Equilibrium Study of Spin-Glass Models: Monte Carlo Simulation and Multi-variate Analysis

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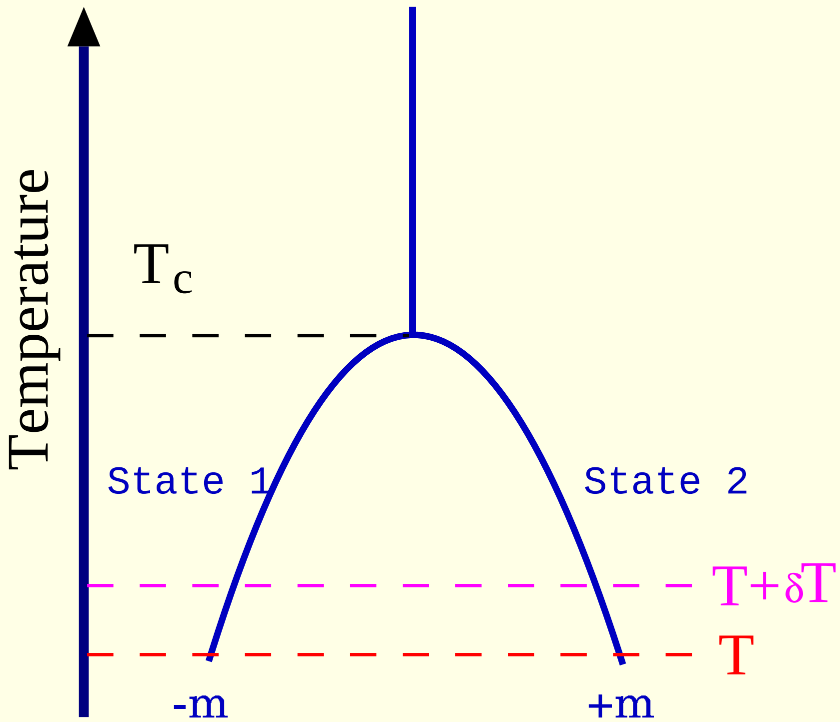
Statistical-Mechanical Approach to Probabilistic Information Processing

Outline

- Stability of the spin-glass state against temperature perturbation
  - Temperature chaos in spin glass state
- Our strategy: Simulation-data analysis
  - Eigenmode anlysis of the susceptibility matrix = PCA
  - application of the analysis to the SK Ising model
- Short-ranged Ising spin glass model
  - Our conclusion :
    spin glass states in four dimensions are very sensitive to temperature change.

Stability or Fragility of the ordered state

- Simplest case： Ising ferromagnetic model below T_c



  - An overlap between two valleys

    $$q^{12} = q^{21} = -m^2(T)$$
    $$q^{11} = q^{22} = +m^2(T)$$

    The overlap distribution becomes trivial delta functions at $q = \pm m^2$.

  - An overlap between equilibrium states at T and $T + \delta T$

    $$q(T, T+\delta T) = \pm m(T)m(T+\delta T),$$

    varying *smoothly* with T.

- The ferromagnetic ordered state is usually stable against temperature change.

Example: Instability of the ordered state against a perturbation

A ground state of 1 dimensional random Ising spin : $H(S_i) = -\sum J_{i,i+1}S_iS_{i+1}$

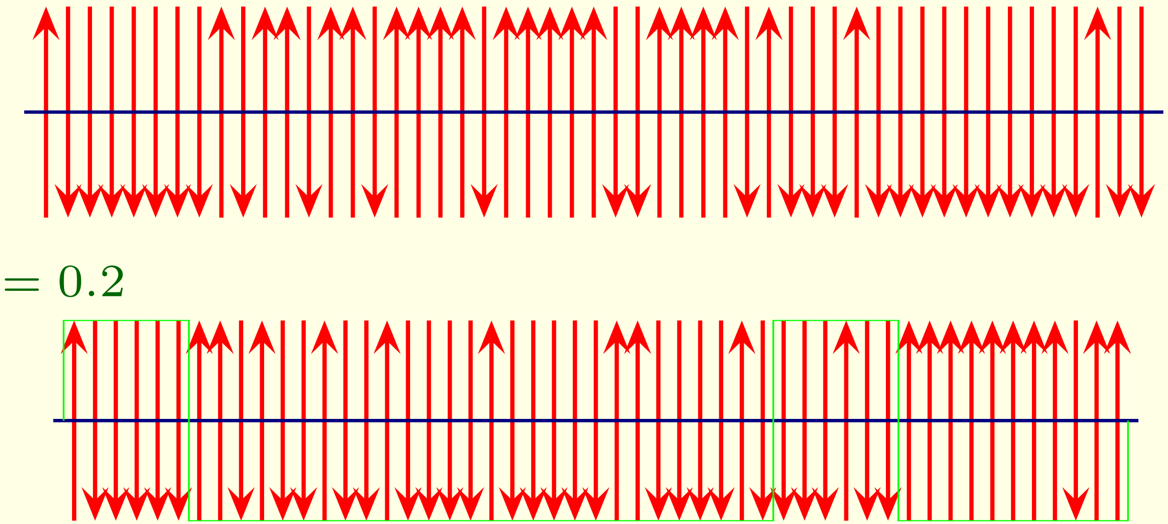
Does the ground state change by adding a random perturbation term $\epsilon J'_{i,i+1}$?

