Dissertation Committee Meeting

<u>Disordered Systems in Hierarchical Networks</u>

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Committee:

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EMORY UNIVERSITY

Outline

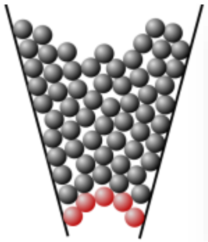
- Review of research
- Project 1: Jamming in Hierarchical Networks
- Project 2: antiferromagnetic Ising model
- Future Plan

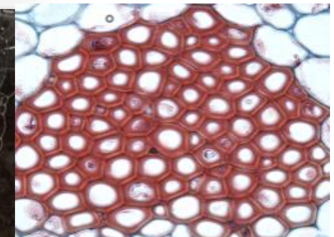
Review of research work

- **Jamming in Hierarchical Networks**
  - *Publication*:
    - X. Cheng and S. Boettcher, *Computer Physics Communications* (Revision submitted);
  - *Conference presentations*:
    - 2014 UGA CSP Workshop,
    - 2014 APS March Meeting;
- **Antiferromagnetic Ising model in Hierarchical Networks**
  - *Publication*: plan to write 1~2 papers according to results
  - *Conference Presentations*:
    - 2015 UGA CSP Workshop,
    - 2015 APS March Meeting;
- Rotation Project: effect of a large number of receptors (Dr. Nemenman)
  - *Publication*:
    - X. Cheng, L. Merchan, M. Tchernookov, I. Nemenman, *Phys. Biol.* **10** 035008 (2013);
  - *Conference presentations*:
    - q-bio 2012;
    - 2013 APS March Meeting;

Jamming in Hierarchical Network

- Jamming is ubiquitous



- Characteristics:
  - Rigid state at high packing density (not highest)
  - Out of equilibrium
  - Extremely slow relaxation
- Still a challenge to understand
  - Extremely long relaxation;
  - No significant structural change;
  - Heterogeneities;

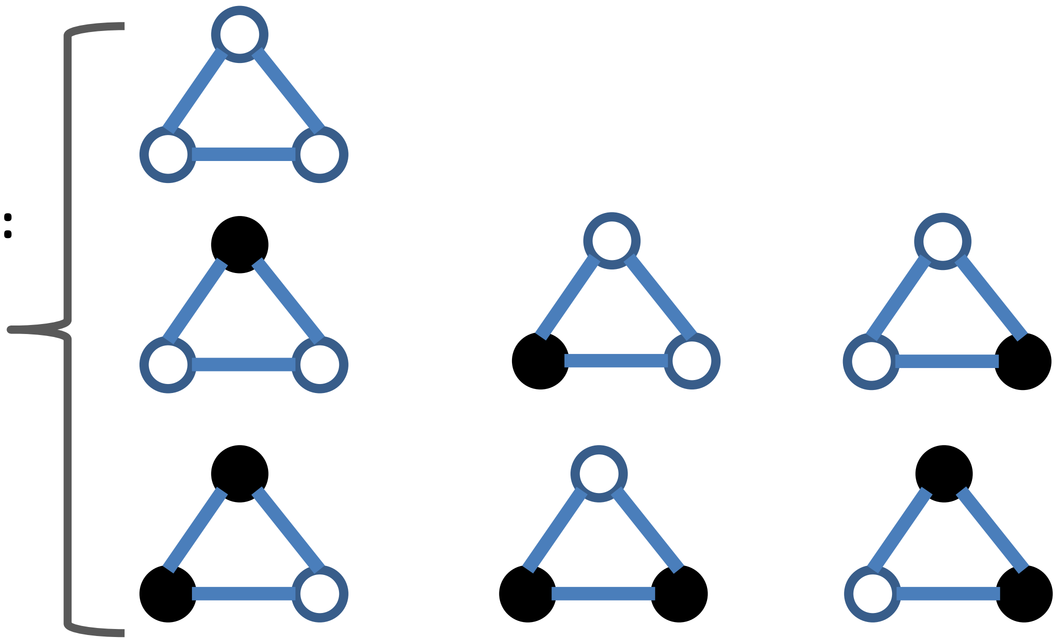
Research Questions

- What causes slow relaxation?
  - Interaction?
  - Geometry?
- Equilibrium real phase transition?
  - “Yes” evidences in mean-field models;
  - Non-mean field models?
- Phase transition necessary for jamming?
  - jamming without phase transition?
  - no published evidence so far

Jamming Model

- Biroli-Mezard Model
  - Each site has $x_i = 0, 1$ particle with μ *(chemical potential)*
  - Rule: at most l $(0, 1, \cdots)$ neighbors

