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Eigenmodes of Susceptibility Matrix
(帯磁率行列の固有モード解析)

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Outline

- Correlation Matrix Spectral Analysis
- New techniques for numerical diagonalization of correlation matrix
  - Dual Trick
  - (On-line Method)
- Applications to spin models
  - three-dimensional fully frustrated Ising model
  - short-range Ising spin glass model

Eigenmode Analysis of Susceptibility Matrix

Susceptibility Matrix ($N \times N$ dense matrix)

$$\boxed{C_{ij} = \langle S_i S_j \rangle} = \begin{cases} \delta_{ij} & (T \to \infty) \\ +1 & (T \to 0 \quad \text{in non-frustrated ferromagnet}) \end{cases}$$

Eigenmode associated with O(N) eigen value : Long range order

$$\chi_{\mathrm{SG}}^{J} \equiv \frac{1}{N} \sum_{ij} \left(\langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle\right)^2 = \frac{1}{N} \sum_{ij} C_{ij}^2 = \mathrm{Tr}\ C^2/N \quad \text{for} \quad T > T_c$$

- Analytical argument of Griffiths phase in random spin systems :

  A.J.Bray and M.A.Moore J. Phys. **C15** (1982) L765.

  A.J.Bray, Phys. Rev. Lett., **59** (1987) 586

- Numerical studies of the Griffiths phase: Nemoto-Yamada, unpublished

- Dynamical correlation matrix:

  H. Takano and S. Miyashita, J. Phys. Soc. Jpn., **64** (1995) 3688.

Correlation-Matrix Analysis in the Spin Glass Phase (1)

- J. Sinova, G. Canright and A. H. MacDonald, Phys. Rev. Lett. **85** (2000) 2609.
- J. Sinova, G. Canright, H. E. Castillo and A. H. MacDonald,
  Phys. Rev. B **85**, (2001) 104427. (J. Sinova and G. Canright, cond-mat/0103071.)

Random Filed Ising Model

Ordering appears in the spectrum of the correlation matrix AS AN EXTENSIVE EIGENVALUE.

There is **RSB** $\longrightarrow$ There must be MORE THAN ONE EXTENSIVE EIGENVALUE in the spectrum of C_{ij}.

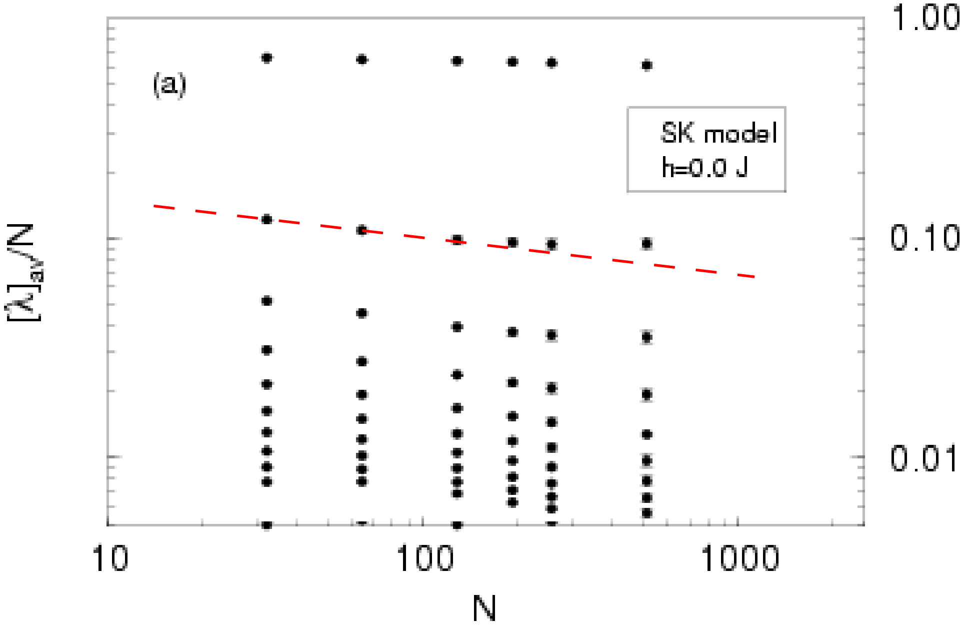
Absence of RSB $\longrightarrow$ There can only be on such extensive eigenvalue.

