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Relaxation Modes in the Two-Dimensional $\pm J$ Ising Spin Glass

Hiroshi TAKANO and Seiji MIYASHITA[1]
Department of Physics, Faculty of Science and Technology, Keio University, Yokohama 223
[1] *Graduate School of Human and Environmental Studies, Kyoto University, Kyoto 606*
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A new method to find slow relaxation modes in random spin systems is applied to the two-dimensional $\pm J$ Ising spin glass below the critical temperature of the corresponding nonrandom ferromagnet. It is found through Monte Carlo simulations that the slow relaxation modes obtained by the method describe the long-time behavior of spins well. The slow relaxation modes are spatially localized and can be regarded as clusters. The distribution of the relaxation rates is consistent with the prediction of the theory which assumes independent motion of clusters.

KEYWORDS: random spin systems, relaxation modes, the Ising spin glass, the Griffiths singularity, spin autocorrelation function, Monte Carlo simulations

1. Introduction

There have been many studies[1-13] on slow relaxation due to the Griffiths singularity.[14] Theories[1-7] have predicted that the relaxation of the averaged spin autocorrelation function in a random spin system becomes anomalously slow at a certain temperature region above the transition temperature $T_c^{\rm rand}$ of the random spin system. The temperature region is called the Griffiths phase.

For a diluted Ising ferromagnet or a $\pm J$ Ising spin glass in d dimensions, the asymptotic long-time behavior of the averaged spin autocorrelation function $q(t)$ at temperatures between $T_c^{\rm rand}$ and $T_c^{\rm pure}$ has been predicted[1,3,7] as

$$q(t) \sim \exp\left[-C\,(\ln t)^{d/(d-1)}\right]. \qquad (1)$$

Here, $T_c^{\rm pure}$ denotes the critical temperature of the corresponding nonrandom (pure) system. For a system of N Ising spins, $q(t)$ is defined as

$$q(t) = \frac{1}{N}\sum_{i=1}^{N} q_i(t) = \frac{1}{N}\sum_{i=1}^{N}\langle S_i(t)S_i(0)\rangle, \qquad (2)$$

where $S_i(t)$ denotes a value of the ith spin at a time t and $\langle\cdots\rangle$ represents the thermal average in the equilibrium.

For diluted Ising ferromagnets and $\pm J$ Ising spin glasses in d dimensions, the long-time behavior of $q(t)$ observed in Monte Carlo simulations[8,10-13] seems to be described by a stretched exponential decay

$$q(t) \sim \exp[-Dt^{\beta}] \qquad (3)$$

with a temperature-dependent exponent $0 < \beta < 1$ rather than the predicted behavior (1). Thus, the results of the simulations are apparently inconsistent with the theoretical predictions based on the independent cluster picture.

For the two-dimensional bond-diluted Ising ferromagnet with a bond concentration below the percolation threshold, the present authors have shown[10] that the distribution of the longest relaxation time for each cluster agrees with the theoretical prediction and that the nonexponential decay of $q(t)$, which seems a stretched exponential decay, can be explained by this distribution. Thus, for the diluted Ising ferromagnet, the simulation results are consistent with the theory. The reason why eq. (1) does not fit the Monte Carlo data well is simply that the theoretical asymptotic behavior (1) is not reached in the time region studied by Monte Carlo simulations. For the $\pm J$ Ising spin glasses, however, no identification of clusters has been made and it remains unsolved whether the relaxation phenomena observed in the simulations can be described by the theory based on the independent cluster picture, although some evidences supporting the cluster theory have been found.[13]

In the kinetic Ising model, the autocorrelation function of the ith spin $q_i(t) = \langle S_i(t)S_i(0)\rangle$ is expressed by a sum of the contributions from relaxation modes as $q_i(t) = \sum_n |\mu_{i,n}|^2 \exp(-\lambda_n t)$. Here, λ_n is the relaxation rate of the nth relaxation mode and $|\mu_{i,n}|^2$ is its contribution to $q_i(t)$. If the long-time dynamics of spins can be described in terms of independent motions of clusters, each cluster is considered to correspond to a slow relaxation mode n and the amplitude $|\mu_{i,n}|^2$ of the mode is expected to be spatially localized. Conversely, if the amplitude $|\mu_{i,n}|^2$ of a slow mode n takes appreciable value only for spins in a localized region, this means that the spins in the region relax cooperatively as a cluster.