Example: triangle
$l = 1$



$1 \cdot \exp[0 \cdot \mu]$

$3 \cdot \exp[1 \cdot \mu]$

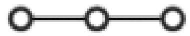
$3 \cdot \exp[2 \cdot \mu]$

$$\Xi = \sum_{n_i=0}^{n_{\max}} g_i \cdot \exp[n_i \cdot \mu]$$

Jamming state:
Particle number $n < n_{\text{equlibrium}}$

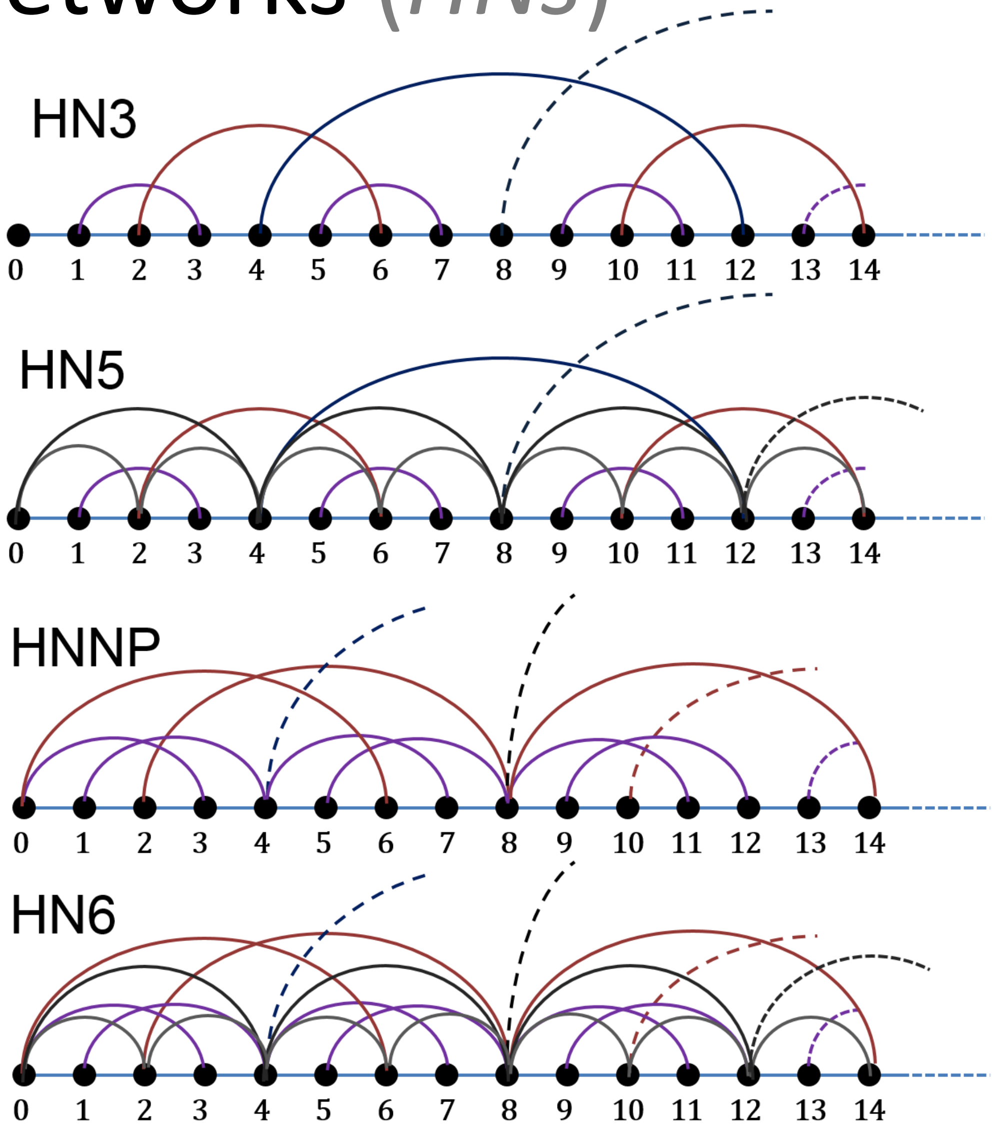
Hierarchical Networks: Hanoi networks

- HN3:

$N = 2^{1} + 1$ 

Hierarchical networks (*HNs*)

- HN3:
  - degree 3
- HN5:
  - average degree 5
- HNNP:
  - average degree 4
  - nonplanar
- HN6
  - average degree 6
  - nonplanar



Why Hierarchical Networks (HNs)?

- Exactly solvable by **R**enormalization **G**roup (RG)

- Lattice-like structure
  - Mean-Field ⇨ HNs ⇨ Regular lattice

- Geometrical effect
  - Different degrees: 3, 4, 5, 6
  - Planar vs non-planar
- Fixed structure: computational efficient
  - Avoid averages over random ensembles

Methods

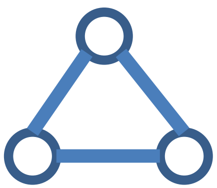
- **S**imulated **A**nnealing (SA) $\longleftrightarrow$ Experiment
  - probe dynamical behaviors
  - Glassy relaxation

- **W**ang-**L**andau Sampling (WL)
  - direct access to *Density of States*
  - partition function $\Rightarrow$ equilibrium quantities

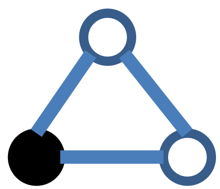
- **R**enormalization **G**roup (RG)
  - Exact solutions in the thermodynamic limit
  - Challenging for $l > 0$

Simulated Annealing

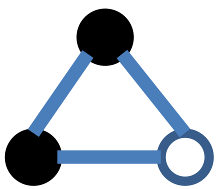
- Monte Carlo Simulation $\leftrightarrow$ Experiment
  - Randomly pick a site i;
  - If $x_i = 0$, add a particle with $P = \min[\,1,\ \ e^{\mu}\,]$ within constraint;
    If $x_i = 1$, remove a particle with a $P = \min[\,1,\ \ e^{-\mu}\,]$
  - Update $\mu \leftarrow \mu + d\mu$ every 1 Monte Carlo sweep (N random steps)
  - Keep packing fraction ρ every sweep



$\mu \to 0$



Small μ



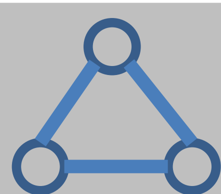
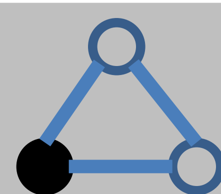
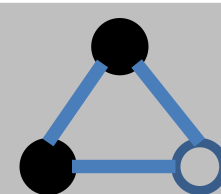
Big μ

Wang-Landau Sampling

- Monte Carlo Methods to find the **density of states**

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

- Fact: random sampling with $P \propto \frac{1}{g_i} \rightarrow$ flat histogram

			
g_i	1	3	3
$\frac{1}{g_i}$	1	1/3	1/3

Flat Histogram

Wang-Landau Sampling

- Monte Carlo Methods to find the **density of states**

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

- Fact: random sampling with $P \propto \frac{1}{g_i} \longrightarrow$ flat histogram
  - 1. Set all unknown $g_i = 1$ (initial guess) and H_i=0 (histogram);
  - 2. Randomly add a particle with $P = \min\left[1, \exp\left(\frac{g_i}{g_{i+1}}\right)\right]$;

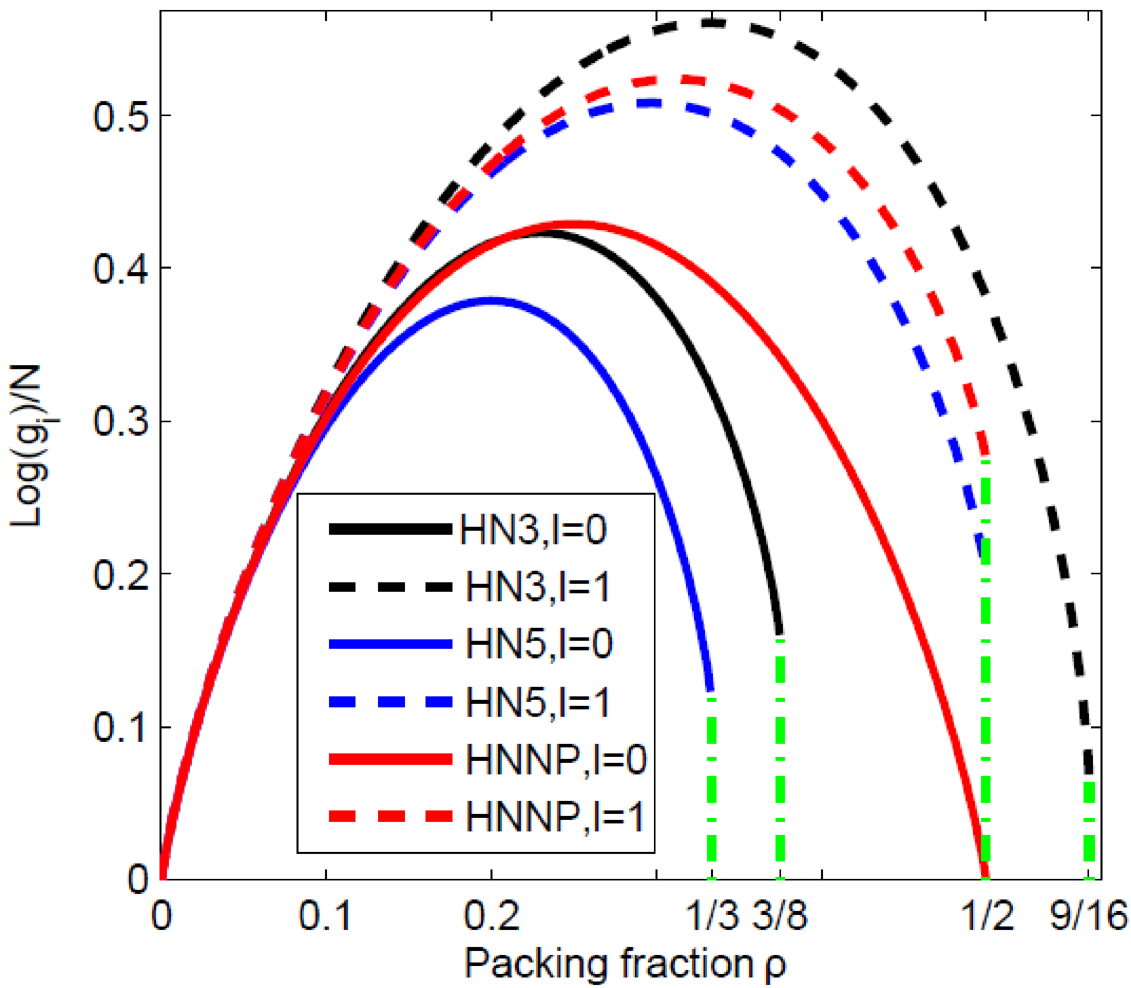
    OR randomly remove one with $P = \min\left[1, \exp\left(\frac{g_{i-1}}{g_i}\right)\right]$;
  - 3. If a state i is visited: $g_i \leftarrow g_i * f$ (modification factor: $f > 1$);

