist;
- No real phase transition;



Summary and Conclusion

	$\boldsymbol{l = 0}$	$\boldsymbol{l = 1}$
HN3	**JT** / **No PT**	**JT** / **No PT** (not sure)
HN5	**JT** / **No PT**	**No JT** / **No PT**
HNNP	**JT** / **No PT** (not sure)	**No JT** / **No PT**

JT: *Jamming Transition;* **PT**: *Phase Transition*

- Glassy dynamics & power-law relaxation & Jamming transition
- Algorithm efficiency improved by more random walk

Summary and Conclusion

	$l = 0$	$l = 1$
HN3	JT / No PT	JT / No PT (not sure)
HN5	JT / No PT	No JT / No PT
HNNP	JT / No PT (not sure)	No JT / No PT

JT: *Jamming Transition;* **PT**: *Phase Transition*

- Glassy dynamics & power-law relaxation & Jamming transition
- Algorithm efficiency improved by more random walk
- **Jamming transition** may not necessarily indicate a real **phase transition**

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- Summary

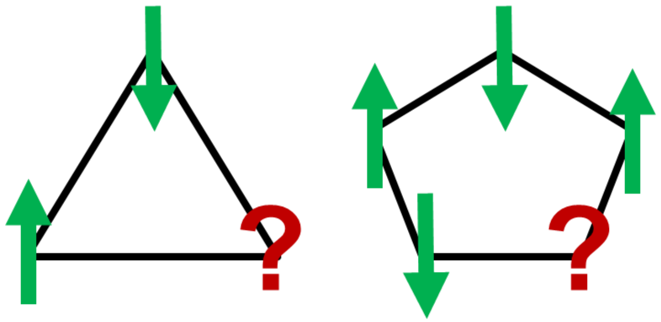
Antiferromagnetic Ising model

- Antiferromagnetic Ising model

$$E = -J \sum S_i S_j \ , J < 0$$

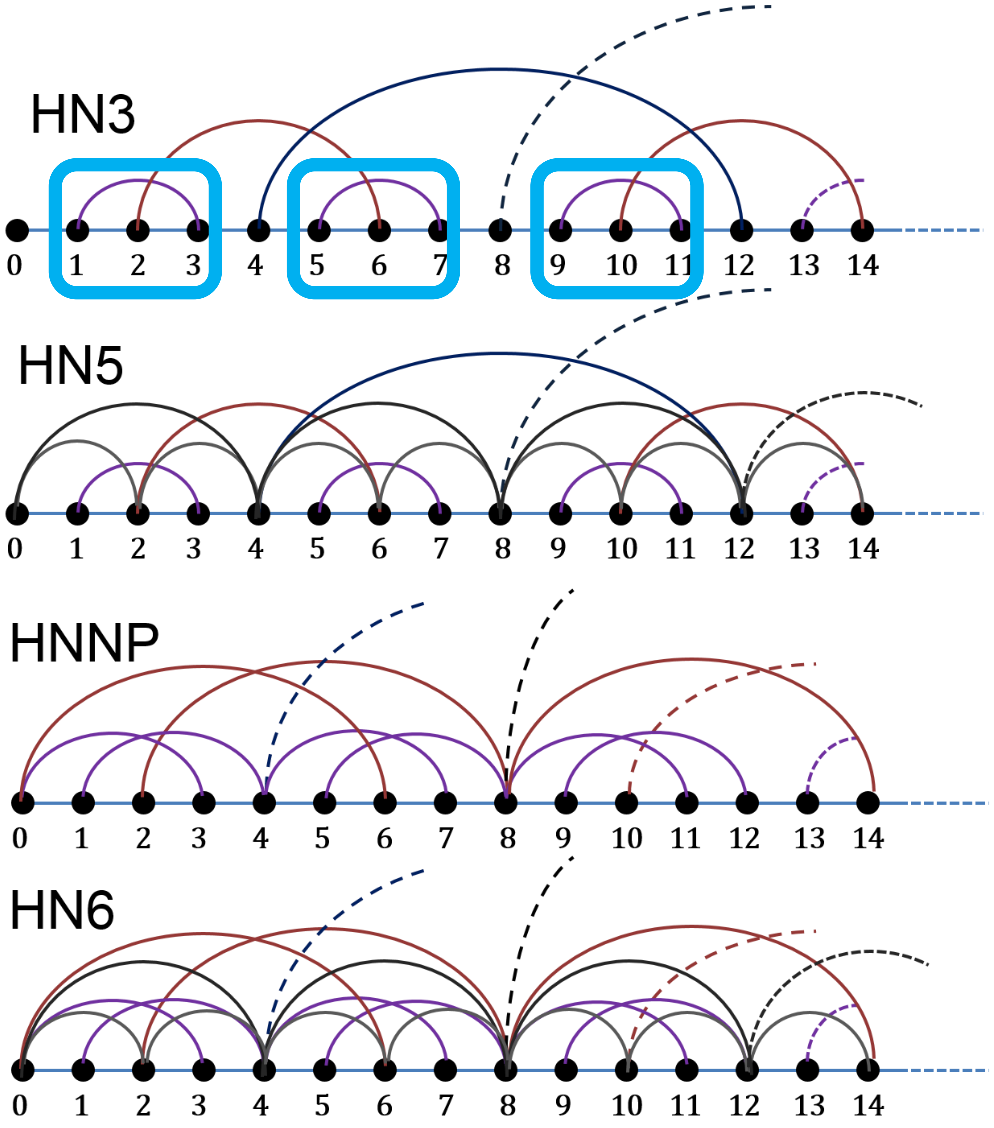
$E = -J > 0$ $\quad$ $E = J < 0$

- Geometric frustration: odd loops



Hierarchical networks (*HNs*)

- HN3
- HN5
- HNNP
- HN6



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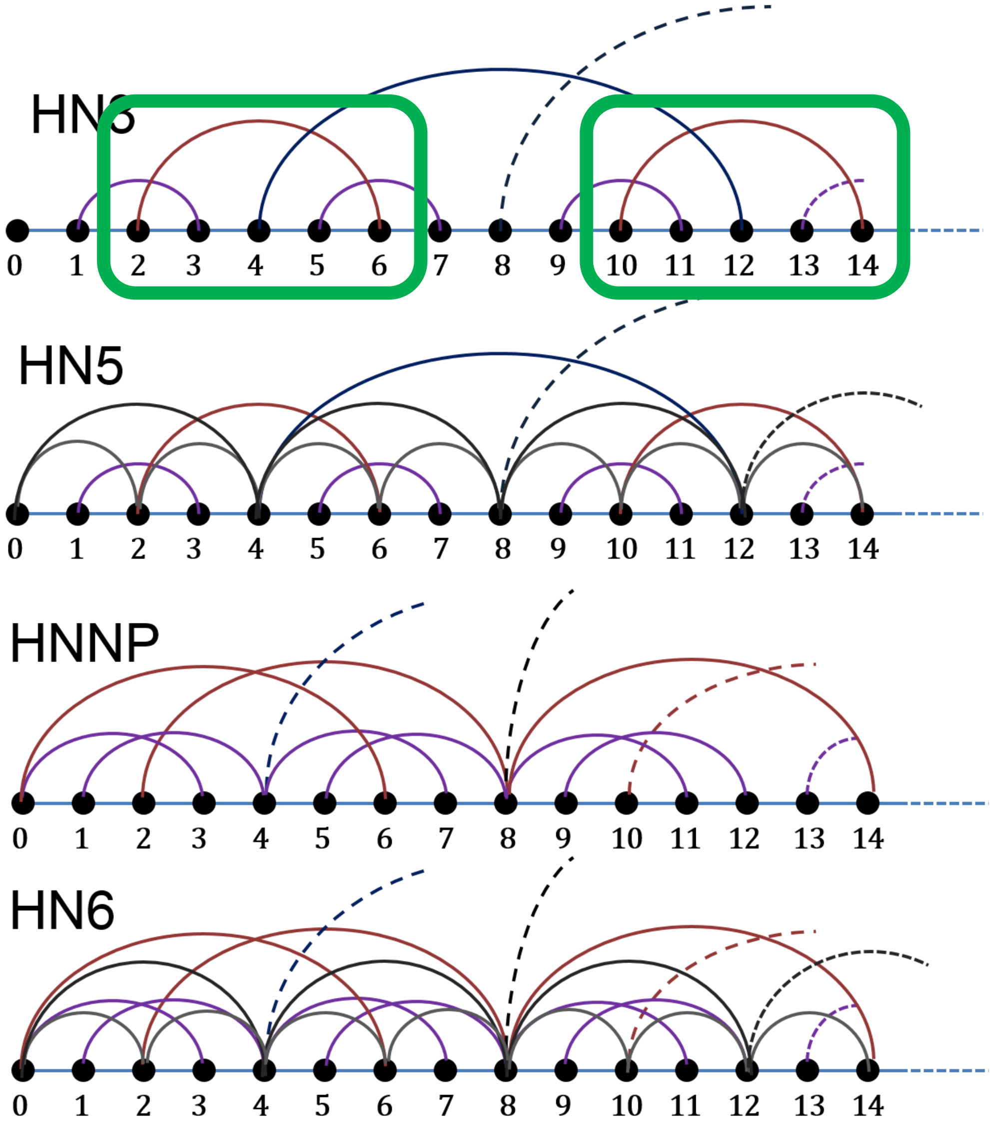

