Eigenmode analysis of the susceptibility matrix of the four-dimensional Edwards-Anderson spin-glass model

Article · August 2002

Source: arXiv

CITATIONS
7

READS
80

2 authors:

Koji Hukushima
The University of Tokyo
148 PUBLICATIONS **4,367** CITATIONS

SEE PROFILE

Yukito Iba
The Institute of Statistical Mathematics
42 PUBLICATIONS **894** CITATIONS

SEE PROFILE

Eigenmode analysis of the susceptibility matrix of the four-dimensional Edwards–Anderson spin-glass model

Koji Hukushima[1,*] and Yukito Iba[2,†]

[1] *Institute for Solid State Physics, University of Tokyo, 5-1-5 Kashiwa-no-ha, Kashiwa, Chiba 277-8581, Japan*

[2] *Department of Prediction and Control, The Institute of Statistical Mathematics 4-6-7, Minami-Azabu, Minatoku 106-8569, Tokyo, Japan*

(Dated: July 4, 2002)

The nature of spin-glass phase of the four-dimensional Edwards-Anderson Ising model is numerically studied by eigenmode analysis of the susceptibility matrix up to the lattice size 10^4. Unlike the preceding results on smaller lattices, our result suggests that there exist multiple extensive eigenvalues of the matrix, which does not contradict replica-symmetry-breaking scenarios. The sensitivity of the eigenmodes with respect to a temperature change is examined using finite-size-scaling analysis and an evidence of anomalous sensitivity is found. A computational advantage of dual formulation of the eigenmode analysis in the study of large lattices is also discussed.

PACS numbers: 75.10.Nr, 02.60.Dc

An essential problem in the study of randomly frustrated systems such as spin glass (SG) is how to choose appropriate order parameters. In these systems, most fluctuating variables depend on both of the sample and the temperature used in an experiment. A traditional way to analyze such systems is introduction of order parameters defined by replica overlap. [1, 2].

An alternative method [3, 4], which is more natural and direct, is to choose a set of bases adaptive to a given sample and temperature. Then, order parameters are defined as projections to them. This approach are also useful for the analysis of Monte Carlo (MC) simulation [5]. Recently, Sinova et al. [6, 7] pointed out a relation between the behavior of eigenvalues of the susceptibility matrix with the increase of system size and the existence of replica symmetry breaking (RSB) [2, 8], which refreshed the interest in this approach. They argue that RSB corresponds to the existence of *multiple extensive eigenvalues* in the thermodynamic limit, while the droplet picture [9] implies the uniqueness of the extensive eigenvalue. Sinova et al. numerically investigated the eigenmodes of the Gaussian Edwards-Anderson (EA) Ising model in four dimensions, for which the existence of RSB is most controversial, and obtained an evidence against the RSB picture.

Although their approach is an attractive one, their study is limited to relatively small size $\leq 6^4$ (=1296) of the system. In the present letter, we extend the analysis to much larger size 10^4 (=10000) and to provide further tests for the RSB scenario. Our results show that the scaling of the second eigenvalue looks different in the region of larger system size $\geq 8^4$ at the temperature region that Sinova et al. studied. It no longer contradicts the RSB picture.

We also argue that there are no reason to restrict ourselves in the analysis of eigenvalues. Information contained in eigenmodes themselves, which are discarded in [6, 7], are also useful when we consider gauge invariant quantities defined by them. As an example, we discuss temperature dependence of the eigenmodes as a measure of fragility of the SG equilibrium states. An evidence of anomalous sensitivity in the SG phase is obtained by a finite-size-scaling analysis.

