

Search for the Heisenberg spin glass on rewired cubic lattices with antiferromagnetic interaction

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Abstract. Spin glass (SG) is a typical magnetic system which is mainly characterized by a frozen random spin orientation at low temperatures. Frustration and randomness are considered to be the key ingredients for the existence of SGs. Previously, Bartolozzi *et al.* [Phys. Rev. B73, 224419 (2006)] found that the antiferromagnetic (AF) Ising spins on scale free network (SFN) exhibited SG behavior. This is purely AF system, a new type of SG different from the canonical one which requires the presence of both FM and AF couplings. In this new system, frustration is purely due to a topological factor and its randomness is brought by irregular connectivity. Recently, it was reported that the AF Heisenberg model on SFN exhibited SG behavior [Surungan *et al.*, JPCS, 640, 012005 (2015)/doi:10.1088/1742-6596/640/1/012005]. In order to accommodate the notion of spatial dimension, we further investigated this type of system by studying an AF Heisenberg model on rewired cubic lattices, constructed by adding one extra bond randomly connecting each spin to one of its next-nearest neighbors. We used Replica Exchange algorithm of Monte Carlo Method and calculated the SG order parameter to search for the existence of SG phase.

1. Introduction

Spin glass (SG) is a fascinating subject in condensed matter physics. It is a random magnetic system having a unique type of order called temporally ordered phase [1] rather than spatially ordered phase. This type of order is associated with frozen random spin configuration at low temperature. From the theoretical point of view, SG is a perfect ground test for several complex problems such as NP-hard and optimization algorithm [2, 3]. SGs have found some technological applications, for example, as a material for giant magneto-resistance (GMR)[4]. The phenomenon of SGs was firstly observed in experiment by Cannella and Mydosh in the early 70s [5]. They reported the presence of a cusp instead of a sharp peak in the plot of ac-susceptibility of transition metal impurities hosted by noble metals (*CuMn* and *AuFe*). These are magnetic alloy with a small concentration of magnetic impurities (*Mn* and *Fe*) randomly substituted into the lattice of non-magnetic hosts (*Cu* and *Au*).

Frustration and randomness are considered to be the pivotal ingredients for the existence of SG. Spins are frustrated if they fail to simultaneously satisfy their nearest neighbors for minimizing the interaction energy. The example of this is a plaquette where both ferromagnetic (FM) and antiferromagnetic (AF) interaction exist, or by an AF triangular unit. Spins interacting ferromagnetically (anti-ferromagnetically) will prefer to be aligned (anti-aligned) to minimize the free energy.



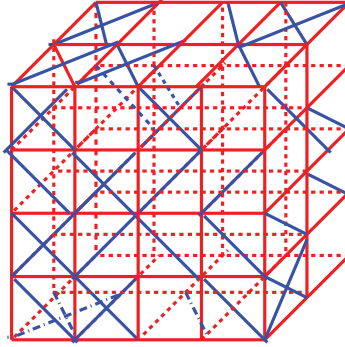


Figure 1. (Color online) An example of a rewired cubic lattice with an extra link randomly connects each spin to one of the next-nearest neighbors.

SGs exhibit many such remarkable phenomena as aging, rejuvenation and memory effects [6], which have been the subject of some recent studies[7, 8]. Due to the randomness and frustration, the ground state configuration is highly degenerate, leads the system to possess finite value ground state entropy, commonly called residual entropy. It is also due to the random frustration that the energy landscape of the system is occupied by a large number of local minima. Accordingly, finding the ground state energy of the systems is extremely difficult and has been a challenge for many optimization algorithms such as genetic and hysteresis algorithms [9, 10].

The so-called non-canonical SG has recently attracted a lot of interest [11, 12, 13, 14]. This is a new type of SGs with purely AF where randomness is in connectivity and the frustration is brought by the topological factor. Its existence was firstly reported on scale free network (SFN) for the Ising model[11]. We have studied this type of model for Heisenberg case and found SG phase transition[13]. As an SFN corresponds to a lattice with very large spatial dimension and due to the importance of dimensionality in phase transition, it is desirable to find the existence of SG phase on finite dimension regular lattices. While our recent study on rewired square lattice found no SG for Heisenberg model [14], we observed SG for the Ising case[15].

We further elaborate this type of models on higher dimensional lattice, the rewired cubic lattice. It is motivated by the notion that larger coordination number should preserve any existing order phase including SGs. The remaining part of the paper is organized as follows: Section II describes the model and method. The result is discussed in Section III. Section IV is devoted to the summary and concluding remarks.