- Ferromagnetic case $(J_{ij} = J)$ is stable when $\epsilon < J$
- Random system : An overlap correlation vanishes in a large length scale

$$\lim_{|i-j|\to\infty} \langle S_i(\epsilon)S_i(0)S_j(\epsilon)S_j(0)\rangle = 0$$

$\epsilon = 0.0$

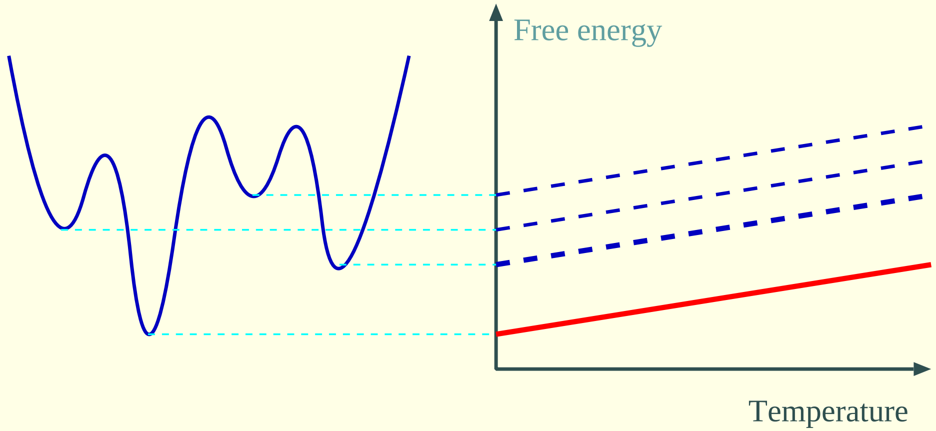
$\epsilon = 0.2$



- Origin of the perturbation term could be due to temperature change.

Fragility of the glassy state in disordered Systems

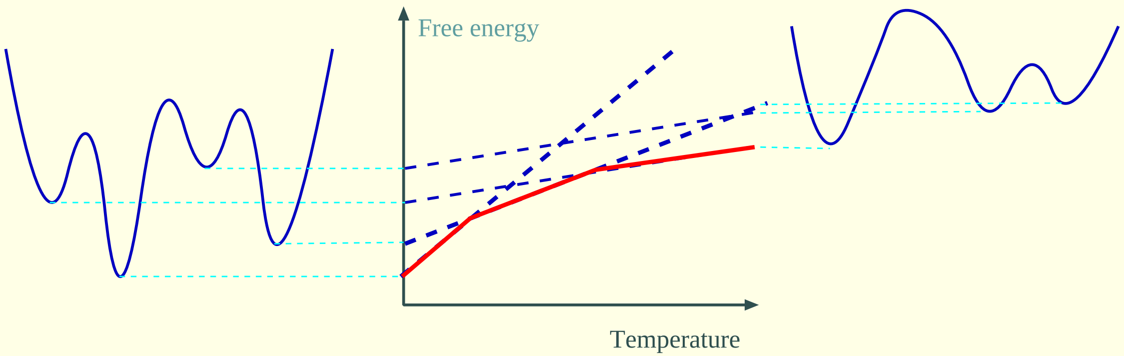
- Stable case



NO LEVEL CROSSING

The lowest free-energy state at T ALSO dominates the partition function at $T + \delta T$.

- Unstable case



LEVEL CROSSING

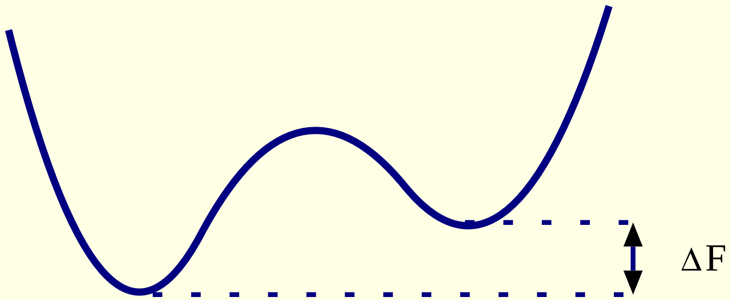
Temperature chaos as level crossings

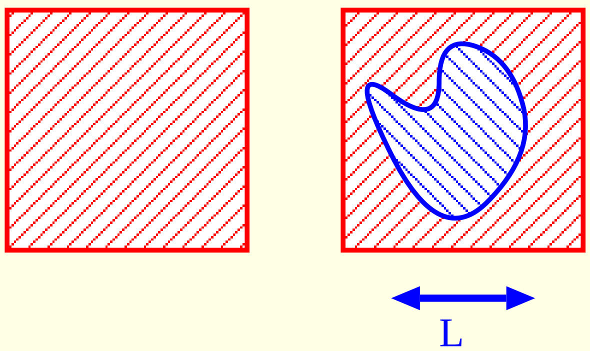
– Temperature Chaos : Stability against temperature perturbation.
The equilibrium states at different temperatures are *TOTALLY DIFFERENT*.
$\Longrightarrow$ The overlap $q(T, T + \delta T)$ is ZERO

"Chaotic Nature of the Spin-Glass Phase"