Let us begin with the definition of the model. The four-dimensional EA model is defined with energy

$$H(S) = -\sum_{\langle ij \rangle} J_{ij} S_i S_j, \tag{1}$$

where the Ising spins $\{S_i\}$ are defined on a hyper-cubic lattice in four dimensions with the total number $N = L^4$ of sites. The strength $\{J_{ij}\}$ of nearest-neighbor interactions is distributed according to the bimodal distribution with equal weights at $J_{ij} = \pm J$. A SG phase transition in this model has been well-established by numerical works. In particular, recent extensive MC studies have estimated the critical temperature $T_{\rm c}$ to be $2.0J$ [10, 11]. The value of stiffness exponent $\theta \sim 0.7$ [11, 12] in four dimension is significantly larger than that in three dimensions, $\theta_{\rm 3D} \sim 0.2$ [13], which makes the study of asymptotic behavior considerably easier.

The susceptibility matrix of the model is written as a covariance form

$$C_{ij} = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle, \tag{2}$$

where the bracket denotes the thermal average. When we perform a MC simulation for the model, it can be approximated by $\tilde{C}_{ij} = \frac{1}{M}\sum_{\mu=1}^{M} X_i^\mu X_j^\mu$, where X_i^μ is defined as $S_i^\mu - 1/M \sum_{\mu=1}^{M} S_i^\mu$ and S_i^μ is the value of a spin $i\,(i = 1 \ldots N)$ in a snapshot $\mu\,(\mu = 1 \ldots M)$. Then, in principle, diagonalization of $\tilde{C}_{ij}$ gives eigenvalues and the corresponding eigenvectors of C_{ij}. In the high temperature limit, the matrix C_{ij} is equivalent to the interaction matrix J_{ij}, which is sparse in short-range models,

but it can be a dense matrix at lower temperatures. An efficient method for the eigenmode analysis used in this study will be explained at the end of the paper.

In this study, we use the exchange MC method [14], which enables equilibration of the system at low temperatures, even in the SG phase. We simulate 32 replicas of different values of temperature simultaneously with the use of the multi-spin coding, and try to exchange replicas at neighboring temperatures after each sweep with single-spin heat-bath flips. The lowest temperature of the replicas is $1.0J \sim 0.5T_c$, whereas the highest temperature is $5.0J \sim 2.5T_c$. The systems of sizes $L = 4$, 6, 8, and 10 are examined. For each value of L, the number of bond samples used is 800, 640, 464 and 372, respectively.

In Fig. 1, we present the average of the largest eight eigenvalues $\lambda_{\rm AVE} = [\lambda]_J$ scaled by the system size N with $[\cdots]_J$ being an average over the quenched randomness J_{ij}. The data for the largest scaled eigenvalue is almost independent of N, implying that the eigenvalue is extensive at $T/J = 1.0$. This is consistent with the assumption that the system is in the SG phase. We are mostly interested in whether the second eigenvalue is extensive or not. It is observed in Fig. 1 that the second eigenvalue apparently follows algebraic decay up to $L \leq 6$, which is consistent with the results of Sinova et al. [6, 7]. The value of the slope in $L \leq 6$ in the double-log plot is also consistent with θ/d expected from the droplet picture [6], when we use the value of θ/d estimated in the previous studies [11, 12]. However, the behavior of the second eigenvalue changes around $L = 8$ and has a tendency to saturate to a certain value in $8 \leq L \leq 10$. Essentially, the same behavior is observed for the typical averaged value, $\lambda_{\rm TYP} \equiv \ln[\exp \lambda]_J$. These observations show that the second eigenvalue is also extensive in the SG phase. That is, more than one eigenvalue is extensive. According to the interpretation by Sinova et al.[6, 7], our results do not contradict the RSB picture.

Note that our findings of the multiple extensive eigenvalues will also be compatible with a recently proposed sponge-like excitation picture [15] (KMPY picture), which argues that there appear to be large-scale low-energy excitations with the fractal dimension d_s less than the bulk dimension d. Since the energy of such an excitation is supposed not to increase with the system size, we expect that it gives an additional extensive eigenvalue of the susceptibility matrix. The standard RSB and the KMPY pictures can only be distinguished by the fractal nature of low-lying excitations.

