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Computational and Theoretical Study of Disordered Systems

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PhD Dissertation Defense

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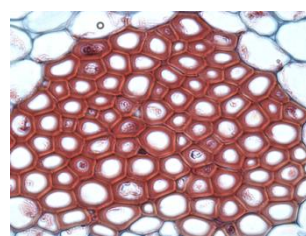
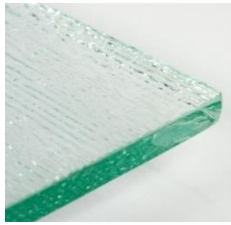


Outline

- 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.



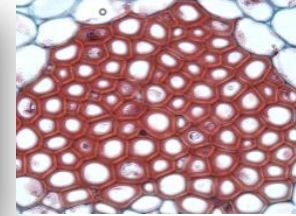
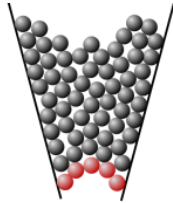
- More unclear questions
- Focus on theoretical models
 - Lattice glass model
 - Antiferromagnetic Ising model
 - Random Field Ising model

Outline

- Introduction of Disordered Systems
- **Jamming in Hierarchical Networks (HNs)**
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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?

Model: lattice glass model

- Biroli-Mezard Model (BM)

Structural disorder → Complex Dynamics

Model: lattice glass model

- Biroli-Mezard Model (BM)

Structural disorder \rightarrow Complex Dynamics

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

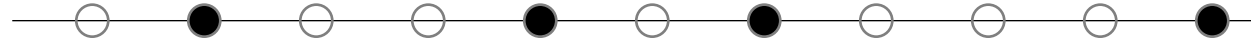
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Example: $l = 0$



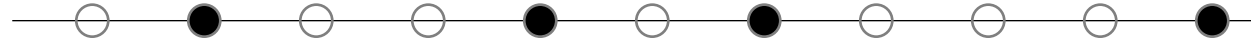
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$$\Xi = \sum_{n=0}^{n_{\max}} g_n \exp(n\beta\mu)$$

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

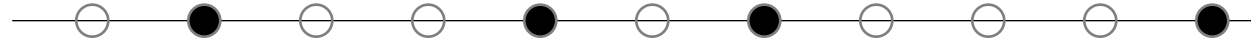
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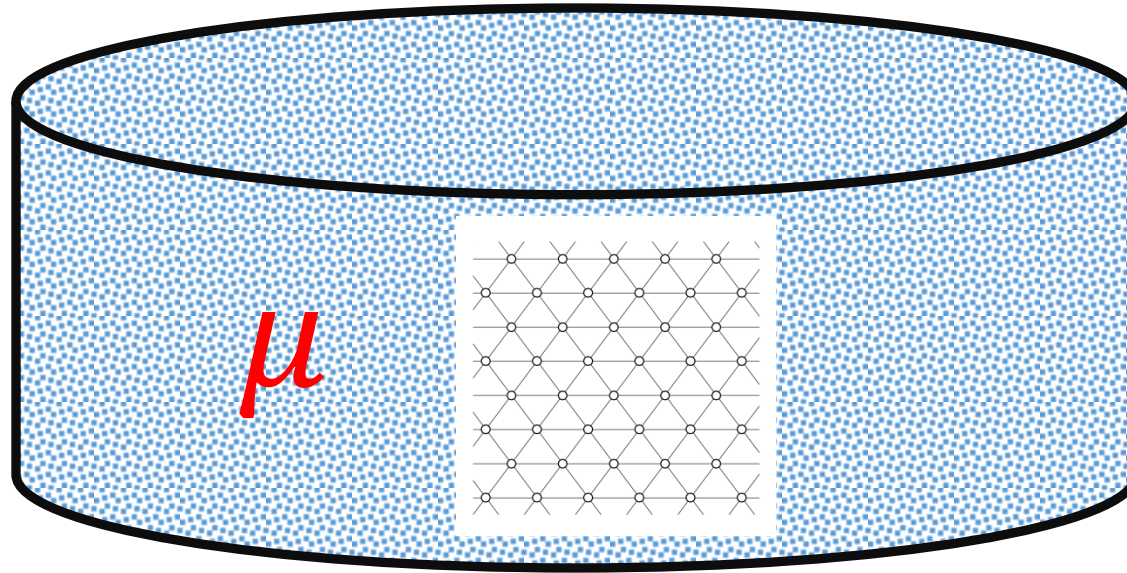
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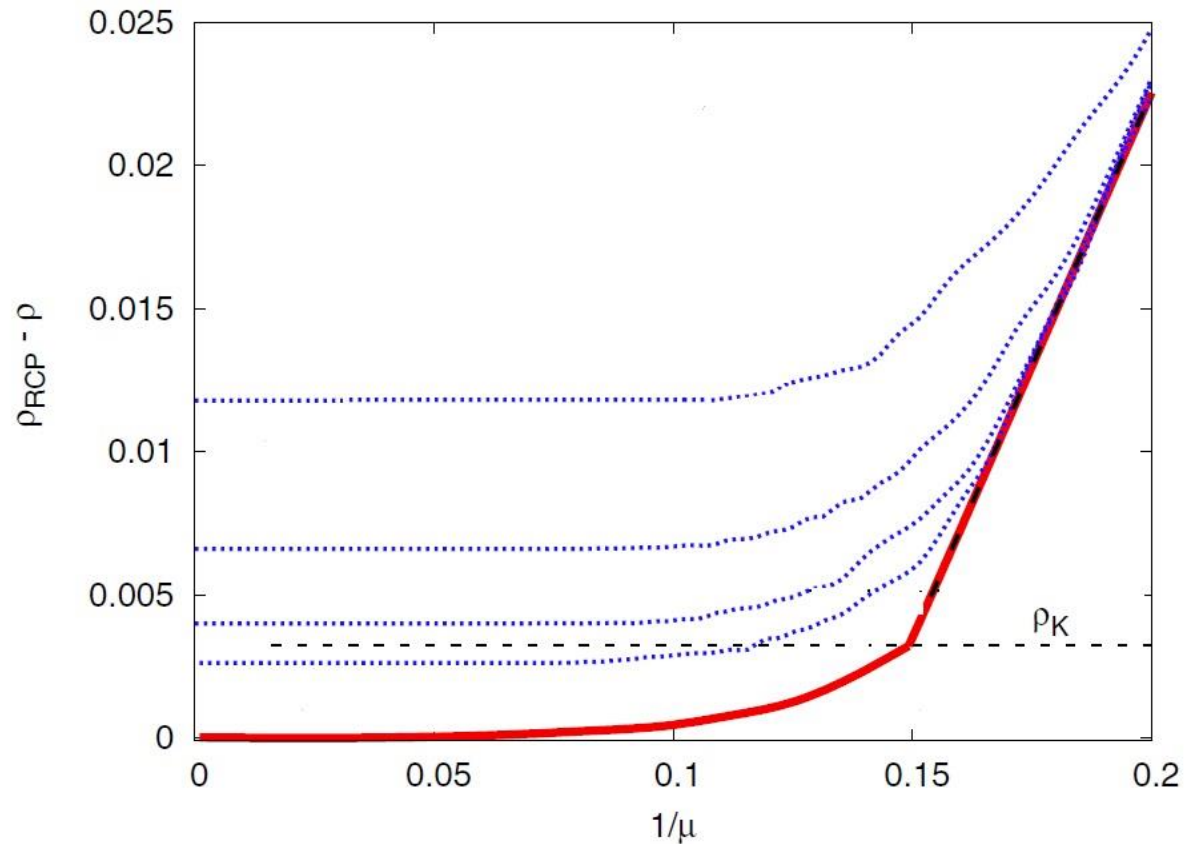
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- g_n is the density of state with n particles

Jamming in lattice glass model



- Bigger $\mu \rightarrow$ higher packing fraction ρ
- μ is big enough \rightarrow non-equilibrium state: **Jamming state**
- Mean field theory \rightarrow phase transition underlying jamming transition

Equilibrium phase transition \iff Jamming Transition?



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

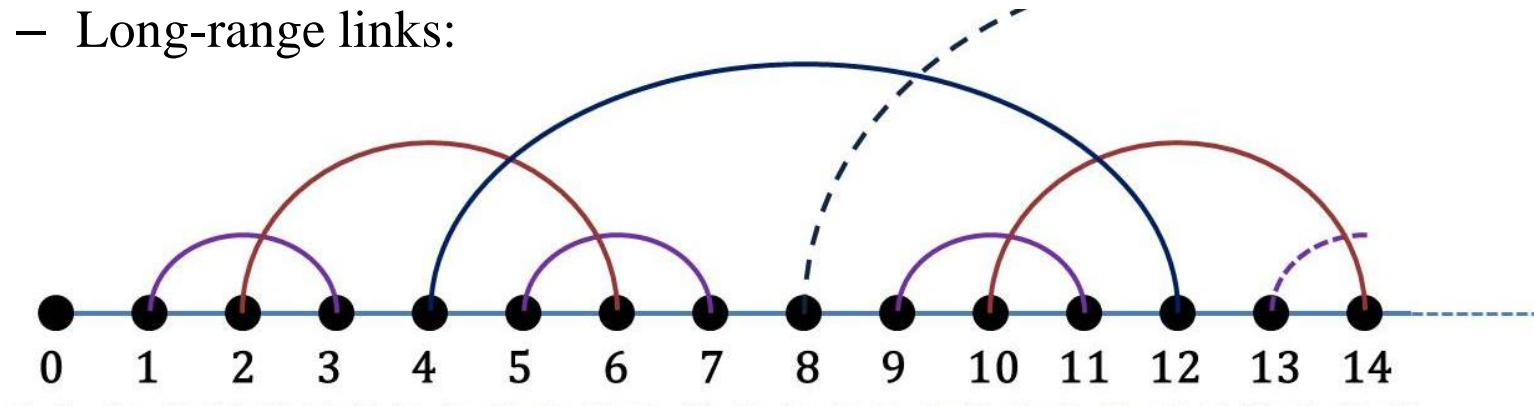
True in non-mean-field model?

Model: Hierarchical Networks

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

Model: Hierarchical Networks

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Model: Hierarchical Networks

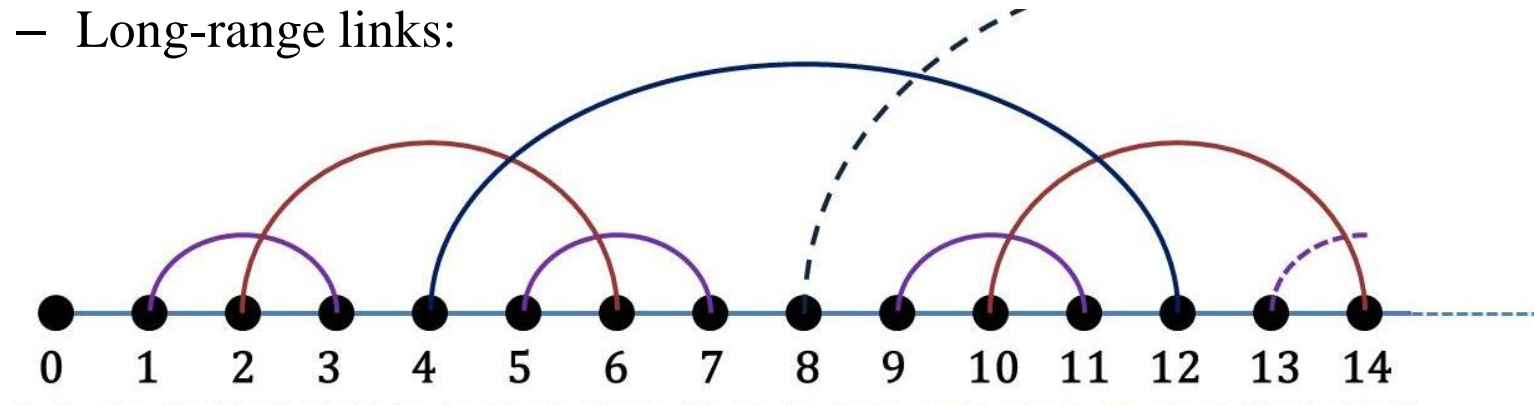
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$$N = 2^1 + 1$$



Model: Hierarchical Networks

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



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

Why Hierarchical Networks (HNs)?

- Exactly solvable by Renormalization Group (RG)
- Lattice-like structure
 - Mean-Field \Rightarrow HNs \Rightarrow 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 → Experiment
randomly add or remove particle with $P(\mu)$;
 μ is increased by $d\mu$ per MC sweep;
 - Wang-Landau Sampling → Density of States g_n

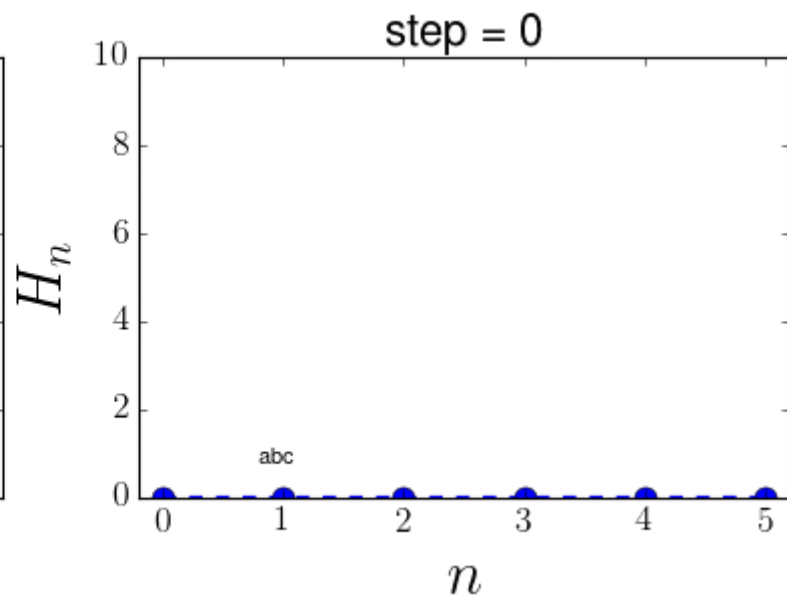
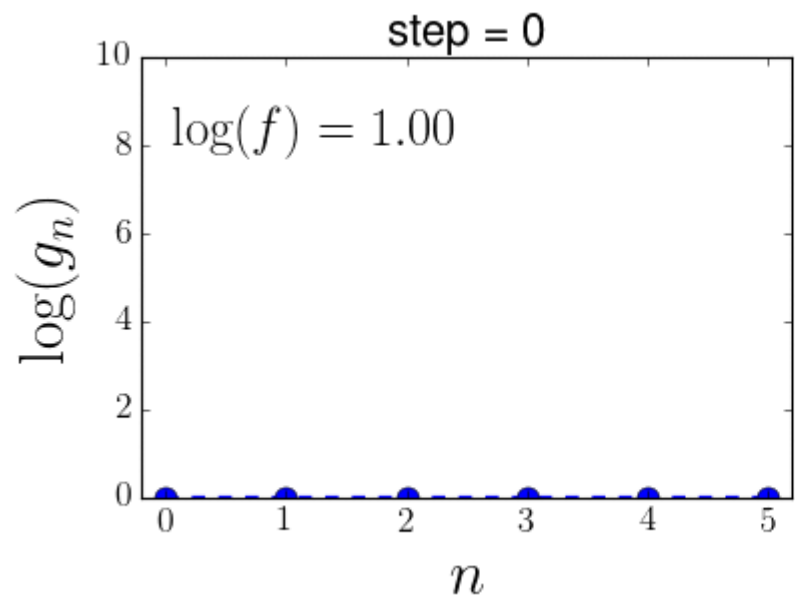
$$\Xi = \sum_{n=0}^{n_{\max}} g_n \exp(n\mu)$$

