Parisi States in a Heisenberg Spin-Glass Model in Three Dimensions

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We have studied low-lying metastable states of the $±J$ Heisenberg model in two ($d = 2$) and three ($d = 3$) dimensions having developed a hybrid genetic algorithm. We have found a strong evidence of the occurrence of the Parisi states in $d = 3$ but not in $d = 2$. That is, in $L^d$ lattices, there exist metastable states with a finite excitation energy of $\Delta E \sim O(J)$ for $L \rightarrow \infty$, and energy barriers $\Delta W$ between the ground state and those metastable states are $\Delta W \sim O(JL^d)$ with $\theta > 0$ in $d = 3$ but with $\theta < 0$ in $d = 2$. We have also found droplet-like excitations, suggesting a mixed scenario of the replica-symmetry-breaking picture and the droplet picture recently speculated in the Ising SG model.

Recently, the Heisenberg spin-glass (HSG) model in three dimensions ($d = 3$) has been attacked a great interest, because evidence of the occurrence of SG phase transition at a finite, no-zero temperature ($T_C \neq 0$) has been given in numerical studies in contrary to a common belief that any phase transition does not occur without some anisotropy [1,2]. Kawamura and his coworkers noticed chiralities of the spins and showed that a chiral glass (CG) phase transition occurs at $T_{CG} \neq 0$, but the spin glass phase is still absent [3–5]. On the other hand, Matsubara et al. examined the stiffness at $T = 0$ and $T \neq 0$ of the $±J$ HSG model on the $L^3$ lattice with open boundaries and suggested that the SG phase transition will occur at $T_{SG} \sim 0.19 J$ [6,7]. They also obtained almost the same transition temperature by using different numerical methods, i.e., an aging effect [8] and the divergence of the SG susceptibility [9]. Recently, Nakamura and Endoh showed that, using nonequilibrium relaxation method, the CG phase transition and the SG phase transition occur at the same temperature of $T_{SG} = T_{CG} \sim 0.21 J$ [10]. Quite recently, Lee and Young presented the same conclusion using a finite size analysis of the correlation length of the spins and chiralities [11].

An interesting question is, then, the nature of the SG phase of the HSG model. In the Ising SG (ISG) models in $d = 3$, two pictures have been extensively discussed: the replica-symmetry-breaking (RSB) picture of Parisi [12] and the droplet picture of Fisher and Huse [13]. An important difference between the RSB and the droplet pictures concerns the nature of large scale excitations. In the RSB picture, there are many metastable states, which involve turning over a finite fraction of the spins and which cost only a finite energy even in the thermodynamic limit. The energy barriers between each of these metastable states and the ground state and also between those metastable states are infinite in the thermodynamic limit. Hereafter we call those metastable states Parisi states. By contrast, in the droplet picture, the lowest excitation which has linear spatial extent $l$ typically costs an energy of order $Jl^\theta$ with $\theta > 0$. Hence, in the thermodynamic limit, excitations which flip a finite fraction of the spins cost an infinite energy.

In this Letter, having developed a hybrid genetic algorithm (HGA) for systems with the XY and Heisenberg spins, we have studied the ground state and low-lying metastable states of the $±J$ HSG on finite lattices of $L^d$ ($d = 2$ and 3). We have found the Parisi states in $d = 3$ but not in $d = 2$. This finding is very important, because it gives a strong support of the presence of the SG phase in $d = 3$. We have also found metastable states with droplet-like excitations near the Parisi states. We hope our findings will help to understand properties of the low temperature phase of the HSG model.

We start with the $±J$ Heisenberg model on the $d$ dimensional lattice of $L^d (\equiv N)$ with periodic boundary conditions. The Hamiltonian is described by

$$H = - \sum_{(ij)} J_{ij} S_i S_j \quad (1)$$

where $S_i$ is the Heisenberg spin of $|S_i| = 1$, and $(ij)$ runs over all nearest-neighbor pairs. The exchange interaction $J_{ij}$ takes on either $+J$ or $-J$ with the same probability of $1/2$.