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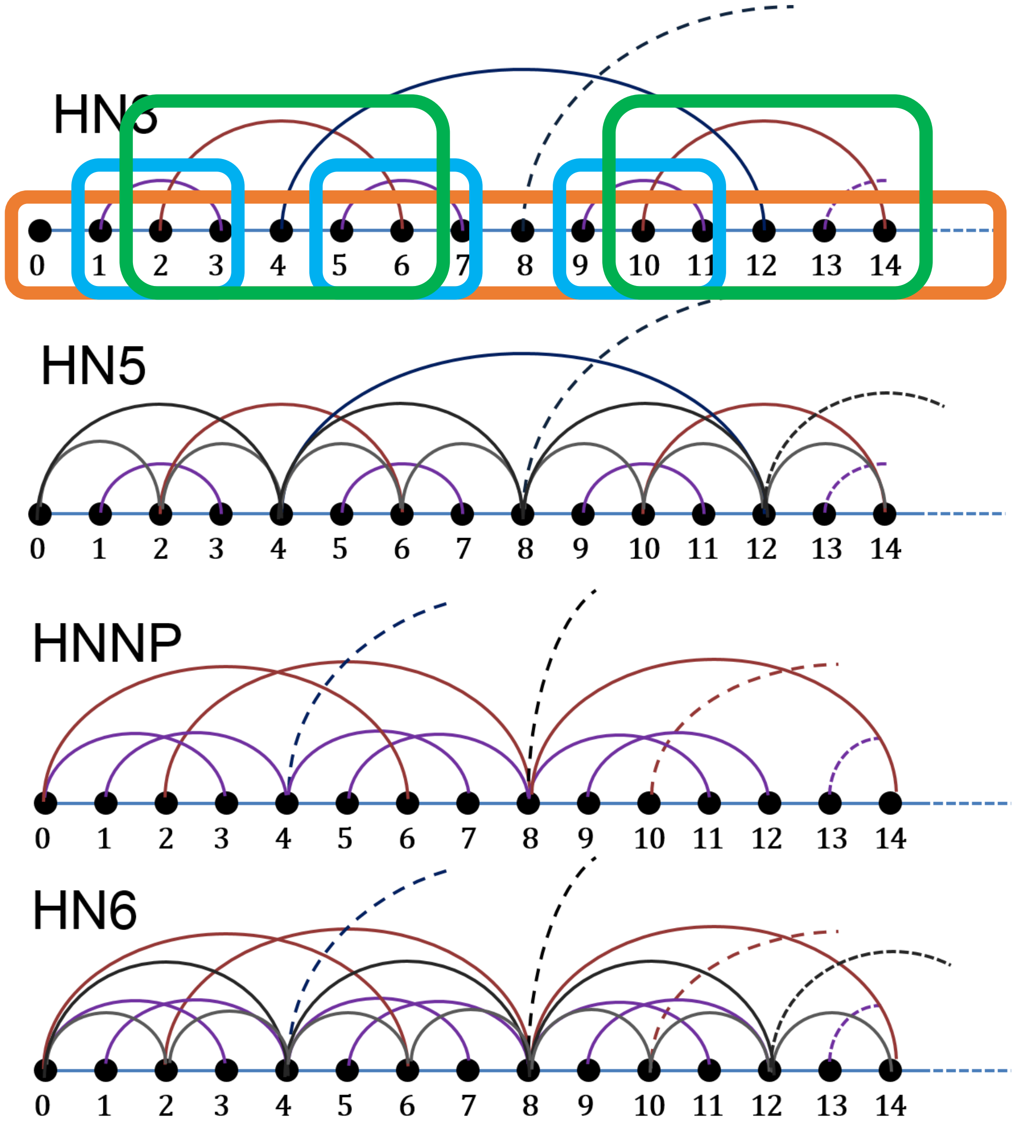
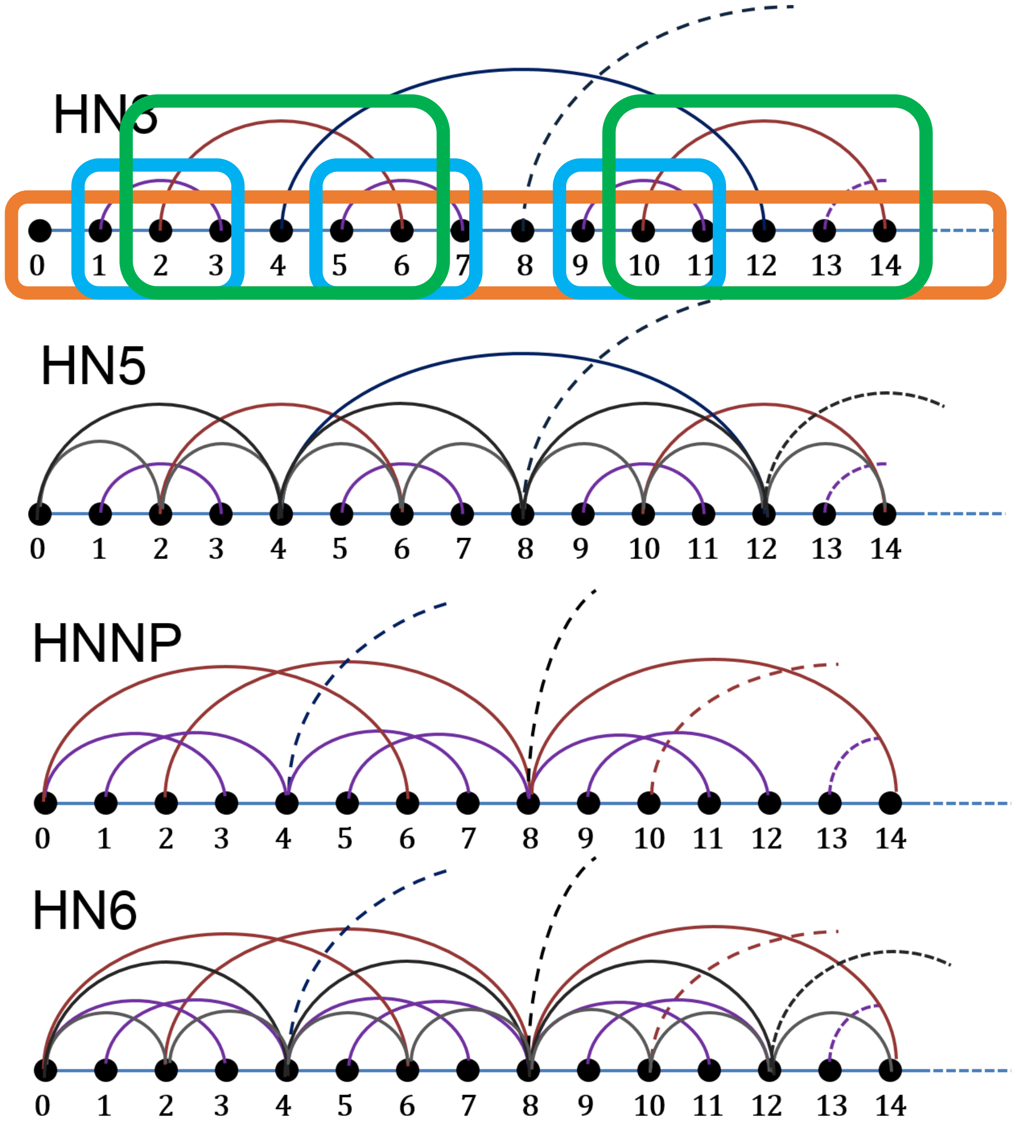


Hierarchical networks *(HNs)*

- HN3
- HN5
- HNNP
- HN6

- Interpolations:
  - Long-range link strength: $y \cdot J$
  - $y = 0$: HNNP
  - $y = 1$: HN6



Research Questions

- Anything interesting in this simple model?
- Glassy dynamics?
- Phase transitions?
  - Spin glass phase?
- Difference to mean-field models?

Methods

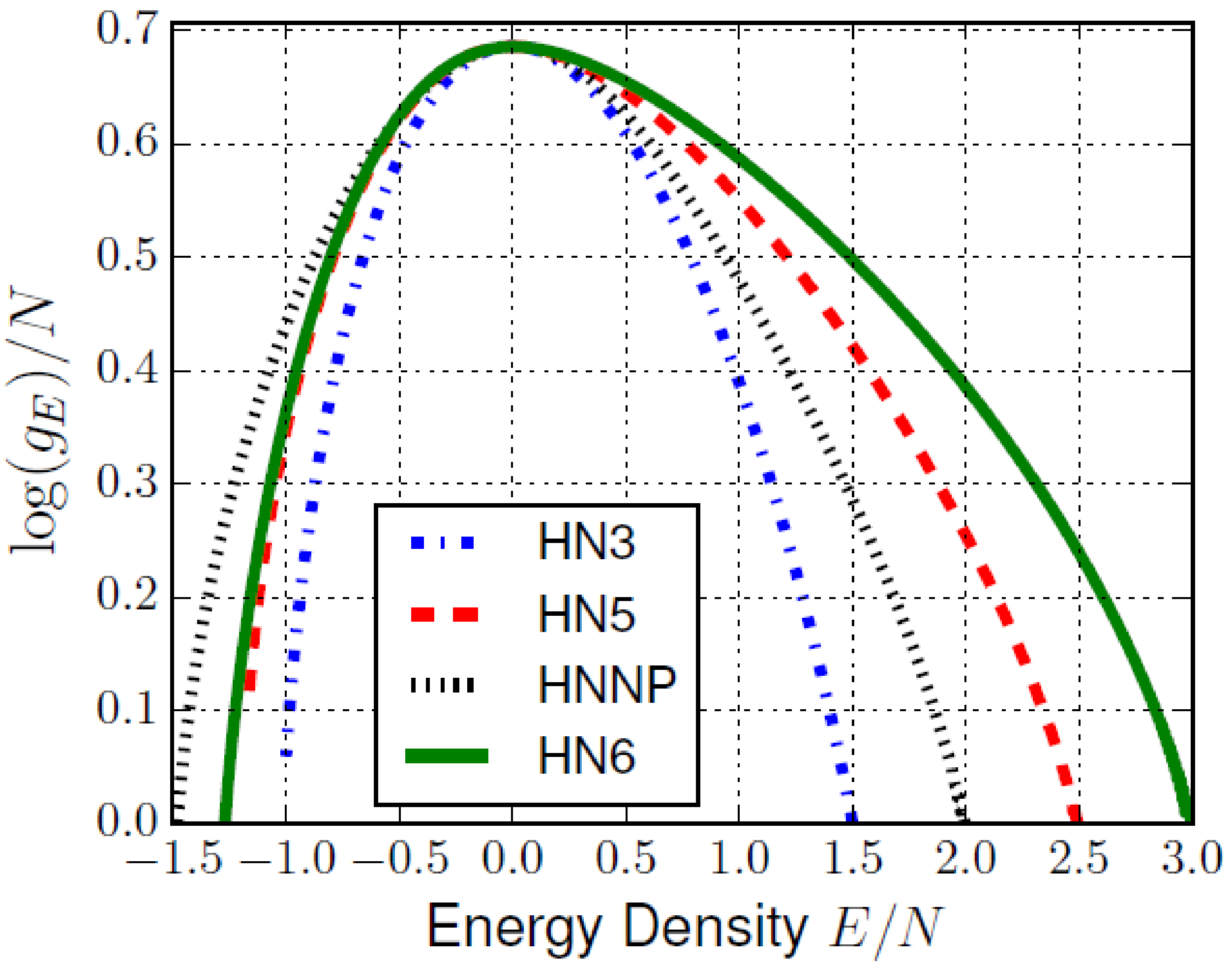
- Monte Carlo Methods:
  - **Simulated Annealing** → Experiment
  - Wang-Landau Sampling → Density of States $\boldsymbol{g_E}$

$$\Xi = \sum_{n=0}^{n_{\max}} \boldsymbol{g_E} \exp(-\beta \boldsymbol{E})$$

- Analytical Method:
  - Renormalization Group (HN3, HN5, HNNP, HN6)

Density of States (WL)

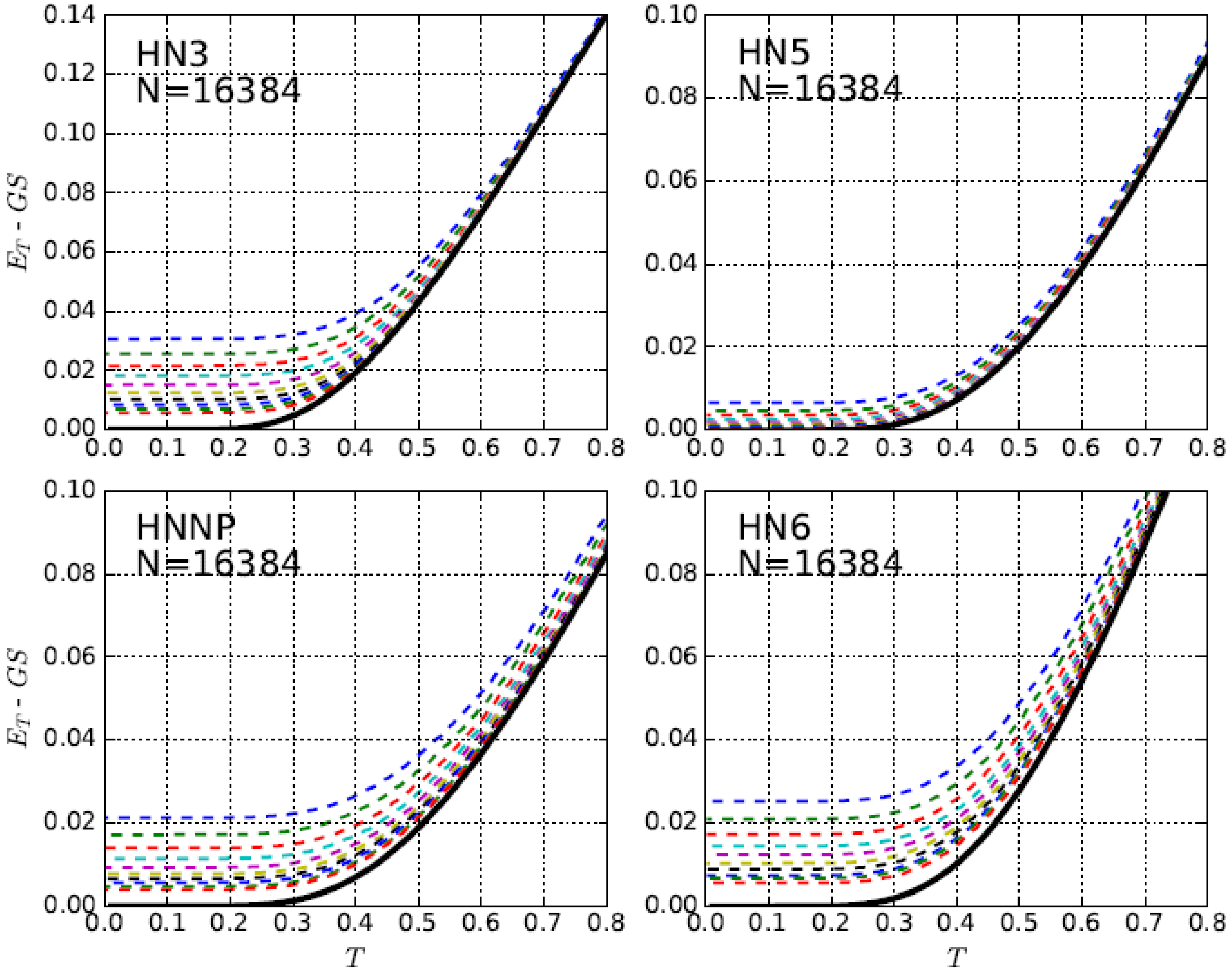
- Planar: HN3, HN5
  Degenerate ground states
- Non-planar: HNNP, HN6
  Unique ground states
- Confirmed by entropy (RG)
- Wang-Landau fails
  - $N > 512$