How our results are affected by the critical fluctuation? One conventionally uses the overlap distribution function $P(q)$ to test the RSB picture in short-range SG systems [1, 2, 10, 16]. A non-zero limiting value of $P(q)$ at $q \simeq 0$ in the thermodynamic limit is considered as an evidence of the RSB phase. According to the droplet picture, $P(q)$ at all q except for the self-overlap *decreases* with increasing L like $L^{-\theta}$. On the other hand, at the

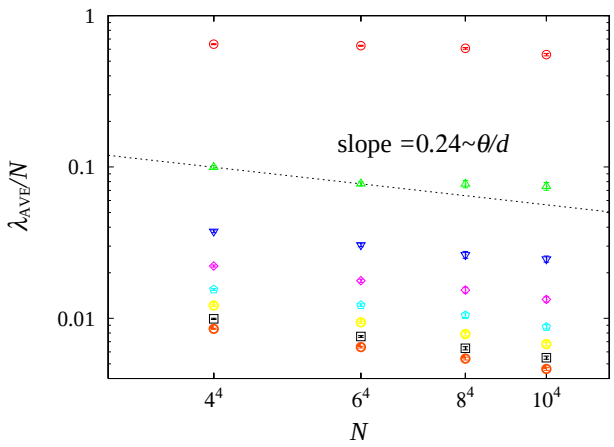

FIG. 1: Size dependence of the first eight eigenvalues of the susceptibility matrix in the four-dimensional EA Ising model at $T/J = 1.0$. The dotted line has the slope $\theta/d \sim 0.24$.

critical temperature, $P(q = 0)$ *increases* with L as $L^{\beta/\nu}$ where β and ν are the critical indices. These contributions, whose signs are opposite, can apparently cancel out for moderate system sizes and give a plateau misidentified as a convergence of $P(0)$ to a non-zero constant [17]. Such cancellation would not be expected in the present approach, because both effects make the scaled eigenvalues λ_i/N of the susceptibility matrix *decrease* with L. Thus, there are no chance of the cancellation even in the critical regions. We have confirmed that a few largest eigenvalues algebraically decay in L near the critical temperature, as expected. Meanwhile, we see no significant decrease of $\lambda_{\rm AVE}/N$ in Fig. 1, which convinces us that $T/J = 1.0$ is already outside the critical region.

So far we focus our attention on the eigenvalues of the susceptibility matrix. Useful information is, however, also contained in the eigenmodes. Here, as an example, we propose the use of temperature dependence of the eigenmodes as a measure of the sensitivity of the thermodynamic states with respect to a temperature change. The overlap between eigenmodes with two different temperatures T_0 and $T_0+\Delta T$ is defined by the scalar product of eigenvectors of the susceptibility matrix

$$r(\Delta T, L) = \left[\left|\frac{1}{N}\sum_i e_i(T_0, L)e_i(T_0 + \Delta T, L)\right|\right]_J , \quad (3)$$

where $e_i(T, L)$ denotes ith component of the eigenvector with the largest eigenvalue. We normalize the length of the eigenvectors e_i to the unity. With this definition, the overlap $r(\Delta T, L)$ is equal to unity when the temperature difference ΔT is zero. In the inset of Fig. 2 we present $r(\Delta T, L)$ calculated with $T_0/J = 1.0$. For a given temperature difference ΔT, the overlap $r(\Delta T, L)$ decreases with increasing size L. We examine an one-parameter scaling $r(\Delta T, L) = R(L/\Delta T^{-1/\zeta})$ for the overlap. As