2. Model and Simulation

The SG model is written with the following Hamiltonian

$$H = - \sum_{\langle ij \rangle} J_{ij} \vec{s}_i \cdot \vec{s}_j \quad (1)$$

where J_{ij} is the coupling interaction between spins residing on sites i -th and j -th of the lattice. For a purely AF model, $J_{ij} = J < 0$. We consider a rewired cubic lattice with one extra link added to each site. The link connects each spin to one of the next-nearest spins. Therefore, a spin can have in maximum up to 13 links. The summation is performed over all directly connected spins of the rewired lattice. Figure 1 shows one particular realization of the lattices. A randomly rewired cubic lattice is a quasi-regular lattice where each site has different number of neighbors. We define an average number of links (ANOL) for this type of lattice, associated with a coordination number n for a regular lattice. As we add only one extra link to each site of the cubic lattice ($n = 3$), then for the resulted lattice, ANOL = 4. In principle we can generate any lattice with fractional ANOL. As shown in Fig. 1, a large number of triangular units exist,

on which spins are frustrated due to AF interaction. Randomly adding extra links is a simple way of transforming a purely AF system into a non-canonical SG model. This type of procedure had been done for example in Ref. [12]. We do not follow this procedure as it breaks totally the translational symmetry of regular lattices, while we want to preserve the notion of spatial dimension.

Monte Carlo simulation is a standard numerical method to study complex systems such as SGs. Due to the presence of local minima in the energy landscape of the system, the performance of the conventional Metropolis algorithm is poor. A random walker can easily get trapped in one of the local minima and suffers from critical slowing down, particularly when approaching critical temperature. Cluster algorithms are commonly used to overcome this phenomenon. However, for SG system, due to the presence of frustration, a cluster algorithm is not applicable. Instead, one implements extended ensemble algorithms, *i.e.*, Replica Exchange (RE) algorithm [16].

The basic idea of RE algorithm is to avoid a random walker being trapped in one local minimum by duplicating the original system into several replicas. Each replica is in contact with a corresponding heat bath and independently treated by a standard Metropolis algorithm. Then, the simulation is run in parallel where replicas of two adjacent temperatures are exchanged. Configurations of pairs in two consecutive trials of exchanges have to be different. For example, if we start with M replicas and a set of invers temperatures β , the first trial of exchange involves pairs of replicas: X_1 and X_2 , X_3 and $X_4, \dots, X_{M-1}$ and X_M ; then followed by the next trial which involves pairs: X_2 and X_3 and X_4 and $X_5 \dots X_{M-2}$ and X_{M-1} . This is important to enable any random walker to escape from any local minimum. An exchange can be performed, for example, in every 5 MCSs.

The final result of the simulation is obtained by combining all results from each replica (temperature). The probability distribution of finding the whole M replicas in a state $\{X\} = \{X_1, X_2, \dots, X_M\}$ is given by,

$$P(\{X, \beta\}) = \prod_{m=1}^M \frac{\exp(-\beta_m H(X_m))}{Z(\beta_m)} \quad (2)$$

where $Z(\beta_m)$ is the partition function for the m -th replica. We can then define an exchange matrix between replicas, $W(X_m, \beta_m | X_n, \beta_n)$, which is the probability to switch the configuration X_m of β_m with the configuration X_n of β_n . With the requirement of keeping the entire system at equilibrium, we use the detailed balance condition on the transition matrix

$$\begin{aligned} & P(\{X_m, \beta_m\}, \dots, \{X_n, \beta_n\}, \dots) \cdot W(X_m, \beta_m | X_n, \beta_n) \\ &= P(\{X_n, \beta_n\}, \dots, \{X_m, \beta_m\}, \dots) \cdot W(X_n, \beta_n | X_m, \beta_m), \end{aligned} \quad (3)$$

along with Eq. (2), so that we have

$$\frac{W(X_m, \beta_m | X_n, \beta_n)}{W(X_n, \beta_n | X_m, \beta_m)} = \exp(-\Delta), \quad (4)$$

where $\Delta = (\beta_n - \beta_m)(H(X_m) - H(X_n))$. With this constraint, we can choose the matrix coefficients according to the standard Metropolis algorithm which gives the following

$$W(X_m, \beta_m | X_n, \beta_n) = \begin{cases} 1 & \text{if } \Delta < 0, \\ \exp(-\Delta) & \text{if } \Delta > 0. \end{cases} \quad (5)$$