    update $H_i \leftarrow H_i + 1$;
  - 4. Repeat 2 and 3 until the sampling reach a roughly flat histogram;

    then reduce f closer to 1; reset $H_i = 0$

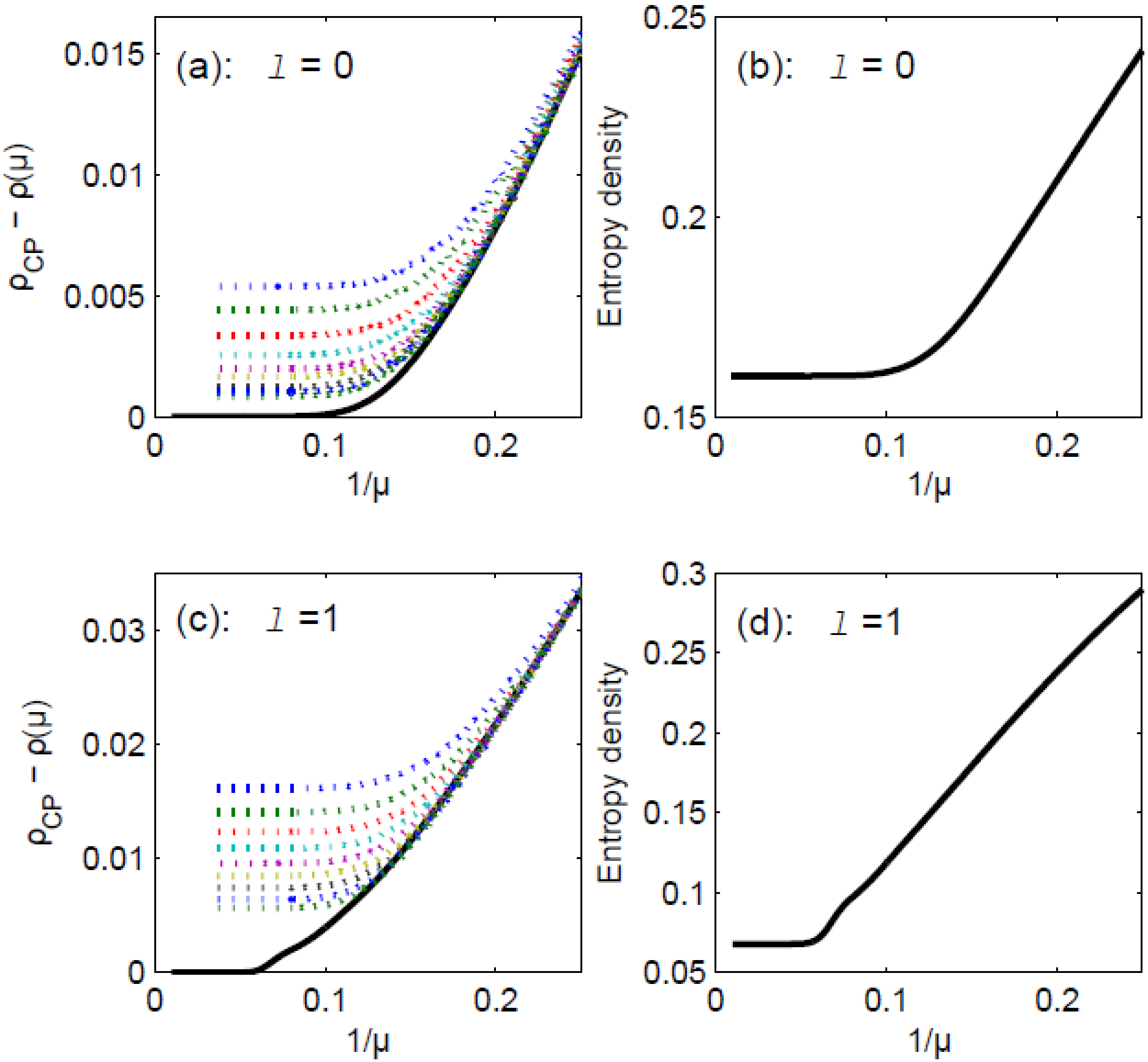
Accuracy of $g_i \propto \ln(f)$;

Density of States



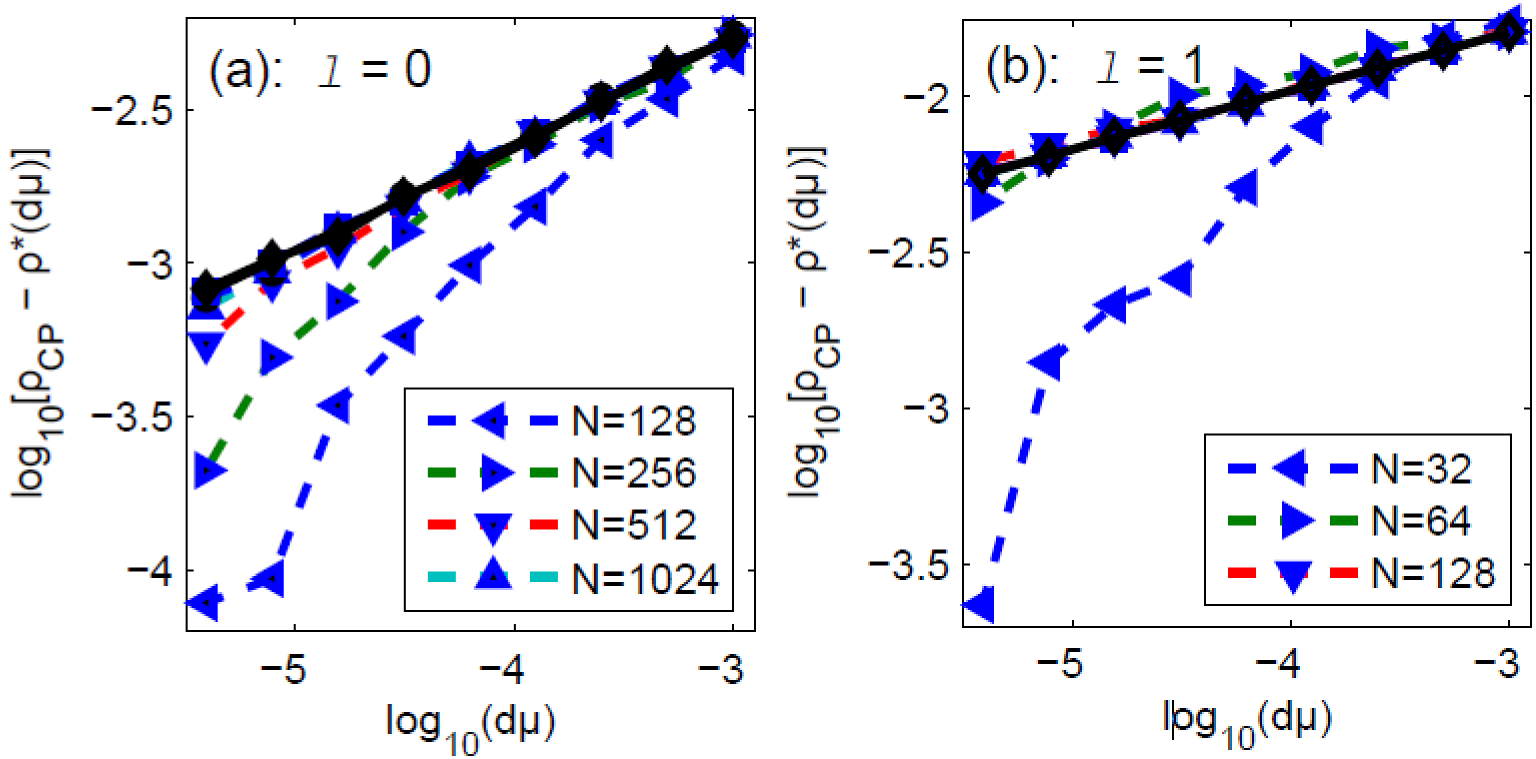
- Non-symmetric
- Mostly no unique ground states
- Failed to converge for $N > 1024$