A. J. Bray and M. A. Moore: Phys. Rev. Lett. **58**, 57 (1987).

D. S. Fisher and D. A. Huse: Phys. Rev. B **38**, 386 (1988).





Free-energy difference at T

$\Delta F(T) = \Delta E - T\Delta S \sim \Upsilon L^{\theta}$

θ: stiffness exponent

Υ: T dependent stiffness constant

Change the temperature to $T + \delta T$

$$\begin{aligned} \Delta F(T+\delta T) &\simeq \Delta E - (T+\delta T)\Delta S \\ &\simeq \Upsilon L^{\theta} - \delta T \Delta S. \end{aligned}$$

Entropy difference of the droplet surface

$\Delta S \sim \pm L^{d_s/2}$: d_s: fractal dimension

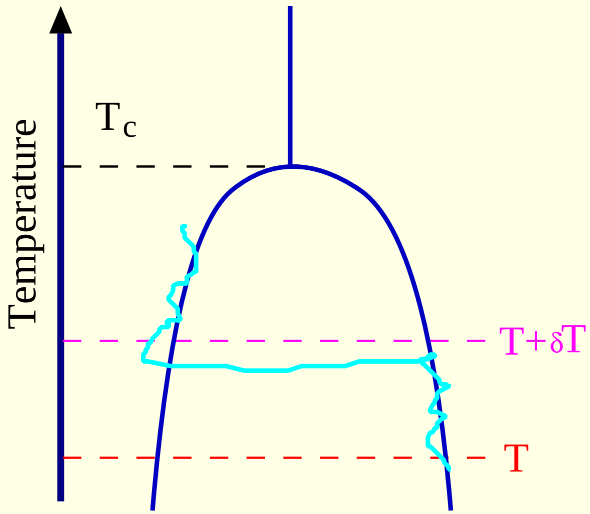
If $d_s/2 > \theta$, $\Delta F(T+\delta T) \simeq \Upsilon L^{\theta} + \delta T L^{d_s/2}$ can CHANGE the sign.

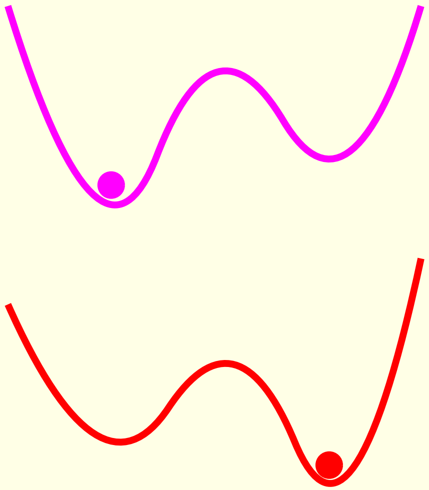
$\Longrightarrow$ The equilibrium state should change on a length scale $L(\delta T) \sim \delta T^{-\frac{1}{d_s/2-\theta}}$.

Chaos exponent ζ and Stiffness Exponent θ

- Chaos exponent: $\zeta = d_s/2 - \theta > 0 \Longrightarrow$ CHAOS .... Lyapunov exponent
- Stiffness exponent θ:
  - mean-field picture (mean-field model): $\theta = 0$.
  - short-ranged SG model in three dimensions: $\theta \simeq 0.2$. (Numerical estimation)

$d_s/2 \geq (d-1)/2 \qquad \Longrightarrow$ Temperature Chaos likely occurs in SG systems.





Against Temperature Chaos...

- I. Kondor, J. Phys. A **22**, L163 (1989)
  On chaos in spin glass

- A. Billoire and E. Marinari, J. Phys. A **33**, L265 (2000),
  Evidences Against Temperature Chaos in Mean Field and Realistic Spin Glasses

- T. Rizzo, J. Phys. A **34**, 5531 (2001),
  Against Chaos in Temperature in Mean-Field Spin Glass Models.

- R. Mulet, A. Pagnani, and G. Parisi, Phys. Rev. B **63**, 184438 (2001),
  Against temperature chaos in naive Thouless-Anderson-Palmer equations

- A. Billoire and E. Marinari, cond-mat/0202473,
  Overlap Among States at Different Temperatures in the SK Model.

Experiment 1: Memory and Chaos Effects in Spin Glasses

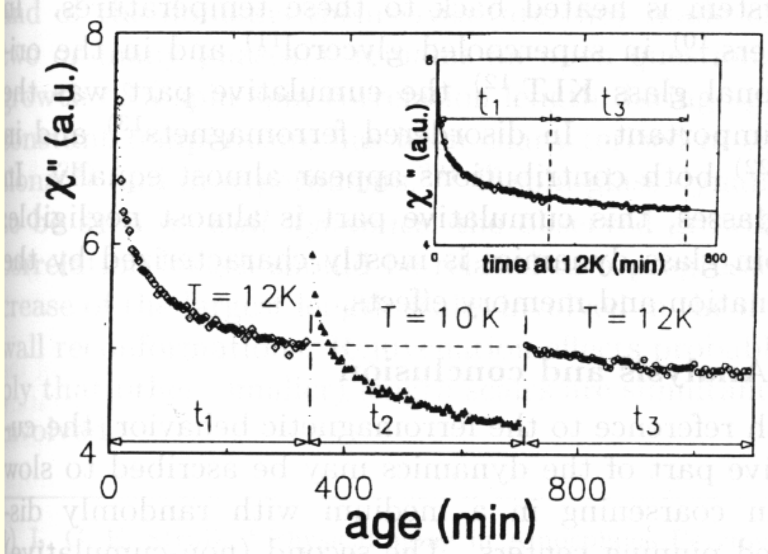
J. Hammann, et al : J.Phys.Soc.Jpn. 69 (2000)Suppl. A, 206–211.
(Saclay-Uppsala experiments, 1992)

- Temeprature cycling experiment

- Rejuvenation(Chaos) effect:
  long relaxation process at T_1 does not play any role for the relaxation at a different temperature.