Due to the fact that the acceptance ratio decays exponentially with $(\beta_n - \beta_m)$, we restrict the exchange temperatures next to each other, *i.e.*, the terms $W(X_m, \beta_m | X_{m+1}, \beta_{m+1})$. In performing the simulation, we define one MC step (MCS) as updating once each spin of each

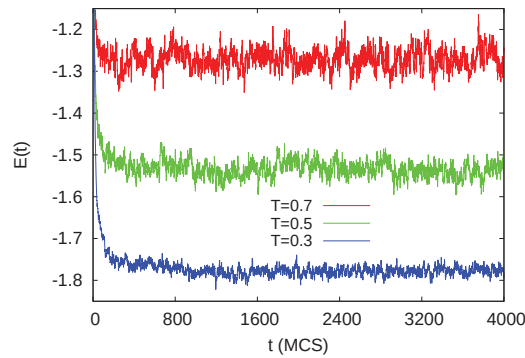


Figure 2. (Color online) Time series of energy at $T = 0.7, 0.5$ and 0.3 for linear size $L = 10$.

replica, either consecutively or randomly. After a number of MCSs, we exchange configurations from pairs of temperatures next to each other based on the probability according to Eq. 5.

For each connectivity realization we start from a random spin configuration. Then, we perform 10^4 MCSs for equilibration before taking a total of 10^4 sample points for the thermal averages. To avoid temporal correlation between samples, we performed several extra MCSs between two sample points. We consider high and low temperatures to search for SG phase transition. The thermal averages obtained for each lattice size then averaged over many lattice connectivities, which is a standard procedure in doing MC simulation for a random system such as SG. In the next section, we present the results of our study.

3. RESULTS AND DISCUSSION

3.1. Energy and the specific heat

We have simulated AF Heisenberg model on rewired cubic lattices with $ANOL = 4.0$ for several linear sizes $L = 8, 10, 12$, and 16 ; the number of spins is L^3 . The periodic boundary condition is imposed so that each site of the native cubic lattice (before being rewired) has six nearest neighbors. For each system size we took many realizations of connectivities, then average the results over the number of realizations. Each realization corresponds to one particular connectivity distribution randomly generated. For the result to be reliable, we have to take a reasonable number of realizations. In our previous study of Heisenberg SG on SFN, we took 1000 realizations. Here we took smaller number of realizations ($N_r = 144$) due to its degree of randomness is less compared to the previous system.

To check the reliability of our simulation we evaluated the energy time series of the system, from which the average energy and specific heat can be extracted. One can tell whether the system is in equilibrium or not by analyzing the energy time series. In MC simulation, time

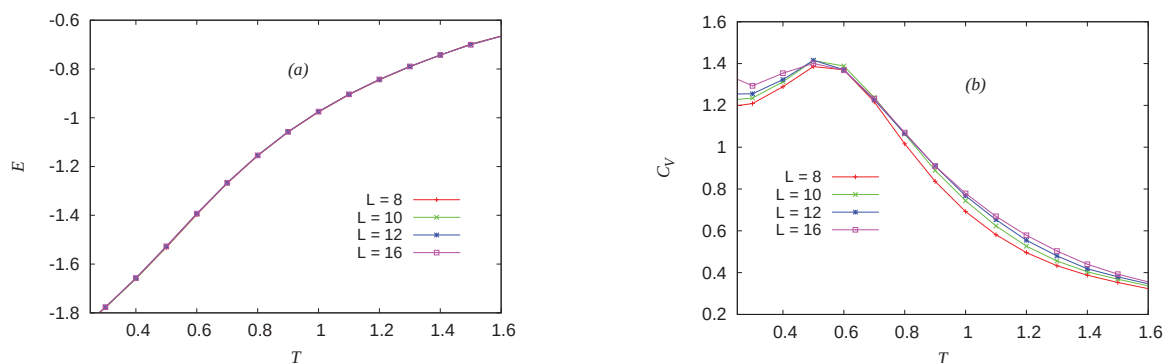


Figure 3. (Color online) (a) Temperature dependence of average energy and (b) specific heat for different sizes.

corresponds to a series of MCSs. We perform M_s MCSs for each temperature and take N_s samples out of M_s . To make sure the system is well equilibrated, we perform enough initial M_i MCSs, usually M_i around 10^4 MCSs, before doing measurement.