Jamming



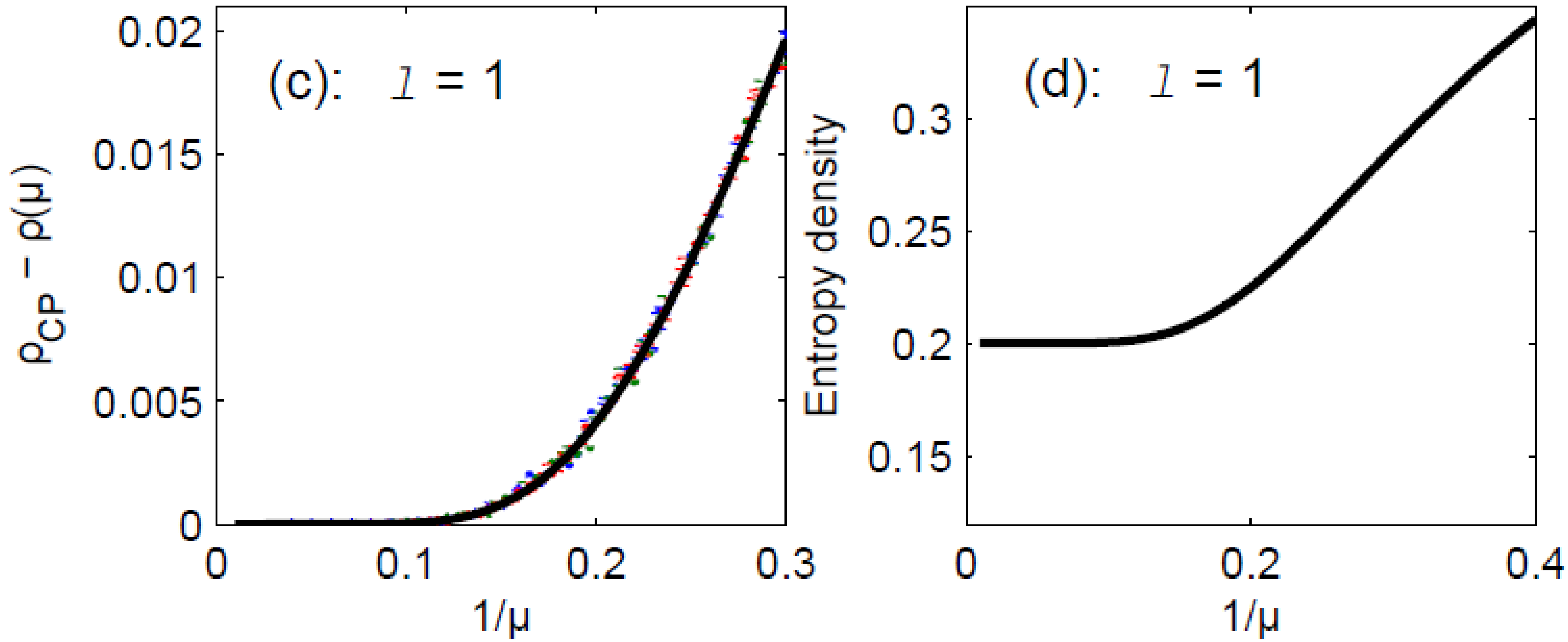
- HN3, $l = 0{,}1$
- Dashed:
  SA: $N = 2^{15}$
- Solid:
  WL: $N = 2^{10}$
- Annealing schedules:
  $0.001, \frac{0.001}{2}, \cdots, \frac{0.001}{512}$
- Jamming exists
- No phase transition: $l = 0$

Power-law relaxation



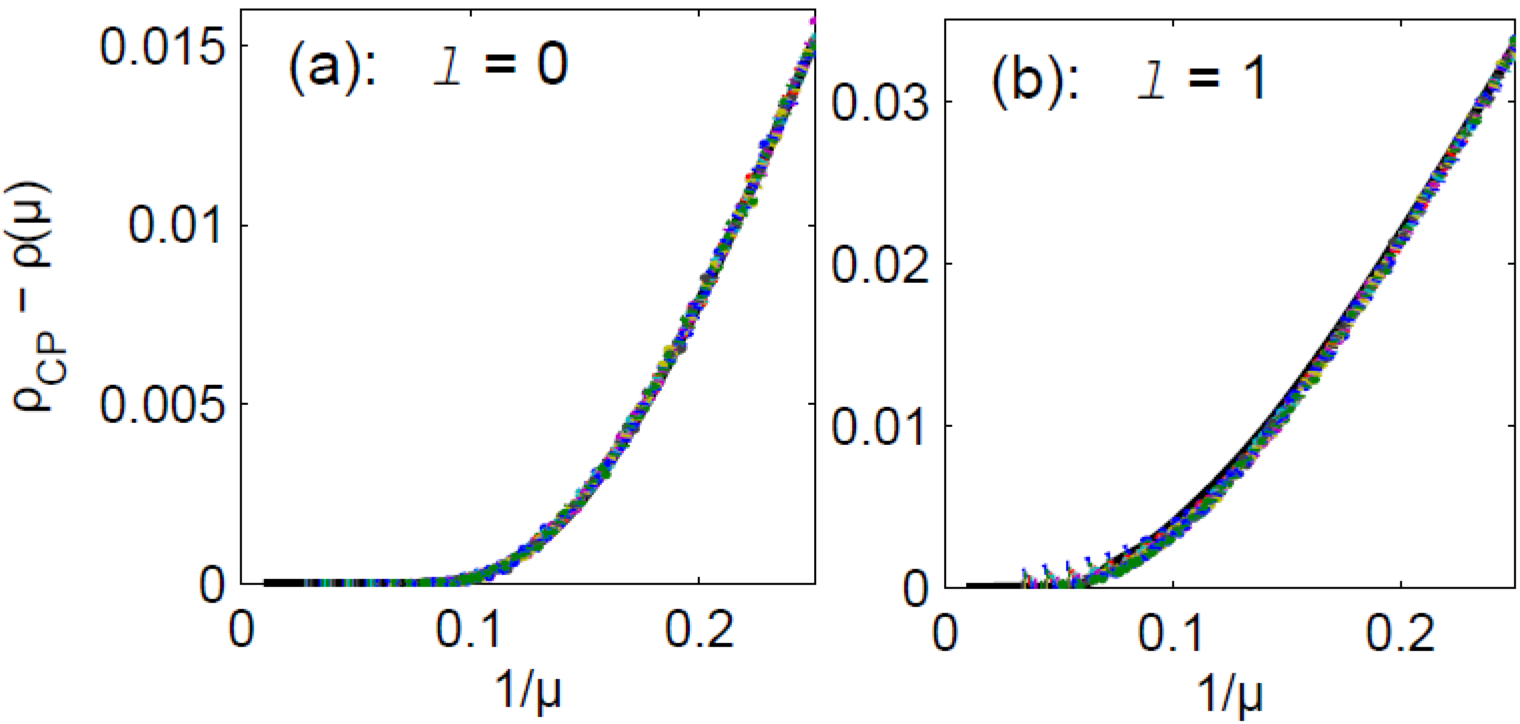
- Slope: 0.34, 0.19
- Similar results: HN5, $l = 0$; HNNP, $l = 0$;