Glassy relaxation (SA)

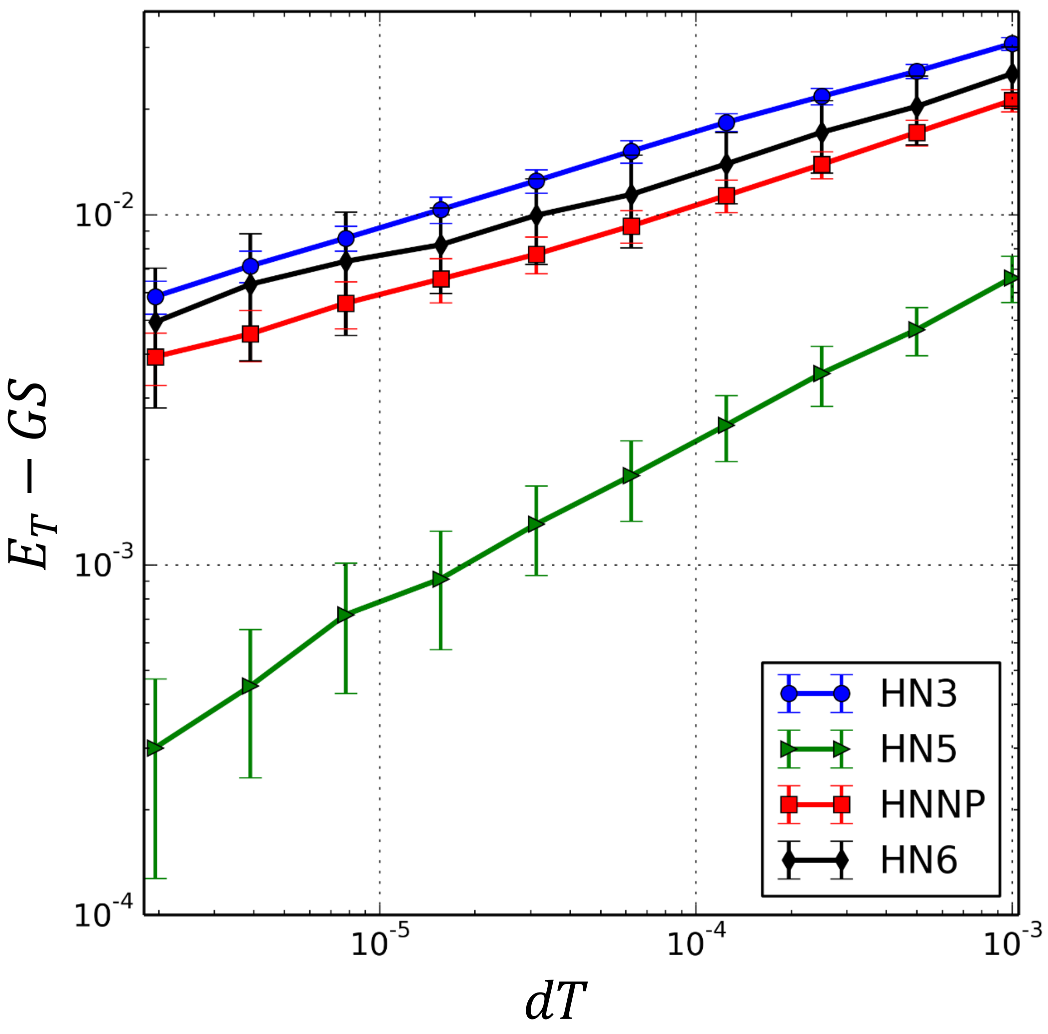
- x axis: T
- y axis: $E_T - GS$

- Extremely slow relaxation at low T



Power-law relaxation (SA)

- Power-law relaxation
- HN3, HNNP, HN6:
  - Slope = ~ 0.27
- HN5 may equilibrate gradually
  - Similar to that in jamming



Spin glass transition (RG)

- Renormalized interaction strength J

  - Recursive equations

Numerical solution

Analytical solution

McKay and Berker, *Phys. Rev. Lett.* **48**, 11 (1982)

Spin glass transition (RG)

- Renormalized interaction strength J
  - <u>Recursive equations</u>

Numerical solution

Analytical solution

- Planar: HN3, HN5
  - stable fixed-point solution
  - no phase transition

McKay and Berker, *Phys. Rev. Lett.* **48**, 11 (1982)

Spin glass transition (RG)

- Non-Planar: HNNP, HN6
  - spin glass transition at low T

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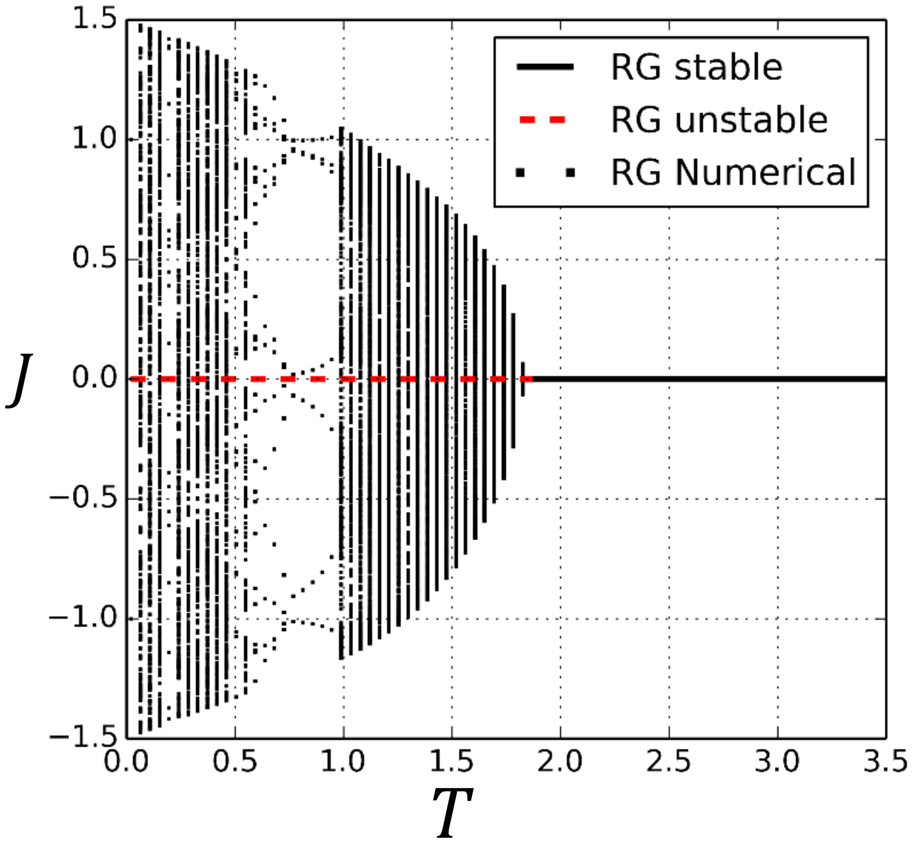
HNNP $(y = 0)$



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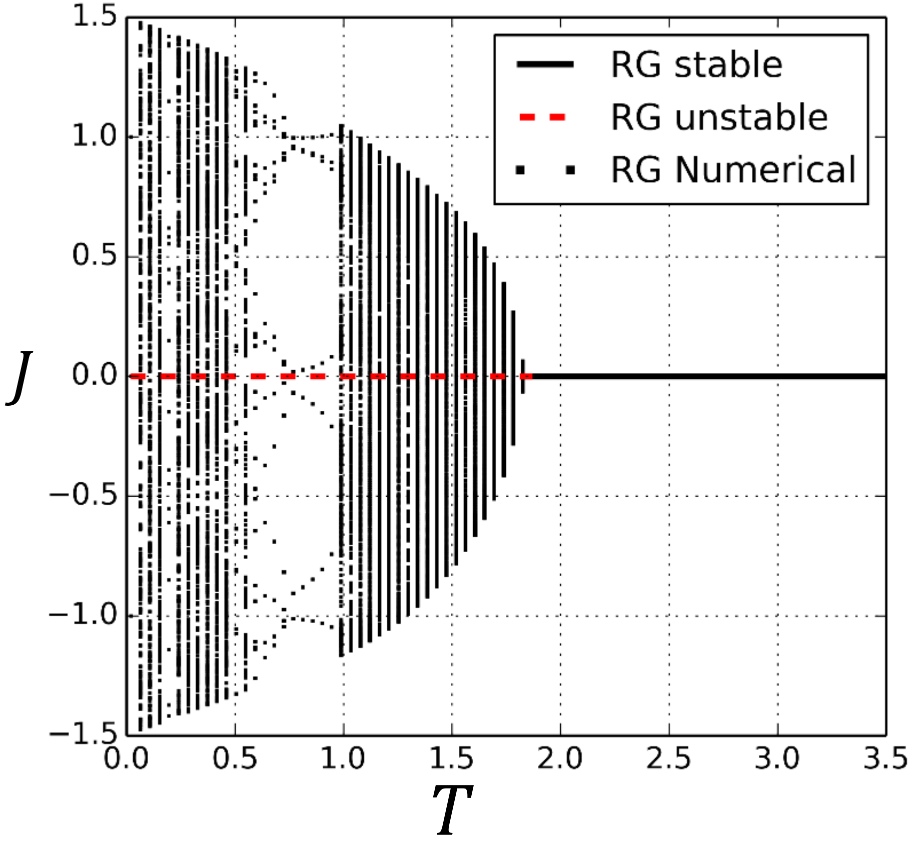
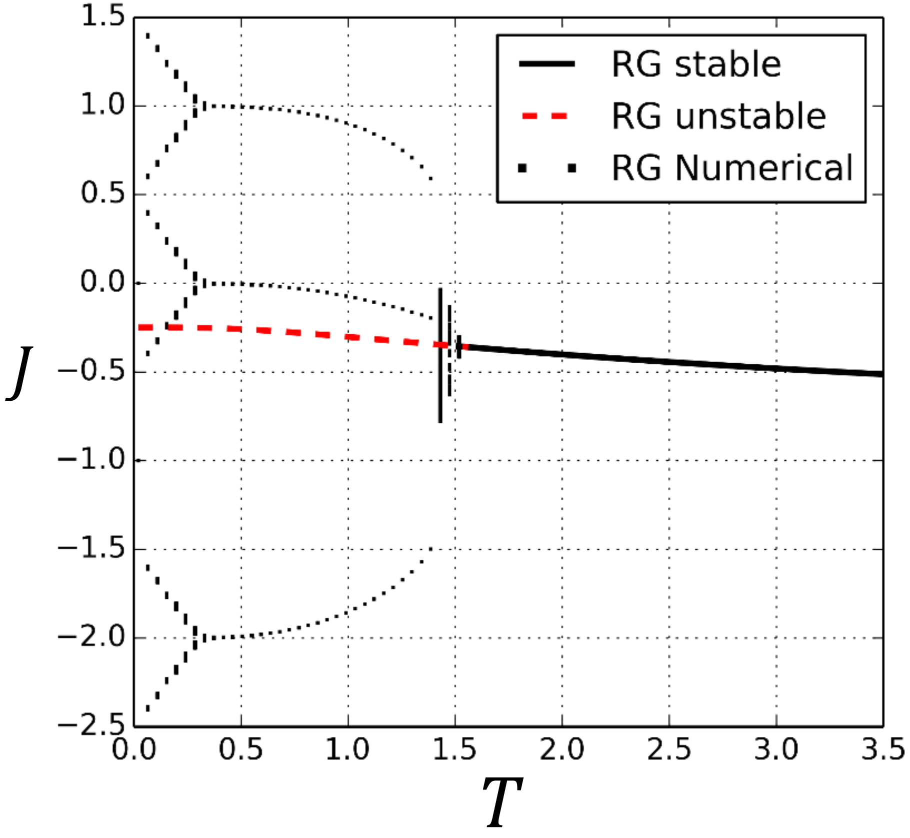