The energy time series (ETS) of three different temperatures, *i.e.*, $T = 0.7, 0.5$ and $T = 0.3$, were taken for linear size $L = 10$. As shown in Fig. 2, the system reaches equilibrium after several MCSs, depending on temperature, which is around 2000 for $T = 0.3$. Fluctuation at larger system size is more pronounced compared to smaller system size. We extracted two quantities from ETS, namely the ensemble average of energy, $\langle E \rangle = \frac{1}{N_s} \sum_{N_s} E_i$, and the specific heat defined as follows

$$C_v = \frac{N}{kT^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right) \quad (6)$$

where $N = L^3$ and k are respectively the number of spins and Boltzmann constant. These quantities are shown in Fig. 3(a) and (b).

As the specific heat plot has a constant peak, which corresponds to critical exponent $\alpha = 0$, it can not precisely signify the presence, neither the absence of spin glass phase transition in the system. A more convincing evidence for the existence or absence of SG phase is obtained from the SG order parameter which is presented in the next sub-section.

3.2. Spin Glass Order Parameter

The existence of SG phase is characterized by the following order parameter [17]

$$q_{EA} \equiv \left[\left\langle \left| \frac{1}{N} \sum_i \vec{s}_i^{(\alpha)} \otimes \vec{s}_i^{(\beta)} \right| \right\rangle \right]_{\text{av}}, \quad (7)$$

where $\vec{s}_i^\alpha$ and $\vec{s}_i^\beta$ are two sets of vector spins from different replicas having the same structure of connectivity. The essence of this parameter is to capture the frozen configuration in SG phase; which is merely introduced for numerical simulation. In real experiment it is almost impossible to obtain two duplicated systems with exactly the same realization of randomness. It is to be noticed that we have additional replicas for the calculation of overlapping parameter, apart from replicas related to the RE method.

The overlapping parameter is much simpler for Ising spins compared to the vector spins which involves tensor product [13, 14]. If system is frozen, their overlapping parameter will give finite value and vanish otherwise. The plot of temperature dependence of q_{EA} for different sizes, $L = 8, 10, 12$, and 16 is shown in Fig. 4. As indicated, the parameter is increasing as temperature decreases. However, the finite values of the parameter at lower temperature decrease as system

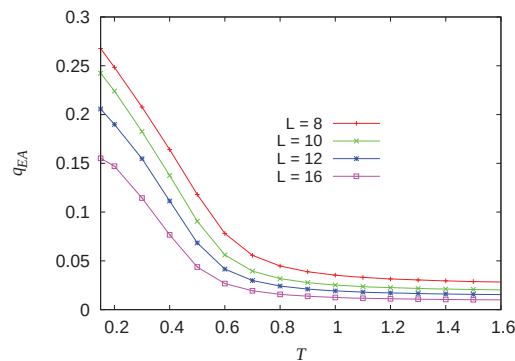


Figure 4. (Color online) Temperature dependence of the overlapping order parameter for various system sizes.

sizes increase. This is the indication of the absence of SG phase on the rewired cubic lattice with $ANOL = 4.0$ in the thermodynamic limit. Therefore, it is desirable to study this type of model with larger value of $ANOL$, associated with system with larger spatial dimension. This argument is comparable with the case in the canonical SG model where the existence of SG phase on cubic lattice remains a controversy, while convincingly found in the structure with four spatial dimensions [18].

4. SUMMARY AND CONCLUSION

We have studied antiferromagnetic Heisenberg model on rewired cubic lattices with average number of links ($ANOL$) or connectivity density 4.0; obtained by adding one extra link to each site of the cubic lattice. Each added link is constrained to connect to one of the next-nearest neighbors of each site. We use Replica Exchange Monte Carlo method which is considered to be very powerful in dealing with complex systems such as SGs. We calculate several physical observables such as energy, specific heat and overlapping SG order parameter.

We observed no finite temperature SG phase transition which is indicated by the decreasing value of the overlapping parameter q_{EA} as the system sizes increase at low temperatures. This result suggested that the AF rewired cubic lattice with $ANOL=4$ can not host the non-canonical Heisenberg SG phase. With our previous report on the existence of this type of SG on SFN[13], which corresponds to regular lattice with very large spatial dimension, the quest for finding lower critical dimension or $ANOL$ for this system still remains. The study of the system with larger $ANOL$ is required. A systematic study of system with larger fractional $ANOL$ is still in progress. The results will be reported elsewhere.

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