Equilibrium study of spin glass models: Monte Carlo simulation and multivariate analysis*

Koji Hukushima†
Department of Basic Science, University of Tokyo

Despite extensive studies over many years, the nature of low-temperature phase in spin glasses remains a controversial issue. There are two theories extensively discussed: the droplet theory and the replica symmetry breaking (RSB) theory. Many numerical studies have been done in an attempt to resolve the controversy. In my talk, I will focus on our numerical results, which are obtained by an extended ensemble Monte Carlo (MC) method recently developed and a multivariate analysis of the simulation data.

An essential problem in the study of randomly frustrated spin systems such as spin glasses is how to choose order parameter. A traditional way to analyze such systems is introduction of order parameters defined by replica overlap. An alternative method, 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. An example of such bases in this direction is eigenmodes of the susceptibility matrix $C_{ij} = \langle S_i S_j \rangle$. This is identical with the principle component analysis. While this approach is also useful for the analysis of MC simulation, one usually encounter certain difficulties in storing the matrix elements and diagonalizing the matrix. In particular, the latter requires $O(N^3)$ operations with N being the matrix size. We have proposed a new algorithm based on an idea of the principal component analysis in order to overcome such difficulties[1]. This algorithm have been successfully applied to finite-dimensional Edwards-Anderson (EA) spin-glass models. In figure 1, we show an example which is application to a two-dimensional $\pm J$ spin glass model with system size 64^2.

Figure 1: An application of the eigenmode analysis to a two-dimensional $\pm J$ spin-glass model with system size 64×64 at temperature $T/J = 0.4$. The eigenvector of the susceptibility matrix with the largest eigenvalue is drawn with shading in real space. Shaded areas represent frozen spins which construct large clusters. It is found that a large cluster includes many small light dots corresponding to fluctuating spins.

Recently, Sinova et al[2] have argued that multiple pure states predicted by RSB picture

*This work has been done in collaboration with Prof. Y. Iba (Institute of Statistical Mathematics).
†E-mail: hukusima@phys.c.u-tokyo.ac.jp

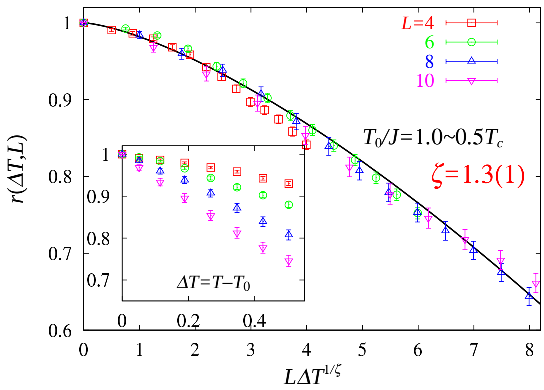

Figure 2: A scaling plot of the first eigenmode overlap between $T = T_0 = 1.0J$ and $T_0 + \Delta T$ against the scaling variable $L\Delta T^{1/\zeta}$ where $\zeta = 1.3(1)$. The model system is the four dimensional $\pm J$ Ising spin glass. The curve represents a fit to the form $r(\Delta T, L) =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

corresponds the existence of multiple extensive eigenvalues of the matrix in the thermodynamics limit. They obtained an numerical evidence against RSB scenario in a four-dimensional EA Ising spin glass model with relatively small size $\leq 6^4$. We have studied the eigenmodes of a similar four-dimensional EA model using the proposed method up to the linear size $L = 10$[1] larger than those investigated in previous studies. Unlike the preceding results on smaller lattices, it is found that the second eigenvalue, as well as the first one, extensive in the low temperature phase. Namely, our results do not contradict RSB scenario.

We also have studied 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 $r(\Delta T, L) = \left[\left|\frac{1}{N}\sum_i e_i(T_0, L)e_i(T_0 + \Delta T, L)\right|\right]_J$, where $e_i(T, L)$ denotes ith component of the eigenvector associated with the largest eigenvalue and $[\cdots]_J$ the average over random realizations of interaction. 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 $T_0/J = 1.0$ well below the transition temperature. 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 shown in Fig. 2, all the data merges into a universal scaling function, which is 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[3]. It is interesting to point out that the scaling exponent ζ defined above is close to the exponent of chaos associated with bond perturbation. Whether this coincidence is accidental or not is left for future studies.

References

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