No Jamming



- Jamming may be geometry-related!

Local dynamics



- Hopping eliminates jamming;
- Local dynamics affects jamming;

- May be useful for stochastic optimizations.

Project 1 Summary

- Phase transition is not necessary for jamming;
- Power-law relaxation near jamming transition;
- Jamming is related to geometry and local dynamics;

- More work for more conclusions
  - Renormalization Group

Antiferromagnetic Ising model

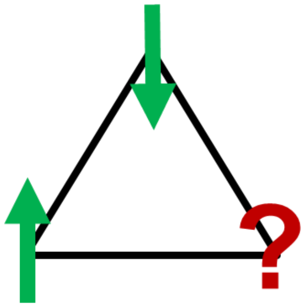
- Antiferromagnetic (AFM) Ising model

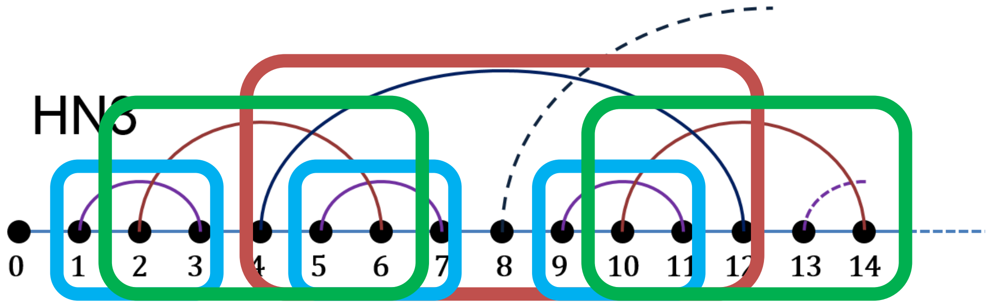
$$E = -J \sum S_i S_j \ , \quad J < 0$$

$\boldsymbol{E = -J > 0}$ $\boldsymbol{E = J < 0}$

  - glassy dynamics

- Geometric frustration: odd loops





Research Questions

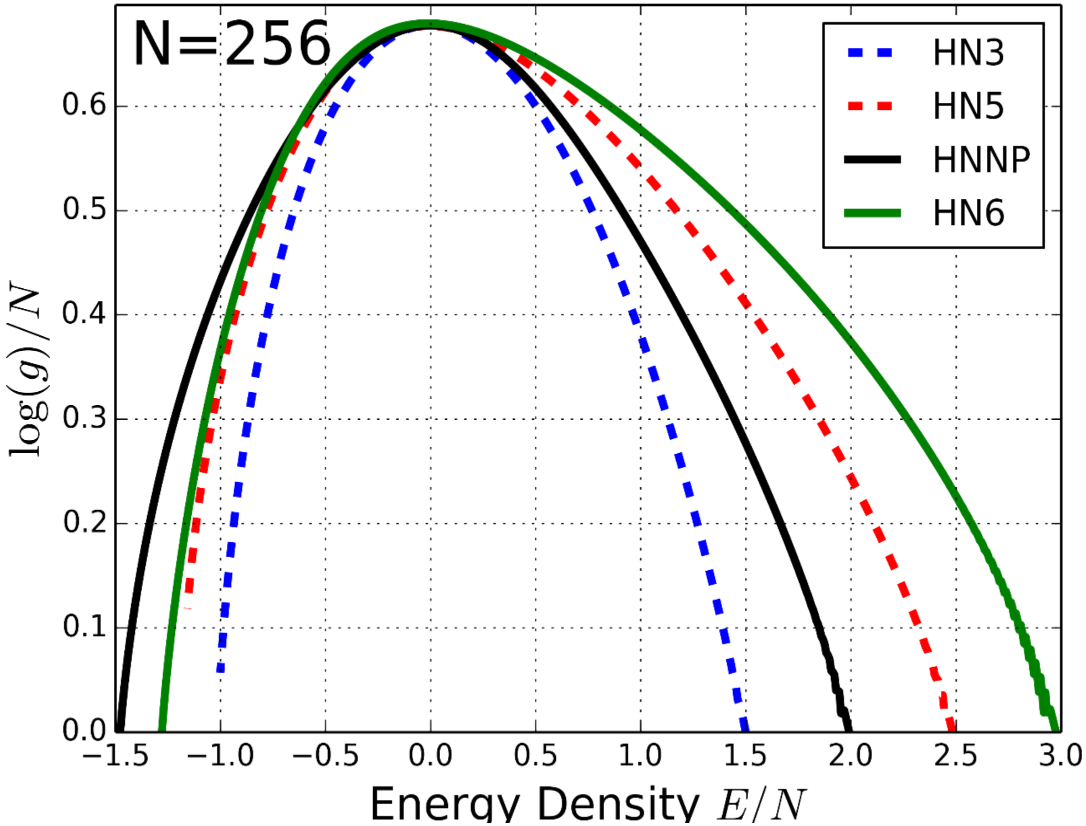
- Phase transitions?
  - Equilibrium/non-equilibrium transition?
  - Spin glass phase?
- Glassy relaxation?
- Influence of geometry?
- Difference to mean-field models?

Methods

- **S**imulated **A**nnealing (SA) ⟷ Experiment
  - probe dynamical behaviors
  - Glassy relaxation
- **W**ang-**L**andau Sampling (WL)
  - direct access to *Density of States*
  - partition function ⟹ equilibrium quantities
- **R**enormalization **G**roup (RG)
  - Exact solutions in the thermodynamic limit

Density of States (WL)

- Planar: HN3, HN5
  Degenerate ground states
- Non-planar: HNNP, HN6
  Unique ground states
- Reference of **SA** & **RG**
- Wang-Landau fails
  - $N > 1024$
  - Geometric frustration?