# of Extensive Eigenvalues → # of pure states.

Correlation-Matrix Analysis in the Spin Glass Phase (2)

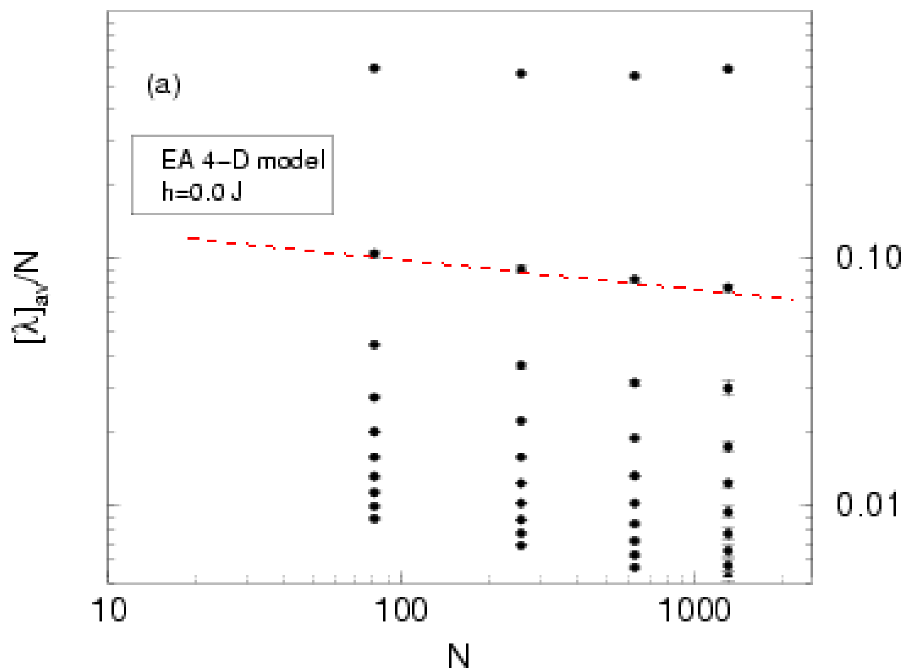
Finite size scaling of the disorder average of the ten largest eigenvalues of C_{ij}

SK model



Multiple extensive eigenvalues in the RSB phase, as expected.

4D Gaussian EA Ising model



A single extensive eigenvalue, consistent with the droplet theory.

Conventional Method for the Eigenmode Analysis

STEP 1: Evaluate susceptibility-matrix using Monte Carlo simulations.

$$C_{ij} = \langle (S_i - \overline{S_i})(S_j - \overline{S_j}) \rangle = \frac{1}{M} \sum_{\mu}^{M} (S_i^{\mu} - \overline{S_i})(S_j^{\mu} - \overline{S_j}) \qquad (1)$$

where $S_i = \frac{1}{M} \sum_{\mu} S_i^{\mu}$ and M is the total number of MC steps.

STEP 2: Diagonalize the matrix C_{ij}

$$\sum_{j}^{N} C_{ij} e_j = \lambda e_i. \qquad (2)$$

Eigenmode Analysis in Physics
Principal Component Analysis (PCA) in Statistics

- $O(N^2)$ memory to storage the matrix element of C_{ij} with $N \times N$.
- $O(N^3)$ time complexity to diagonalize C_{ij} by Householder method.

$$\Longrightarrow \begin{cases} \text{Nemoto } \textit{et al} & N \leq 28^2 = 784 \\ \text{Sinova } \textit{et al} & N \leq 6^4 = 1296 \rightarrow 13\text{MB} \end{cases}$$

New Methods for Eigenmode Analysis

Don't keep the matrix elements of C_{ij}.

Proposed Methods

1. **Dual Trick**
   - Memory : $O(N)$
   - Time: $O(N)$
   - Drawback: diagonalization of $M \times M$ matrix
2. **One-line Trick**
   - Memory: $O(N \times K)$, K is a number of our desired eigenmodes.
   - Time: $O(N \times K^2)$
   - Drawback: Need iteration for many times.