  The ordered states seem to depend on temperature. $\rightarrow$ Temperature Chaos??

- Memory effect:
  The system keeps information that relaxation has previously been done during the interval t_1 at T_1.



ig. 7. $CdCr_{1.7}In_{0.3}S_4$ spin glass ($T_g = 16.7K$): effect of a negative temperature cycling $12K- > 10K- > 12K$ on the time dependence of χ'' (f=0.01Hz). The inset shows the relaxation measured during t_3 plotted in continuation of the initial relaxation during t_1 (the solid line is a relaxation at $0.72T_g$ without temperature cycling).

Our strategy: Eigenmode Analysis of susceptibility matrix

- Conventional approach: Overlap between two temperatures T_1 and $T_2 = T_1 + \delta T$.
  - TAP solution (equation of states) in mean-field models:

$$q'(T_1, T_2) \equiv \left[\frac{1}{N} \sum_i m_i(T_1) m_i(T_2) \right]_J$$

  - MC simulation:

$$q^{(2)}(T_1, T_2) \equiv \left[\left\langle \left(\frac{1}{N} \sum_i S_i(T_1) S_i(T_2) \right)^2 \right\rangle_{T_1, T_2} \right]_J$$

- **Our approach**: Eigenmodes of the susceptibility matrix and their temperature dependence.

$$\chi_{ij} = \frac{\partial^2}{\partial h_i \partial h_j} F(\{h_i\}) \Big|_{h=0} = \frac{\partial}{\partial h_i} \langle S_j \rangle \Big|_{h=0} = \beta \langle S_i S_j \rangle$$

Our strategy (2): Eigenmode Analysis of susceptibility matrix

STEP 1: Monte Carlo Simulation

- Perform MC simulation
  - use the extended ensemble method to avoid extremely slow relaxation in random systems.
    - Multicanonical MC (Berg–Neuhaus)
    - Simulated tempering (Marinari–Parisi)
    - Exchange MC (Hukushima–Nemoto, Parallel tempering)

- Generate M spin configurations $\Longrightarrow \{S_i^1\}, \{S_i^2\}, \{S_i^3\}, \cdots, \{S_i^M\}$

STEP 2: Multivariate analysis of the simulation data

- Eigenmode analysis = Principal component analysis (PCA)
- Calculate Susceptibility matrix (or Hamming distance matrix)

$$C_{ij} = \frac{1}{M}\sum_{\mu}^{M}(S_i^\mu - \overline{S_i})(S_j^\mu - \overline{S_j}) \text{ with } \overline{S_i} = \frac{1}{M}\sum_\mu S_i^\mu.$$

- diagonalize the matrix

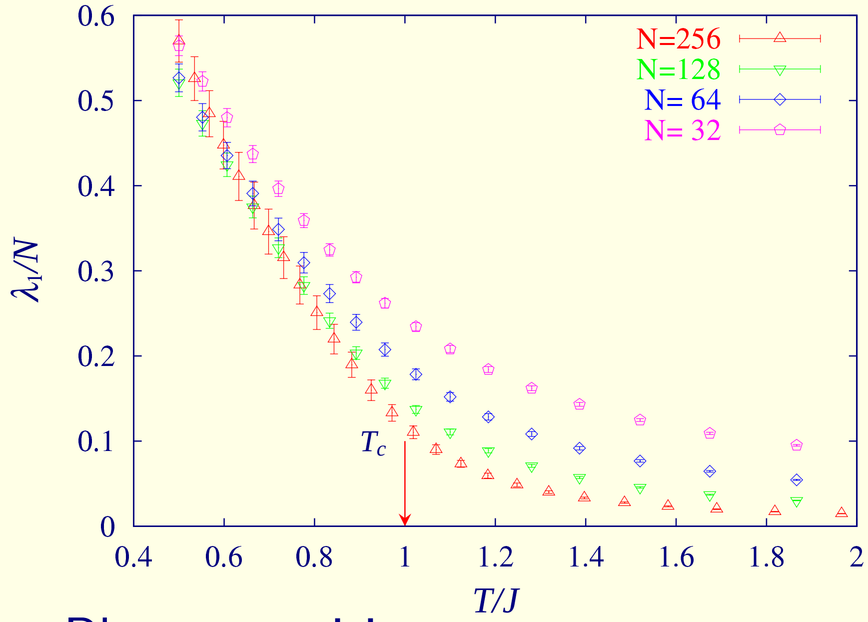
Multivariate Analysis of Simulation data

