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LETTER TO THE EDITOR

Parisi states in a Heisenberg spin-glass model in three dimensions

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Abstract
Having developed a hybrid genetic algorithm, we have studied low-lying excited states of the $\pm J$ Heisenberg model in two ($d = 2$) and three ($d = 3$) dimensions. We have found 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 $L \to \infty$, and energy barriers ΔW between the ground state and those metastable states are $\Delta W \sim O(JL^\theta)$ with $\theta > 0$ in $d = 3$ but with $\theta < 0$ in $d = 2$. This finding favours the replica-symmetry-breaking or the trivial–nontrivial scenario of the SG phase over the droplet scenario.

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Recently, the Heisenberg spin-glass (HSG) model in three dimensions ($d = 3$) has generated great interest, because evidence of the occurrence of SG phase transition at a finite, non-zero temperature ($T_C \neq 0$) has been given in numerical studies contrary to a common belief that no phase transition occurs without anisotropy [1, 2]. Kawamura and his coworkers took note of 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 $\pm J$ Heisenberg model on the L^3 lattice with open boundaries and suggested that the SG phase transition will occur at $T_{SG} \sim 0.19\,\mathrm{J}$ [6, 7]. They also obtained almost the same transition temperature by using different numerical methods, i.e. an ageing effect [8] and the divergence of the SG susceptibility [9]. Recently, Nakamura and Endoh showed that, using a non-equilibrium relaxation method, the CG phase transition and the SG phase transition occur at the same temperature of $T_{SG} = T_{CG} \sim 0.20\,\mathrm{J}$ [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 important question is, then, the nature of the SG phase of the HSG model. In the Ising SG (ISG) models in $d = 3$, two scenarios have been extensively discussed: the replica-symmetry-breaking (RSB) scenario of Parisi [12] and the droplet scenario of Fisher and Huse

[13]. An important difference between the RSB and the droplet scenarios concerns the nature of large-scale excitations. In the RSB scenario, there are many excitations, which involve turning over a finite fraction of the spins and which cost only a finite energy $\Delta E \sim O(J)$ even in the thermodynamic limit. The energy barriers between each of those excitations and the ground state, and also between those excitations, are infinite in the thermodynamic limit. Hereafter, we call those excitations *Parisi states*. By contrast, in the droplet scenario, the lowest excitation which has linear spatial extent l typically costs an energy $\Delta E \sim Jl^{\theta}$ with $\theta > 0$. Hence, in the thermodynamic limit, excitations which flip a finite fraction of the spins cost an infinite energy. In addition, the surface of the excitations in the droplet scenario is fractal with a fractal dimension $d_s < d$, whereas in the RSB scenario the surface is space filling, i.e. $d_s = d$. Recently, a trivial–nontrivial (TNT) scenario has been presented on the basis of numerical results [14, 15], that is, the surface of large-scale excitations appears to be fractal and only a finite amount of energy is needed to excite them (i.e. the Parisi states). Our primary question is whether the Parisi states (the RSB or the TNT scenario) exist or not in the HSG model.

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 excited states of the $\pm J$ Heisenberg model 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 favours the RSB or the TNT scenario over the droplet scenario. We should note, however, that our results also imply the occurrence of small scale droplet-like excitations around the Parisi states. We hope our finding will stimulate studies of the low temperature phase of the HSG model.

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

$$H = -\sum_{\langle ij \rangle} J_{ij} \boldsymbol{S}_i \boldsymbol{S}_j \qquad (1)$$

where $\boldsymbol{S}_i$ is the Heisenberg spin of $|\boldsymbol{S}_i| = 1$, and $\langle ij \rangle$ runs over all nearest-neighbour pairs. The exchange interaction J_{ij} takes on either $+J$ or $-J$ with the same probability of 1/2.

First we consider the ground state. The search for the ground state of the HSG is a very difficult problem, because many metastable states exist in the system. Usually, the ground state of the HSG model is obtained by using a spin quench (SQ) method with many different initial spin configurations [3, 16]. However, the number N_i of initial spin configurations which is needed for obtaining the ground state increases rapidly as the size of the lattice increases. Here we use a HGA which is analogous to the one used in the Ising SG model [17]. Starting with a population N_p of random spin configurations (parents) $\{C_l\}$, new configurations (offspring) are generated by recombination of different parents C_l and $C_m (l \neq m)$, where we use a single-point crossover. Then, after some fraction r of the spins are refreshed (mutation), the SQ method is applied to optimize the offspring. The population N_p is updated in such a way that three-fourths of the parents with higher energy are exchanged for the offspring which are selected in order of the lower energy. This procedure is repeated many times (generation number N_g). In the Heisenberg SG, we should pay special attention to optimize the interface energy in the recombination of C_l and C_m when one generates the offspring. 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. 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 spin configuration $\left\{\boldsymbol{S}_i^G\right\}$ and the energy E_G is determined, one can search for excited states A with the spin configuration $\left\{\boldsymbol{S}_i^A\right\}$ and the energy E_A.