HN6 $(y = 1)$



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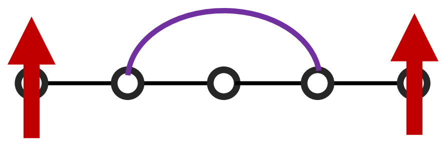
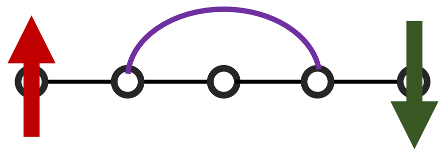
Free energy chaos

- Boundary conditions
  - Parallel: up-up



  - Anti-parallel: up-down



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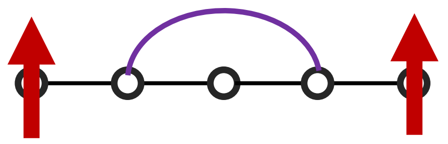

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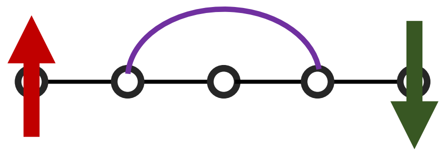

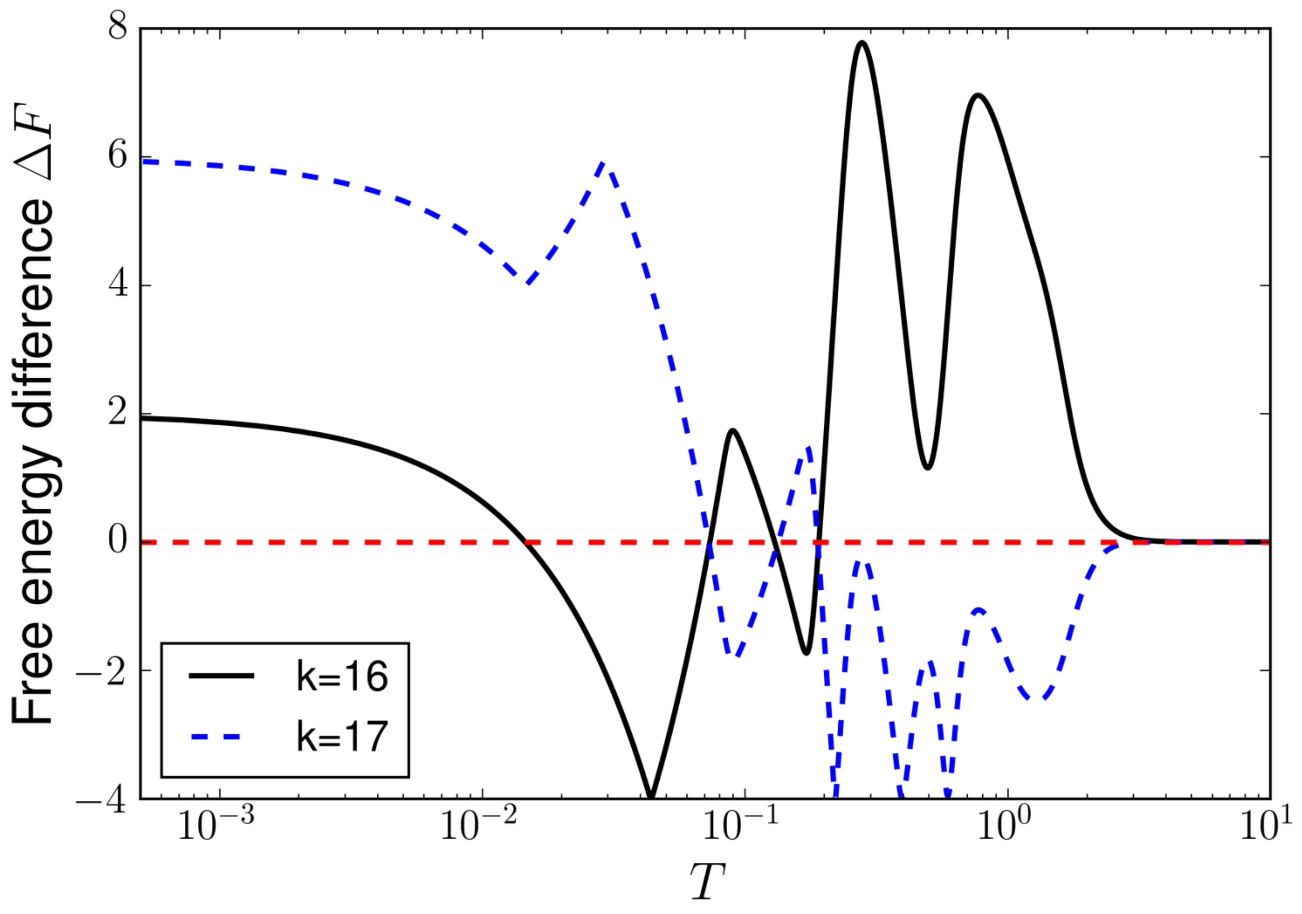

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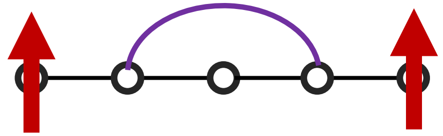

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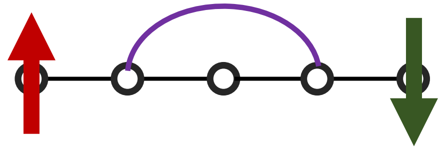
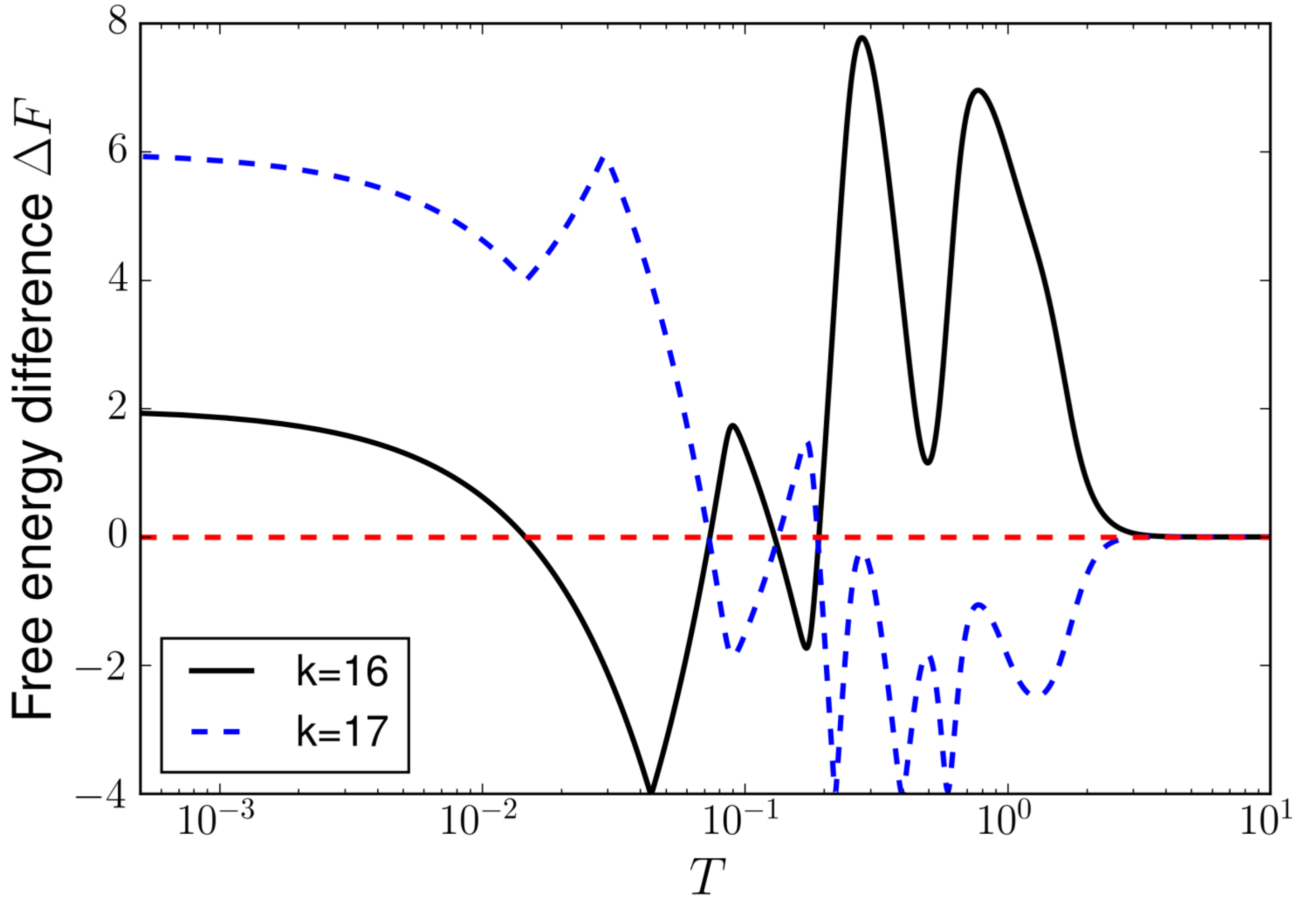


- Crossings N_C



Free energy chaos

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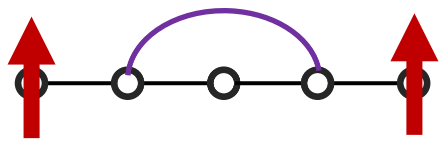