In this report, we apply an approximate method to find slow relaxation modes and their relaxation rates[15] to the two-dimensional $\pm J$ Ising spin glass in the Griffiths phase through Monte Carlo simulations. The method can find clusters as localized relaxation modes. The consistency between the results of the Monte Carlo simulations and the cluster theory is examined. In §2, the model and the method is explained. In §3, the results of the application of the method to the two-dimensional $\pm J$ Ising spin glass are presented. Summary is given in the last section.

2. Model and Method

In this report, the $\pm J$ Ising spin glass is considered on an $L \times L$ square lattice with periodic boundary con-

ditions. The Hamiltonian of the system including the factor $-1/(k_{\rm B}T)$, where $k_{\rm B}$ and T are the Boltzmann constant and the temperature, respectively, is given by $\mathcal{H} = -\frac{1}{k_{\rm B}T}H = \frac{1}{k_{\rm B}T}\sum_{\langle i,j\rangle} J_{i,j}S_iS_j = \sum_{\langle i,j\rangle} K_{i,j}S_iS_j$. Here, $S_i = \pm 1$ denotes an Ising spin at the ith site and $\sum_{\langle i,j\rangle}$ denotes the summation over all the nearest-neighbor pairs. Each coupling constant $K_{i,j}$ is an independent quenched random variable which is equal to K with probability p or $-K$ with probability $1-p$.

The dynamics of the system is assumed to be described by the single-spin-flip kinetic Ising model.[16,17] The probability $P(S;t)$ that the system has a spin configuration $S = \{S_i\}$ at time t obeys a master equation

$$\frac{\partial}{\partial t}P(S;t) = \sum_i [-W_i(S)P(S;t) + W_i(F_iS)P(F_iS;t)] = -\sum_{S'}\Gamma(S|S')P(S';t), \quad (4)$$

where F_iS denotes a spin configuration obtained from S by flipping the ith spin and $\Gamma(S|S')$ is the time-evolution matrix. The transition probability per unit time $W_i(S)$ for the ith spin to flip in a configuration S is chosen to be of heat bath type (Glauber type):[16,17] $W_i(S) = \frac{1}{2}(1 - S_i\tanh E_i)$ with $E_i = \sum_j^{\langle i\rangle} K_{i,j}S_j$, where $\sum_j^{\langle i\rangle}$ denotes the summation over all nearest-neighbor sites of the ith site.

Let $\phi_n(S)$ be a left eigenvector of Γ with an eigenvalue λ_n: $\sum_S \phi_n(S)\Gamma(S|S') = \lambda_n\phi_n(S')$. Then, the corresponding right eigenvector $\psi_n(S)$, which satisfies $\sum_{S'}\Gamma(S|S')\psi_n(S') = \lambda_n\psi_n(S)$, is expressed as $\psi_n(S) = \phi_n(S)P_{\rm eq}(S)$. We choose the eigenvectors to satisfy the orthonormal condition $\sum_S \phi_n(S)\psi_n(S) = \sum_S \phi_n(S)\phi_m(S)P_{\rm eq}(S) = \delta_{n,m}$. The equilibrium time correlation functions of ϕ_n are given by $\langle\phi_n(t)\phi_m(0)\rangle = \delta_{n,m}\exp(-\lambda_n t)$. The equilibrium distribution $P_{\rm eq}(S)$ is a right eigenvector of Γ with zero eigenvalue. The corresponding left eigenvector is unity. For systems of finite size, all other eigenvalues are positive. In the following, a left eigenvector $\phi_n \neq 1$ and its eigenvalue $\lambda_n > 0$ are called a relaxation mode and its relaxation rate, respectively.

Let $T_t(S|S')$ denote the conditional probability for the system to take a configuration S at time $t_0 + t$ and S' at t_0. This $T_t(S|S')$ is given as $T_t(S|S') = {\rm e}^{-\Gamma t}(S|S')$, which is the $(S|S')$ component of the matrix ${\rm e}^{-\Gamma t}$. The eigenvalue problem for Γ can be rewritten as that for T_t: $\sum_S \phi_n(S)T_t(S|S') = \exp(-\lambda_n t)\phi_n(S')$ and $\sum_{S'} T_t(S|S')\psi_n(S') = \exp(-\lambda_n t)\psi_n(S)$.