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

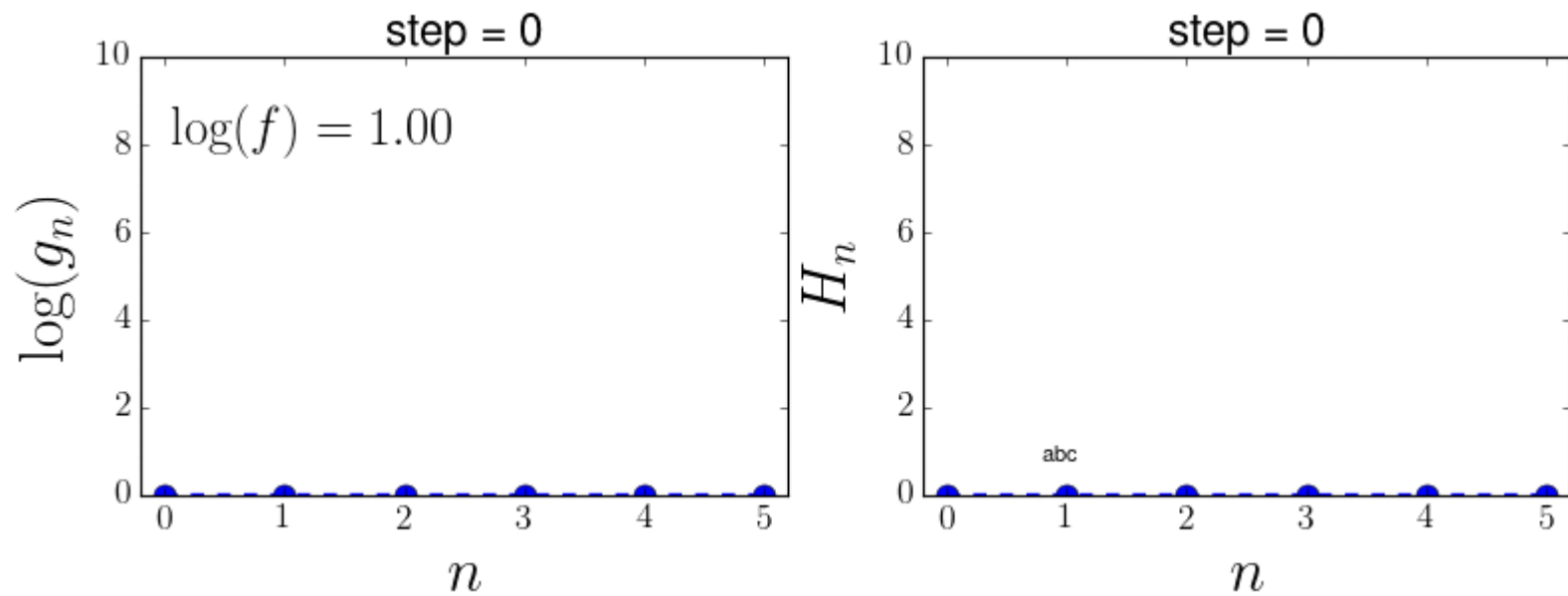
Wang-Landau sampling

- Histogram method
 - Sampling with probability $\hat{P} \propto 1/P \rightarrow$ **flat histogram**
 - Non-thermodynamic, Non-Markov-Chain Monte Carlo
- Procedure
 - Initial guess: flat $g_n \{1, 1, 1, 1, \dots\}$ and flat $H_n \{0, 0, 0, 0, \dots\}$
 - 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. $H_n = H_n + 1$; $g_n = g_n \times f$
 - 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

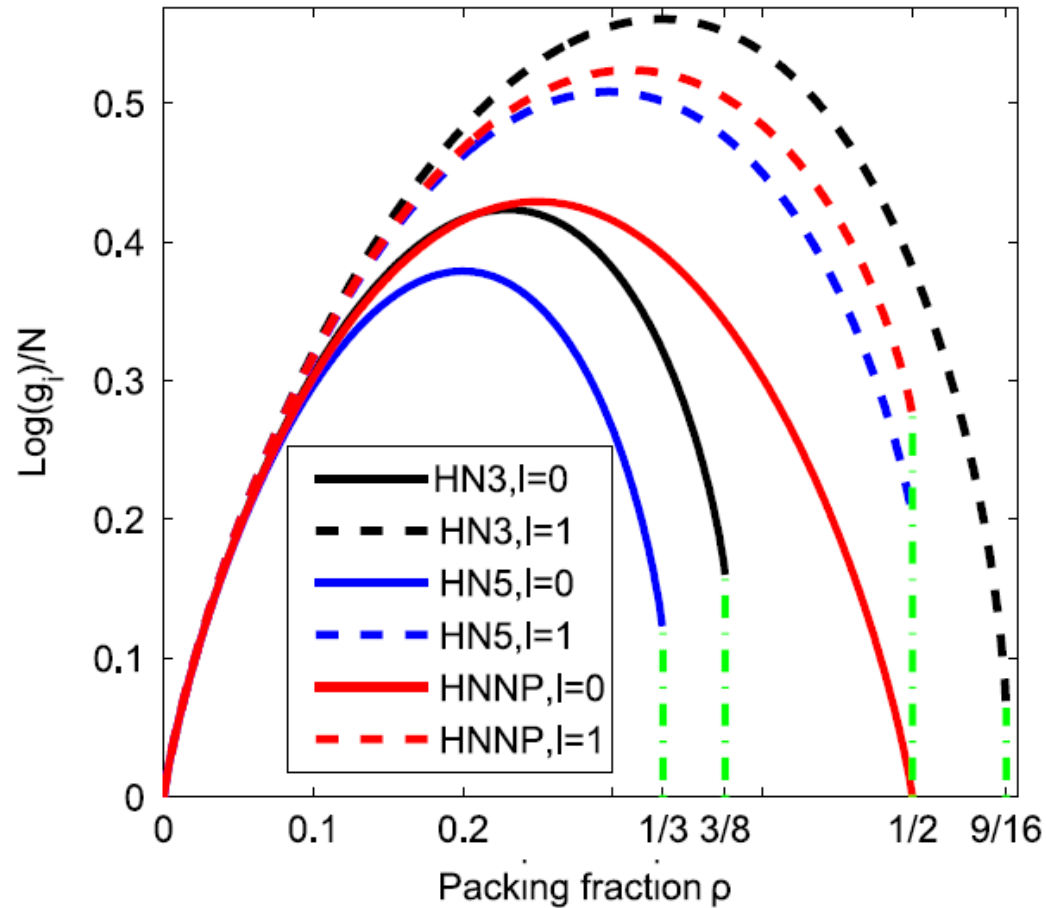


Extremely slow for large system size

Wang-Landau sampling

- Histogram method
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 - Randomly pick a site i
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 - **Exchange particle with an empty site**
 - Update g_n and H_n of the current state, i.e. $H_n = H_n + 1$; $g_n = g_n \times f$
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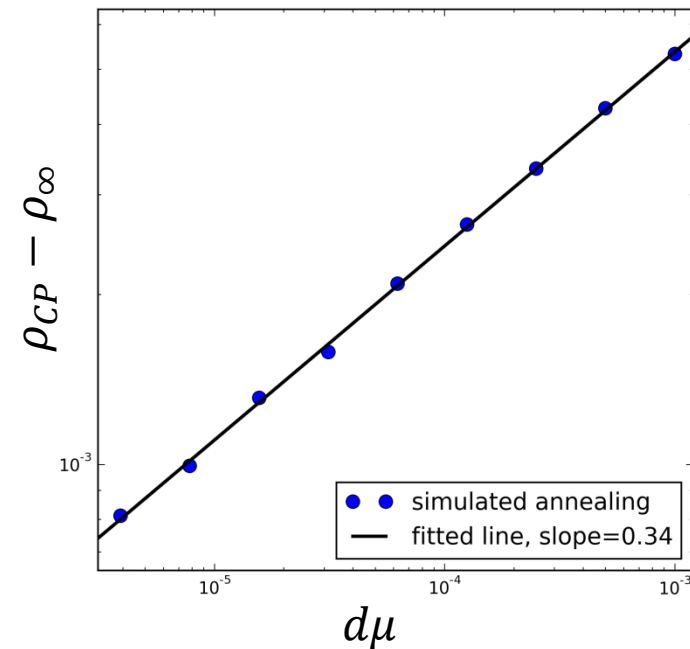
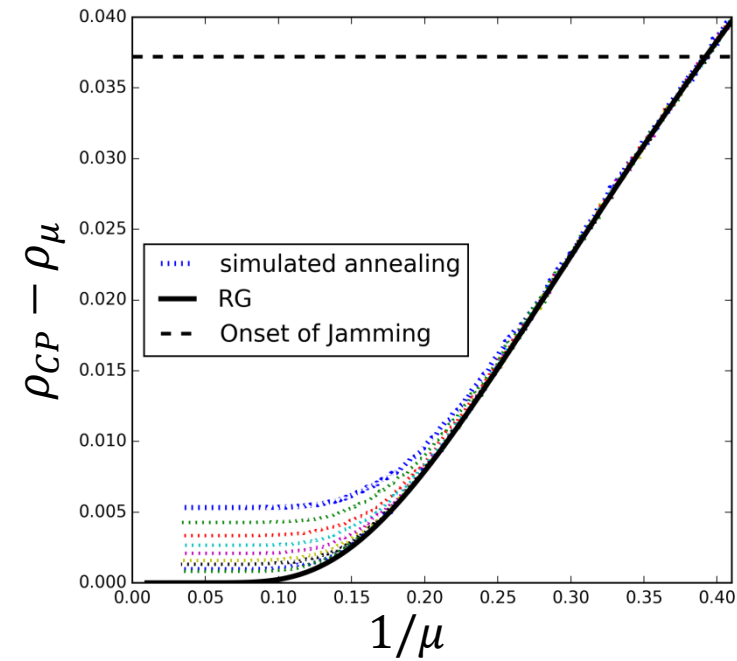
Results of Wang-Landau sampling



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

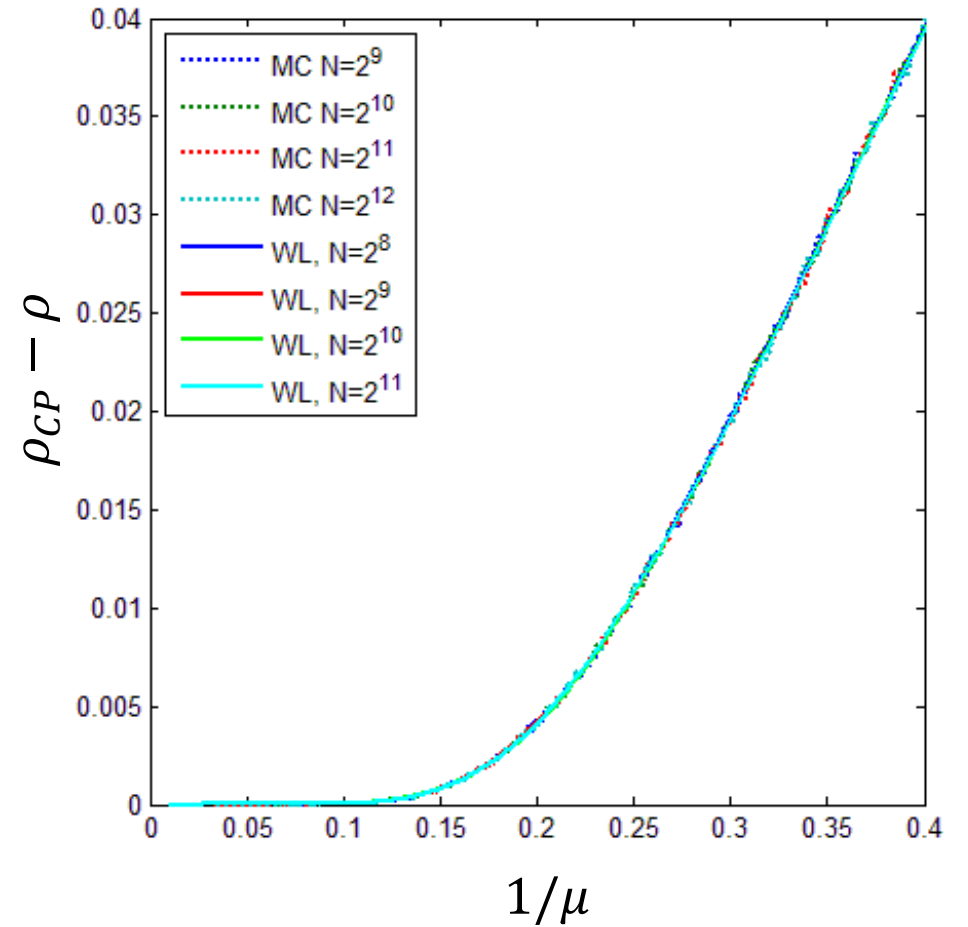
Results of $l = 0$ for HN3

- 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

	$l = 0$	$l = 1$
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

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**

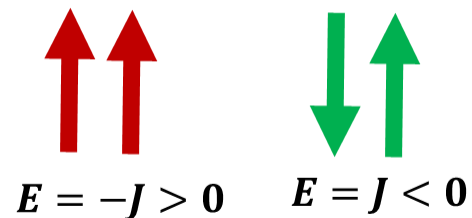
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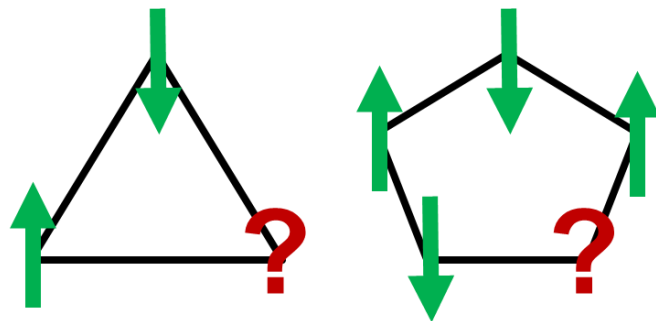
Antiferromagnetic Ising model