Before analyzing the model, we briefly mention properties of the Heisenberg SG model. First we should note that the model has the $SO(3) (\equiv SU(2)/C_2)$ symmetry. So the ground state has a two-fold degeneracy. We call these two spin configurations as $G_1$ and $G_2$ and describe them $\{S_i^{G_1}\}$ and $\{S_i^{G_2}\}$. Note that, if $G_1$ is obtained, one can readily obtain $G_2$ by reversing all the spins of $G_1$, i.e., $\{S_i^{G_2}\} = \{-S_i^{G_1}\}$, and vice versa. The energy of the model is unchanged under any uniform rotation of the system. Then the spin configuration of the Heisenberg SG model is characterized by a set of pair-spin correlations $\{S_i S_j\}$. That is, the SG order parameter space
is constructed by this set and the distance between two spin configurations $A$ with $\{S^A_i\}$ and $B$ with $\{S^B_i\}$ is described as

$$S(A, B) = \frac{1}{N^2} \sum_{i,j} (S^A_i S^A_j - S^B_i S^B_j)^2.$$  \hspace{1cm} (2)

Hereafter we take the ground state as the datum point and consider the distance $\Delta S$ of the spin configuration $A$ from the ground state spin configuration $G_1$ or $G_2$, i.e., $\Delta S \equiv S(A, G_1) = S(A, G_2)$. Note that, since the ground states $G_1$ and $G_2$ share the same point in the SG order parameter space, hereafter we omit the subscript. Note also that, if $\{S^A_i\}$ is independent of $\{S^G_i\}$, $\Delta S \sim \sqrt{\frac{1}{2N} \sum_{i,j} ((S^A_i S^A_j)^2 + (S^G_i S^G_j)^2)} \rightarrow \sqrt{\frac{2}{3}} \int \cos(\theta)^2 d\Omega = \sqrt{2/3}$ for $L \rightarrow \infty$.

Usually, the ground state of the HSG is searched by using a spin quench (SQ) method [3,14]. However, the number $N_i$ of initial spin configurations which are needed to get the ground state increases rapidly as the size of the lattice increases. Here we develop a hybrid genetic algorithm (HGA) to search the ground state and low-lying metastable states. Starting with a population $N_p$ of random spin configurations (parents) $\{B_l\}$, new configurations (offsprings) are generated by recombination of different parents $B_l$ and $B_m$ ($l \neq m$) (quadruple crossover). Then some fraction $r$ of the spins are refreshed (mutation). This algorithm is hybridized with a local optimization (the SQ method) of the offsprings. The population $N_p$ is updated by replacing $3N_p/4$ parents with higher energy by $3N_p/4$ offsprings which are selected in order of the lower energy. This procedure is repeated for many times (generation number $N_g$). This algorithm is analogous to that used in the Ising SG model [15]. In the Heisenberg SG, however, we should pay a special attention to optimize the interface energy between two parents $B_l$ and $B_m$ when one generates the offsprings. This problem can be resolved by applying a uniform rotation to all the spins of one of the parents. Having used this algorithm, we have been able to obtain the ground state of the HSG model on larger lattices of $12 \times 12 \times 12$. The HGA also works well in the XY SG models. Details of the HGA will be reported elsewhere.

Once the ground state $G$ with the energy $E_G$ are determined, one can obtain metastable states $A$ with $E_A$. We use the distance $\Delta S$ and the excitation energy $\Delta E(\equiv E_A - E_G)$ to distinguish different metastable states. We may use two different methods for searching those states: (i) the usual SQ method and (ii) the HGA. Both methods have their own merit. In the former, we can get different metastable states. However, we have to start with many different initial spin configurations to get low-lying metastable states, e.g., $N_i \sim 10^6$ for $L = 10$ in $d = 3$. On the other hand, the latter is appropriate to search the lowest metastable state in a given range of $\Delta S$. We are enough to give a smaller number of parents, e.g., $N_p \sim 100$ for $L = 10$ in $d = 3$. In Figs. 1 (a) and (b), we present results of distribution of the metastable states of typical bond realizations (samples) in $d = 3$. In fact, by using the two methods we can get the same lowest metastable state in a given range of $\Delta S$ (here $\Delta S > 0.4$). Usual excitation energies $\Delta E$’s increase with $\Delta S$ and also with $L$. A remarkable point is that $\Delta E$’s of the low-lying metastable states are much smaller than those usual excitation energies. In particular, we often see metastable states with finite $\Delta S$ which have a very small $\Delta E$ (see Fig.1(b)). This result implies the presence of the Parisi states. We will discuss this problem considering an energy barrier between the ground state and those low-lying metastable states on the basis of a domain wall picture. Another remarkable point is that, near the ground state, there are many metastable states the energy of which increases as $\Delta S$ increases. This result suggests the occurrence of some localized excitation the excitation energy of which increases as the scale of the excitation is increased [16]. That is, the excitation will be droplet-like. The same is true for the excitations in metastable states near the Parisi states. We will get back to this point to consider properties of the low temperature phase.
for $\Delta S > 0.4$ indicated by the symbol $\circ$. It is interesting to see that $\Delta W$'s are much higher than $\Delta E$.