Let $S_i(S)$ denote the value of the ith spin in a configuration S. By expanding $S_i(S)$ as $S_i(S) = \sum_n \mu_{i,n}\phi_n(S)$, the correlation matrix $C_{i,j}(t) = \langle S_i(t)S_j(0)\rangle$ and the autocorrelation $q_i(t) = \langle S_i(t)S_i(0)\rangle$ are expressed as $C_{i,j}(t) = \sum_n \mu_{i,n}\mu_{j,n}\exp(-\lambda_n t)$ and $q_i(t) = \sum_n |\mu_{i,n}|^2\exp(-\lambda_n t)$.

In the following, an approximate method to find slow relaxation modes[15] is explained. Although the explanation is given for the kinetic Ising model, the generalization to other spin systems is straightforward.

For the $\pm J$ Ising spin glass in the Griffiths phase, the previous study[13] has revealed the following. In the Griffiths phase of the $\pm J$ Ising spin glass, slowly relaxing spins form cluster structure and one cluster approximately corresponds to a unfrustrated region. For a unfrustrated region corresponding to a cluster, the correlation function $\langle m_{\rm M}(t)m_{\rm M}(0)\rangle$ of the Mattis order[20] $m_{\rm M}$ of the region decays almost exponentially. This suggests that a cluster of spins which relax cooperatively can be identified with a localized relaxation mode similar to the Mattis order $m_{\rm M}$. Therefore, we use a generalization of the Mattis order

$$\phi_n(S) = \sum_i f_{n,i}S_i(t_0/2;S) \quad (5)$$

as an approximate relaxation mode ϕ_n,[15] where $S_i(t;S) = \sum_{S'} S_i(S')T_t(S'|S)$ is the expectation value of the ith spin after a period t starting from a configuration S. Here, $f_{n,i}$ are assumed to be a real number. Based on the variational formulation of the eigenvalue problem for T_t, a relaxation mode $\{f_{n,i}\}$ and its relaxation rate λ_n is determined by a generalized eigenvalue problem

$$\sum_j C_{i,j}(t_0+t)f_{n,j} = \exp(-\lambda_n t)\sum_j C_{i,j}(t_0)f_{n,j} \quad (6)$$

with the orthonormal condition

$$\sum_{i,j} f_{n,i}C_{i,j}(t_0)f_{m,j} = \delta_{n,m}. \quad (7)$$

The expansion coefficients $\mu_{i,n}$ of $S_i(S)$ are given by

$$\mu_{i,n} = \sum_j C_{i,j}(t_0/2)f_{n,j}. \quad (8)$$

Here, $C_{i,j}(t) = \langle S_i(t)S_j(0)\rangle$ is the correlation matrix, which is real and symmetric. Because the trial eigenvector (5) contains only N independent parameters, this eigenvalue problem (6) has N eigenvectors, while the original eigenvalue problem has 2^N eigenvectors. Note that the approximation is considered to become better as t_0 becomes larger.

3. Results for $\pm J$ Ising Spin Glass

In this section, the method explained in the previous section is applied to the two-dimensional $\pm J$ Ising spin glass by means of Monte Carlo simulations. In the following, the parameters are chosen as $L = 32$, $p = 0.5$ and $K = 0.6$. The two-dimensional $\pm J$ Ising spin glass with $p = 0.5$ is believed to undergo no phase transition at finite temperatures. The critical coupling $K_{\rm c}^{\rm pure}$ for the pure system ($p = 1$ or 0) is given by $K_{\rm c}^{\rm pure} \simeq 0.44$. Thus, the present value $K = 0.6$ corresponds to the Griffiths phase of the system $K > K_{\rm c}^{\rm pure}$.

A standard Monte Carlo method which uses discrete time steps and updates spins in random sequence is used to generate a sample of the time evolution of spin configurations described by the master equation (4). The unit time in the master equation (4) corresponds to one update per spin in the present Monte Carlo method, which is called one Monte Carlo step per spin (MCS).

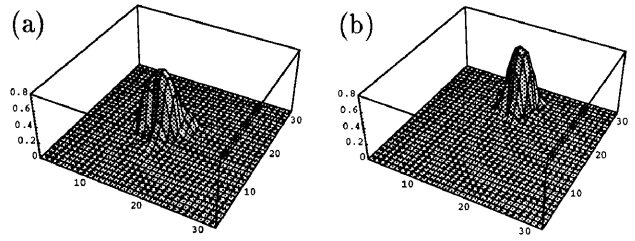

Fig. 1. The spatial distribution of the amplitude $|\mu_{i,n}|^2$ for (a) $n = 1$ and (b) $n = 2$.