- Antiferromagnetic Ising model

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

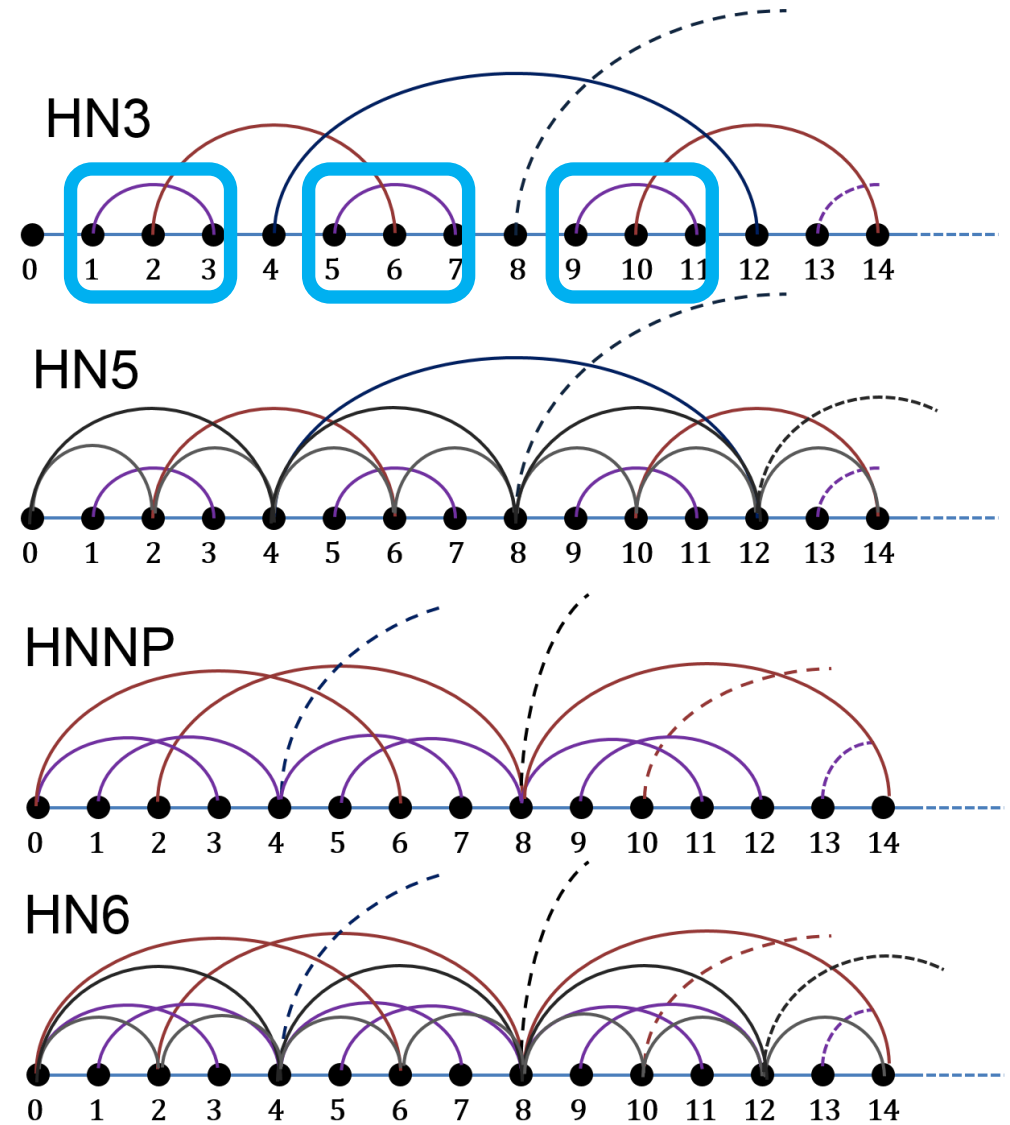


- Geometric frustration: odd loops



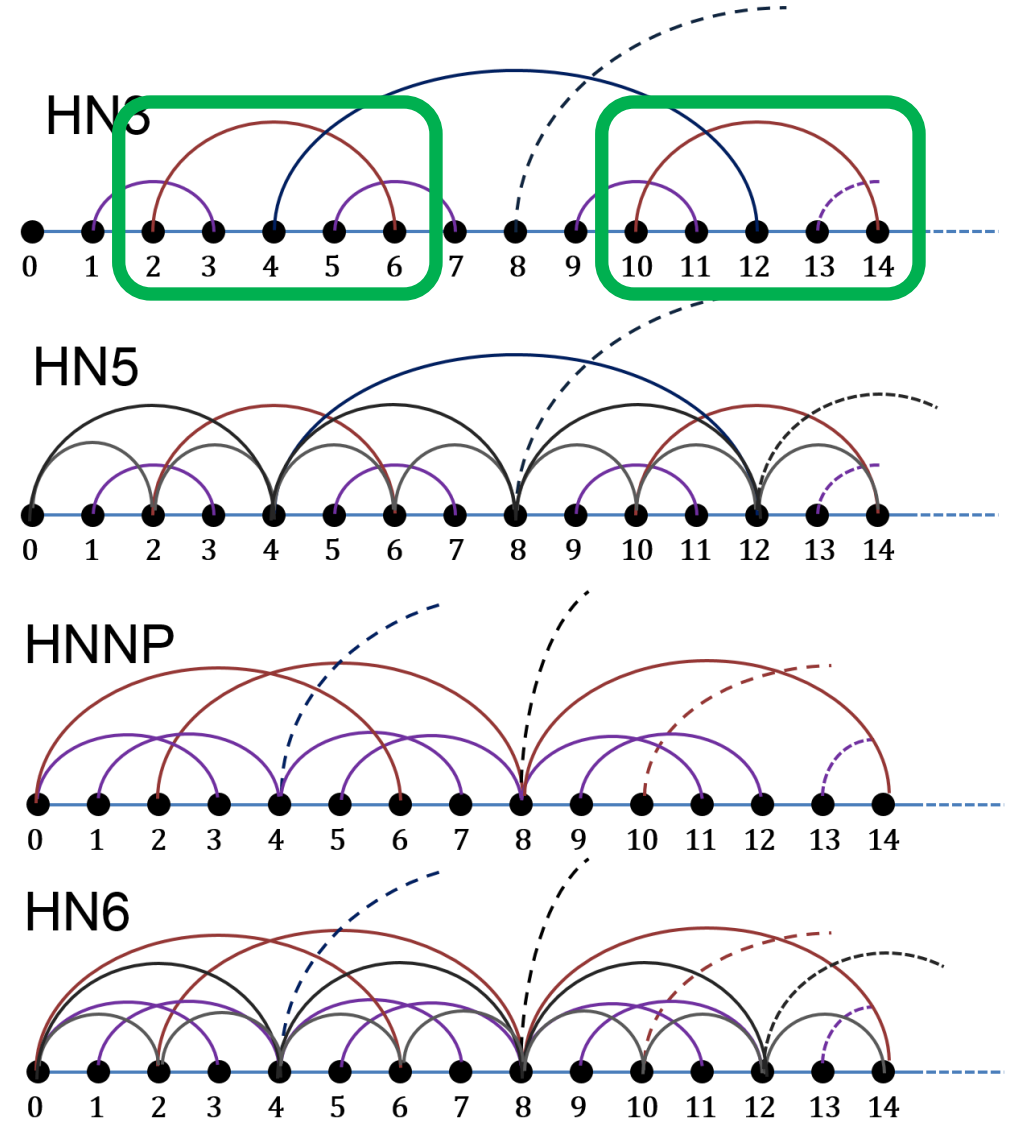
Hierarchical networks (*HNs*)

- HN3
- HN5
- HN6



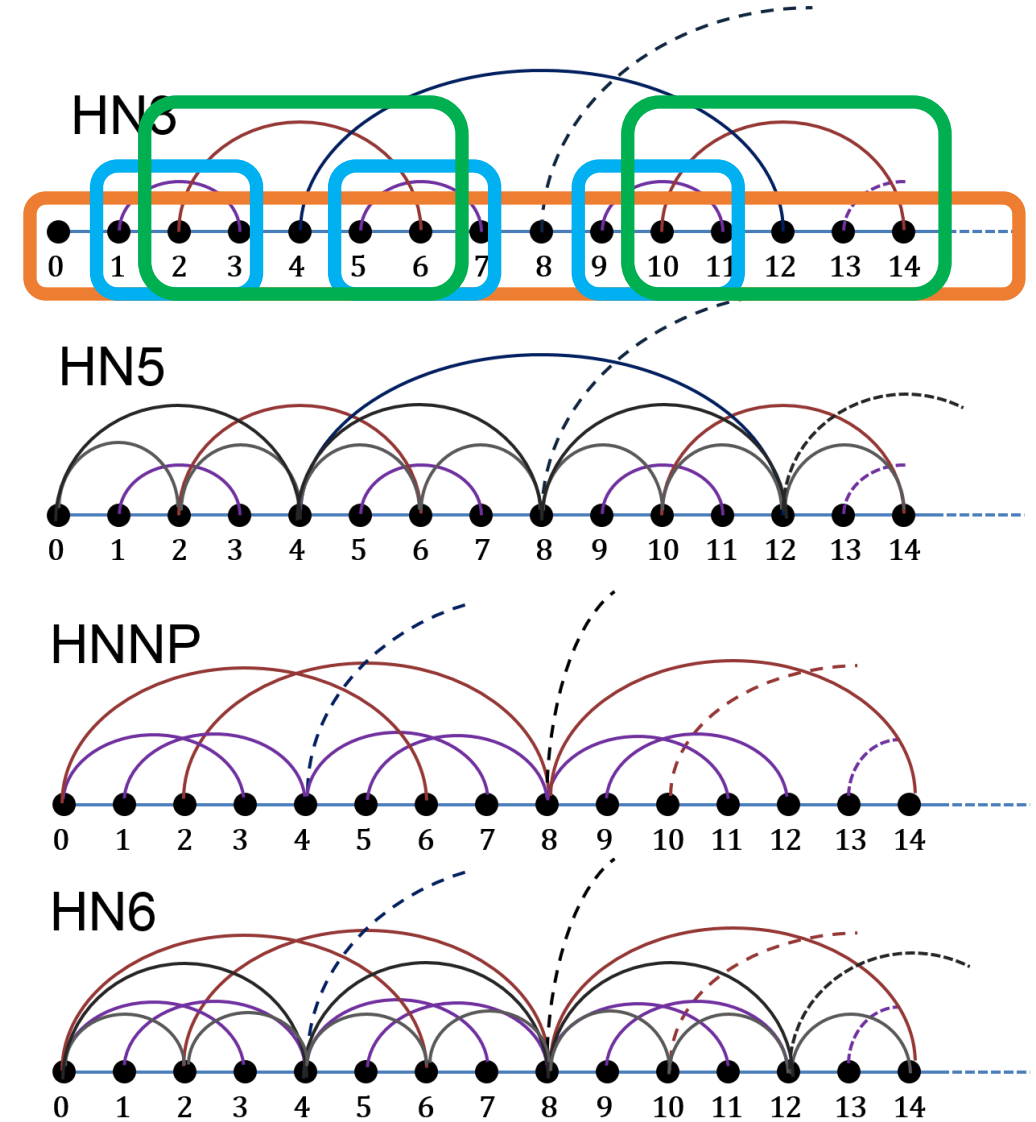
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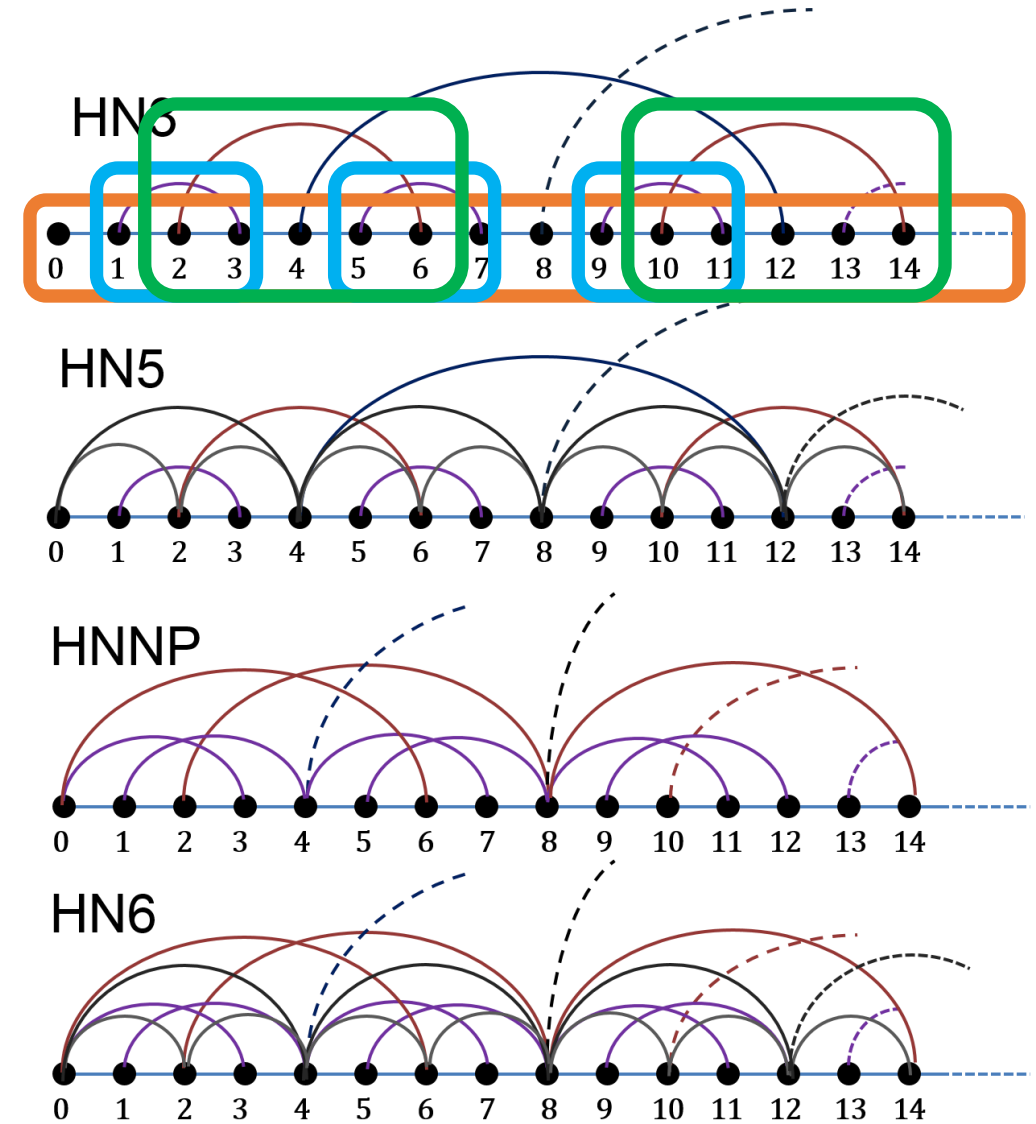
Hierarchical networks (*HNs*)