Now we consider the domain wall energies between the ground state and the lowest metastable state in a given range of $\Delta S$ for different samples. Here we consider the case $0.4 < \Delta S < 0.6$, because we are interested in large scale excitations. We denote the excitation energy of the lowest metastable state in this range as $\Delta E_0$. Our attention is paid to the minimum domain wall energy $\Delta W_{\text{min}}(\equiv \min(\Delta W's))$ for each of those samples. The calculation has been performed in $d = 2$ and $d = 3$ by using the HGA. The linear sizes of the lattice are $L = 10 \sim 24$ in $d = 2$ and $L = 6 \sim 11$ in $d = 3$, and the numbers of the samples are $N_s = 1024$ in both $d = 2$ and $d = 3$ except for the largest lattices ($N_s = 512$ for $L = 24$ ($d = 2$), and $N_s = 256$ for $L = 11$ ($d = 3$). The following numbers of $N_p$ and $N_g$ are chosen with a common mutation ratio $r = 0.4$. In $d = 2$, $N_p = 16, 32, 64, 128, 256$ for $L = 10, 12, 16, 20, 24$, respectively, and $N_g = 5$ for $L \leq 16$ and $N_g = 16, 32$ for $L = 20, 24$, respectively. In $d = 3$, $N_p = 16, 32, 64, 128, 256, 512$ for $L = 6, 7, 8, 9, 10, 11$, respectively, and $N_g = 5$ for $L \leq 8$ and $N_g = 8, 16, 32$ for $L = 9, 10, 11$, respectively. Note that, metastable states are not always found in this range of $\Delta S$ by using the HGA with $r = 0.4$ [17], especially in smaller lattices. In Fig. 2, we plot ($\Delta E_0, \Delta W_{\text{min}}$) for different samples in $d = 3$. A remarkable point is that, as $L$ is increased, the distribution of $\Delta W_{\text{min}}$ considerably spreads to the higher energy side, while the distribution of $\Delta E_0$ slightly shifts to the lower energy side. Note that, in $d = 2$, the distributions in both $\Delta E_0$ and $\Delta W_{\text{min}}$ shift to the lower energy side with increasing $L$. 

![FIG. 1. Distributions of metastable states (dots) in the $(\Delta S, \Delta E)$ plane for typical samples with (a) $L = 6$ and (b) $L = 10$ in $d = 3$ obtained by using the SQ method with $N_s = 2 \times 10^4$ ($L = 6$) and $2 \times 10^6$ ($L = 10$). $\circ$ indicates the lowest metastable state for $\Delta S > 0.4$ obtained by using the HGA and $\times$ denote the domain wall states described in the text. $G$ indicates the position of the ground state.](image-url)
We calculate average values \( \langle \Delta E_0 \rangle \) and \( \langle \Delta W_{\text{min}} \rangle \) over different samples and show them in Figs. 3 and 4 for \( d = 2 \) and \( d = 3 \), respectively, as functions of \( L \). In \( d = 2 \), in fact, \( \langle \Delta E_0 \rangle \) and \( \langle \Delta W_{\text{min}} \rangle \) decrease slightly, and \( \langle \Delta W_{\text{min}} \rangle \) increases with \( L \). We could fit data for larger \( L \) as \( \langle \Delta W_{\text{min}} \rangle \propto J L^\theta \) with \( \theta = 0.53 \pm 0.08 \). These results strongly suggest the presence of the Parisi states. That is, in the thermodynamic limit, there are metastable states which have a finite excitation energy \( \Delta E_0 \), probably \( \Delta E_0 \ll J \), and which are separated from the ground state with an infinite energy barrier. The exponent \( \theta \) is the measure of the domain wall height. It is interesting to find that the value of \( \theta \sim 0.53 \) is compatible with the stiffness exponent of \( \theta = 0.4 \sim 0.8 \) estimated recently [6,7].

In summary, we have studied low-lying metastable states of the \( \pm J \) Heisenberg model in two \((d = 2)\) and three \((d = 3)\) dimensions having developed a hybrid genetic algorithm. We have found the Parisi states in \( d = 3 \). Since the Parisi states occur in the SG phase, we suggest that the SG phase really occurs in the HSG in \( d = 3 \). We have also found metastable states with droplet-like excitations near the Parisi states. So the SG phase of this HSG model will be characterized by a mixed scenario of the RSB picture and the droplet picture analogous to one [18] that was speculated previously in the Ising SG model [19]. In this scenario, the system at \( T = 0 \) is located in one of the Parisi states and dynamical properties of the system at low temperatures may be described by using the droplet-like excitations thermally activated in that Parisi state. In the Ising model, aging dynamics of the SG model in \( d = 3 \) has been reported to be well described by using the droplet picture [20], although the model has large scale excitations with finite excitation energy [21,22]. We hope that the present findings stimulate studies of aging dynamics of the HSG as well as the equilibrium properties of the real SG systems.

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