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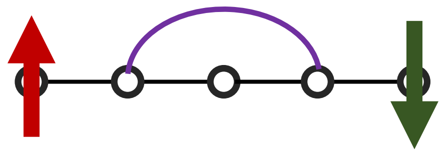
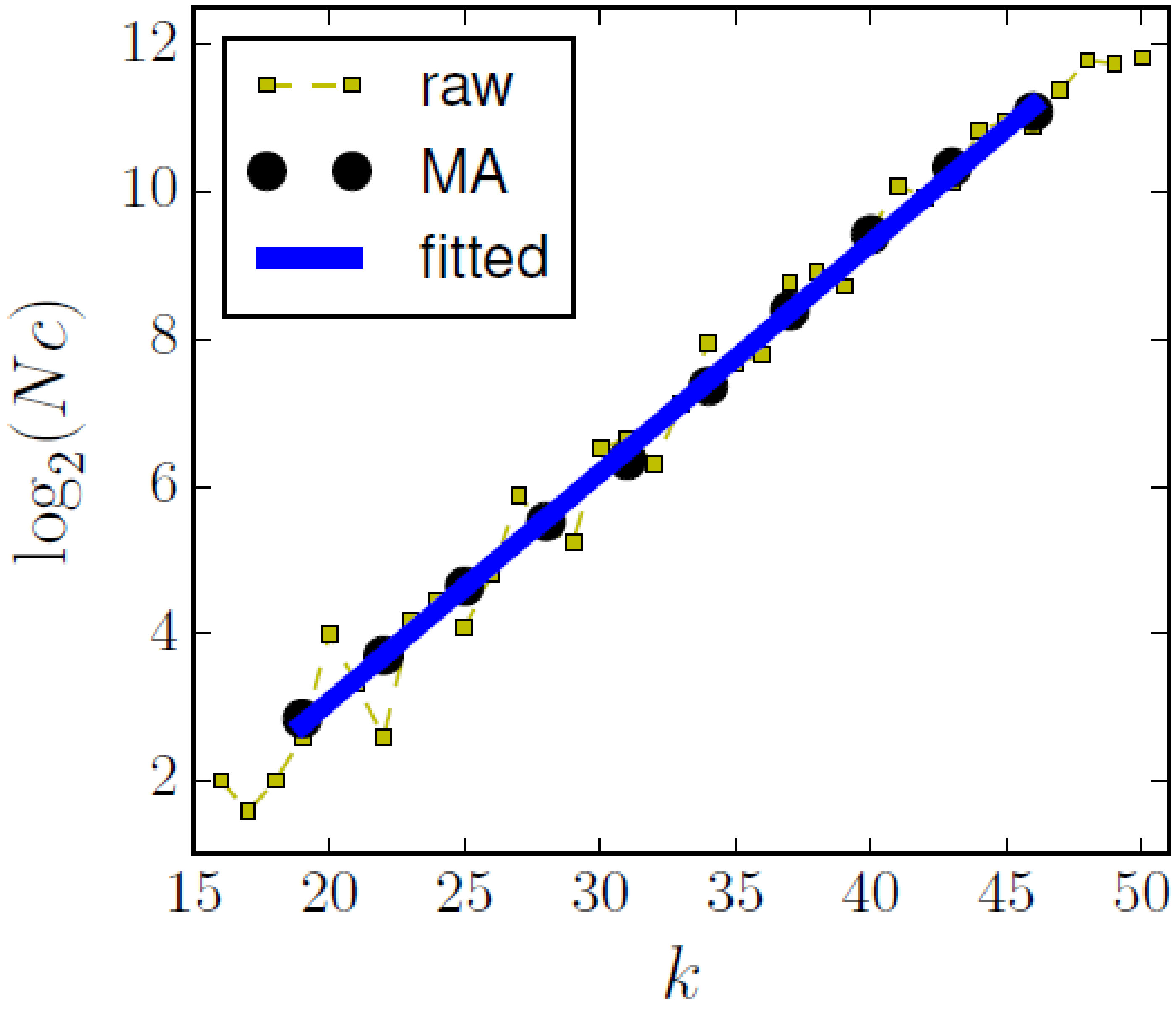
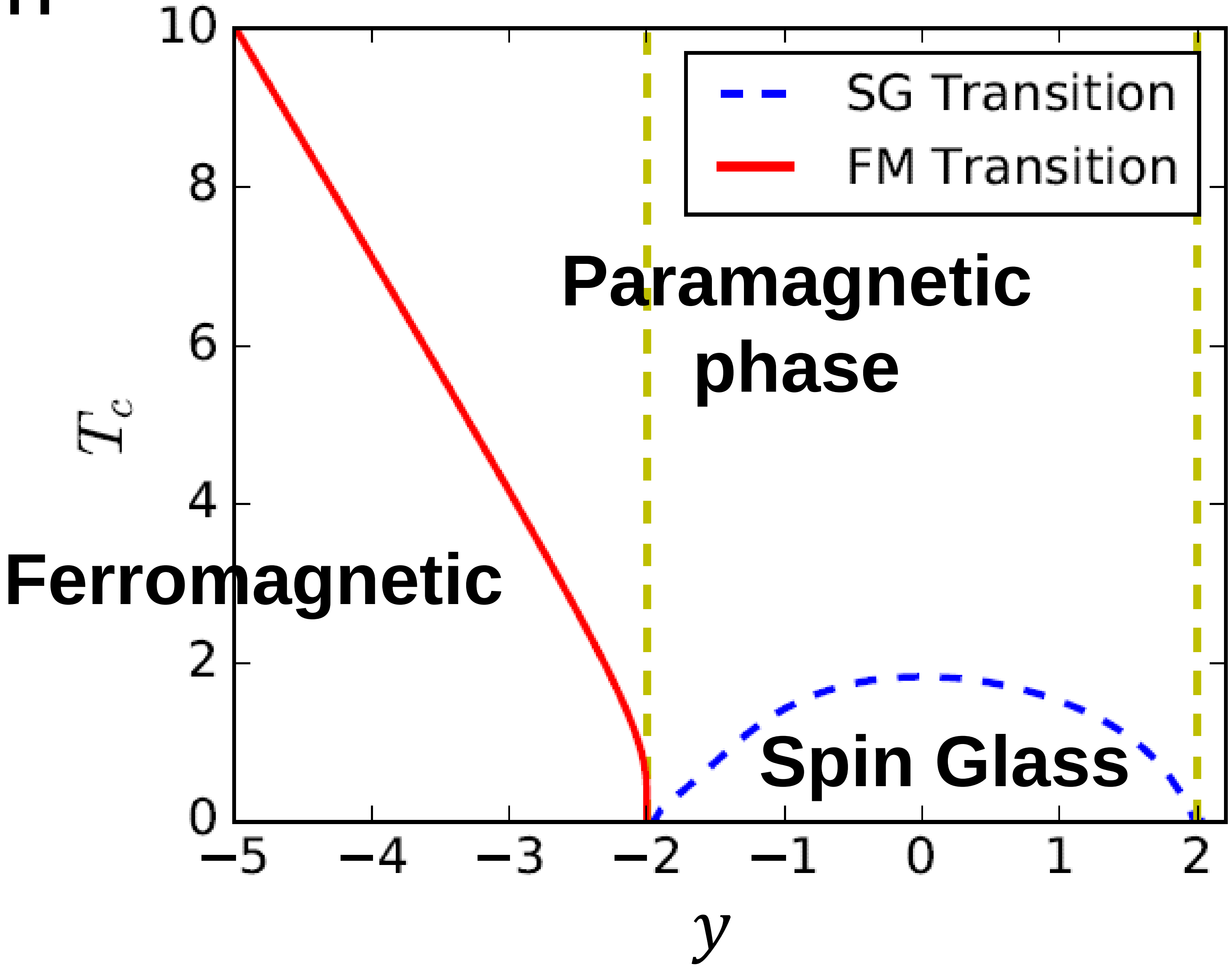


- Crossings N_C
  - Power-law scaling

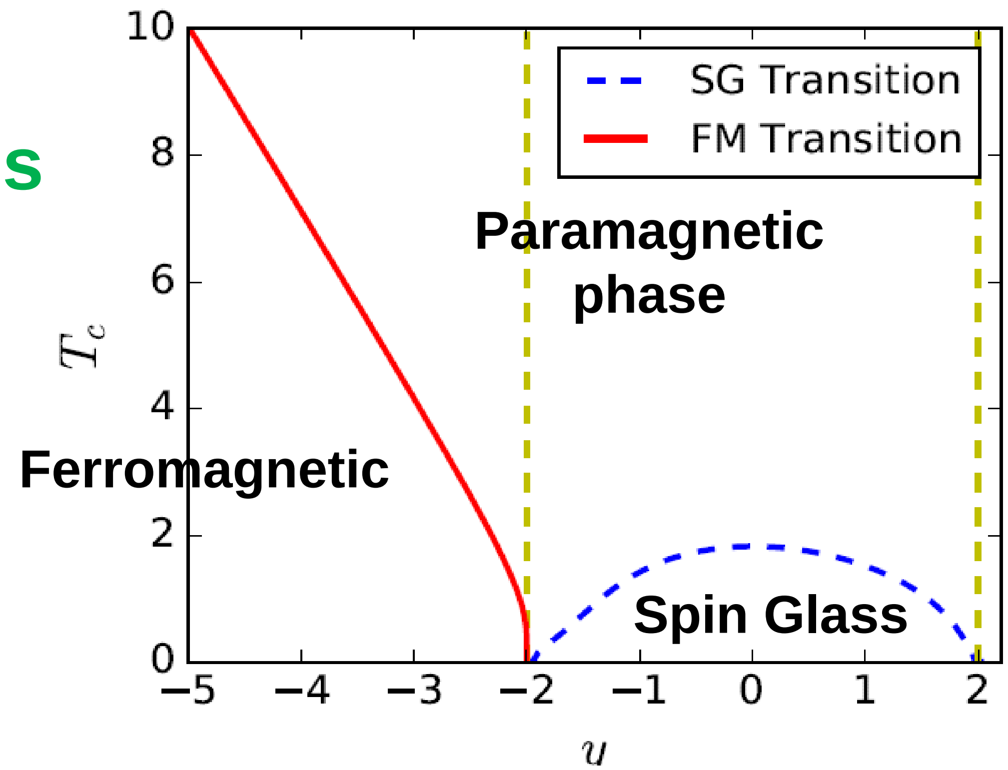


Phase Diagram



Summary and Conclusion

- Glassy dynamics and power-law relaxation
- Free energy chaos in non-planar networks
- Spin glass phase transition
- **Simple model → rich findings**

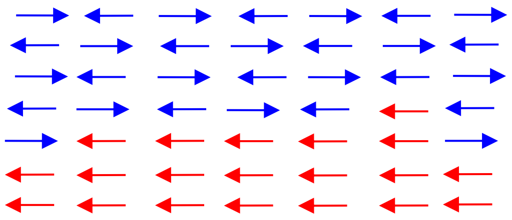


Outline

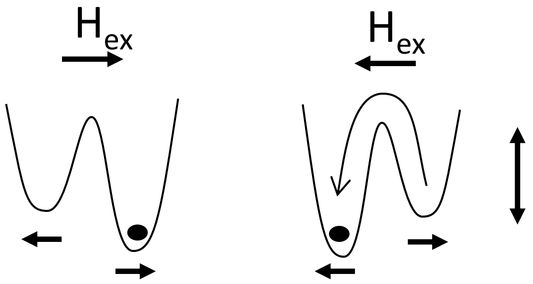
- Introduction of Disordered Systems
- Jamming in Hierarchical Networks (HNs)
- Antiferromagnetic Ising model in HNs
- Aging in Random Field Ising Model
- Summary

Motivation

Quenched disorder at F-AF interface



Arrhenius activation of magnetic domains*

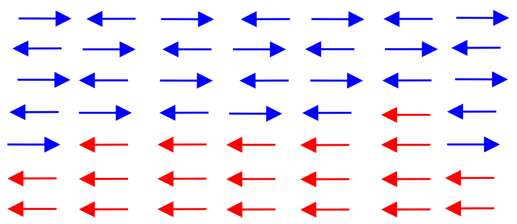


$$\tau = \tau_0 \exp\left(\frac{E}{k_B T}\right)$$

* E. Fulcomer, S.H. Charap, JAP 1972, and many more thereafter

Motivation

Quenched disorder at F-AF interface



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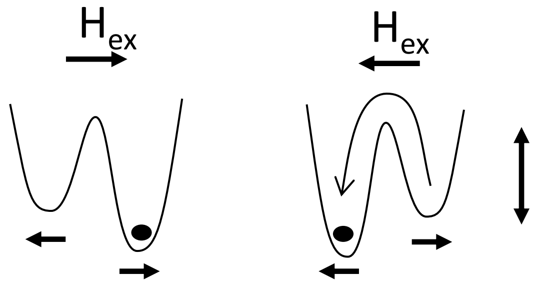


$$\tau = \tau_0 \exp\left(\frac{E}{k_B T}\right)$$

In the experiment:

Power-law relaxation; small exponent

* E. Fulcomer, S.H. Charap, JAP 1972, and many more thereafter

Random Field Ising Model

- Proposed by Imry and Ma in 1975
- Studied experimental systems:
  - diluted antiferromagnets, impure substrates, magnetic alloys
- simulate aging in thin-film F/AF bilayers

$$H = -J \sum_{<ij>} s_i s_j + \sum_i \boldsymbol{h_i} s_i$$

  - $J = 1$: coupling constant
  - $\boldsymbol{h_i}$: quenched random field

Imry and Ma, *PRL*, 35-21 (1975).