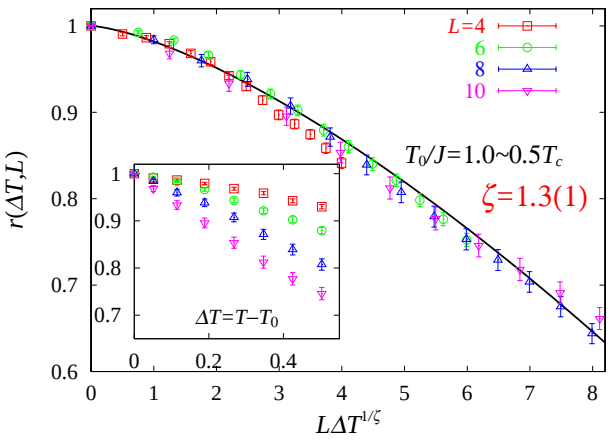

FIG. 2: A scaling plot of the first eigenmode overlap between $T = T_0 = 1.0J$ and $T_0 + \Delta T$ against the scaling variable $L\Delta T^{1/\zeta}$ where $\zeta = 1.3(1)$. The curve represents a fit to the form $r(\Delta T, L) = 1 - CL^{\zeta}\Delta T$ [24] with $C \sim 0.02$. The inset presents raw data as a function of temperature difference ΔT with different sizes.

shown in Fig. 2, all the data merges into a universal scaling function, which is a monotonically decreasing with the increase of the scaling variable $L\Delta T^{1/\zeta}$. The result implies that a pair of eigenmodes with the largest eigenvalue at infinitesimally different temperatures are not correlated with each other in the thermodynamic limit, that is, extreme sensitivity to a temperature perturbation. This peculiar feature never occur in a simple ferromagnet where the largest eigenmode always corresponds to the uniform state. It reminds us of "chaotic nature" of equilibrium SG states [18, 19]. It is interesting to point out that the scaling exponent ζ defined above is close to the exponent of chaos associated with bond perturbation [21]. Whether this coincidence is accidental or not is left for future studies.

Let us give a comment on the numerical method for calculation of the eigenmodes, which relaxes the numerical difficulty of treating a covariance matrix of large dimensions. In this method, *dual algorithm*, we diagonalize a $M \times M$ matrix $\tilde{D}$ defined by

$$\tilde{D}_{\mu\nu} = \frac{1}{N}\sum_{i=1}^{N} X_i^{\mu} X_i^{\nu}, \tag{4}$$

instead of diagonalizing the $N \times N$ matrix $\tilde{C}$. We denote eigenvectors of the matrices $\tilde{C}$ and $\tilde{D}$ as $\{e_i\}^{(n)}$ and $\{e^{\mu}\}^{(m)}$, respectively, where n and m are the indices of eigenvectors. It is easy to show the following primal–dual relations: (1) $\sum_i X_i^{\mu} e_i^{(n)}$ is an eigenvector of $\tilde{D}$ if it is not the null vector, and (2) $\sum_{\mu} X_i^{\mu} e^{\mu(m)}$ is an eigenvector of $\tilde{C}$ if it is not the null vector. Note that when $N > M$, the matrix $\tilde{C}$ is singular and has at least $N - M$ zero eigenvalues, and, conversely, when $M > N$, the matrix $\tilde{D}$ is singular and has at least $M - N$ zero eigenvalues. With this relation, we can replace the diagonalization of the covariance matrix $\tilde{C}$ with that of the sample-overlap matrix $\tilde{D}$, which reduces the amount of computation when $N > M$. Both algorithms give the same results for the same set of samples within numerical accuracy. We should use a sufficient large number M which gives a good approximation of the susceptibility matrix. In the present study, we have tested convergence of the eigenvalues with different values of M and have confirmed that the algorithm shows good convergence. The dual algorithm has been known in the field of multivariate analysis and already used in simulation studies of proteins. In the field of spin glasses, however, it seems less known and used. While a dual plot for visualizing hierarchical structures of low-energy valleys is recently introduced by [25], they did not stress the advantage of the dual formulation as a tool for efficient computation.

To summarize, we numerically explored the eigenmodes of the susceptibility matrix of the four-dimensional Edwards-Anderson Ising spin glass model. First, we studied the eigenvalues of systems larger than those investigated in the previous study and found a strong evidence that the second eigenvalue is extensive in the thermodynamic limit. This no longer conflicts with the RSB pictures. Secondly, we discuss the sensitivity of the normalized eigenmodes against temperature perturbation and found extreme sensitivity to the variation of the temperature. Finally, we mention to a technique with the primal–dual relation used in this study, which will be useful for the study of large systems.