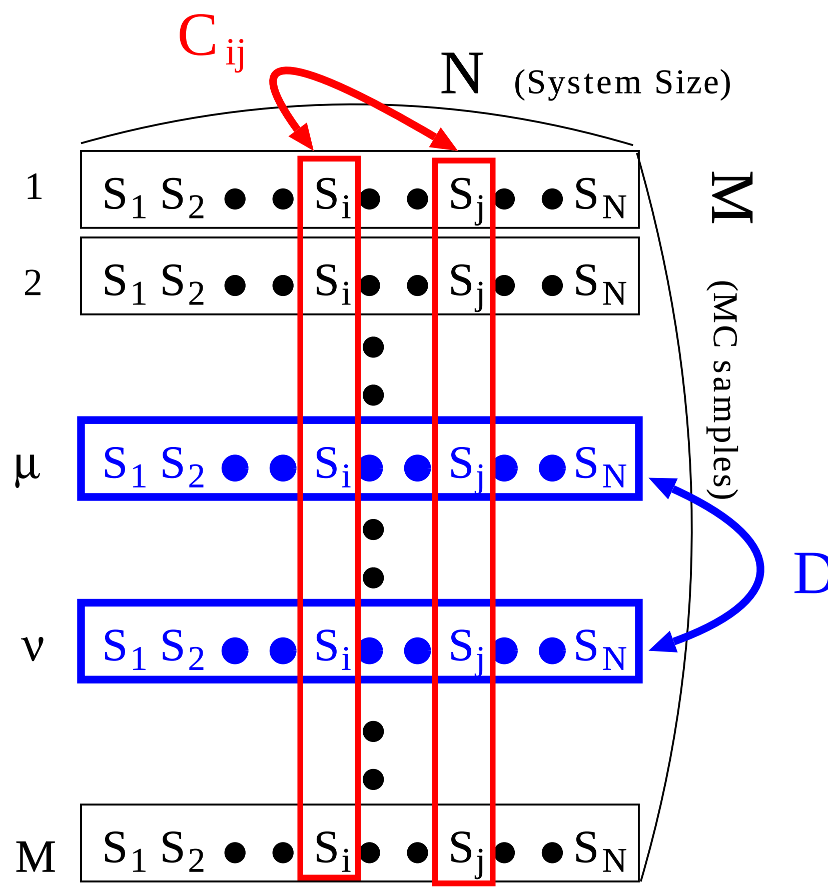
Dual Trick Method

Step 1: Evaluate **Hamming-distance Matrix** $D^{\mu\nu}$ between data obtained by MC simulation

$$D^{\mu\nu} = \frac{1}{N}\sum_i^N (S_i^\mu - \overline{S_i})(S_i^\nu - \overline{S_i}).$$

Step 2: Diagonalize the Matrix $D^{\nu\mu}$ **(Dual Problem)**

$$\sum_\nu^M D^{\mu\nu}\hat{e}_\nu = \lambda \hat{e}_\mu.$$



Dual to Original Problem

- Dual relation

primary	$\sum_j^N C_{ij} e_j = \lambda e_i.$	$(N \times N)$
dual	$\sum_\nu^M D^{\mu\nu} \hat{e}_\nu = \lambda \hat{e}_\mu.$	$(M \times M)$
DATA	$X_i^\mu = (S_i^\mu - \langle S_i \rangle)$	$(M \times N)$

$$e_i = \sum_{\mu=1}^{M} X_i^\mu \hat{e}^\mu$$

Eigenvector with the eigenvalue λ/M of the correlation matrix C_{ij}

- Paradox: Missing rank ?