Monte Carlo Simulation

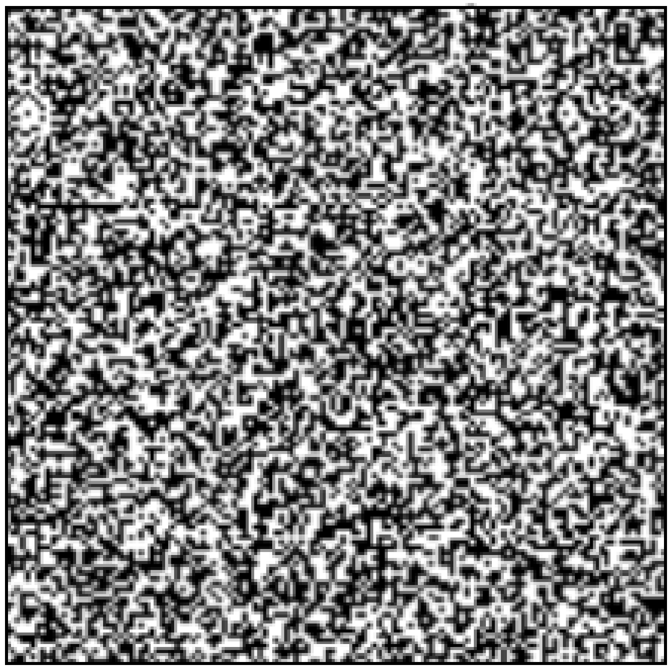
Experiment

- 1. Thin film

Simulation

- 1. 2D square lattice

1. Initial State



Monte Carlo Simulation

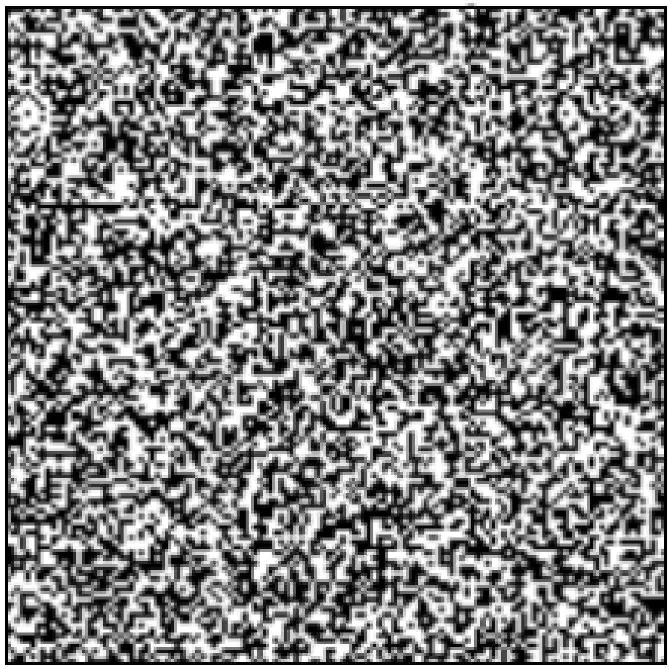
Experiment

- 1. Thin film
- 2. Cool down slowly

Simulation

- 1. 2D square lattice
- 2. Simulated annealing

1. Initial State



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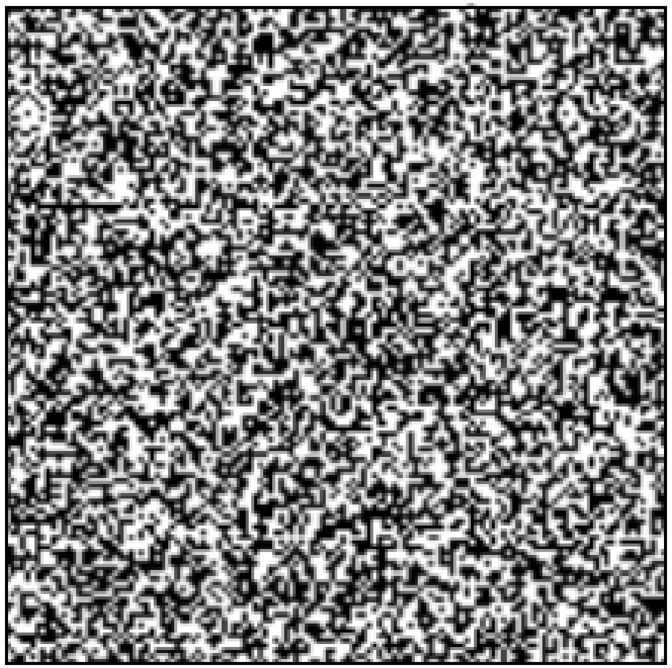


2. After Annealing

Monte Carlo Simulation

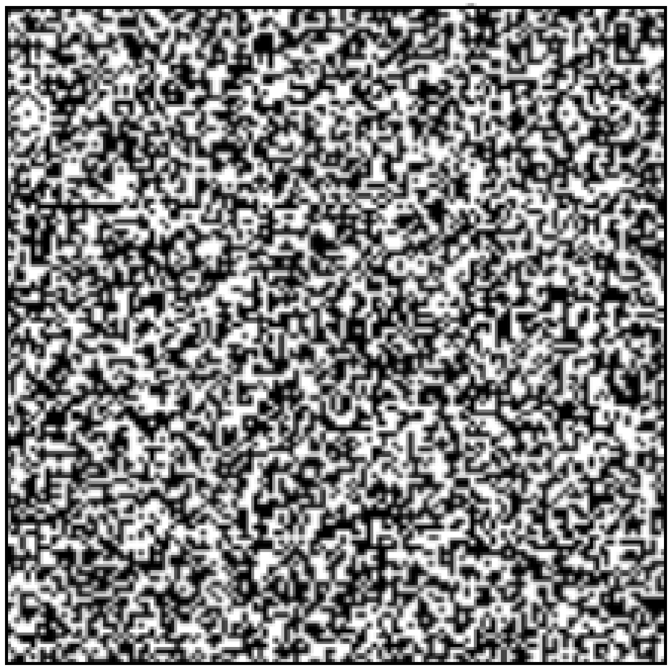
Experiment

- 1. Thin film
- 2. Cool down slowly
- 3. Measure resistance

Simulation

- 1. 2D square lattice
- 2. Simulated annealing
- 3. Measure energy

1. Initial State



2. After Annealing

Monte Carlo Simulation

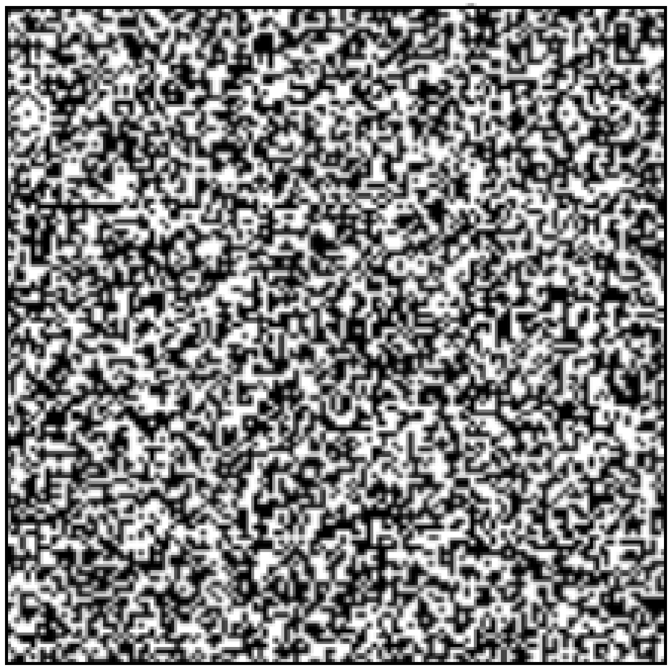
Experiment

- 1. Thin film
- 2. Cool down slowly
- 3. Measure resistance
- 4. Flip external field

Simulation

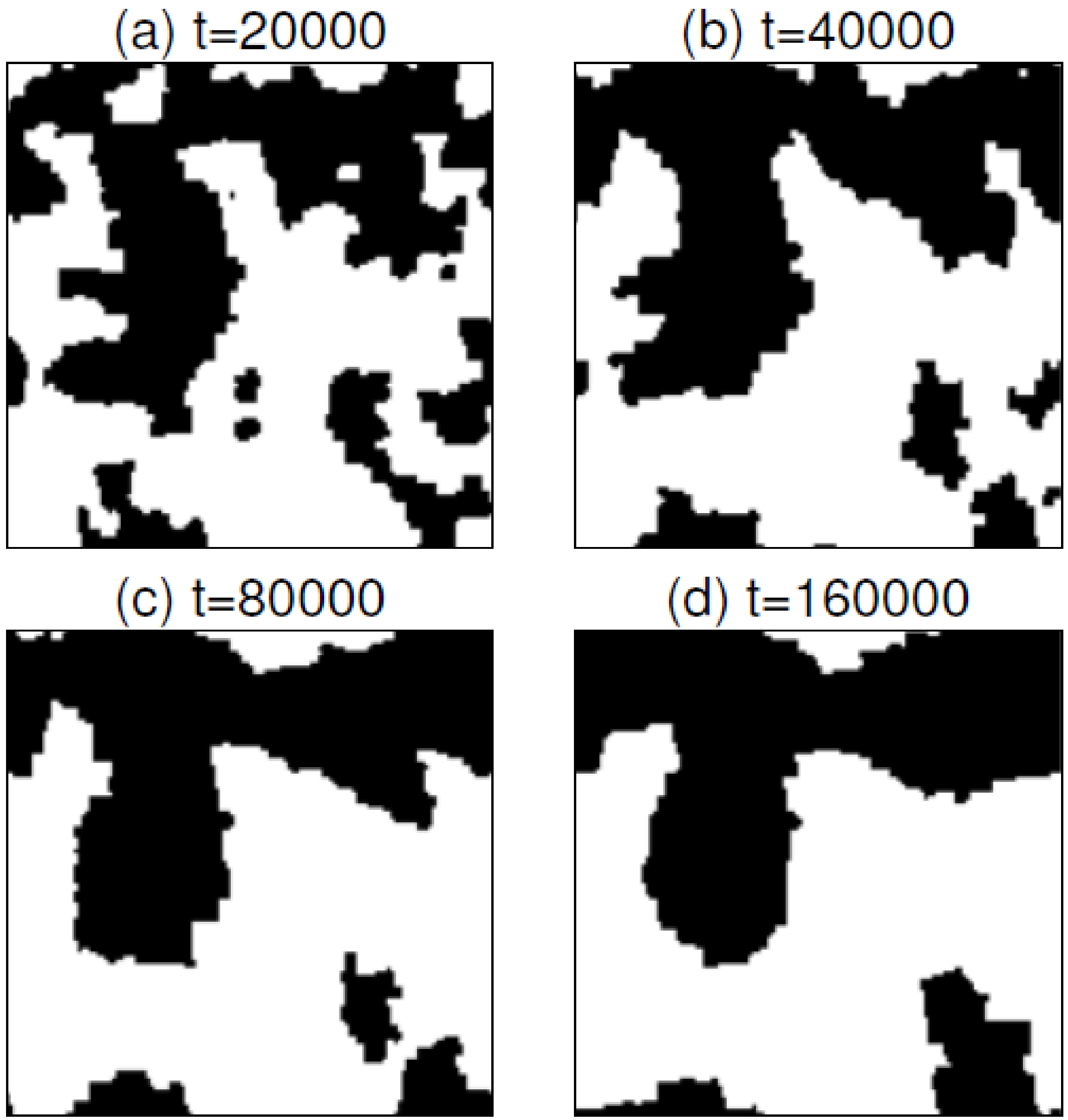
- 1. 2D square lattice
- 2. Simulated annealing
- 3. Measure energy
- 4. Flip random fields

