

PHASE TRANSITION BEHAVIOUR OF ISING SPIN GLASS ON THE FCC LATTICE

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Received 09 July 2013;

Accepted for publication 31 August 2013

Abstract. *In this work, we study the nature of phase transition in a face centered cubic (FCC) antiferromagnet with Ising spins. The spin-glass character depends on the concentration p of ferromagnetic bonds randomly generated into the system. We introduce a new quantity M_Q combined by the Edwards-Anderson order parameter Q and the standard magnetization M . Note that, it is impossible to obtain the susceptibility defined by the variance of Q or M , but we can do that for M_Q . Using the standard Monte-Carlo and powerful Wang-Landau flat-histogram methods, we carry out in this work intensive simulations with many value of p . We show that the first-order transition has been destroyed with a tiny amount of ferromagnetic bond $p \sim 0.01$. With increasing p , the antiferromagnetic phase changes into a spin glass, and then to ferromagnetic phase.*

I. INTRODUCTION

A spin glass is a disordered magnet with random interactions, both ferromagnetic and also antiferromagnetic bonds are randomly distributed with comparable frequency. The term "glass" comes from an analogy between the magnetic disorder in a spin glass and the positional disorder of a conventional, chemical glass, a window glass. Spin glasses have many metastable structures, so it is very difficult to explore experimentally or in simulations.

Phase transition in spin glasses is a subject of intensive investigation since four decades. The main difficulties in such systems come from the combination of the frustration and the bond disorder. The most popular Ising spin glass model have been introduced by Sherrington and Kirkpatrick [1, 2]. This is a classical mean field model with random interactions between the spin pairs.

The phenomena of slow dynamics or slow relaxation near the phase transition have been the subject of many theoretical [3–6] and experimental [7–10] studies, it presents many interesting features that reflect the nature of the phase transition.

The paper is organized as follows. Sec. II is devoted to a description of our model and the simulation method. Results are shown in Sec. III. Conclusions are given in Sec. IV.

II. THE MODEL

We consider the FCC lattice with Ising spins of magnitude $S = 1$. The Hamiltonian is given by

$$H = - \sum_{\langle i,j \rangle} J_{ij} (S_i S_j), \quad (1)$$

where S_i is the Ising spin at the lattice site i , $\sum_{\langle i,j \rangle}$ is made over the NN spin pairs S_i and S_j with interaction J_{ij} . Hereafter we suppose that $J_{ij} = -J$ ($J > 0$) for antiferromagnetic bonds and $J_{ij} = J$ for ferromagnetic bonds. The three-dimension (3D) lattice is composed of L^3 FCC-cells each with four spins (L being the number of cells in each direction). The four sublattices are shown in Fig. 1. The total number of spins of the lattice is $N = 4L^3$. The number of NN bond per spin is 12, thus the total number of bond of the system is $N_b = 12 \times N/2 = 24L^3$. We use the periodic boundary conditions.

To create a spin glass, we introduce a number of ferromagnetic bonds N_b^F in a random manner into the pure antiferromagnetic state. We define the ferromagnetic bond concentration p by $p = N_b^F/N_b$. The phase transition behavior of the system depends on the parameter p ($0 \leq p \leq 1$), i.e., it changes from pure antiferromagnetic phase (at $p = 0$) to pure ferromagnetic phase at ($p = 1$) passing through the spin glass phase.

In order to investigate the nature of the phase transition at various p , we use the standard Monte Carlo method and the Wang-Landau technique of simulation. Wang and Landau [11] recently proposed a MC algorithm for classical statistical models which allowed to study systems with difficultly accessed microscopic states. In particular, it permits to detect with efficiency weak first-order transitions [12, 13] The algorithm uses a random walk in energy space in order to obtained an accurate estimate for the density of states (DOS), call it $g(E)$, which is defined as the number of spin configurations for any given E . This method is based on the fact that a flat energy histogram $H(E)$ is produced if the probability for the transition to a state of energy E is proportional to $g(E)^{-1}$. We

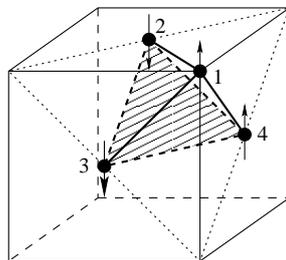


Fig. 1. The FCC cell with four sublattices.

