Search for the non-canonical Ising spin glass on rewired square lattices

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Abstract. A spin glass (SG) of non-canonical type is a purely antiferromagnetic (AF) system, exemplified by the AF Ising model on a scale free network (SFN), studied by Bartolozzi et al. [Phys. Rev. B73, 224419 (2006)]. Frustration in this new type of SG is rendered by topological factor and its randomness is caused by random connectivity. As an SFN corresponds to a large dimensional lattice, finding non-canonical SG in lattice with physical dimension is desirable. However, a regular lattice can not have random connectivity. In order to obtain lattices with random connection and preserving the notion of finite dimension, we costructed rewired lattices. We added some extra bonds randomly connecting each site of a regular lattice to its next-nearest neighbors. Very recently, Surungan et al., studied AF Heisenberg system on rewired square lattice and found no SG behavior [AIP Conf. Proc. 1719, 030006 (2016)]. Due to the importance of discrete symmetry for phase transition, here we study similar structure for the Ising model ($Z_2$ symmetry). We used Monte Carlo simulation with Replica Exchange algorithm. Two types of structures were studied, firstly, the rewired square lattices with one extra bonds added to each site, and secondly, two bonds added to each site. We calculated the Edwards-Anderson paremter, the commonly used parameter in searching for SG phase. The non-canonical SG is clearly observed in the rewired square lattice with two extra bonds added.

1. Introduction
Spin glass (SG) system is an interesting subject to study, both theoretically and experimentally due to its wide range applications. It is considered for example as a candidate material for giant magneto-resistance (GMR)[1]. From the view point of computational (theoretical) physics, SG is a very good ground test for several such complex problems as NP-hard and optimization [2, 3]. This type of system is different from the usual magnet as it does not possess total magnetization at any temperature. It is grouped as a magnetic system due to the frozen random spin configuration at low temperatures. The frozen configuration is regarded as a typical ordered, called a temporally ordered phase rather than spatially ordered phase [4]. The SG phenomenon was first reported in experiment in the early 70s by Cannella and Mydosh who observed the presence of cusp instead of sharp peak in ac-susceptibility [5] of alloys composed from transition metal impurities hosted by nobel metals ($CuMn$ and $AuFe$). In these materials, magnetic impurities ($Mn$ and $Fe$) with small concentration randomly occupy the sites of the non-magnetic hosts ($Cu$ and $Au$).

Frustration and randomness are two main ingredients for a system to exhibit SG phase. Spins are frustrated if fail to simultaneously satisfy all their nearest neighbors in minimizing the interaction energy. This is firmly exemplified by spins on an AF triangular unit. Spins with
ferromagnetic (FM) couplings (anti-ferromagnetically) will prefer to align in parallel to each other and anti-parallel for AF couplings, in order to minimize the free energy.

The ground state (GS) configuration of the system is highly degenerate due to random frustration; leads the system to possess GS entropy, well known as residual entropy. It is also due to this factor that makes the system exhibiting many remarkable phenomena such as aging, rejuvenation and memory effects [6]. Due to the existence of a large number of local minima in the energy landscape, finding the GS energy of the systems is challenging for many optimization algorithms[7, 8]. Most SGs studied in literature are of canonical type, being characterized of having both FM and AF interactions. The so-called non-canonical SG has recently received significant interest [9, 10, 11, 14]. It is a new type of SG which is is purely AF, possessing random connectivity and its frustration is brought by the topological factor. This kind of SG was firstly reported for the Ising model on scale free network (SFN)[9]. Recently, we studied Heisenberg model on SFN with AF interaction and found SG phase transition[11].

The SFN corresponds to large dimensional regular lattices. A profound behavior of such network is small-world connectivity, where two spins randomly chosen are always connected by a shortcut distance in maximum, for example, of six units[13]. With this behavior, the notion of spatial dimension is lost. It is therefore desirable to probe this type of SG in reasonable spatial dimension. Very recently we studied Heisenberg model on rewired square lattice and found no SG transition[14]. Due to the importance of discreteness in phase transition [15, 16], here we study Ising model on rewired square lattices. The remaining part of the paper is organized as the following: We describe in Section II the model and method; discuss the result is in Section III. Section IV is devoted for summary and concluding remarks.

2. Model and Simulation

We study the Ising model which is written in the following Hamiltonian

\[ H = -J \sum_{\langle ij \rangle} s_i s_j \]  

(1)

where \( J \) characterizes the interaction between the Ising spin \( s_i \) residing respectively on \( i \)-th site of the lattice. We consider a pure AF system, so that \( J < 0 \). The summation is performed over all nearest neighbor spins, including the newly added neighbors due to rewiring. Regular lattices such as the square and cubic, all spins have the same number of neighbours, associated with a definite coordination number. Here, we studied two types of structures: (i) rewired square lattice with one extra bond added to each spin, and (ii) two extra bonds added. The first added bond connects a spin to one of its diagonal neighbours, while the second one connects each spin to one of the next-next nearest spins. Therefore, for the first structure, spins can have five, six or seven bonds. Particular realizations of these lattices are shown in Fig. 1.