- theory: Eigenmode of the susceptibility matrix in spin glasses.
  - A. J. Bray and M. A. Moore, J. Phys. **C15** (1982) L765.
- Numerical Examination
  - Nemoto-Yamada, Bussei-Kenkyu (Kyoto) **74** (2000) 122.
  - J. Sinova, G. Canright and A. H. MacDonald, Phys. Rev. Lett. **85** (2000) 2609.
- Cluster analysis of the simulation data
  - E. Domany, G.Hed, M. Palassini and A.P.Young, Phys. Rev. B **64** (2001) 224406.
- Finite mixture,
  - Iba-Hukushima, Prog. Theor. Phys. 138 (2000) 462.
  - Marinari-Martin-Zuliani, cond-mat/0103534
- Protein, ... PCA

Application to the SK model 1

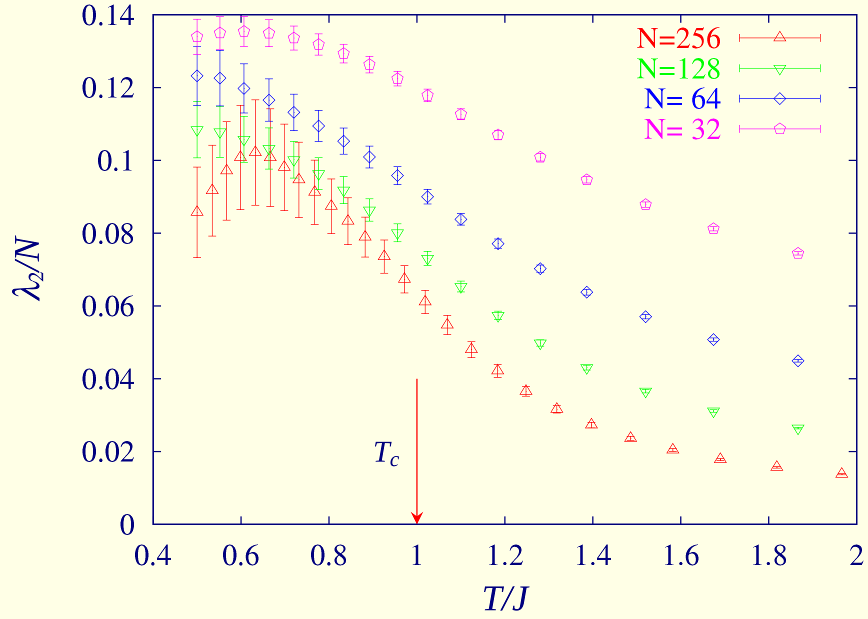
Temp. dep of 1st Eigenvalue

λ_1/N vs T/J



Temp. dep of 2nd Eigenvalue

λ_2/N vs T/J



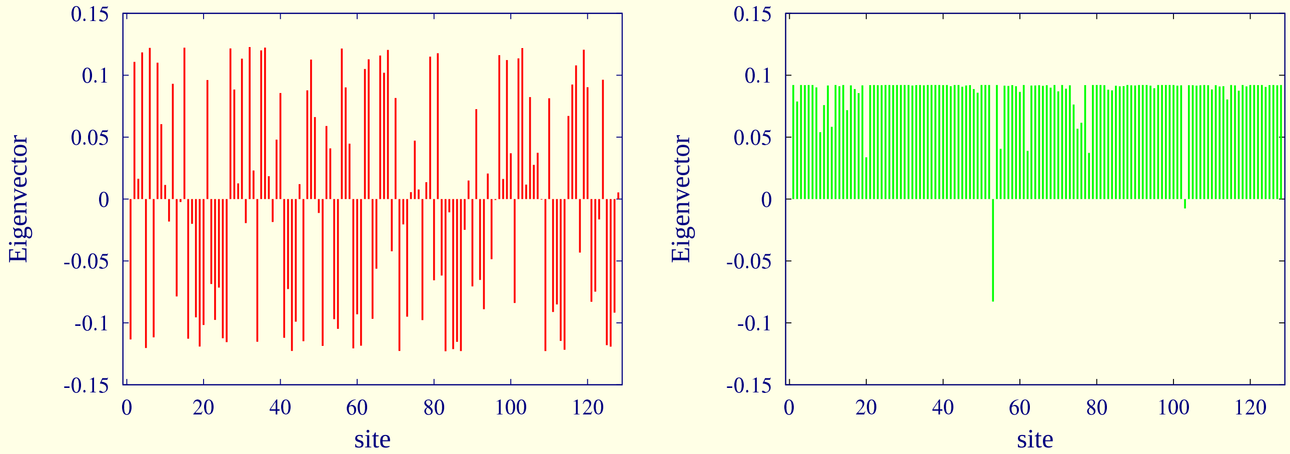
- Phase transition :
  SG transition is characterized by
  $$\chi_{\mathrm{SG}}^J = \frac{1}{N}\mathrm{Tr}C^2.$$
  – disordered phase : $\lambda \sim O(1)$
  – ordered phase : $\lambda \sim O(N)$

$$\frac{1}{N}\mathrm{Tr}C = 1$$

The next largest eigenvalue also has a finite contribution even in $N \to \infty$.