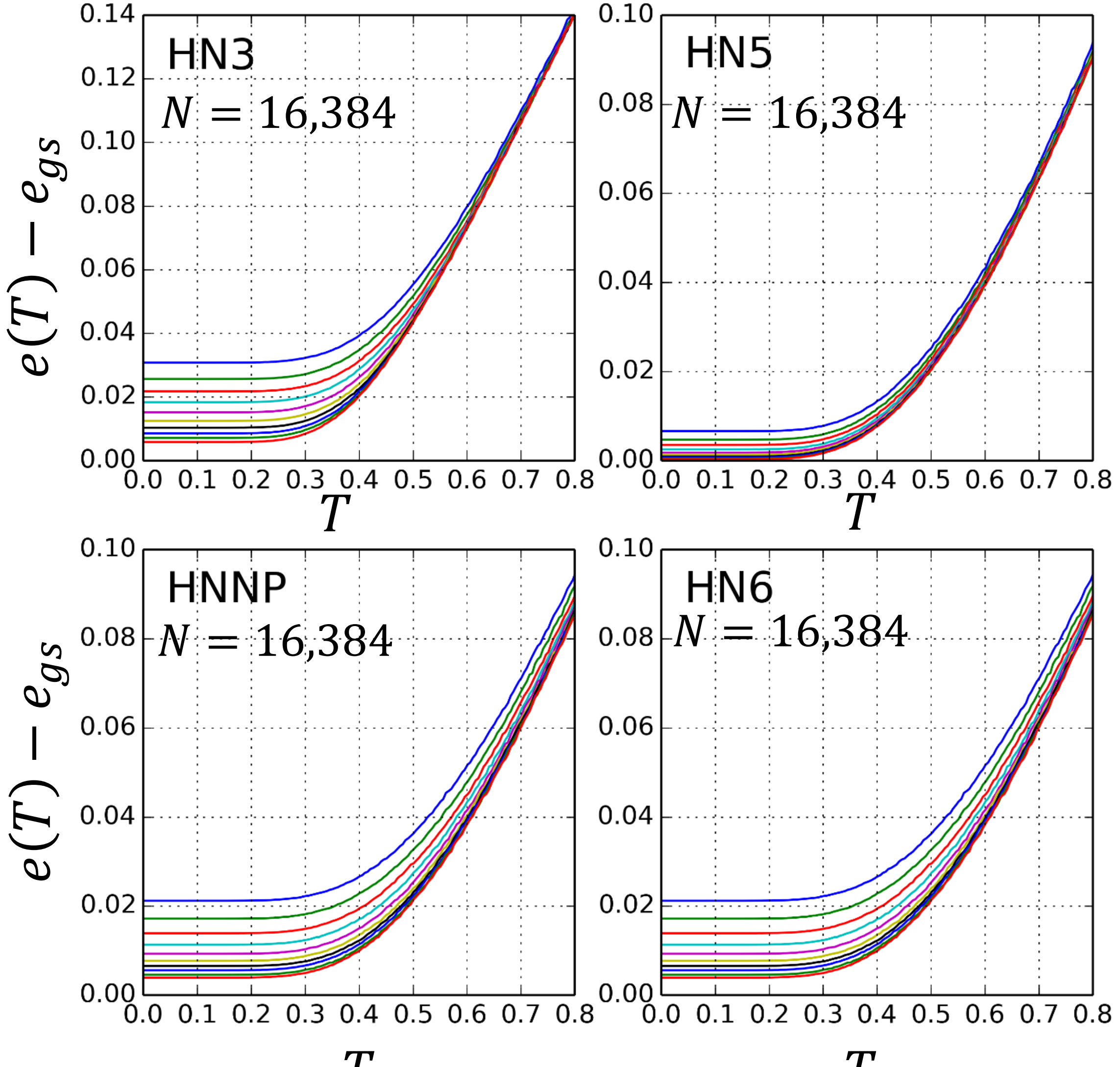
Glassy relaxation (SA)

- x axis: T
- y axis: $e(T) - e_{gs}$

- Annealing schedules:

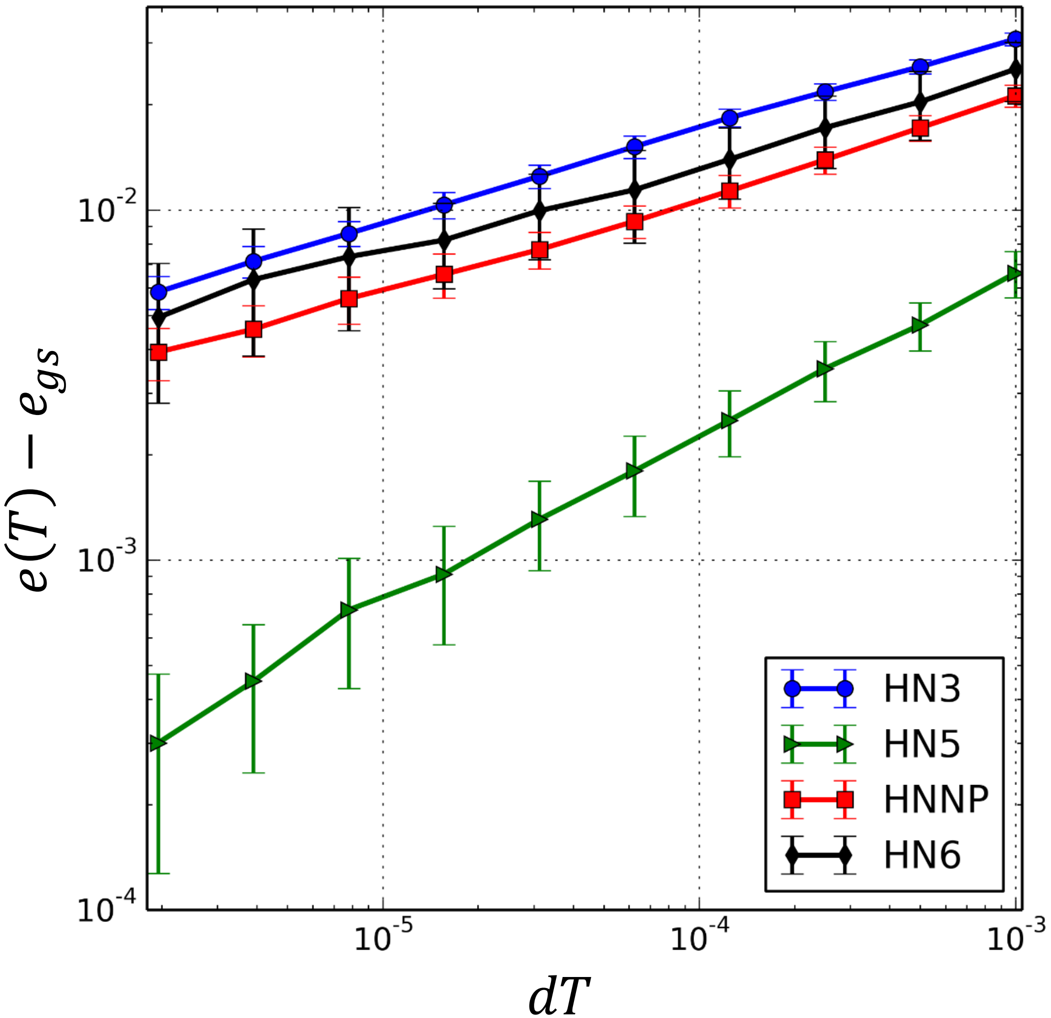
$$\frac{dT}{dt} = \frac{10^{-3}}{1}, \frac{10^{-3}}{2}, \cdots, \frac{10^{-3}}{512}$$