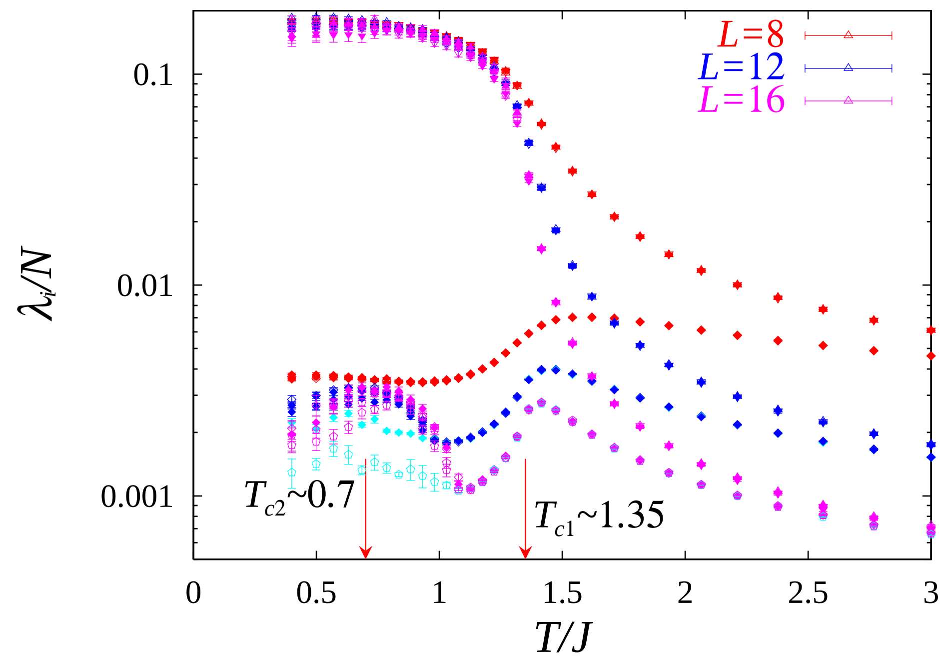
$$[rank] = \min(N, M)$$

Application to $3d$ Fully Frustrated Ising Model

$3d$ Fully Frautrated Ising Model

using **On-line trick method**

- Multiple pure states
  - Phase Transition 1:
    $T_{c1}/J \sim 1.35$
    16-hold states
  - Phase Transition 2:
    $T_{c2}/J \sim 0.7$
    24-hold states



Temperature dependence of the eigenvalues.

Application to Ising Spin Glass Model

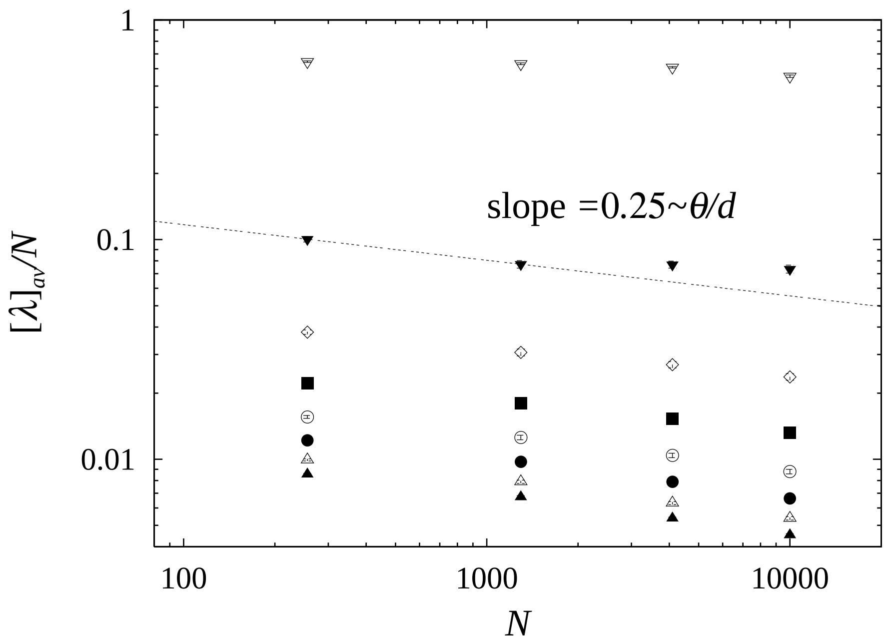
$4d \pm J$ Ising EA Model using **the dual trick method**