1. Initial State

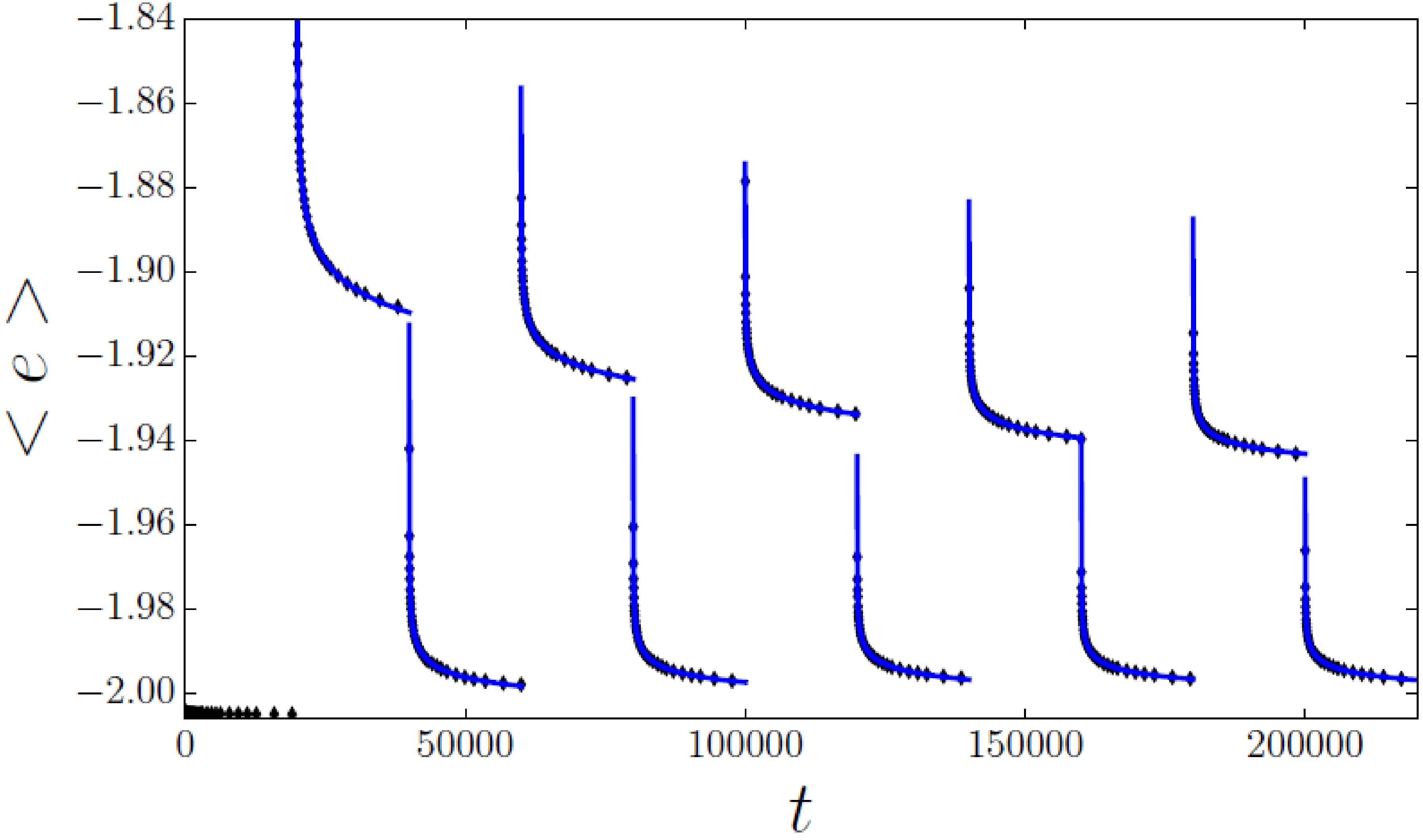


2. After Annealing

Monte Carlo Simulation

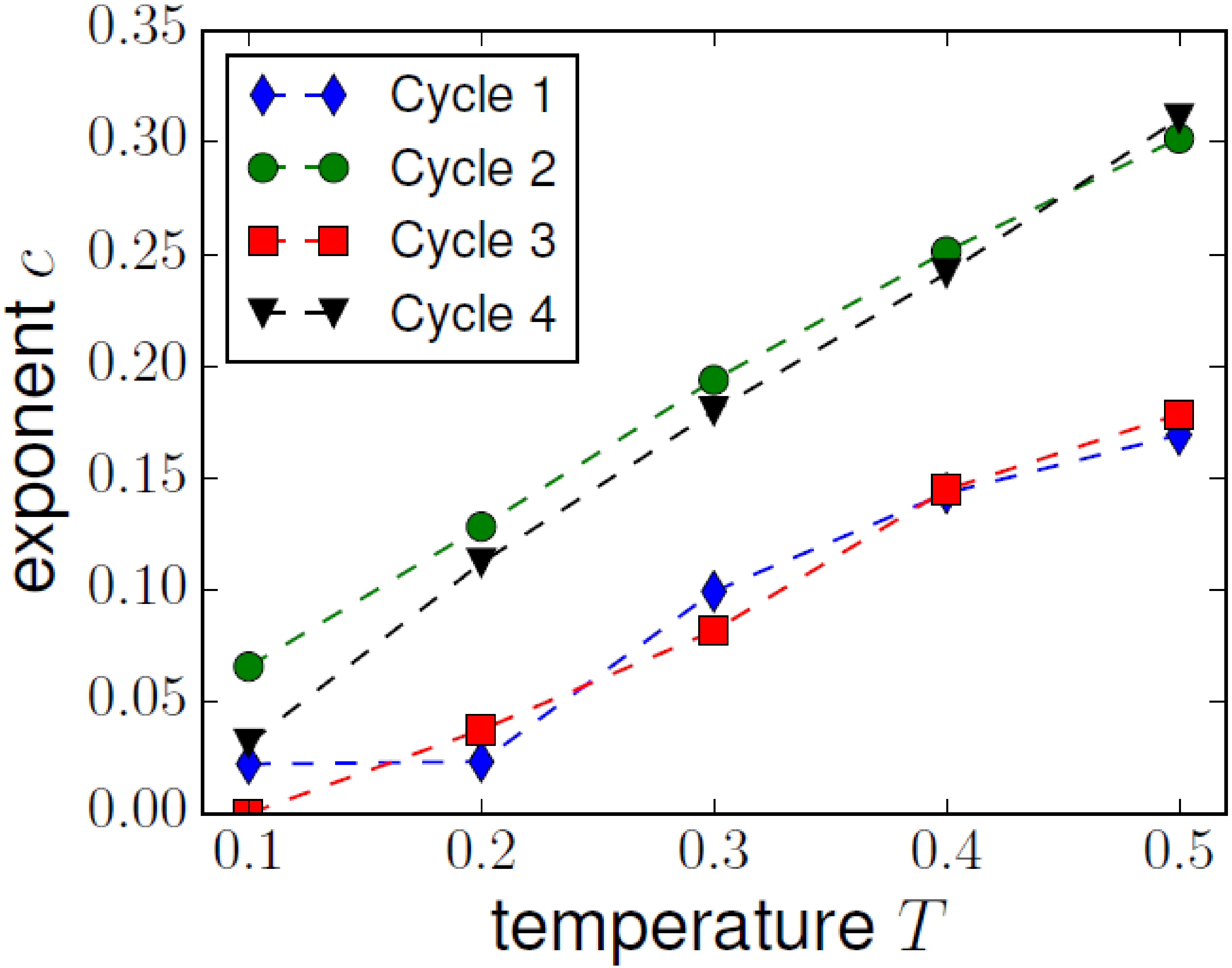


Monte Carlo Simulation



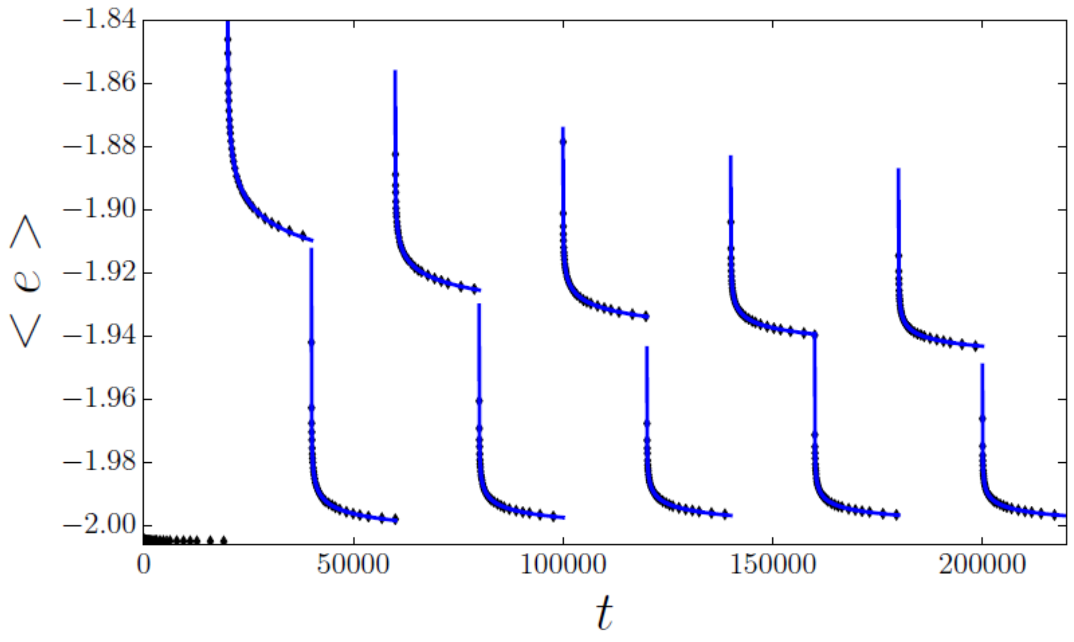
$$\langle e \rangle = e_0 + A \cdot t^{-c}$$

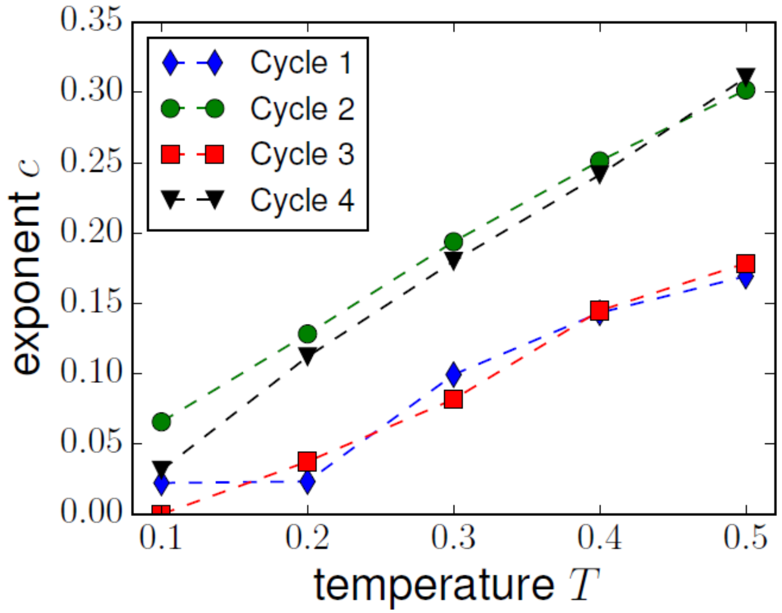
Power-law relaxation



Summary and Conclusion

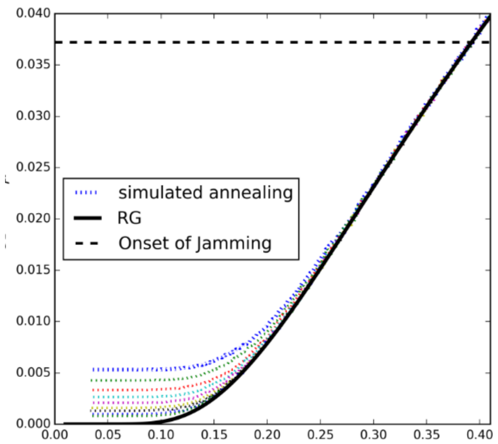
- Simulations agree well with experiments
- Power-law relaxation is confirmed
- Help understand experiment: interface frustration driven

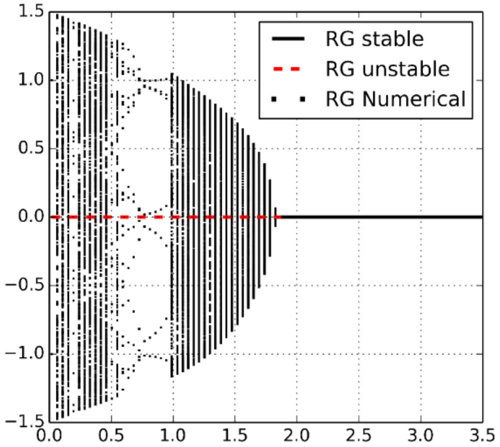


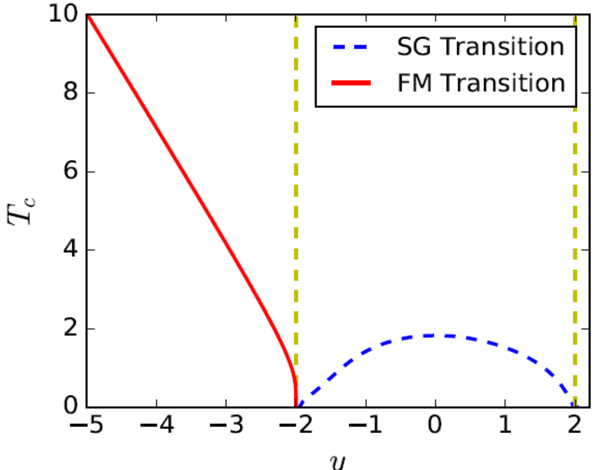


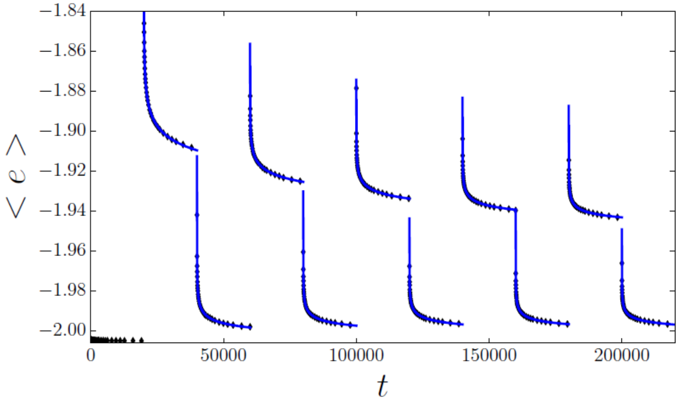
Summary and Conclusion

- 3 Disordered Systems
  - Lattice glass model: dynamics- & geometry-induced disorder
  - Antiferromagnetic Ising model: geometry-induced disorder
  - Random field Ising model: quenched disorder
- Glassy dynamics & power-law relaxation
- Equilibrium phase transition is not necessary
- Glassy dynamics & chaos indicate computational complexity