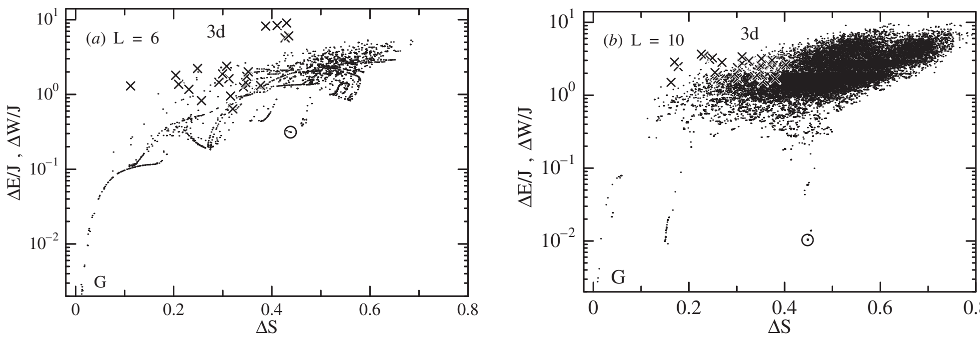

Figure 1. Distributions of excited states (dots) in the $(\Delta S, \Delta E)$ plane for typical samples with (a) $L = 6$ and (b) $L = 10$ in $d = 3$ obtained by using the SQ method with $N_i \sim 2 \times 10^4$ $(L = 6)$ and 2×10^6 $(L = 10)$. $\bigcirc$ indicates the lowest excited state for $\Delta S > 0.4$ obtained by using the HGA, and $\times$ denotes the domain wall states between the ground state and the lowest excited state. G indicates the position of the ground state.

To distinguish each excited state, we consider the excitation energy ΔE and the distance ΔS from the ground state:

$$\Delta E = E_A - E_G \tag{2}$$

$$\Delta S = S(A, G) \tag{3}$$

where

$$S(A, B) = \sqrt{\frac{1}{N^2} \sum_{i,j} \left(\boldsymbol{S}_i^A \boldsymbol{S}_j^A - \boldsymbol{S}_i^B \boldsymbol{S}_j^B \right)^2}. \tag{4}$$

Note that, since the model has a rotational symmetry, we use a set of pair-spin correlations $\{\boldsymbol{S}_i \boldsymbol{S}_j\}$ for describing the spin structure. Note also that, if $\left\{\boldsymbol{S}_i^A\right\}$ is independent of $\left\{\boldsymbol{S}_i^G\right\}$, $\Delta S \sim \sqrt{\frac{1}{N^2} \sum_{ij} \left(\left(\boldsymbol{S}_i^A \boldsymbol{S}_j^A\right)^2 + \left(\boldsymbol{S}_i^G \boldsymbol{S}_j^G\right)^2 \right)} \rightarrow \sqrt{\frac{2}{4\pi} \int \cos(\theta)^2 \, \mathrm{d}\Omega} = \sqrt{2/3} \sim 0.82\,(\equiv \Delta S_\infty)$ for $L \rightarrow \infty$.

We may use two different methods for searching the excited states: (i) the usual SQ method and (ii) the HGA. Both methods have their own merit. In the former, we can get various excited states. However, we have to start with many different initial spin configurations to get low-lying ones, e.g., $N_i \sim 10^6$ for $L = 10$ in $d = 3$. On the other hand, the latter is appropriate for searching the lowest one in a given range of ΔS.[3] We can start with a smaller number of the parents, e.g., $N_p \sim 100$ for $L = 10$ in $d = 3$. In figures 1(a) and (b), we present distributions of the excited states of typical individual samples in $d = 3$ obtained in the SQ method, together with the lowest excited state for $\Delta S > 0.4$ in the HGA. In fact, using these two methods we can get the same lowest excited state. Usual excitation energies ΔE increase with ΔS and also with L. A remarkable point is that ΔE of low-lying excited states are much smaller than those usual excitation energies. In particular, we often find low-lying excited states with finite ΔS which have a very small excitation energy $(\Delta E \ll J)$ (see figure 1(b)). Note that some of the low-lying excited states, including the lowest excited state seen above, are metastable states, because their energies no longer reduce when the SQ

[3] We can get the lowest excited state in any range of ΔS, if we choose the offspring in that range.

algorithm is applied further[4]. Another remarkable point is that, near the ground state, there are many excited states whose energy increases rapidly as ΔS increases. The same is true for excited states near the lowest excited state. The former point implies the presence of the Parisi states. Here we discuss this problem considering *an energy barrier between the ground state and those low-lying excited states on the basis of a domain wall scenario*. The latter point implies the occurrence of droplet-like excitations.This point will be discussed in a separate paper.