The rewired lattices can be regarded as a quasi regular lattice. By excluding the double counting, the average number of bonds (ANOB) for the first and second structure is 3.0 and 4.0, respectively. In principle one can generate any lattice with fractional ANOB. As indicated in in Fig. 1, abundance of triangular units exist, rendering frustration due to AF couplings. Adding extra bonds up to certain number corresponds to increasing the degree of frustration. In principle, it is possible to define the degree of frustration and study its effect on SG properties. This is done for example in Ref. [10] which randomly rewired any pairs of spins. This procedure of rewiring totally breaks the translational symmetry of regular lattices. We do not take such procedure as the notion of spatial dimension needs to be preserved. Although the current developed model is purely theoretical, it may be implemented in growing AF-based SG material by introducing impurity, which was done for example in several References[19, 20, 21].

We performed Monte Carlo (MC) simulation using the Replica Exchange algorithm [17]. This algorithm is exceptionally suitable to overcome the slow dynamics due to the existence
Figure 1. (Color online) Examples of rewired square lattices with (a) an extra bond and (b) two extra bonds; added to each spin. The bonds represented by dashed lines randomly connect each spin to the next-nearest or the next-next nearest neighbors.

of local minima in the energy landscape. The slow dynamics is a common problem in dealing with complex systems such as SGs where a random walker tends to get trapped at certain local minima. The basic procedure of this algorithm is to duplicate the original systems into several replicas, each will be independently treated by a standard Metropolis algorithm. The final results of the calculation is obtained by combining all those separated calculations. During the calculation, replicas belonging to two adjacent temperatures are exchanged; enabling a random walker to stay away from any local minima.

If we start with $M$ replicas; each is in equilibrium with a heat bath of temperature, then given a set of invers temperatures $\beta$, the distribution of probability in finding the entire system in a state $\{X\} = \{X_1, X_2, \ldots, X_M\}$ is given by,

$$P(\{X, \beta\}) = \prod_{m=1}^{M} \tilde{P}(X_m, \beta_m),$$  \hspace{0.5cm} (2)

with

$$\tilde{P}(X_m, \beta_m) = Z(\beta_m)^{-1} \exp(-\beta_m H(X_m)),$$  \hspace{0.5cm} (3)

and the partition function $Z(\beta_m)$ is associated with the $m$-th replica. An exchange matrix between replicas is defined as $W(X_m, \beta_m|X_n, \beta_n)$, which is the probability to exchange the configuration $X_m$ of $\beta_m$ with the configuration $X_n$ of $\beta_n$. With the requirement of preserving the entire system at equilibrium, we apply the detailed balance condition to the transition matrix

$$P(\{X_m, \beta_m\}, \ldots, \{X_n, \beta_n\}, \ldots) \cdot W(X_m, \beta_m|X_n, \beta_n)$$

$$= P(\{X_n, \beta_m\}, \ldots, \{X_m, \beta_n\}, \ldots) \cdot W(X_n, \beta_m|X_m, \beta_n),$$  \hspace{0.5cm} (4)

along with Eq. (3), so that we have

$$\frac{W(X_m, \beta_m|X_n, \beta_n)}{W(X_n, \beta_m|X_m, \beta_n)} = \exp(-\Delta),$$  \hspace{0.5cm} (5)
where $\Delta = (\beta_n - \beta_m)(H(X_m) - H(X_n))$. With this constraint, we can choose the matrix coefficients following the standard Metropolis algorithm which gives

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

(6)

Since the ratio of acceptance exponentially decays with $(\beta_n - \beta_m)$, the exchanges of temperatures are allowed only between temperatures next to each other, e.g., the terms $W(X_m, \beta_m|X_{m+1}, \beta_{m+1})$.

In doing the simulation, one MC step (MCS) is defined as randomly visiting all spins at each replica, either consecutively or randomly, and performing update based on MC rule. After a number of MCSs, pairs of configurations belonging to corresponding temperatures next to each other are exchanged following the probability written in Eq. 6. Two consecutive exchanges are assigned as odd and even. For an odd exchange, we swap the pairs of replicas $X_1$ and $X_2$; $X_3$ and $X_4$; · · ·; $X_{M-1}$ and $X_M$; while for the even one we exchange $X_2$ and $X_3$; · · ·; $X_{M-2}$ and $X_{M-1}$.

For each realization of connectivity we start from a random spin configuration. Then, we run $10^3$ MCSs to equilibrate the system before taking a total of $4 \times 10^4$ sample points for the ensemble averages. Several extra MCSs between sample points were taken to avoid temporal correlation. We probe the high and the low temperatures to search for SG phase transition. The ensemble averages obtained for each size of lattice 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 the AF Ising model on randomly rewired square lattices with ANOB = 3.0 and 4.0 for several linear sizes $L = 16, 24, 32, 48$, and 64. The periodic boundary condition is applied so that every site of the original square lattice possesses similar number of nearest neighbors. For each system size we took large number of realizations of connectivities. The result is obtained by averaging over these realizations. Each realization is associated with one particular randomly generated connectivity distribution. For the results to have better statistics, we took large number of realizations. Previous study of Heisenberg SG on SFN took 1000 realizations. Here we took smaller number of realizations (N=250) due to its degree of randomness is less compared to the previous system.