For a sample of bond configuration $\{K_{i,j}\}$, the correlation matrix $C_{i,j}(t) = \langle S_i(t)S_j(0)\rangle$ is calculated for several values of t. In a Monte Carlo simulation, the initial 10^5 MCS are discarded for equilibration. Then, about 4×10^6 MCS are used for the calculation of the time average. In practice, $C_{i,j}(t)$ for $i \neq j$ is calculated as $C_{i,j}(t) = (\langle S_i(t)S_j(0)\rangle + \langle S_j(t)S_i(0)\rangle)/2$ because $C_{i,j}(t)$ is symmetric.

By using the correlation matrices $C_{i,j}(2)$ and $C_{i,j}(1)$ calculated by the Monte Carlo simulation, the eigenvalue equation (6) is solved for $t_0 = 1$ and $t = 1$ under the orthonormality condition (7). Each eigenvector $\boldsymbol{f}_n = (f_{n,i})$ represents a relaxation mode $\phi_n(S)$ through eq. (5) and the corresponding eigenvalue $\exp(-\lambda_n t)$ gives the relaxation rate λ_n of the relaxation mode. Here, the obtained solutions $\boldsymbol{f}_n$ and λ_n are numbered from $n = 1$ to $n = 1024$ in increasing order of the relaxation rate λ_n: $0 < \lambda_1 \leq \lambda_2 \leq \cdots$.

The coefficient $\mu_{i,n}$ is calculated through eq. (8). The amplitude $|\mu_{i,n}|^2$ represents the contribution of the nth relaxation mode to the autocorrelation function $q_i(t)$. It is found that only a few modes have large contribution to a single spin. Figure 1 shows i-dependence of $|\mu_{i,n}|^2$, that is, the spatial distribution of the amplitude of the nth mode, for $n = 1$ and 2. These slow modes are clearly localized in space and can be regarded as clusters.

In order to see how the estimated relaxation rates and modes can predict the long-time behavior of the system,

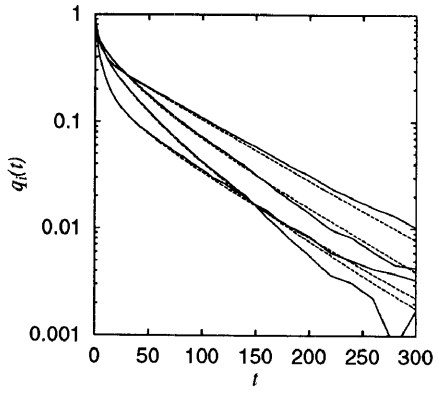

Fig. 2. A semilog plot of $q_i(t)$ versus t for several spins. Solid and dotted lines represent $q_i(t)$ calculated by the Monte Carlo method and that reconstructed from the estimated λ_n and $\mu_{i,n}$, respectively.

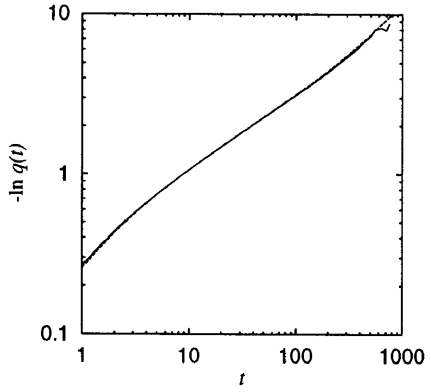

Fig. 3. A log-log plot of $\ln q(t)$ versus t. Solid and dotted lines represent $q(t)$ calculated by the Monte Carlo method and that reconstructed from the estimated λ_n and $\mu_{i,n}$, respectively.

the spin autocorrelation function $q_i(t)$ is reconstructed from the estimated λ_n and $\mu_{i,n}$ and compared with that calculated from Monte Carlo simulation. The results are shown in Fig. 2 for several examples of $q_i(t)$. The agreement between the reconstructed $q_i(t)$ and that calculated by the Monte Carlo method is very good. The same comparison is made in Fig. 3 for the averaged autocorrelation function $q(t) = \frac{1}{N}\sum_i q_i(t)$. Again, the reconstructed $q(t)$ is in very good agreement with that calculated by the Monte Carlo method. This shows the reliability of the present estimation of the relaxation rates and modes.