SG and Ferromagnetic phase in the SK model with $N = 128$

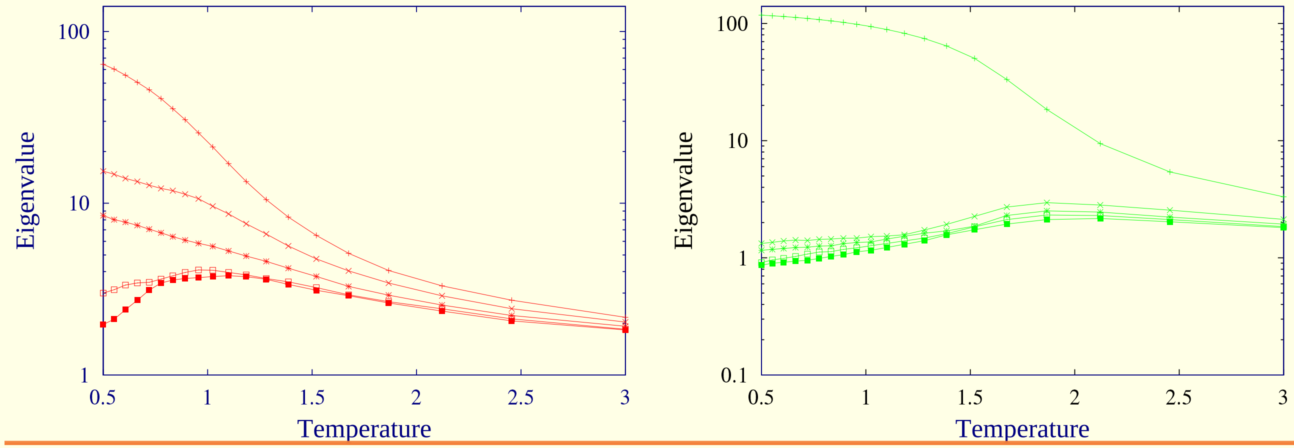
Eigenvector of the largest eigenvalue at $T/J = 0.5$ and $J_0 = 0$ and $J_0 = 1.2$.



Eigenvector corresponds to the ordering pattern.

- SG phase: random vector
- F Phase : uniform

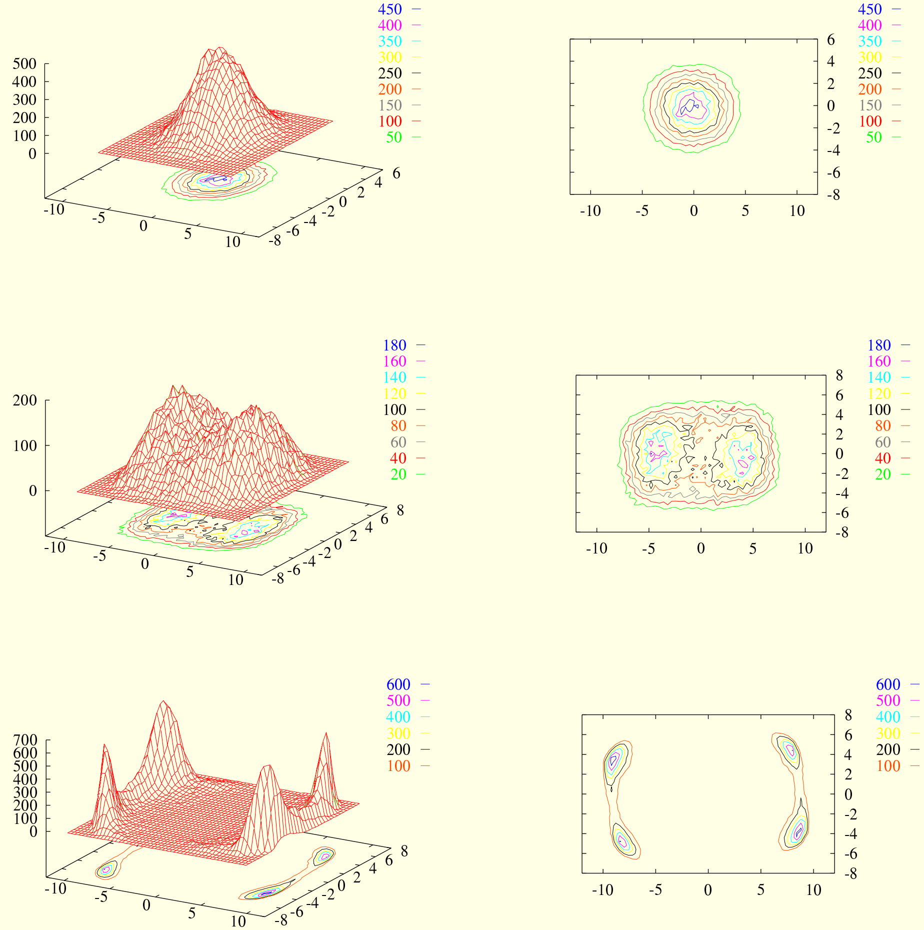
Temperature dependence of the largest 5 eigenvalues



Ferromagnetic phase has a couple of degenerate eigenmodes.

Application to the SK model 3

- PCA plot
  Histogram of the MC simulation data projected onto;
  - x axis:
    the largest eigenvector
    $$x^\mu = \sum_i S_i^\mu e_i^{1st}$$
  - y axis:
    the next largest eigenvector
    $$y^\mu = \sum_i S_i^\mu e_i^{2nd}$$
- Free-energy landscape?