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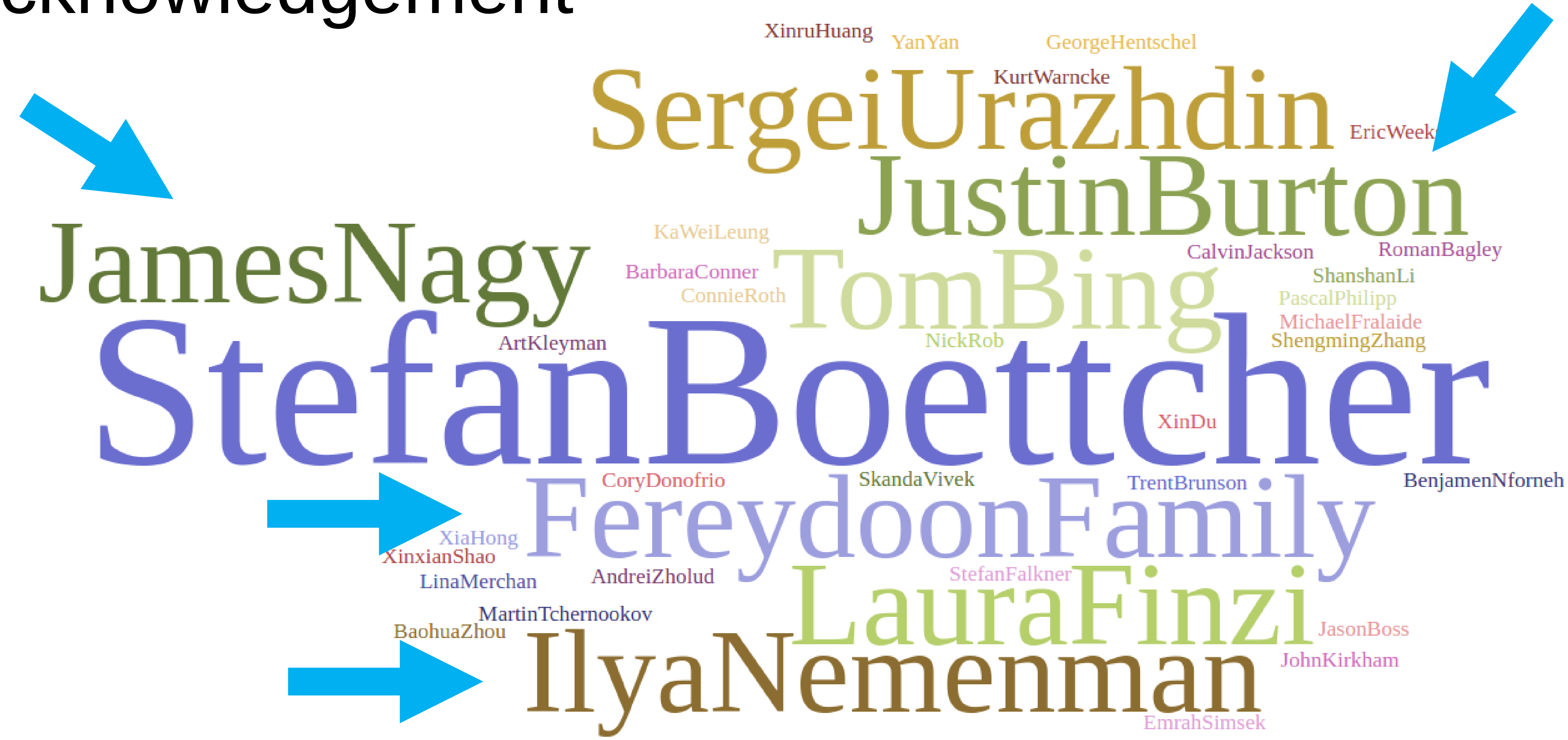

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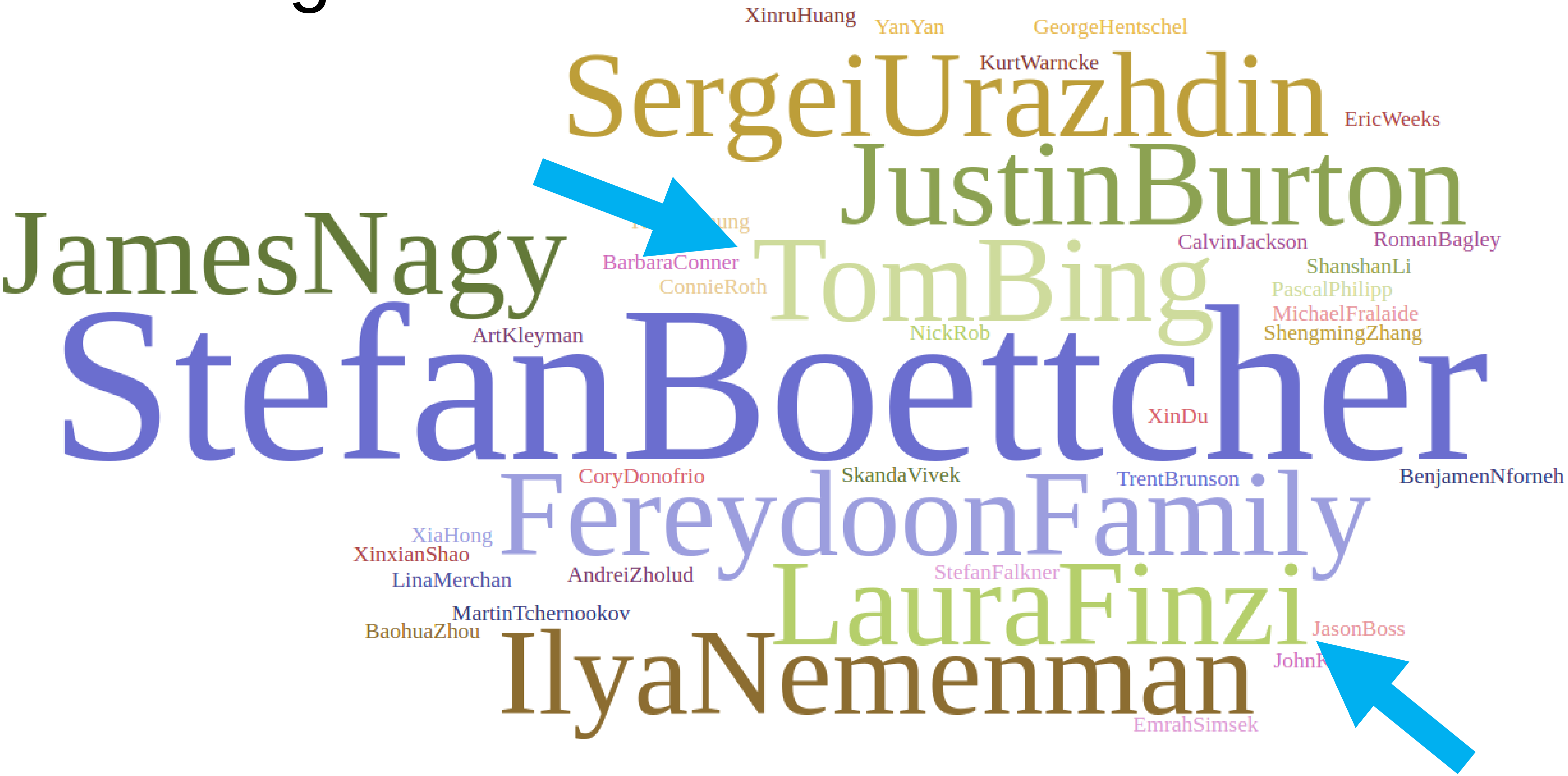

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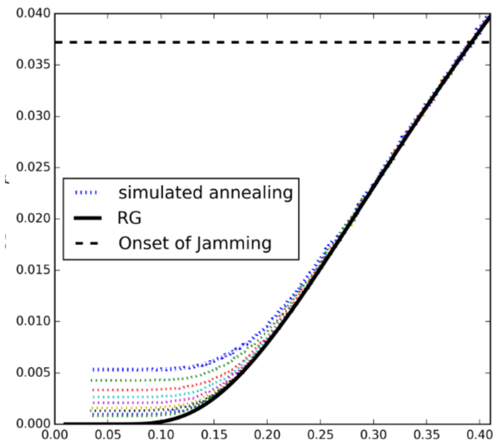

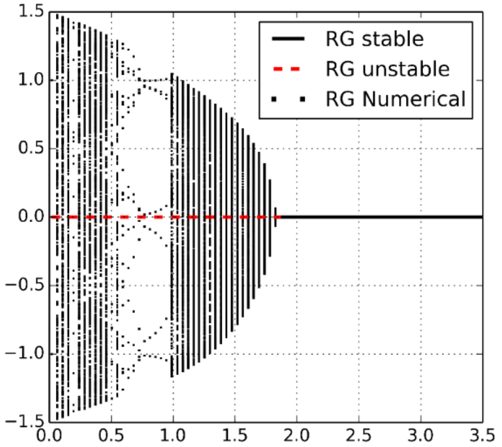

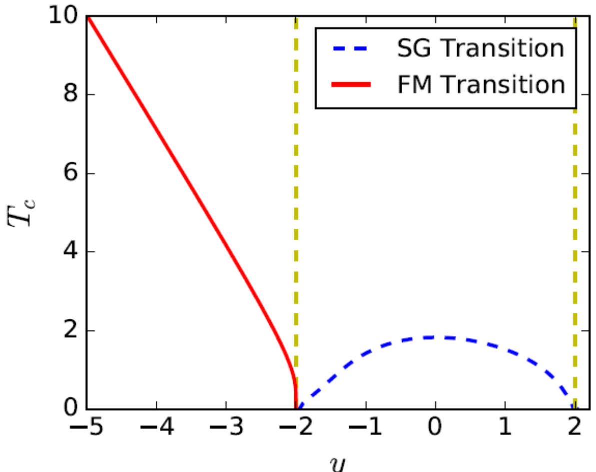

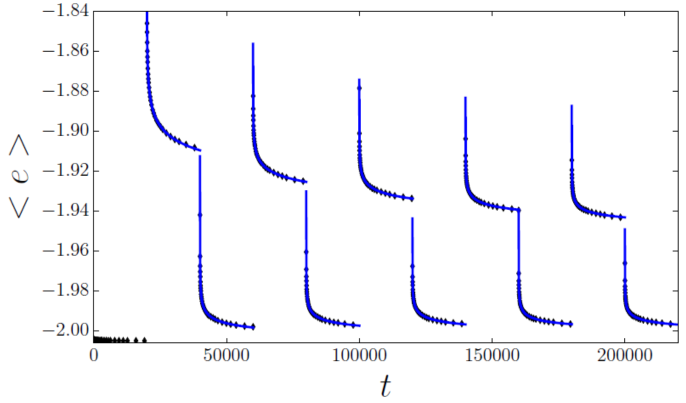

Chaos

- Chaos results from
  - dissimilar configurations
  - Similar free energies
  - Different energy and entropy
- $\Delta F = \Delta E - T\Delta \mathrm{S}$
- Spin glass chaos: ΔE, ΔS are big