Suppose that, in addition to the ground state G with E_G, some low-lying metastable state A is given. The domain wall energy ΔW between G and A may be estimated by the following procedure. (i) We divide the L^d lattice into two parts H_1 and H_2, which are composed of $[(L+1)/2]$ and $[L/2]$ layers, respectively, where each layer has L^{d-1} lattice sites and $[x]$ means the largest integer which does not exceed x. (ii) Fill H_1 with the spins of G and H_2 with the spins of A, and apply a uniform rotation to all the spins on H_2 to minimize the interface energy. (iii) For each part of H_1 and H_2, fix all the spins on the middle layer. Under this restriction, the SQ method is applied to get the spin configuration W which gives the minimum energy E_W of the L^d lattice. (iv) We consider W a domain wall state when $S(W, G), S(W, A) > S(A, G)/4$ is satisfied, and define the domain wall energy $\Delta W = E_W - E_G$, where $S(W, G)$ and $G(W, A)$ are the distances between the states W and G, and between the states W and A, respectively. Note that the restriction for the state W is given to rule out the possibility that it comes close to either G or A. The number of possible divisions of the L^d lattice into H_1 and H_2 is $d \times L$ and the chirality freedom of 2 exists [3, 4]. So we repeat this procedure $2dL$ times. In figures 1(*a*) and (*b*), we have added ΔW of these domain wall states. It is interesting to see that ΔW are much higher than ΔE.

Now we consider the domain wall energies between the ground state and the lowest metastable state in the range of $\Delta S > 0.4$ ($\sim \Delta S_\infty/2$) for different samples. We denote the excitation energy of this metastable state as ΔE_0. Our attention is focussed on the lowest domain wall energy, i.e. $\Delta W_{\min}$ ($\equiv \min(\Delta W)$), 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 $L = 10$–24 in $d = 2$ and $L = 6$–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 $L \leqslant 16$ 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 $L \leqslant 8$ and $N_g = 8, 16, 32$ for $L = 9, 10, 11$, respectively. We calculate average values $\langle \Delta E_0 \rangle$ and $\langle \Delta W_{\min} \rangle$ over different samples and show them in figures 2 and 3 for $d = 2$ and $d = 3$, respectively, as functions of L. In $d = 2$, in fact, $\langle \Delta E_0 \rangle$ and $\langle \Delta W_{\min} \rangle$ decrease with increasing L. These results clearly reveal the absence of the SG phase. By contrast, in $d = 3$, $\langle \Delta E_0 \rangle$ decreases slightly, and $\langle \Delta W_{\min} \rangle$ increases with L. We could fit data for larger L as $\langle \Delta W_{\min} \rangle \propto JL^\theta$ 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 ΔE_0, probably $\Delta E_0 \ll J$, and which are separated from the ground state with an infinite energy barrier. The exponent θ is

[4] Here, we applied the SQ algorithm for $M = 1000$ and $M = 2000$ times for $L = 6$ and $L = 10$, respectively. When we applied the algorithm for several times as large as those numbers of M, almost all excited states near the ground state disappear. Also all low-lying excited states, except for several whose energy is locally minimized, disappear. It should be noted that, nevertheless, the distribution of those excited states is important, because the low temperature property of the model will be governed by them.

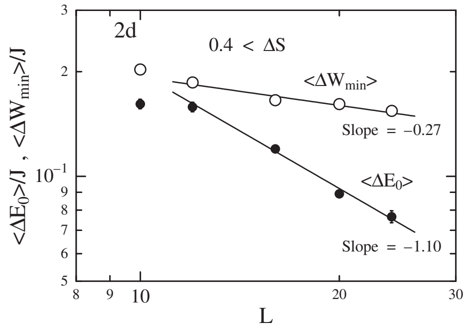

Figure 2. Average values of the lowest excitation energy $\langle \Delta E_0 \rangle$ and the lowest domain wall energy $\langle \Delta W_{\min} \rangle$ in $d = 2$ as functions of the linear lattice size L.

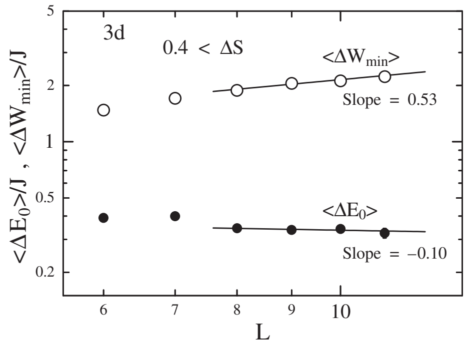

Figure 3. Average values of the lowest excitation energy $\langle \Delta E_0 \rangle$ and the lowest domain wall energy $\langle \Delta W_{\min} \rangle$ in $d = 3$ as functions of the linear lattice size L.

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 $\theta = 0.4$–0.8 estimated recently [6, 7].

In summary, we have studied low-lying excited 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 $d = 3$. We suggest, hence, that the SG phase really exists in the HSG model in $d = 3$. Our result favours the RSB or the TNT scenario over the droplet scenario. The next question is, then, whether the TNT scenario holds or not in the Heisenberg model. We are currently examining this problem calculating a link overlap q_l [14, 15]. Another question is whether droplet-like excitations occur or not around the Parisi states in the thermodynamic limit. That is, localized excitations which have linear spatial extent l ($\ll L$) and which cost an energy of $\Delta E \sim J l^{\theta}$ with $\theta > 0$. If so, the SG phase of this HSG model may be characterized by a mixed scenario of the RSB and the droplet analogous to the one that was speculated in the Ising SG model [18]. This problem will be discussed in a future paper.

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