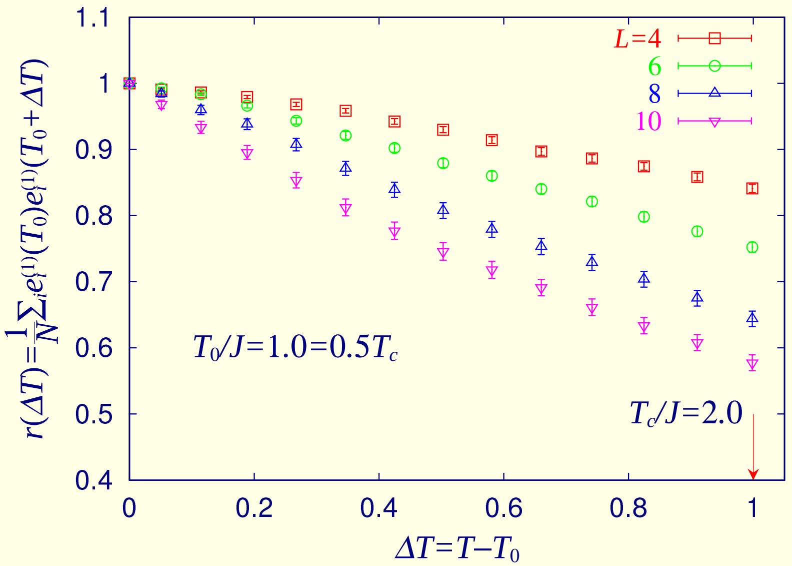
...a spin-glass model in finite dimensions.

Temp. dep. of eigenmode in SG phase : the first eigenvector

4 dimensional $\pm J$ Ising EA Model using **the dual trick method**

Overlap between two eigenvectors

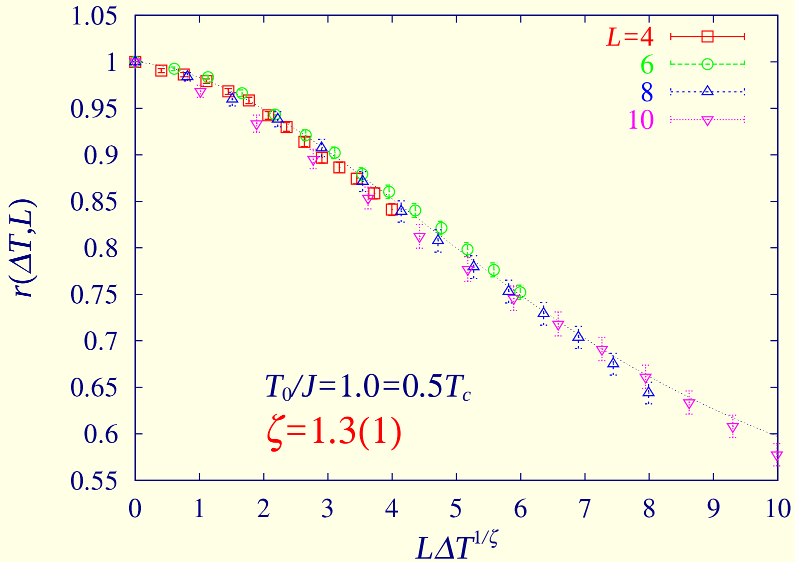
$$r_{T_0}(\Delta T) \equiv \left| \frac{1}{N} \sum_i e_i^{(T_0)} e_i^{(T_0+\Delta T)} \right|$$



The overlap decreases with increasing L.

Finite size scaling

$$r_{T_0}(\Delta T, L) = F(L/L_{\rm ovl}) \text{ with}$$
$$L_{\rm ovl} = \Delta T^{1/\zeta}$$



$r_{T_0}(\Delta T) \to 0$ in the thermodynamic limit($L \to \infty$).

$\Longrightarrow$ Eigenmode (Ordering pattern) significantly depends on temperature.

The second eigenvector...

$4d \pm J$ Ising EA Model using **the dual trick method**

The second eigenvalue is also of order N, namely *Extensive*.

Green Overlap of 1st eigenvec.