To probe the equilibrium properties which is essential for the calculation ensemble average of physical quantities, we evaluated the energy time series (ETS). The average energy and specific heat can be extracted from ETS. Whether the system is in equilibrium or not can be characterized by analysing the energy time series. In MC simulation, time is associated with series of MCS’s. We run $M_s$ MCS’s for every temperature and take $N$ sample points out of $M_s$. To guarantee that the system is well equilibrated, initial MCSs is performed before doing measurement, normally around 10000 MCSs.

From the energy time series (ETS), We extracted two quantities, namely the ensemble average of energy, $\langle E \rangle = \frac{1}{N} \sum_N E_i$, and the specific heat is written as the following

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

(7)

where $k$ and $N$ are the Boltzmann constant and the number of spins, respectively. The temperature dependence of this quantity is shown in Fig. 2 and Fig. 3.

The temperature dependence of specific heat does not have diverging peak for lattice with ANOB = 3.0, and increasing with system size for lattice with ANOB = 4.0. This clearly signify
an absence of (the presence of) phase transition in the first (second) type of lattice. For a more convincing analysis, we calculate the Edwards-Anderson parameter which is presented in the next sub-section.

3.2. Spin Glass Order Parameter
The existence of SG phase transition is characterized by the overlapping parameter, also known as Edwards-Anderson (EA) parameter [18] defined as follows

\[ q_{EA} = \left[ \frac{1}{N} \sum_i s_i^{(\alpha)} s_i^{(\beta)} \right]_{av}, \]

where two sets of systems \( s_i^{(\alpha)} \) and \( s_i^{(\beta)} \) having similar connectivity distribution. The aim of this parameter is to detect the frozen configuration when system is in SG phase; which is merely introduced for numerical simulation. It is almost impossible in experiment to obtain two duplicated systems with similar coupling distribution.

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will be finite and vanish otherwise. The temperature dependence of $q_{EA}$ for various sizes, $L = 16, 24, 32, 48$ and $64$ is depicted in Fig. 4. As indicated, $q_{EA}$ increases as temperature decreases. However, the two systems exhibit different trends. For lattices with ANOB = 3, the finite value of $q_{EA}$ at lower temperature systematically decreases as system sizes increases. This is the indication of the absence of SG phase in the thermodynamic limit. In contrast, for lattices with ANOB = 4.0, the finite value of the parameter at lower temperature remains, indicating the existence of SG phase in the thermodynamic limit. There is a significant increase of $q_{EA}$ for system sizes $L = 16, 24$ and 32, which is a clear sign for the existence of SG phase in the rewired square lattices for ANOB=4.0. Although for larger sizes, i.e., $L = 48$ and 64, the value of the parameter at lower temperature decreases as system sizes increases, similar to the trend for the case of ANOB = 3.0, they are not systematic. The conflicting trends shown by the smaller and larger sizes for lattices with ANOB=4.0, signify the importance of dimensionality (coordination number) for the existence of ordered phase. The lattices with smaller sizes, i.e., $L < 48$, inherit the small-world behavior, which corresponds to properties of larger dimensional lattices. Therefore, although there is a sign for the existence of SG phase in the rewired square lattices for ANOB=4.0, we believe that a more convincing indication should be clearer for lattices with ANOB>4.0. Further study with larger ANOB, presently probed, is required.

4. Summary and Conclusion
We have studied antiferromagnetic Ising model on rewired square lattices with connectivity density (ANOB) 3.0 and 4.0; obtained by adding one and two extra bonds to each site of the original square lattice. The first added bond is constrained to connect to one of the next-nearest neighbors while the second one to one of the next-next-nearest neighbors. We use Replica Exchange Monte Carlo method which is considered very powerful in dealing with randomly frustrated systems such as SGs. Several physical quantities such as energy, specific heat and overlapping SG order parameter were calculated.

An indication SG phase transition is observed in the lattices with ANOB = 4.0 and not for ANOB = 3.0. This is indicated by a clear crossing point in the plot of overlapping parameter $q_{EA}$. There is no crossing point in the plot of the quantity for ANOB=3.0. A clear crossing point in the plot of $q_{EA}$ for smaller sizes is indicative to the effect of small-world behavior of the lattice. In search for a clear indication of SG phase, we need to study lattices with connectivity density, ANOB > 4.0. A more comprehensive study of system with larger fractional value of ANOB is in progress. The results will be reported elsewhere.

![Figure 4](image.png)

Figure 4. Temperature dependence of the overlapping order parameter for lattices with (a) ANOB = 3.0 and (b) 4.0 for various system sizes.
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