- HN3
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Hierarchical networks (*HNs*)

- HN3
- HN5
- HN6
- HN6
- Interpolations:
 - Long-range link strength: $y \cdot J$
 - $y = 0$: HN6
 - $y = 1$: HN6



Research Questions

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

Methods

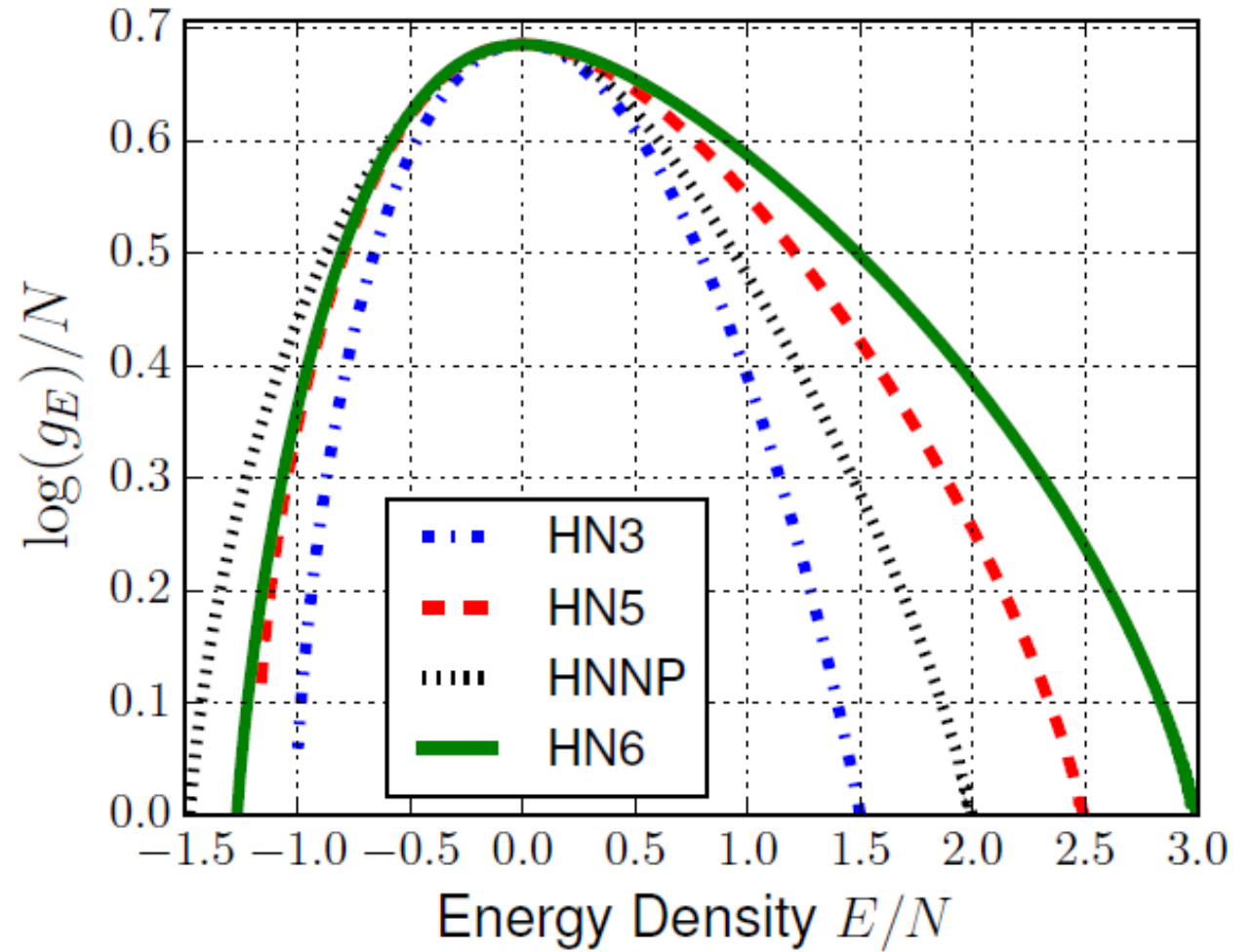
- Monte Carlo Methods:
 - Simulated Annealing → Experiment
 - Wang-Landau Sampling → Density of States g_E

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

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

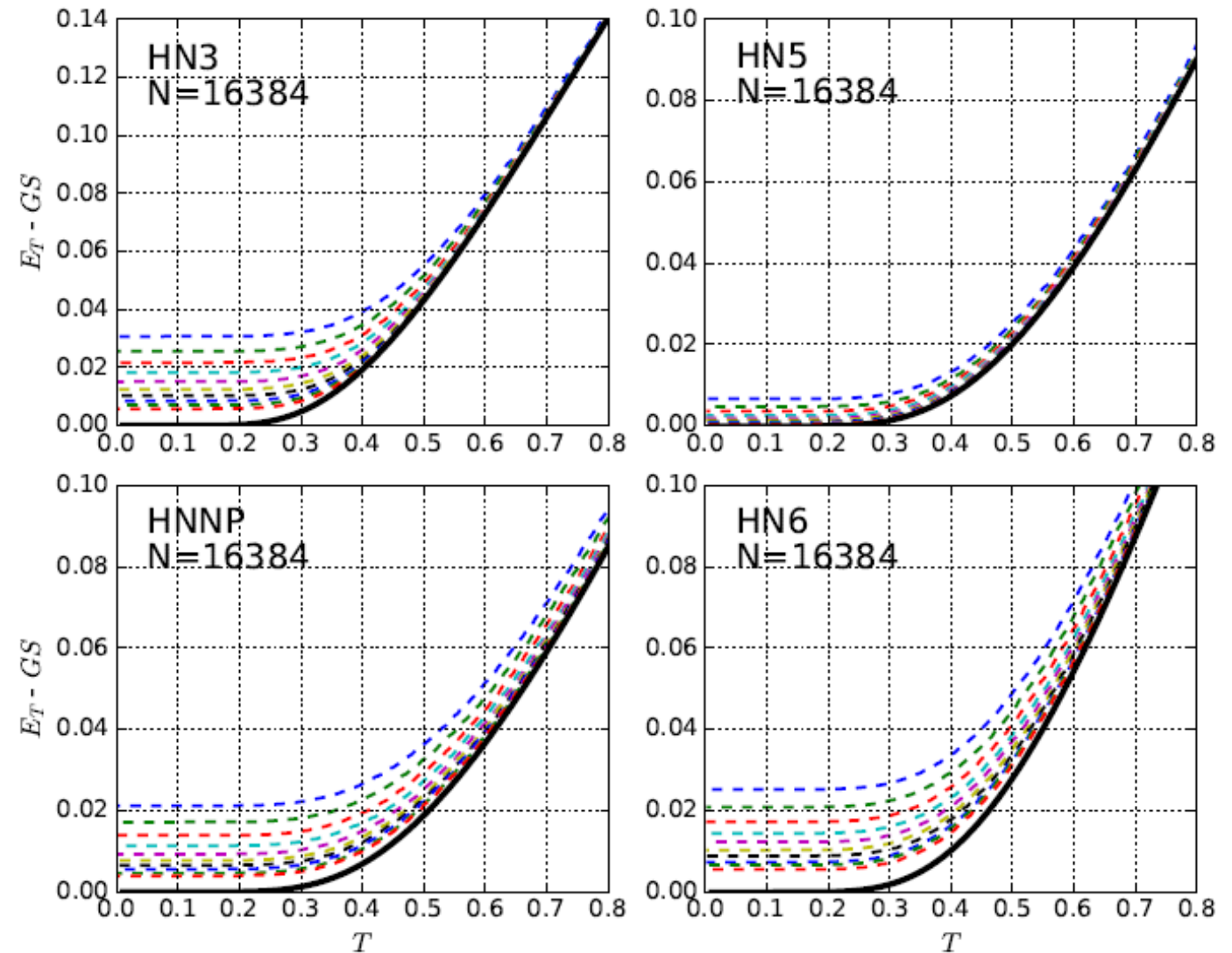
Density of States (WL)

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



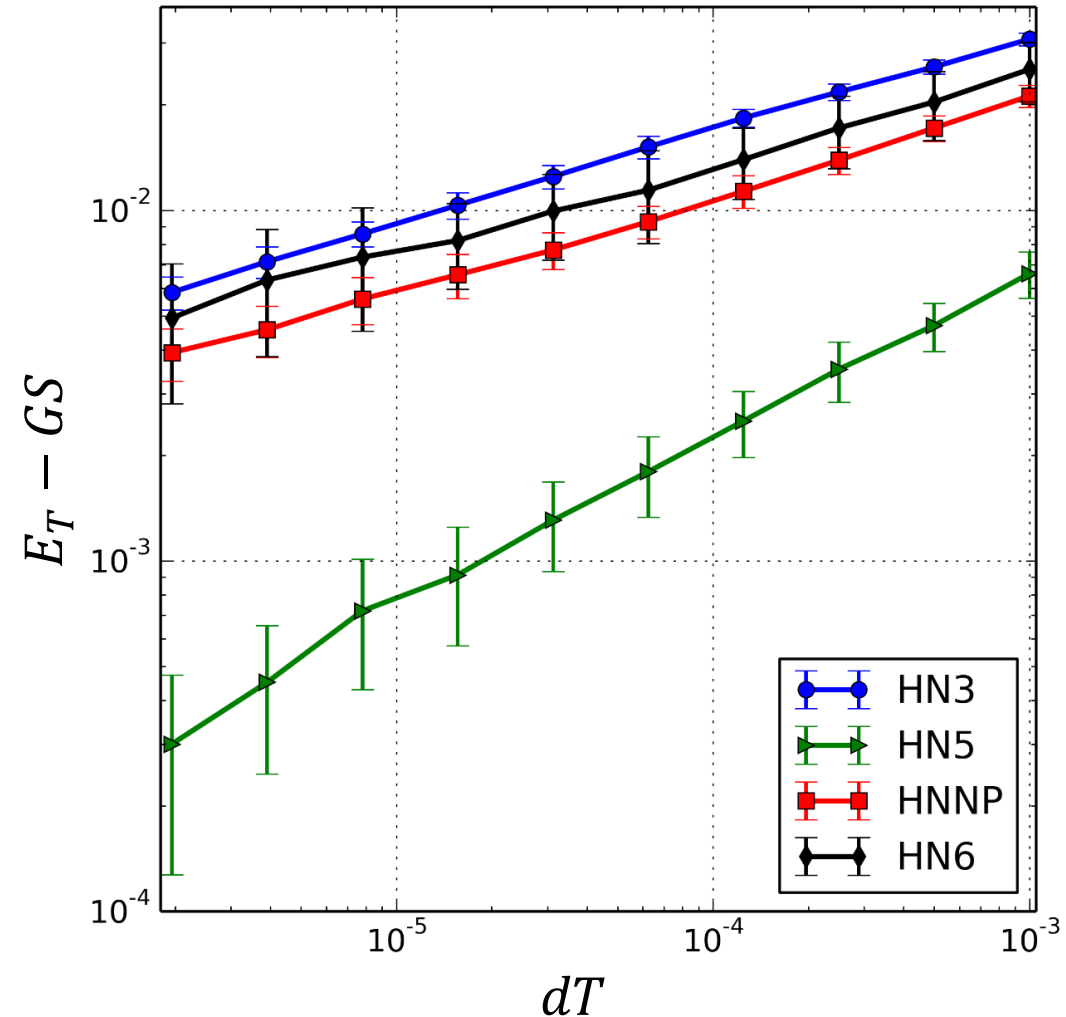
Glassy relaxation (SA)

- 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



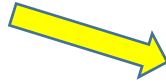
Spin glass transition (RG)

- Renormalized interaction strength J

- Recursive equations



Numerical solution

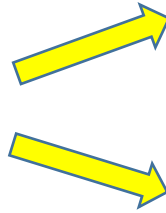


Analytical solution

Spin glass transition (RG)