In the cluster theory of the Griffiths phase of d-dimensional random Ising systems,[1-7] the longest relaxation time of a cluster is given as[6,21]

$$\tau(n) \sim \exp\left[\sigma n^{(d-1)/d}\right] \tag{9}$$

by the size n of a spherical region which can be regarded as a pure system of finite size in the cluster. The probability $P(n)\mathrm{d}n$ that a given spin belongs to such a region of size $n \sim n + \mathrm{d}n$ behaves as

$$P(n) \sim \exp[-cn] \tag{10}$$

in the large n limit. Let $m_{\mathrm{M}}(n)$ denote the Mattis order of the above-mentioned region of size n. In the large n

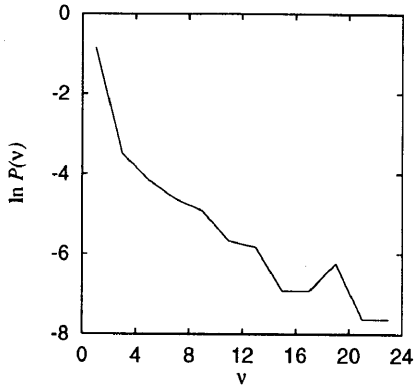

Fig. 4. A plot of $\ln P(\nu)$ versus ν.

limit, $m_{\mathrm{M}}(n)$ should approach a constant m_{M}:

$$m_{\mathrm{M}}(n) \sim m_{\mathrm{M}}. \tag{11}$$

In the Griffiths phase, the long-time behavior of the averaged autocorrelation $q(t)$ is given as

$$q(t) \sim \int \mathrm{d}n P(n) m_{\mathrm{M}}^2(n) \exp\left[-\frac{t}{\tau(n)}\right]. \tag{12}$$

The saddle point estimation of eq. (12) with eqs. (9)–(11) leads to the asymptotic behavior (1) of $q(t)$.

Corresponding to eq. (9), an effective size ν of a cluster (a relaxation mode) is defined through the relaxation time τ of the cluster as[10,13]

$$\nu = (\ln \tau)^{d/(d-1)} \tag{13}$$

or

$$\tau = \exp\left[\nu^{(d-1)/d}\right]. \tag{14}$$

The probability $P(\nu)\Delta\nu$ for a relaxation mode to have an effective size between $\nu - \Delta\nu/2$ and $\nu + \Delta\nu/2$ is estimated from the distribution of the relaxation times $\tau = 1/\lambda$. Figure 4 shows a semilog plot of $P(\nu)$ versus ν. Here, $\Delta\nu$ is chosen to be 2. For large values of ν, $P(\nu)$ seems to behave as

$$P(\nu) \propto \exp(-\gamma\nu), \tag{15}$$

which corresponds to eq. (10).

Let a_n denote the total amplitude of a mode n:

$$a_n = \sum_i |\mu_{i,n}|^2. \tag{16}$$

This a_n can be regarded as an effective number of spins contained in the mode n. Figure 5 shows a plot of a_n versus ν_n for all modes. It can be seen that a_n is approximately proportional to ν_n:

$$a_n \propto \nu_n. \tag{17}$$

This relation between the effective size (the relaxation time) of a mode and the effective number of spins contained in the mode is consistent with the cluster theory.

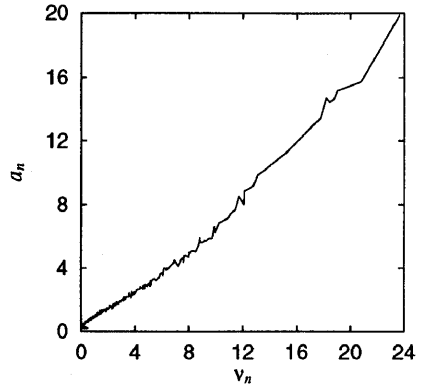

Fig. 5. A plot of a_n versus ν_n.

4. Summary

In this report, we have studied the slow relaxation in the Griffiths phase of the two-dimensional $\pm J$ Ising spin glass. By solving the eigenvalue problem for the correlation matrices, approximate relaxation modes and their relaxation rates are estimated. The relaxation modes and rates obtained describe the long-time behavior of spins well. The slow relaxation modes are localized in space and can be regarded as clusters. This supports the independent cluster picture of the theory. The distribution of the relaxation rates is also consistent with the cluster theory. Thus, for the two-dimensional $\pm J$ Ising spin glass, the simulation results are consistent with the theory. As in the case of the diluted Ising ferromagnet, the reason why the theoretical prediction (1) does not fit the Monte Carlo data well is that the asymptotic behavior (1) is not reached in the time region studied by Monte Carlo simulations.

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