summarize how this algorithm is implied here. At the beginning of the simulation, the density of states $g(E)$ is unknown so all densities are set to unity, $g(E) = 1$. We begin a random walk in energy space (E) by choosing a site randomly and flipping its spin with a transition probability

$$p(E \rightarrow E') = \min [g(E)/g(E'), 1], \quad (2)$$

where E is the energy of the current state and E' is the energy of the proposed flip. Each time an energy level E is visited, the DOS is modified by a modification factor $f > 0$ whether the spin flipped or not, i.e. $g(E) \rightarrow g(E)f$. At the beginning of the random walk, the modification factor f can be as large as $e^1 \simeq 2.7182818$. A histogram $H(E)$ records the number of times a state of energy E is visited. Each time the energy histogram satisfies a certain "flatness" criterion, the visits histogram $H(E)$ is then reset to zero, and the modification factor reduced, typically to the square root of the previous factor, to produce a finer estimate of $g(E)$. The reduction process of the modification factor f is repeated several times until a final value f_{final} which close enough to one. The histogram is considered as flat if

$$H(E) \geq x\% \cdot \langle H(E) \rangle \quad (3)$$

for all energies, where $x\%$ is chosen between 90% and 95% and $\langle H(E) \rangle$ is the average histogram.

The thermodynamic quantities [11, 14] can be evaluated by

$$\langle E \rangle = \frac{1}{Z} \sum_E g(E) E \exp(-E/k_B T), \quad (4)$$

$$C_v = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2}, \quad (5)$$

$$\langle M^n \rangle = \frac{1}{Z} \sum_E M^n g(E) \exp(-E/k_B T), \quad (6)$$

$$\chi = \frac{\langle M^2 \rangle - \langle M \rangle^2}{k_B T}, \quad (7)$$

where Z is the partition function defined by

$$Z = \sum_E g(E) \exp(-E/k_B T).$$

The canonical distribution at any temperature can be calculated simply by

$$P(E, T) = \frac{1}{Z} g(E) \exp(-E/k_B T).$$

In this work, we consider a energy range of interest [15, 16] ($E_{\text{min}}, E_{\text{max}}$). We divide this energy range to R subintervals, the minimum energy of each subinterval is E_{min}^i for $i = 1, 2, \dots, R$, and maximum of the subinterval i is $E_{\text{max}}^i = E_{\text{min}}^{i+1} + 2\Delta E$, where ΔE can be chosen large enough for a smooth boundary between two subintervals. The WL algorithm is used to calculate the relative DOS of each subinterval ($E_{\text{min}}^i, E_{\text{max}}^i$) with the modification factor $f_{\text{final}} = \exp(10^{-9})$ and flatness criterion $x\% = 95\%$. We reject the suggested spin flip and do not update $g(E)$ and the energy histogram $H(E)$ of the current energy level E

if the spin-flip trial would result in an energy outside the energy segment. The DOS of the whole range is obtained by joining the DOS of each subinterval $(E_{\min}^i + \Delta E, E_{\max}^i - \Delta E)$.

III. THE SIMULATION RESULTS

We used the system size of $N = 4 \times L^3$ where $L = 12$, p varies from 0 up to 1. Periodic boundary conditions are used in the three directions. The magnetization and the susceptibility is obtained by standard Monte-Carlo simulation with the equilibrating time is $t_e = 2,000,000$ MC steps/spin and the averaging time is $t_a = 4,000,000$ MC steps/spin. The energy, specific heat and energy histograms are obtained by WL technique.

For $p = 0$, it is well-known that the bulk FCC antiferromagnet with Ising spins shows a very strong first-order transition [17–20]. The phase transition in the Heisenberg model also shows a first-order character [21,22]. Other similar frustrated antiferromagnets such as the HCP antiferromagnet show the same behavior [23,24]. In Fig. 2, we show the energy and the magnetization versus temperature T where the discontinuous vertical lines indicate the discontinuities at the transition temperature T_C . This is the case of pure FCC antiferromagnet. Specific heat and susceptibility as a function of temperature are shown in Fig. 3.

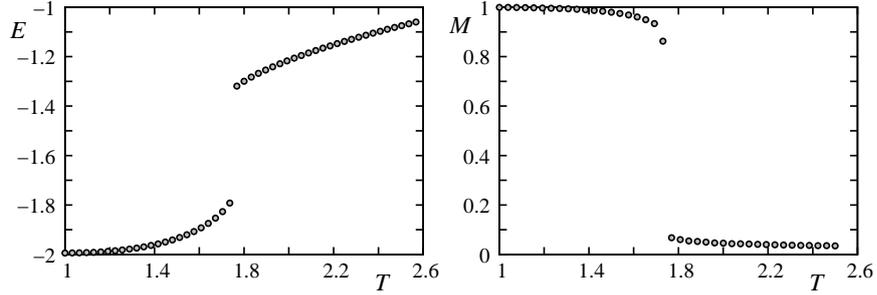


Fig. 2. Energy (left) and magnetization (right) vs temperature for $p = 0$ and $L = 12$.