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Numerical solution

Analytical solution

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

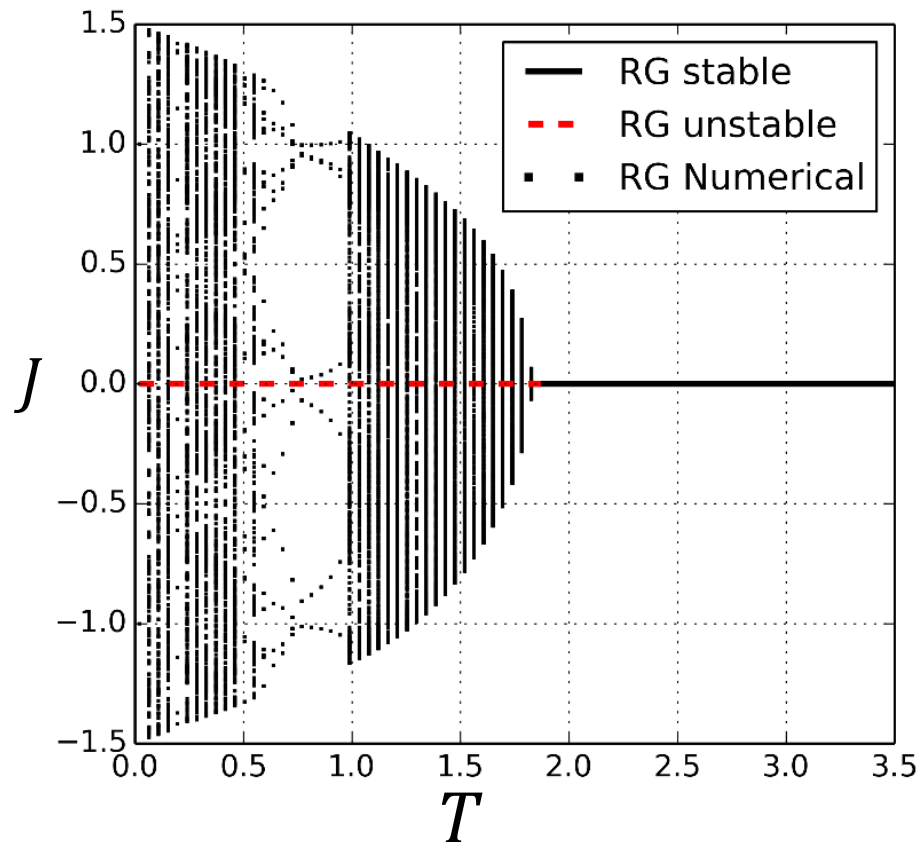
Spin glass transition (RG)

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

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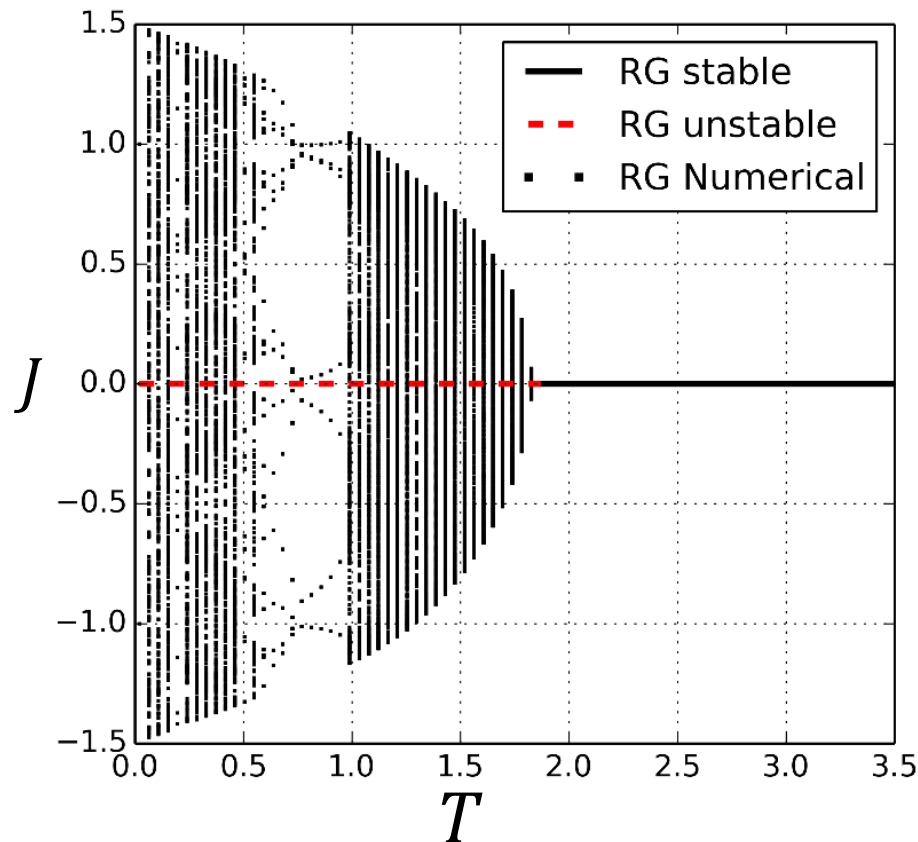
HNPN ($y = 0$)



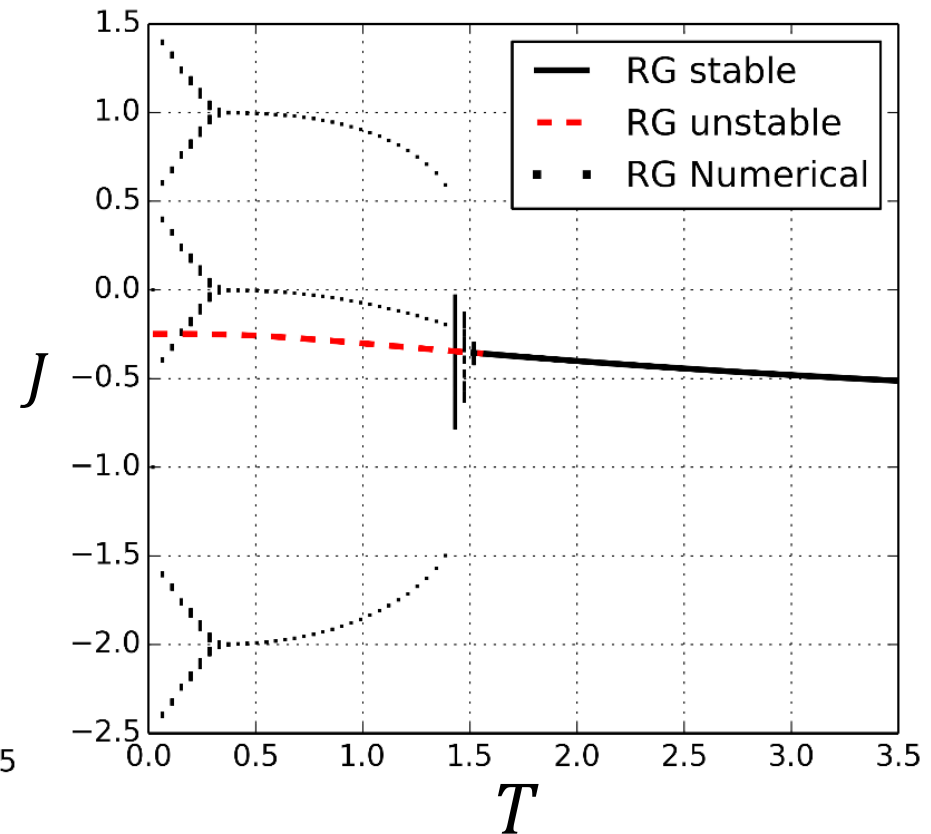
Spin glass transition (RG)

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HNNP ($y = 0$)



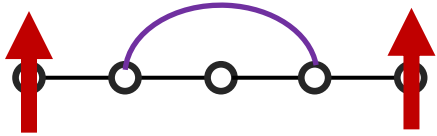
HN6 ($y = 1$)



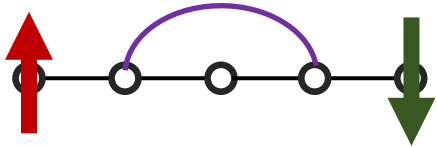
Free energy chaos

- Boundary conditions

- Parallel: up-up



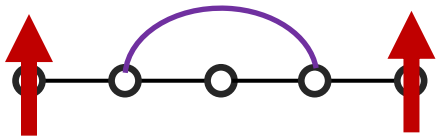
- Anti-parallel: up-down



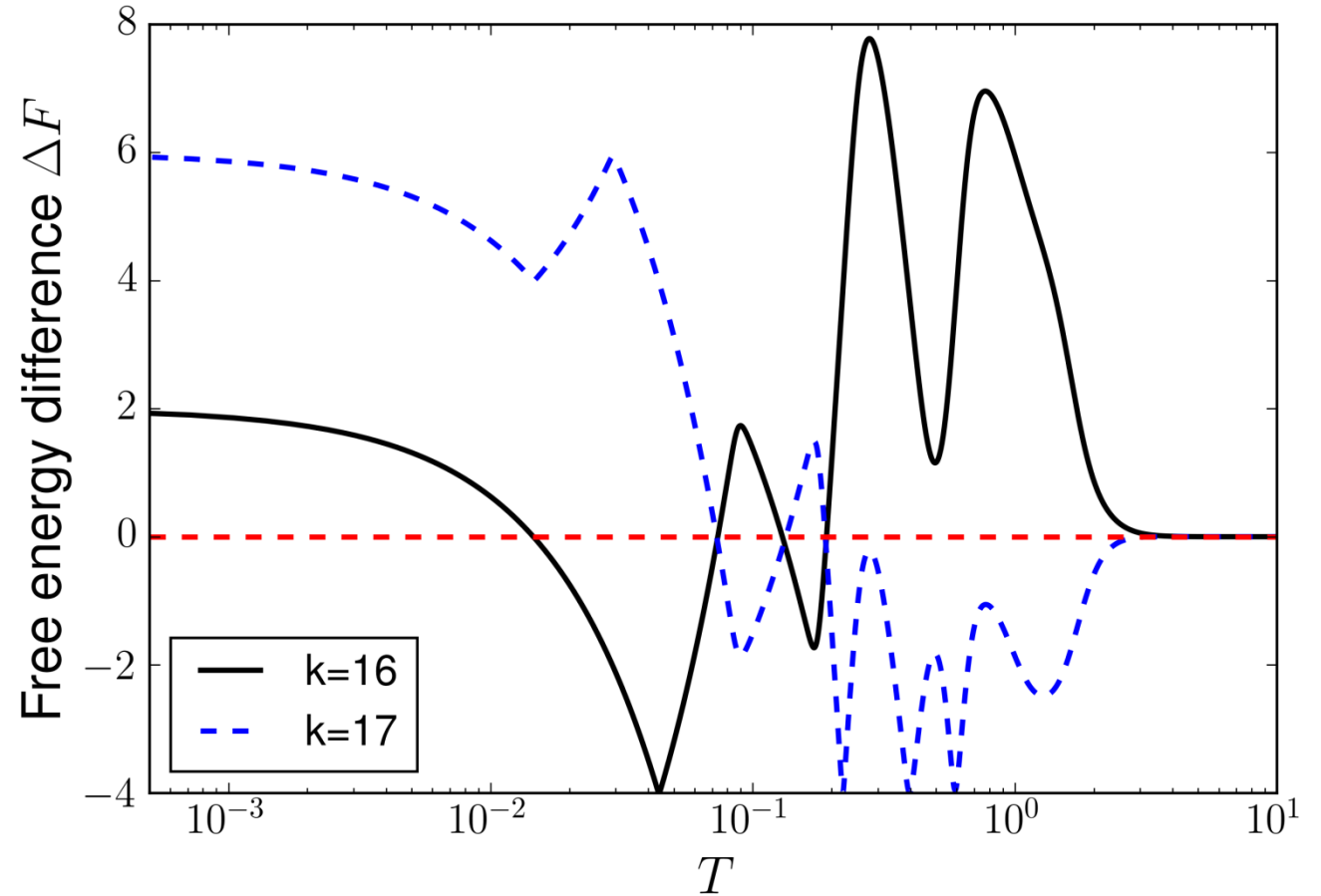
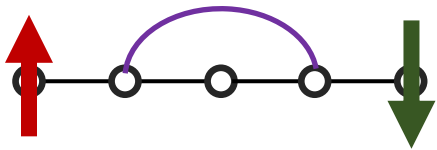
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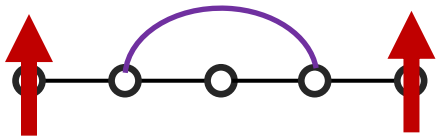
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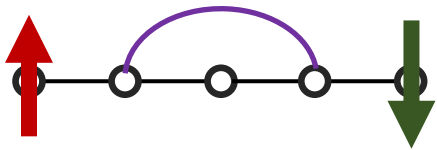
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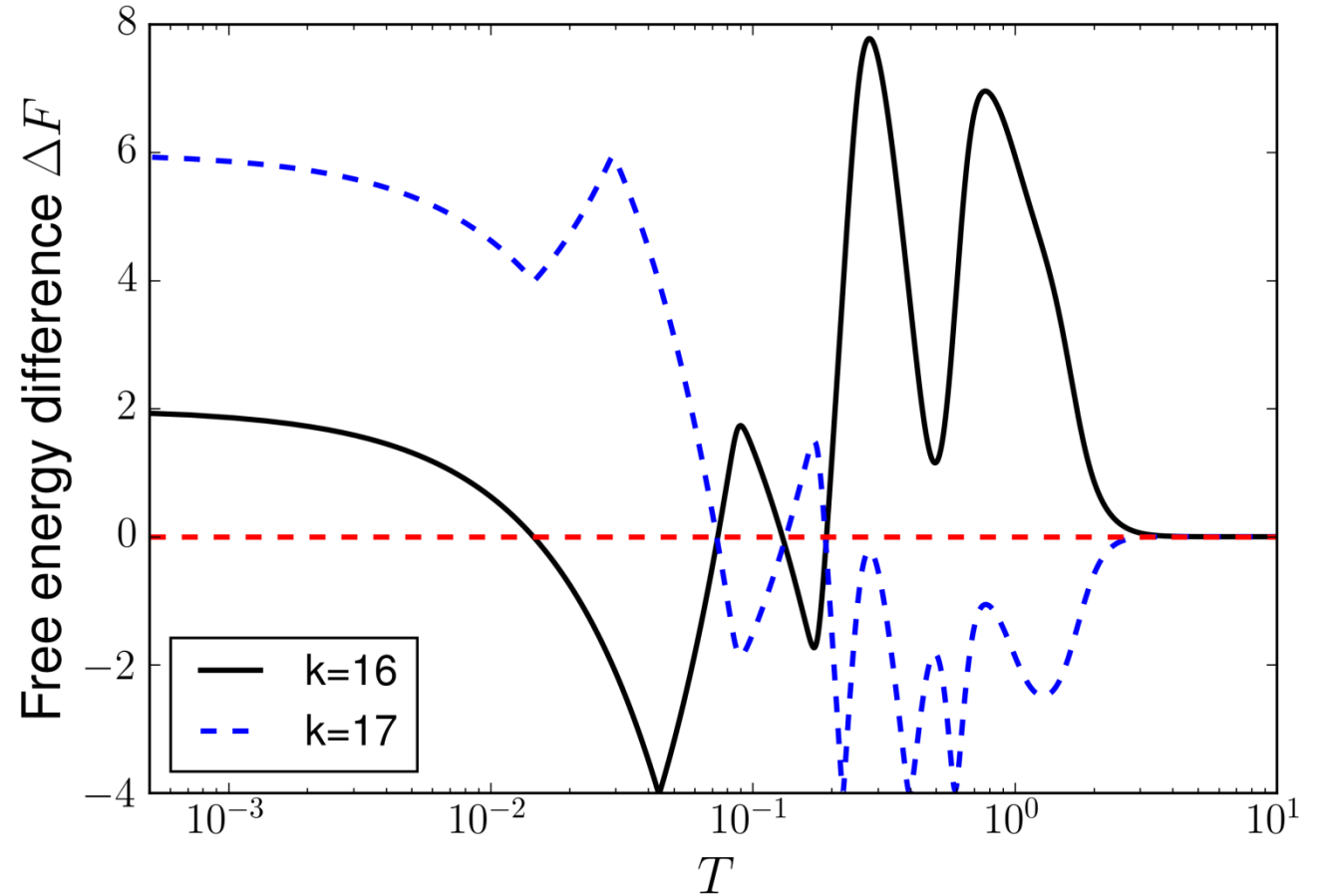
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- Anti-parallel: up-down