We would like to thank K. Nemoto, who kindly introduced us to this topic and gave us a number of important suggestions. We are grateful to H. Yoshino for suggesting the functional form of scaling in Fig. 2. We also thank H. Takayama for fruitful discussions and continuous encouragement. K.H. acknowledges a Grant-in-Aid for the Encouragement of Young Scientists (#13740233) from the Ministry of Education, Culture, Sports, Science and Technology of Japan. The present simulations have been performed on SGI 2800/384 at the Supercomputer Center, Institute for Solid State Physics, the University of Tokyo.

* Electronic address: hukusima@issp.u-tokyo.ac.jp
† Electronic address: iba@ism.ac.jp

[1] K. Binder and A. P. Young, Rev. Mod. Phys. **58**, 801 (1986).
[2] M. Mézard, G. Parisi and M. A. Virasoro, *Spin Glass Theory and Beyond* (World Scientific, Singapore, 1987).
[3] P. W. Anderson, Mat. Res. Bull. **5**, 549 (1970).
[4] A. J. Bray and M. A. Moore, J. Phys. C **15**, L765 (1982).
[5] K. Nemoto, private communication. K. Nemoto, Bussei-Kennkyu (Kyoto) **74**, 122 (2000) (in Japanese). Their

studies with this approach are traced back to more than ten years ago. Unfortunately, most of them remain unpublished.
[6] J. Sinova, G. Canright and A. H. MacDonald, Phys. Rev. Lett. **85**, 2609 (2000).
[7] J. Sinova, G. Canright, H. E. Castillo and A. H. MacDonald, Phys. Rev. B **63**, 104427 (2001).
[8] G. Parisi, Phys. Rev. Lett. **43**, 1753 (1979); Phys. Rev. Lett. **50**, 1946 (1983).
[9] D. S. Fisher and D. A. Huse, Phys. Rev. B **38**, 386 (1988); D. S. Fisher and D. A. Huse, Phys. Rev. B **38**, 373 (1988).
[10] E. Marinari and F. Zuliani, J. Phys. A **32**, 7447 (1999).
[11] K. Hukushima, Phys. Rev. E **60**, 3606 (1999).
[12] A. Hartmann, Phys. Rev. E **60**, 5135 (1999).
[13] A. Hartmann, Phys. Rev. E **59**, 84 (1999); A. J. Bray and M. A. Moore, J. Phys. C **17**, L463 (1984); W. L. McMillan, Phys. Rev. B **30**, 476 (1984).
[14] K. Hukushima and K. Nemoto, J. Phys. Soc. Jpn. **65**, 1604 (1996).
[15] F. Krazakala and O. C. Martin, Phys. Rev. Lett. **85**, 3013 (2000); M. Palassini and A. P. Young, Phys. Rev. Lett. **85**, 3017 (2000).
[16] J. D. Reger, R. N. Bhatt and A. P. Young, Phys. Rev. Lett. **64**, 1859 (1990).
[17] M. A. Moore, H. Bokil and B. Drossel, Phys. Rev. Lett. **81**, 4252 (1998).
[18] A. J. Bray and M. A. Moore, Phys. Rev. Lett. **58**, 57 (1987).
[19] The chaotic nature has been established for a change of the random bond J_{ij} and magnetic field [20, 21], while the chaos arising from the temperature change still remains very controversial [22, 23].
[20] F. Ritort, Phys. Rev. B **50**, 6844 (1994).
[21] M. Ney-Nifle, Phys. Rev. B **57**, 492 (1998).
[22] A. Billoire and E. Marinari, J. Phys. A **33**, L265 (2000).
[23] F. Krzakala and O. C. Martin, to be published in Euro. Phys. J. B (cond-mat/0203449).
[24] According to the scaling argument [9, 18], the probability of large scale excitations induced by the perturbation is given by $\Delta T L^{\zeta}$. It leads to this fitting formula, if the function $1-r(\Delta T, L)$ is determined by the probability of the large scale excitations.
[25] E. Domany, G. Hed, M. Palassini and A. P. Young, Phys. Rev. B **64**, 224406 (2001).