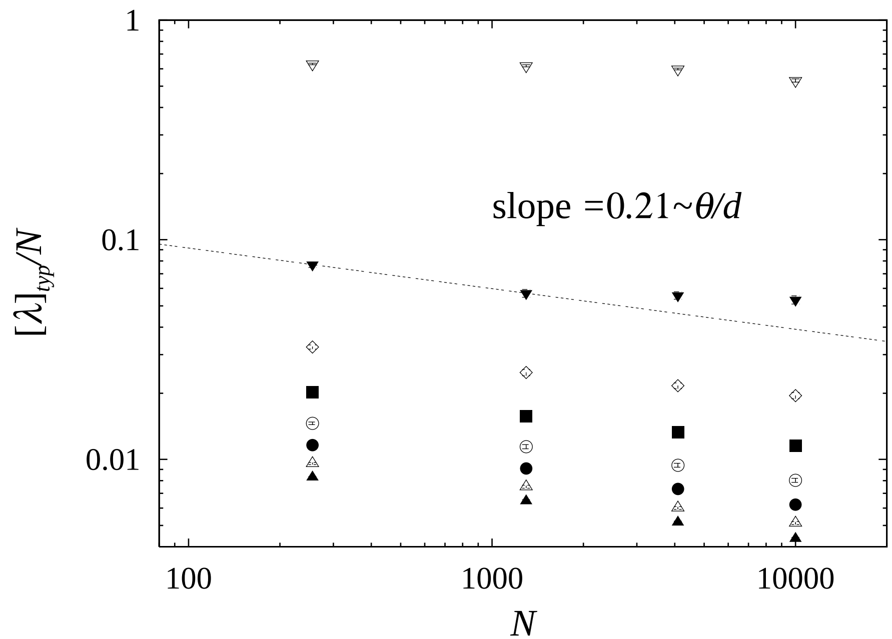
System Size: $N \leq 10^4 = 10,000$ (800MB in conventional method)

Temprature: $T/J = 1.0 \sim 0.5T_c$

Average

Typical ($[\lambda]_{\text{type}} \equiv \exp[\ln \lambda_i]_{\text{av}}$)





The secont eigenvalue is found to be **extensive** for $N > 6^4$.

$\Longrightarrow$ **Multiple Pure States**

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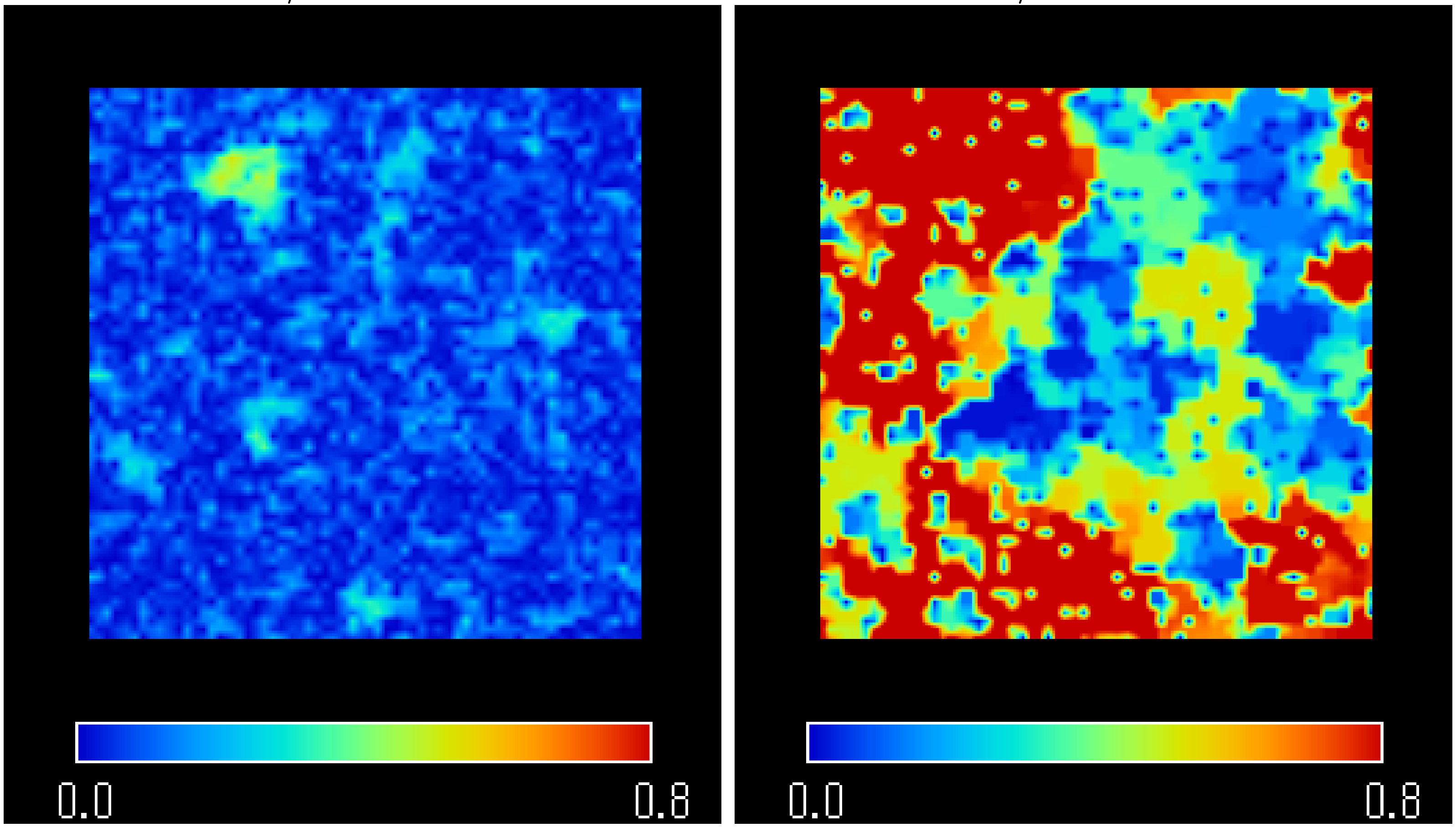
Summary