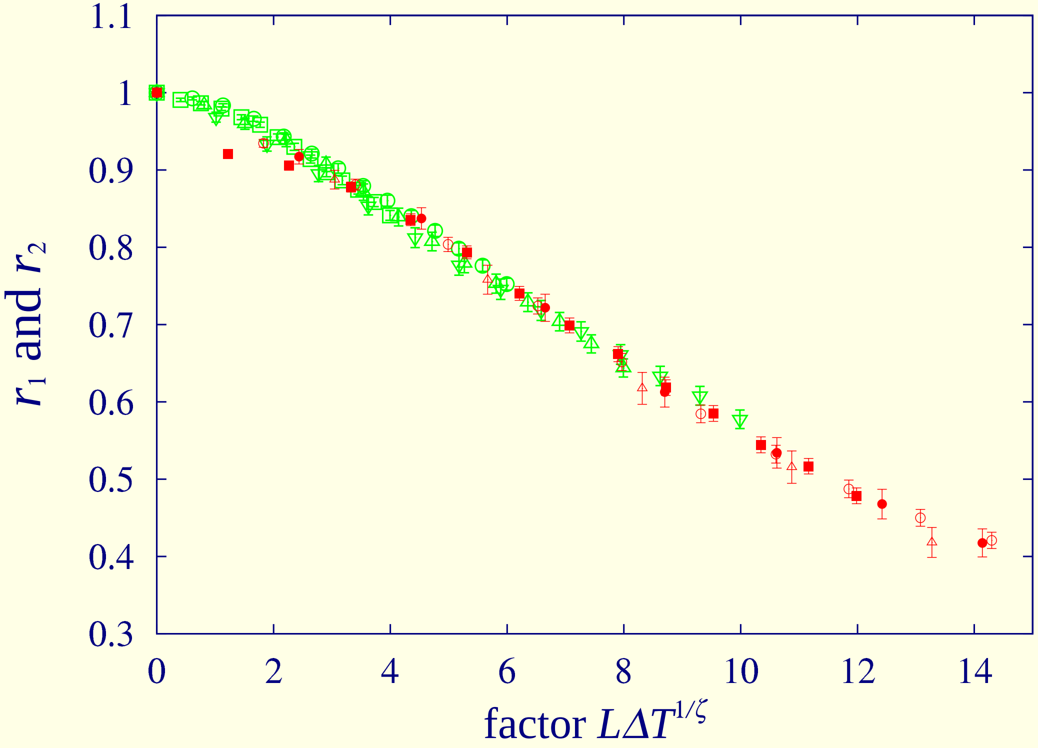
Red Overlap of 2nd one.

one adjustable parameter for the scaling axis.

- the same scaling function.
- And, the exponent $\zeta \simeq 1.3$ agrees with that of bond perturbation in the same model (M. Ney-Nifle,PRB57, 492(1998)).

Finite size scaling

$r_{T_0}(\Delta T, L) = F(L/L_{\rm ovl})$ with $L_{\rm ovl} = \Delta T^{1/\zeta}$



About the scaling function...

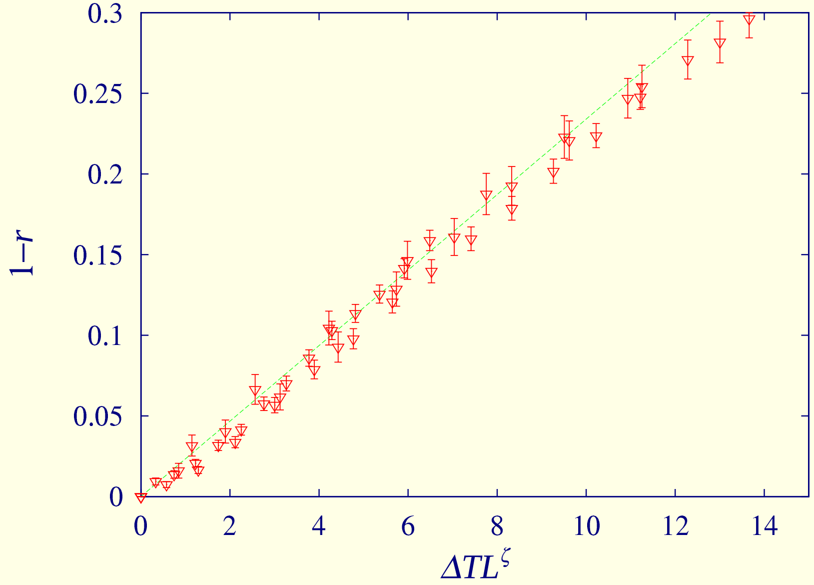
- The overlap $r(\Delta T)$ is unity when $\Delta T = 0$.
- According to Bray-Moore argument, the deviation from unity, $1 - r(\Delta T)$ is due to a droplet excitation with size L, whose probability by entropy gain is expressed as

$$p \sim \frac{\Delta T L^{d_s/2}}{\Upsilon L^{\theta}} = \frac{L^{\zeta}\Delta T}{\Upsilon}$$

- When the droplet size is of order of the system size, the deviation of $r(\Delta T)$ becomes $O(1)$. Thus,

$$1 - r \propto p = \frac{L^{\zeta}\Delta T}{\Upsilon}$$

Scaling function $1 - r$ vs $L^{\zeta}\Delta T$



$f(x) \equiv 1 - r(x)$ is linear in $x = L^{\zeta}\Delta T$ for $x \ll 1$.

Summary

- We have investigated the fragility of the spin glass state in four dimensions :
  - from an new view point, which is temperature dependence of eigenmode of the susceptibility matrix (=PCA).
  - Using the finite-size scaling, the eigenmode is found to be very sensitive to the temperature change, suggesting Temperature Chaos
  - The value of the scaling exponent ζ is consistent with that obtained by other perturbation.

  - Against 'the against ...'
    * F. Krzakala and O .C .Martin, cond-mat/0203449, Eur. Phys. J. B**28** (2002) 199. *"Chaotic temperature dependence in a model of spin glasses"*.
    * K. Hukushima and Y. Iba, cond-mat/0207123.
    * T. Aspelmeier, A. J. Bray, M. A. Moore, cond-mat/0207300, PRL**89**,(2002) 197202. *"Why temperature chaos in spin glasses is hard to observe"*
    * T.Rizzo and A. Crisanti, PRL **90**, (2003) 137201. *"Chaos in Temperature in the SK model"*... 9th order perturbation theory.