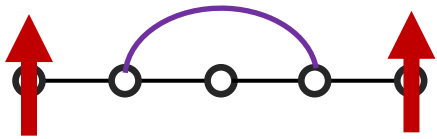
- Crossings N_C



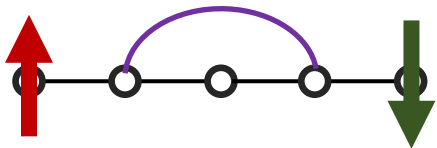
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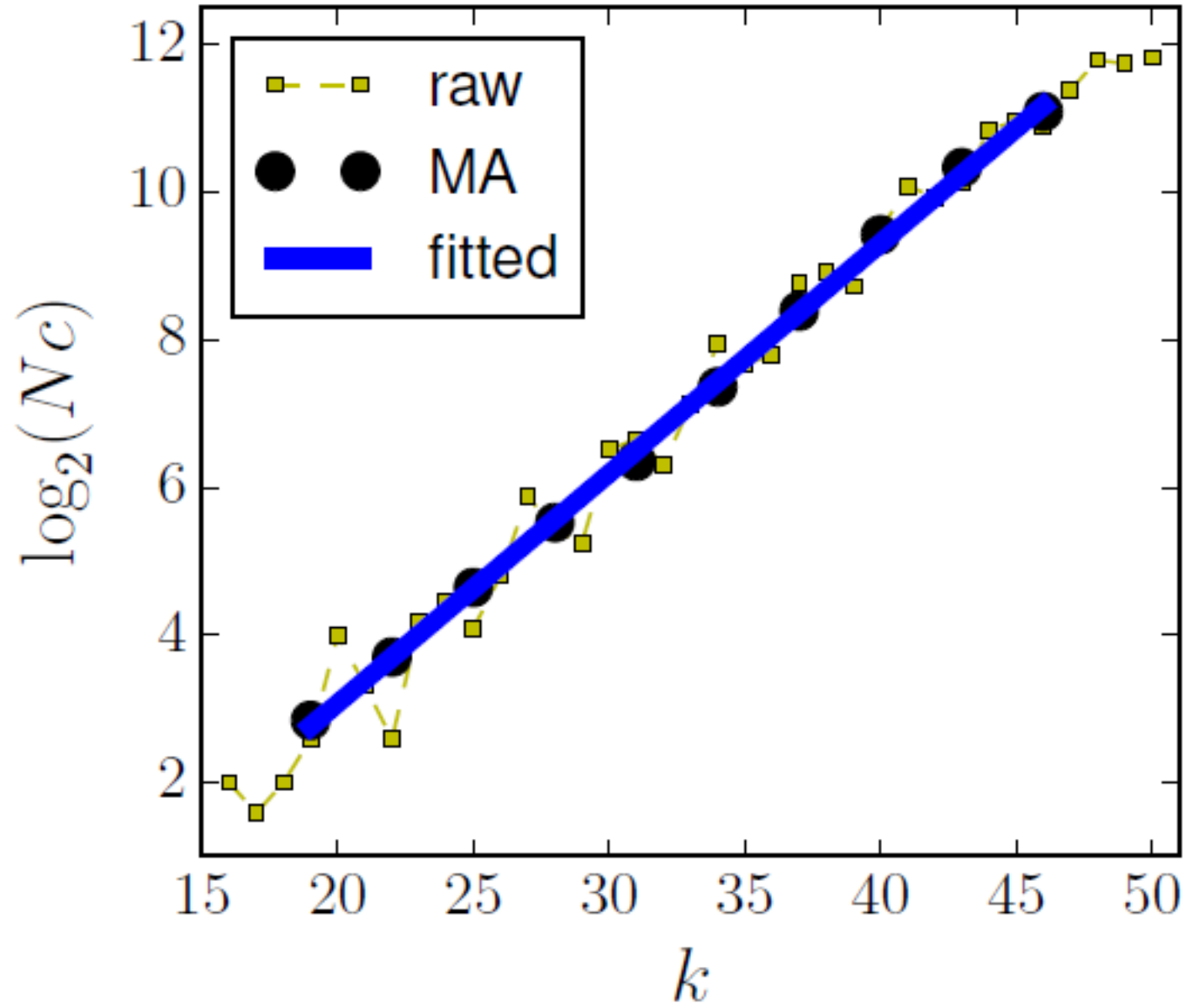


- Anti-parallel: up-down

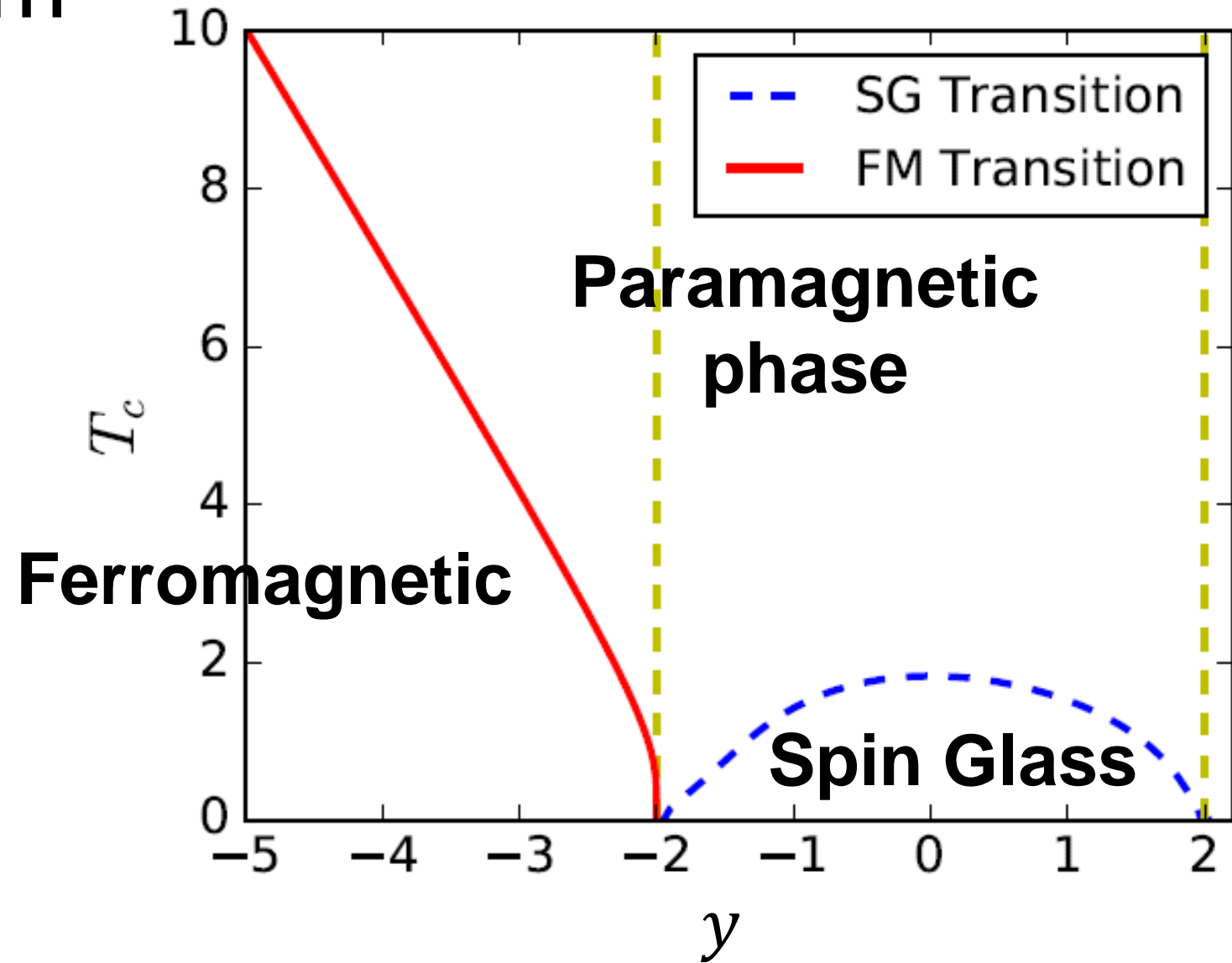


- Crossings N_C

- Power-law scaling

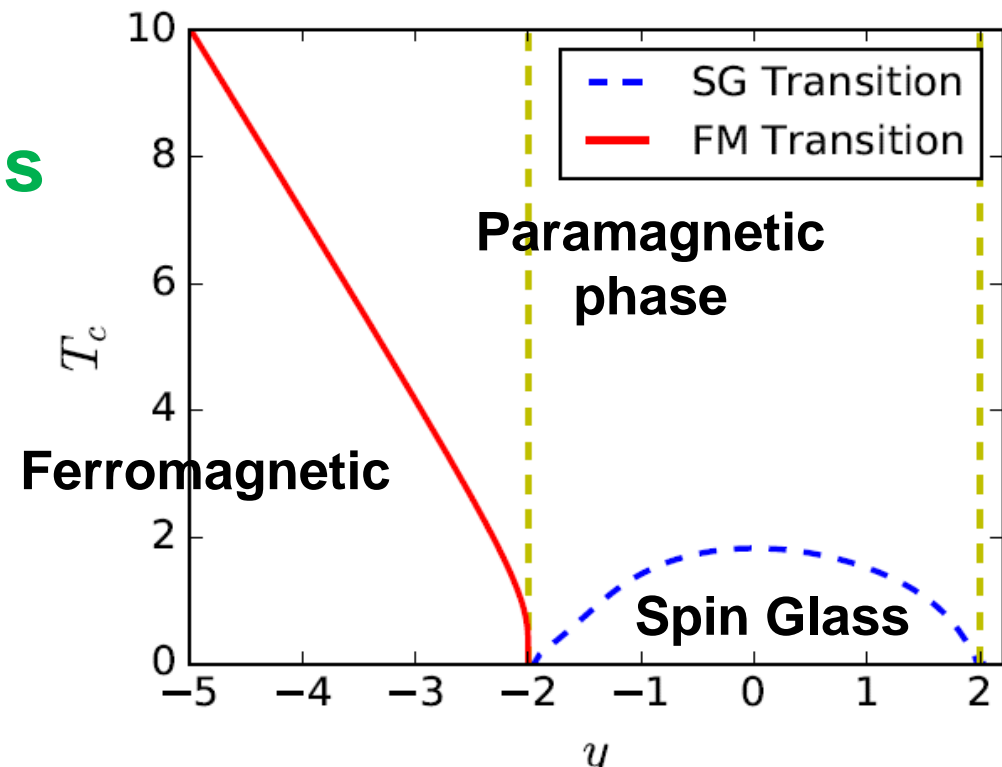


Phase Diagram



Summary and Conclusion

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

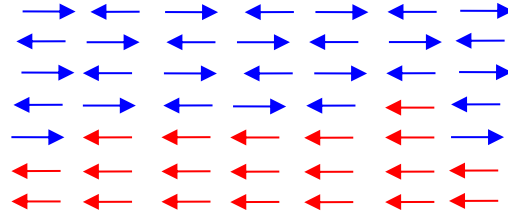


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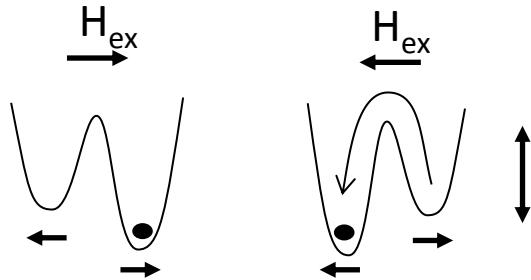
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Motivation

Quenched disorder at F-AF interface



Arrhenius activation of magnetic domains*

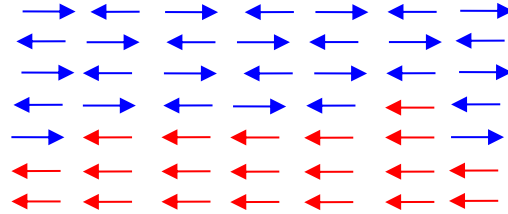


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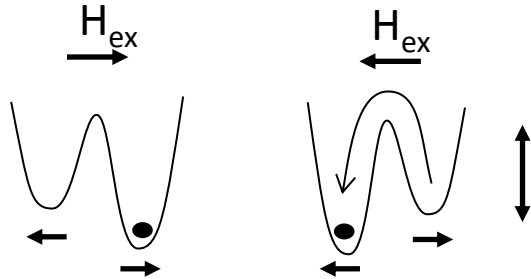
* E. Fulcomer, S.H. Charap, JAP 1972, and many more thereafter

Motivation

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In the experiment:
Power-law relaxation; small exponent