- New technique for Eigenmode Analysis to correlation-matrix
  - Dual Trick
    from Hamming-distance matrix to spin-correlation matrix
  - (On-line Trick)
- Application to $4d \pm J$ Ising EA model
  The second eigenvalue is also extensive at low temperatures.
  $\Longrightarrow$ Multiple pure states
- Furture problems
  - Eigenvector $\longrightarrow$ Ordering pattern, Site magnetization
    - $*$ Direct observation of Low-energy excitations like droplet

Application to $2d$ Ising Spin Glass Model

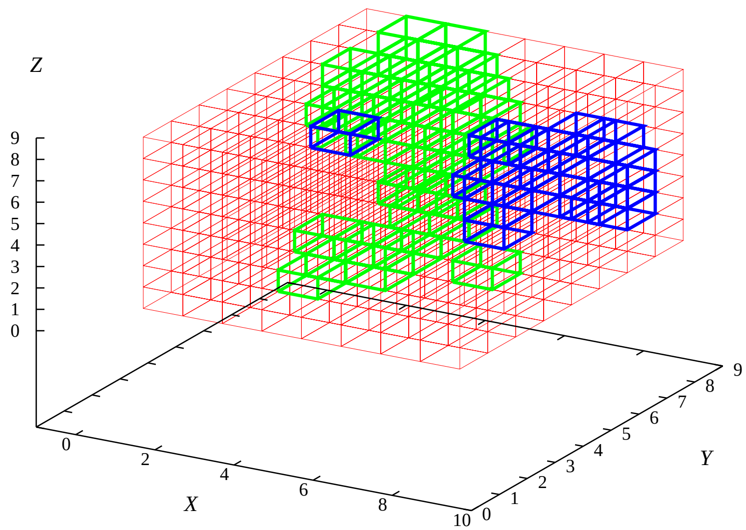
The first eigenvector of a sample with $N = 64^2$

$T/J = 1.8$ $\qquad$ $T/J = 0.4$



Application to $3d\pm$ Ising Spin Glass Model

Three eigenvecors of a sample at $T/J = 0.4$



Real space plot of spin sites with large amplitude of the first(red), second(blue) and third(green))eigenvectors.

Overlap between data and eigenvector.