- Out of Equilibrium at low T
- Extremely slow relaxation at low T



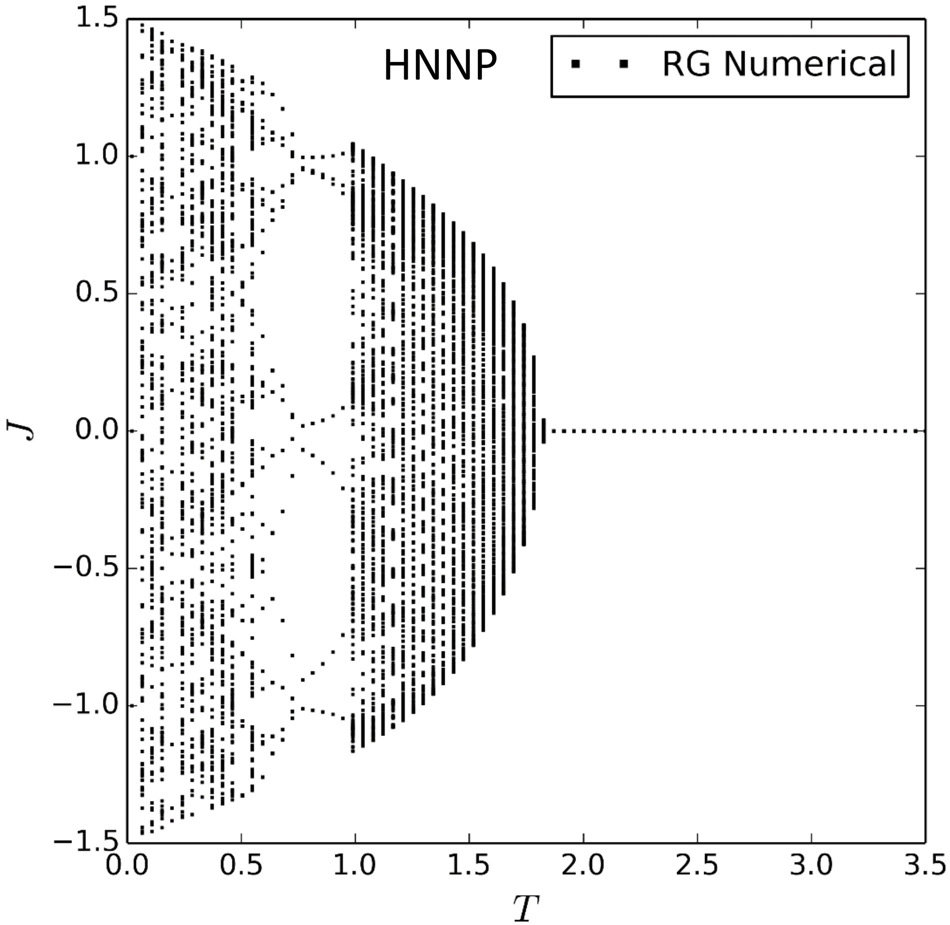
Power-law relaxation (SA)

- Power-law relaxation
- HN3, HNNP, HN6:
  - Slope = ~ 0.27
- HN5 may equilibrate gradually



Spin glass transition (RG)

- Non-Planar: HNNP, HN6
  - partially stable fixed-point solution
  - possible spin glass transition



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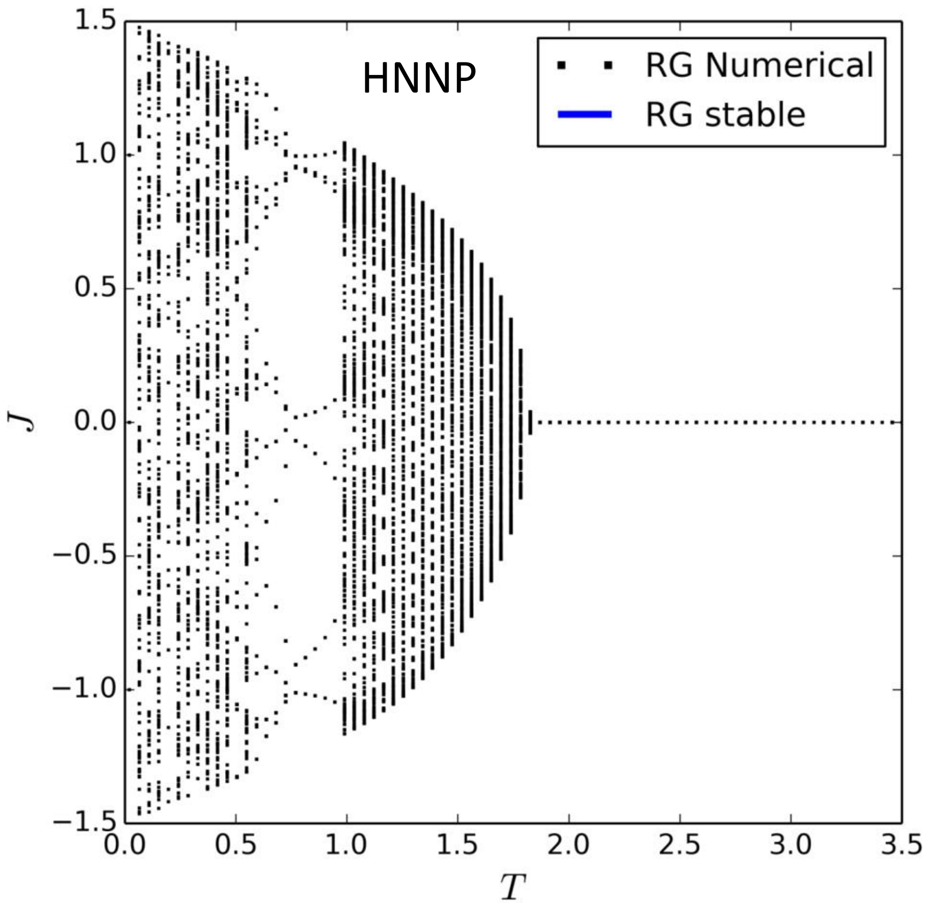

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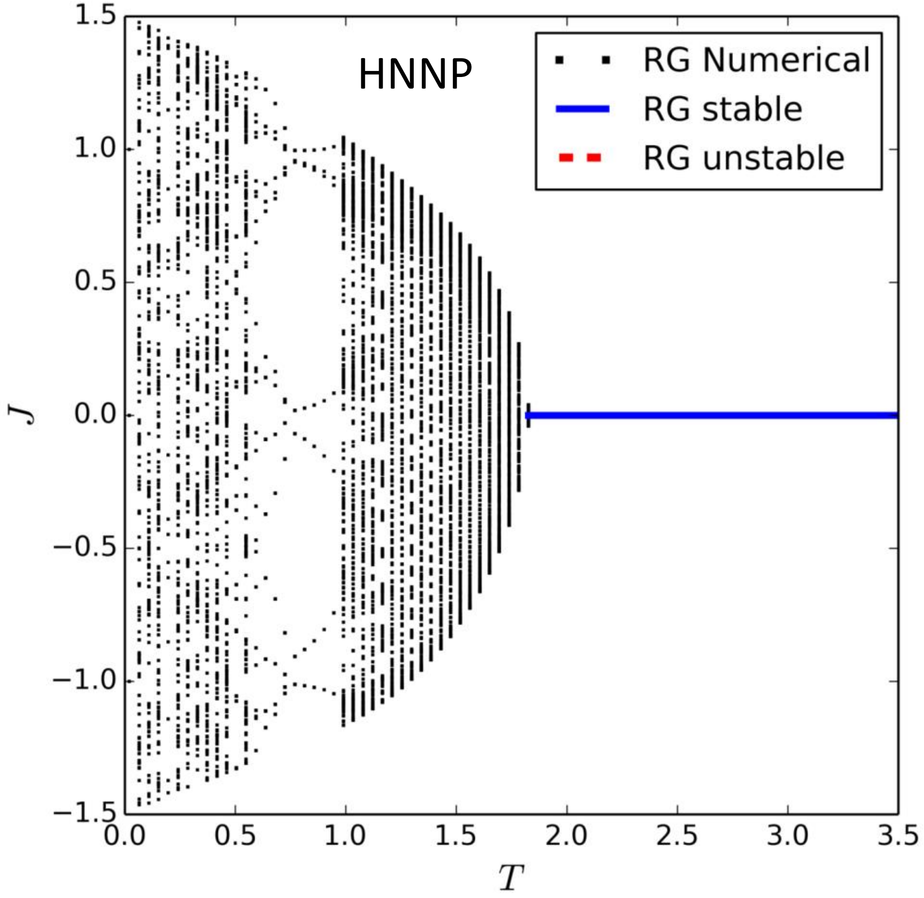