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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

$$H = -J \sum_{\langle ij \rangle} s_i s_j + \sum_i \mathbf{h}_i s_i$$

- $J = 1$: coupling constant
- \mathbf{h}_i : quenched random field

Monte Carlo Simulation

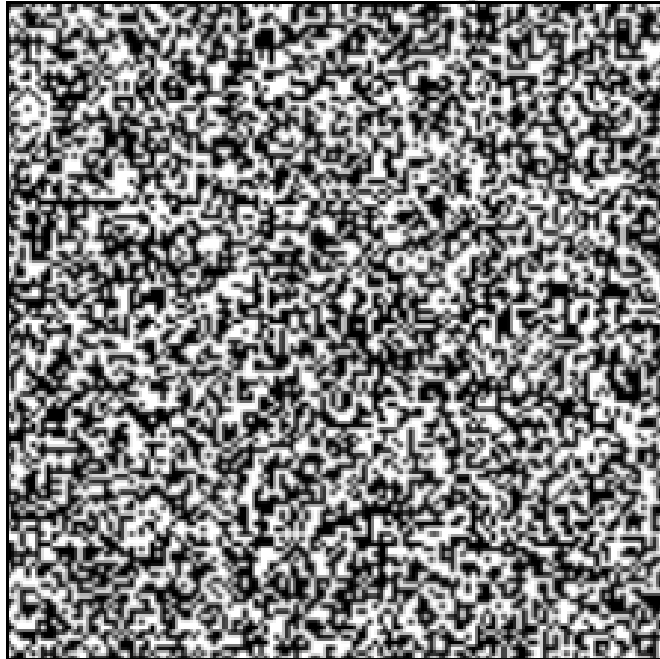
Experiment

- 1. Thin film

Simulation

- 1. 2D square lattice

1. Initial State



Monte Carlo Simulation

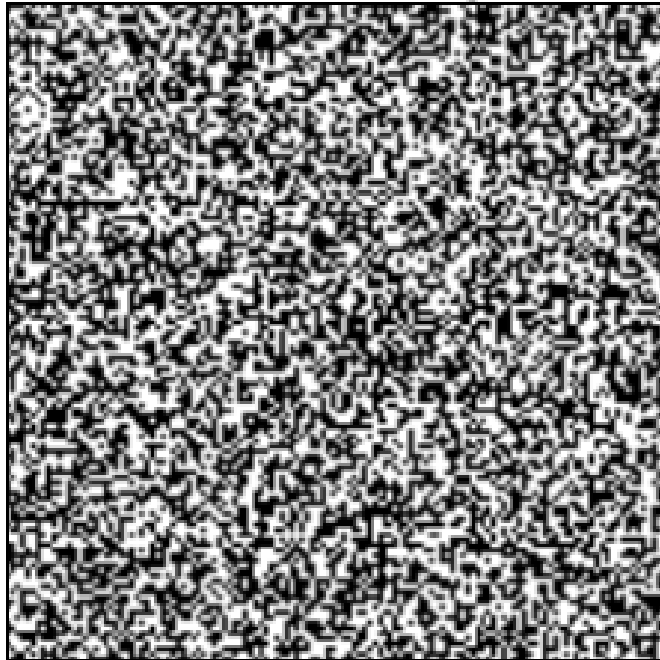
Experiment

- 1. Thin film
- 2. Cool down slowly

Simulation

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

1. Initial State



Monte Carlo Simulation

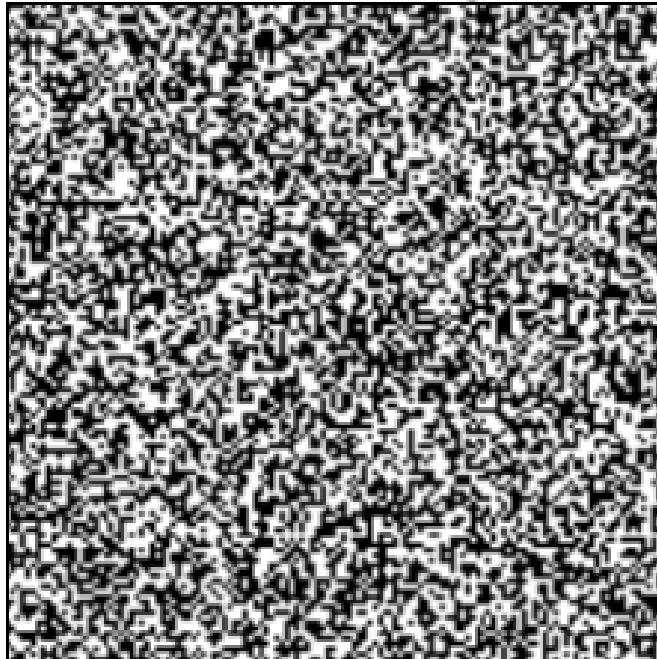
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- 2. Simulated annealing

1. Initial State



2. After Annealing



Monte Carlo Simulation

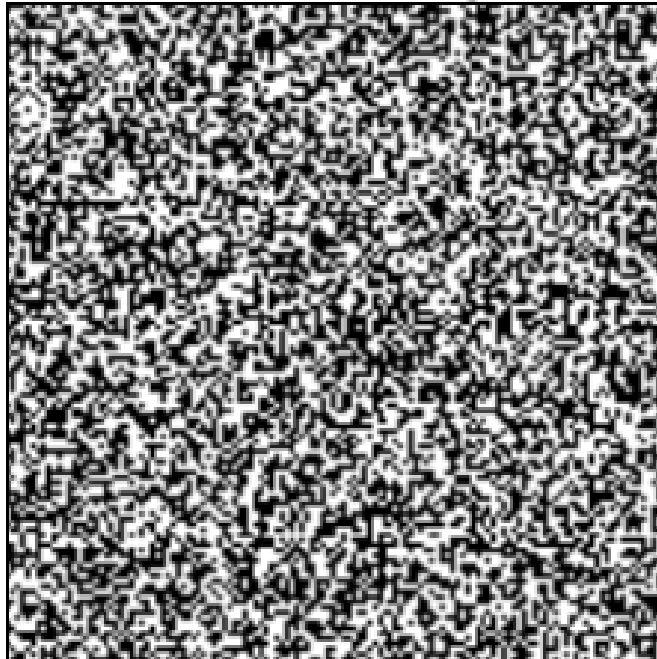
Experiment

- 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

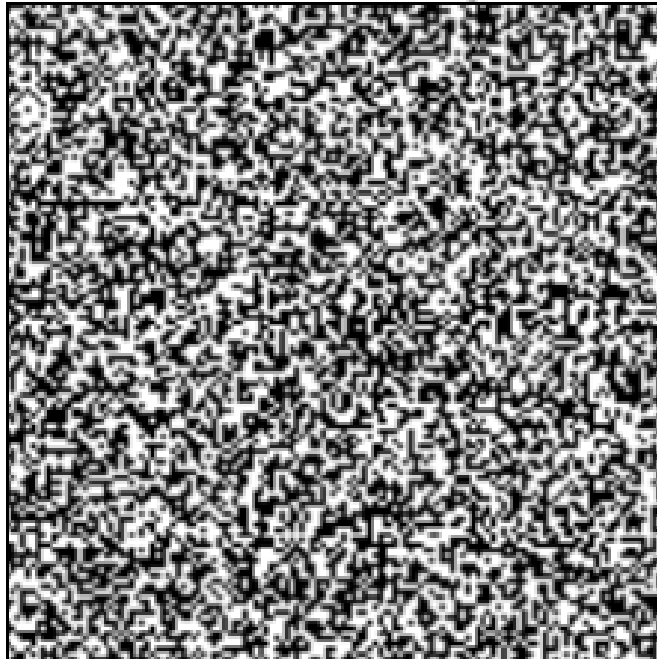
Experiment

- 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

(a) $t=20000$



(b) $t=40000$



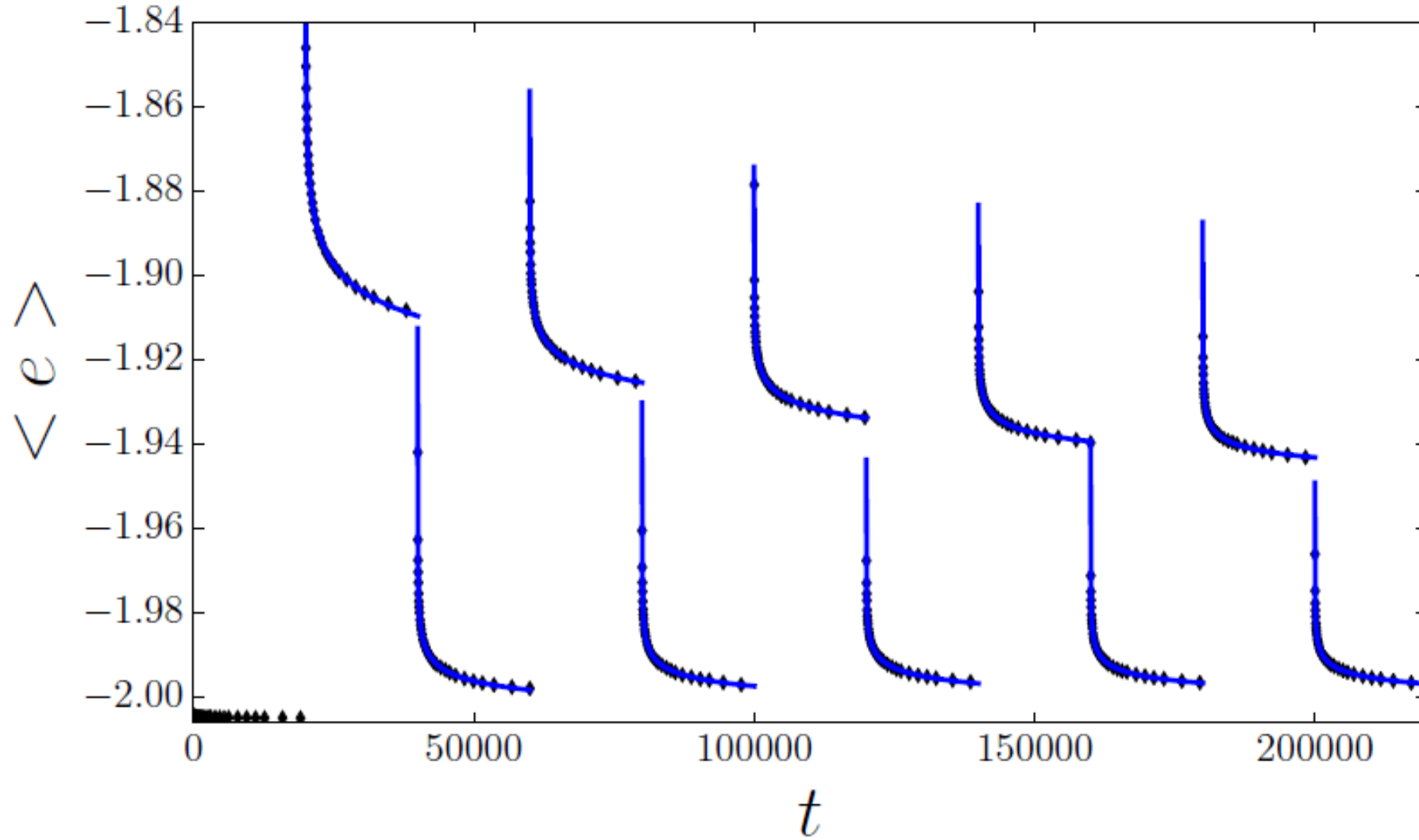
(c) $t=80000$



(d) $t=160000$

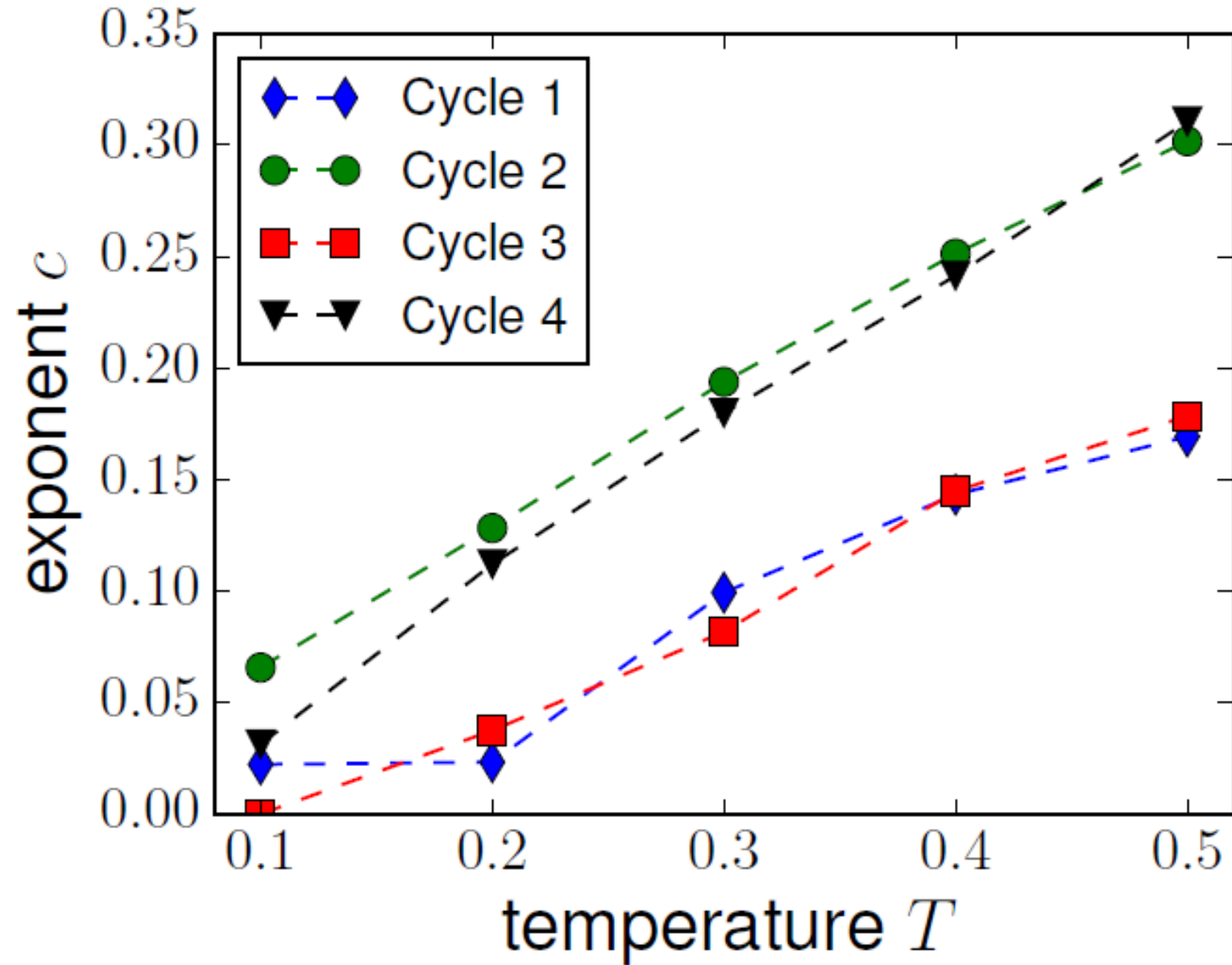


Monte Carlo Simulation



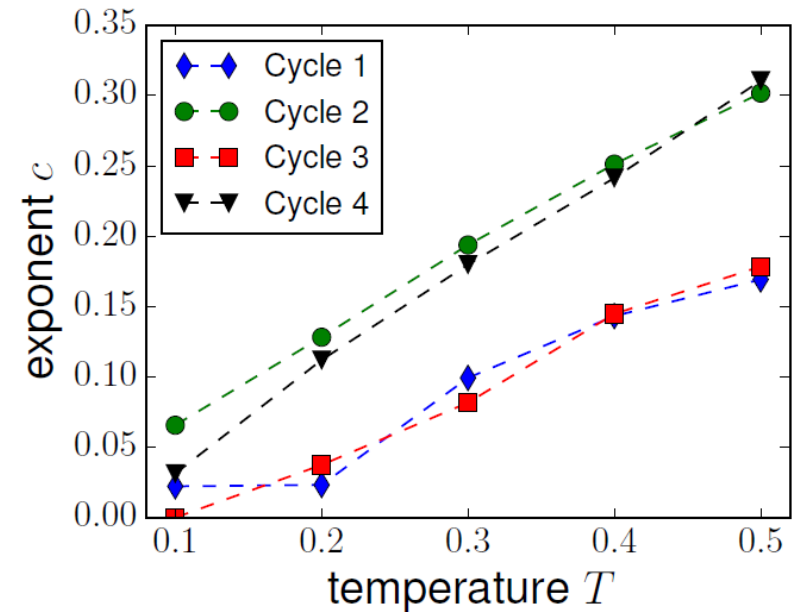
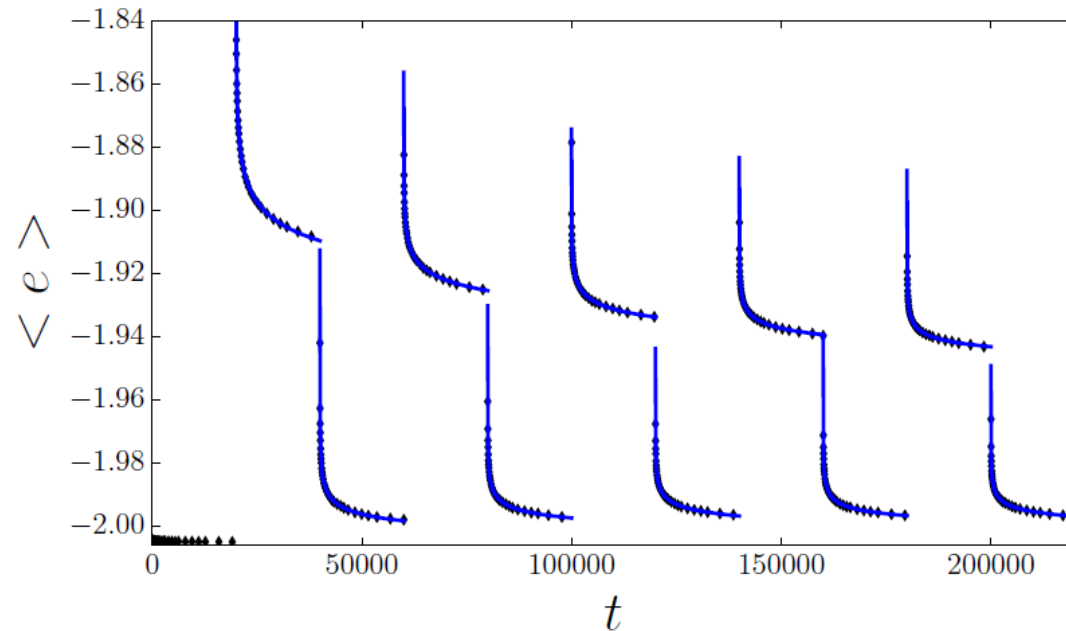
$$\langle e \rangle = e_0 + A \cdot t^{-c}$$

Power-law relaxation



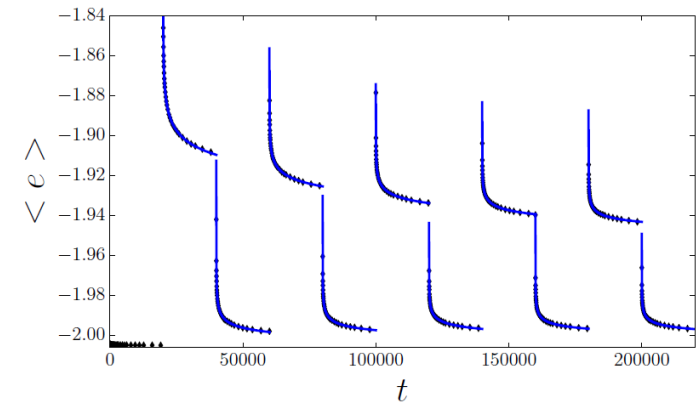
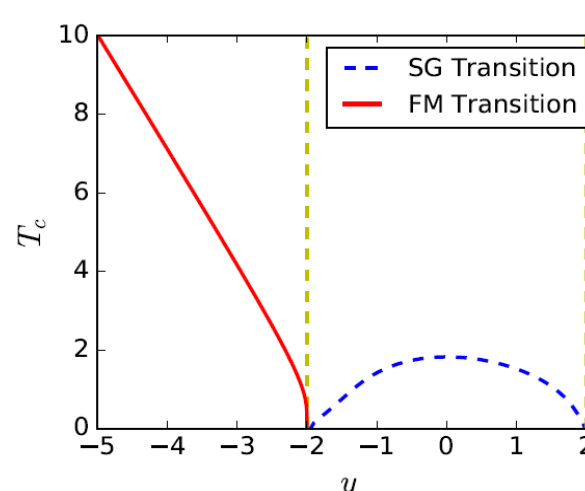
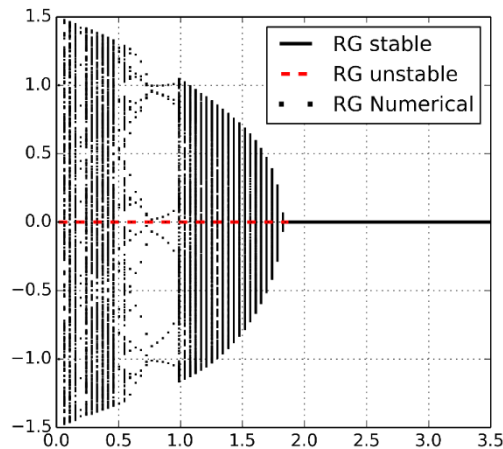
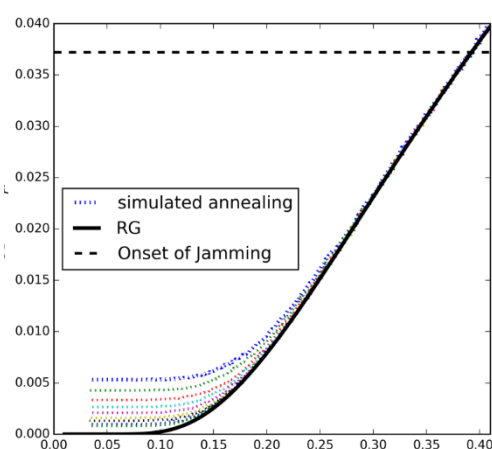
Summary and Conclusion

- 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
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- Equilibrium phase transition is not necessary
- Glassy dynamics & chaos indicate computational complexity



Acknowledgement

A word cloud of names in various colors and sizes, arranged in a roughly circular pattern. The names are: Stefan Boettcher (largest, blue), Justin Burton (green), Tom Bing (light green), James Nagy (green), Fereydoon Family (blue), Laura Finzi (green), Ilya Nemenman (brown), Sergei Urazhdin (yellow), Kurt Warncke (brown), George Hentschel (yellow), Yan Yan (yellow), Xinru Huang (yellow), Eric Weeks (brown), Roman Bagley (purple), Shanshan Li (purple), Pascal Philipp (yellow), Michael Fralade (red), Shengming Zhang (red), Calvin Jackson (purple), Nick Rob (yellow), Art Kleyman (blue), Barbara Conner (purple), Ka Wei Leung (yellow), Connie Roth (yellow), Cory Donofrio (red), Skanda Vivek (green), Trent Brunson (blue), Benjamin Nforneh (blue), Xin Du (red), Xia Hong (blue), Xinxian Shao (red), Lina Merchan (blue), Andrei Zholud (blue), Martin Tchernookov (blue), Baohua Zhou (blue), Stefan Falkner (purple), Jason Boss (purple), John Kirkham (purple), and Emrah Simsek (purple).

Stefan Boettcher

Justin Burton

Tom Bing

James Nagy

Fereydoon Family

Laura Finzi

Ilya Nemenman

Sergei Urazhdin

Kurt Warncke

George Hentschel

Yan Yan

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Stefan Boettcher

Acknowledgement



Acknowledgement



A word cloud of names in various colors and sizes. Two blue arrows point to 'Sergei Urazhdin' and 'Ilya Nemenman'. The names are arranged in a way that some are larger and more prominent than others.

Names included in the word cloud:

- XinruHuang
- YanYan
- GeorgeHentschel
- KurtWarncke
- EricWeeks
- SergeiUrazhdin
- JustinBurton
- JamesNagy
- KaWeiLeung
- BarbaraConner
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- MartinTchernookov
- BaohuaZhou
- LauraFinzi
- JasonBoss
- JohnKirkham
- EmrahSimsek
- IlyaNemenman

A word cloud of names in various colors and sizes. The names are arranged in a roughly circular pattern. Two blue arrows point to specific names: one points to 'Sergei Urazhdin' and the other points to 'Jason Boss'. The names include: Sergei Urazhdin, Justin Burton, Tom Bing, Stefan Boettcher, Fereydoon Family, Laura Finzi, Ilya Nemenman, James Nagy, Barbara Conner, Connie Roth, Art Kleyman, Nick Rob, Calvin Jackson, Roman Bagley, Shanshan Li, Pascal Philipp, Michael Fralaid, Shengming Zhang, Xin Du, Cory Donofrio, Skanda Vivek, Trent Brunson, Benjamin Nforneh, Xia Hong, Xinxian Shao, Lina Merchan, Andrei Zholud, Martin Tchernookov, Baohua Zhou, Emrah Simsek, John, and Jason Boss.

Acknowledgement

A word cloud of names, with 'Stefan Boettcher' being the largest and most central. Four blue arrows point to 'James Nagy', 'Justin Burton', 'Laura Finzi', and 'Ilya Nemenman'. Other names are arranged in a circular pattern around the center, with varying font sizes.

Names in the word cloud include:

- XinruHuang
- YanYan
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- KurtWarncke
- EricWeeks
- SergeiUrazhdin
- JustinBurton
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- SkandaVivek
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- ConnieRoth
- KayLeung
- JamesNagy

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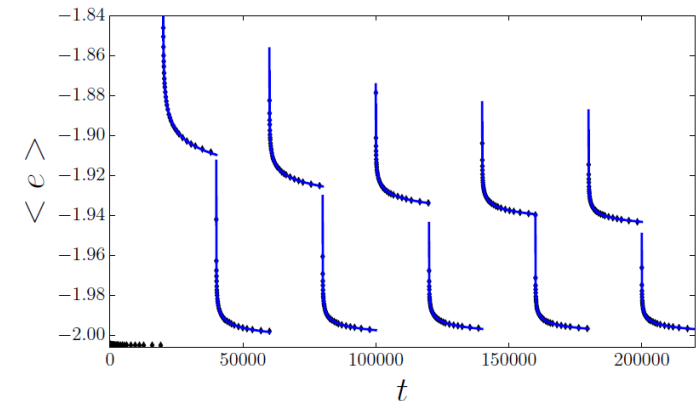
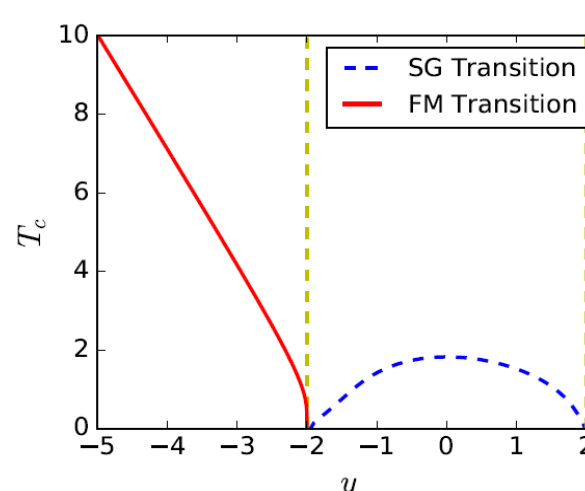
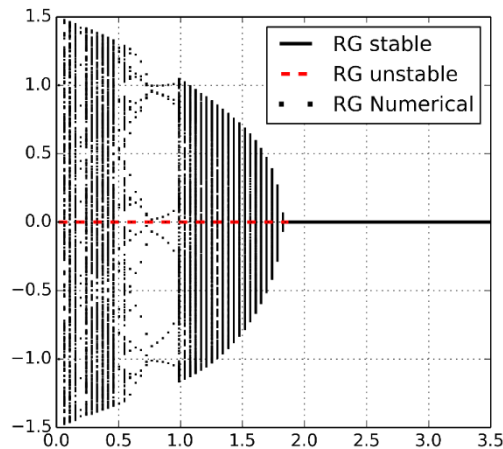
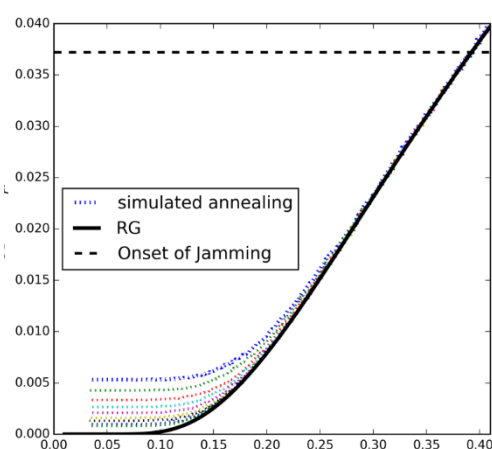
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Chaos

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