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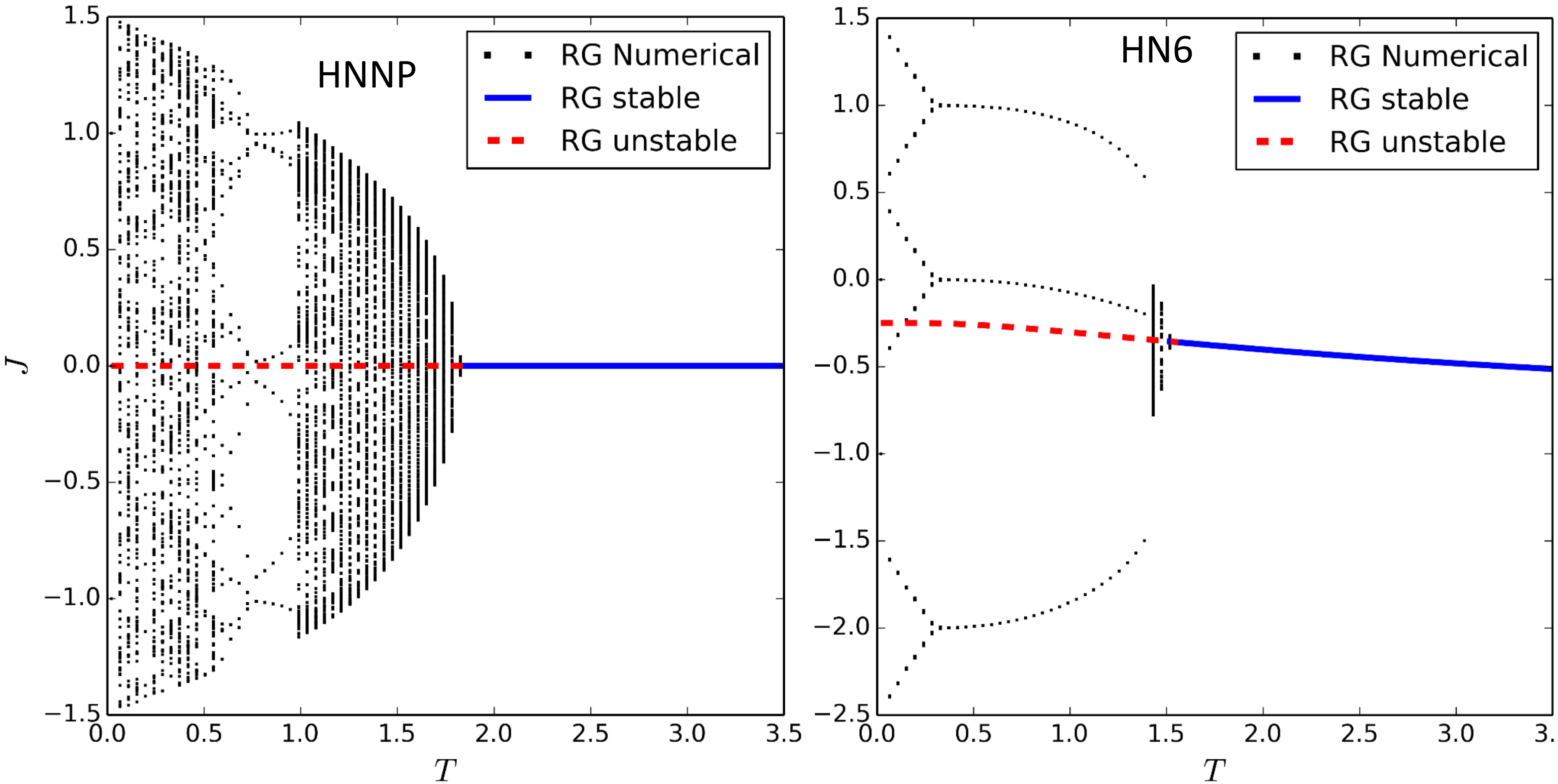
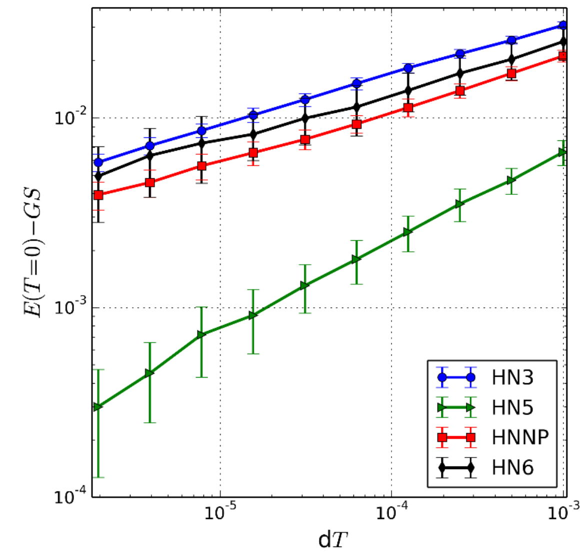
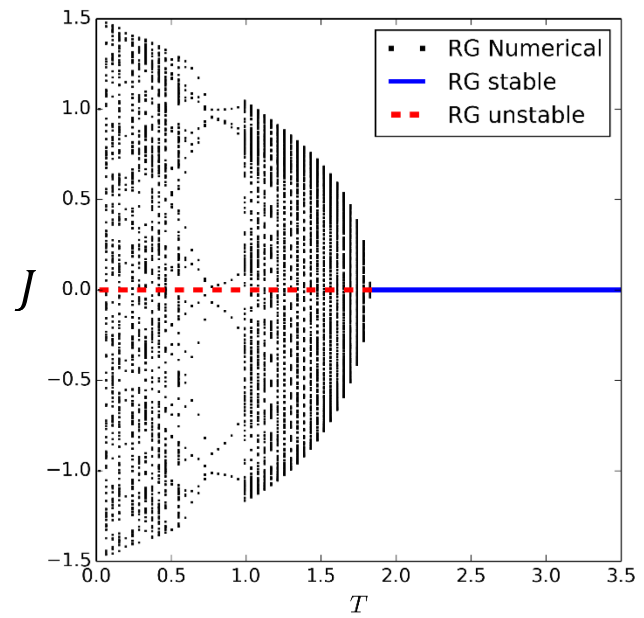


McKay and Berker, *Phys. Rev. Lett.* **48**, 11 (1982)

Project 2 Summary

- Out of equilibrium at low T
- Power-law relaxation
- Spin glass transition
- Future work:
  - $C_v,\ m,\ \chi$ using RG
  - Spin glass ⟺ geometry?





Future Plan

- Research
  - Renormalization group of Ising model
  - 1~2 papers about AFM Ising model
  - Renormalization group of Jamming
- Graduation
  - Computer Science MS (Computational Science)
  - Dec 2015 OR May 2016