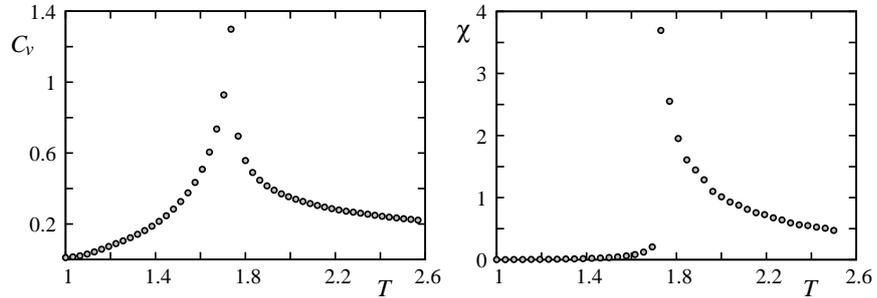


Fig. 3. Specific heat (left) and susceptibility (right) vs temperature for $p = 0$ and $L = 12$.

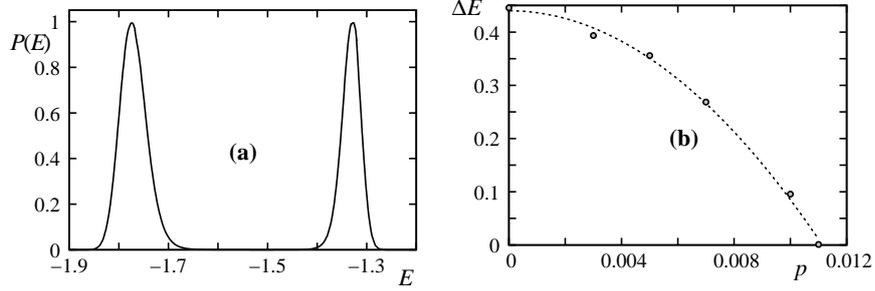


Fig. 4. (a) Energy histograms as a function of energy at $T = 1.75114$ with $p = 0$. (b) The latent heat vs p for $L = 12$.

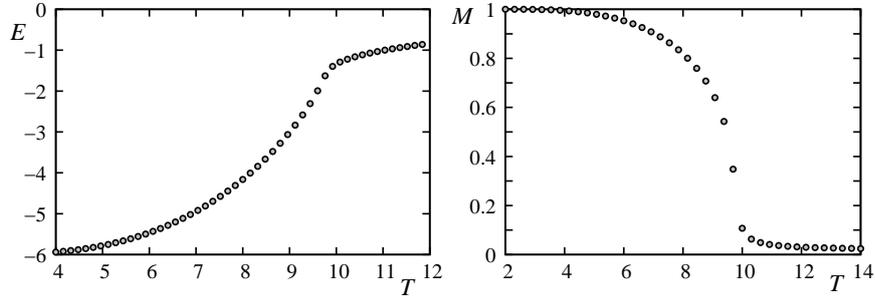


Fig. 5. Energy (left) and magnetization (right) vs temperature for $p = 1.0$ and $L = 12$.

Fig. 4 (a) shows a double peak of the energy distribution at T_C which is another signature of the first-order behavior. The latent heat ΔE is defined by the energy separation of the two peaks in the energy distribution. When the transition is of second order, the energy is continuous, namely $\Delta E = 0$. As shown in Fig. 4 (b) the first order transition remains as long as $p \leq 0.011$. For $p > 0.011$, the phase transition is continuous.

For the case of pure ferromagnet, i.e. $p = 1$, we plot in Fig. 5 the energy and the magnetization. The transition is a second-order one as expected for a 3D Ising ferromagnet.

Let us consider intermediate values of p where the spin-glass phase is expected. The spin-glass phase is determined by the Edwards-Anderson freezing order parameter defined as

$$Q = \sum_i^N \left| \sum_{t=t_e}^{t_e+t_a} S_i(t) \right|. \quad (8)$$

The averaging time t_a is taken as long as possible (at least several millions of MC per spin). The magnetization is defined as

$$M = \sum_{t=t_e}^{t_e+t_a} \sum_i^N S_i(t). \quad (9)$$

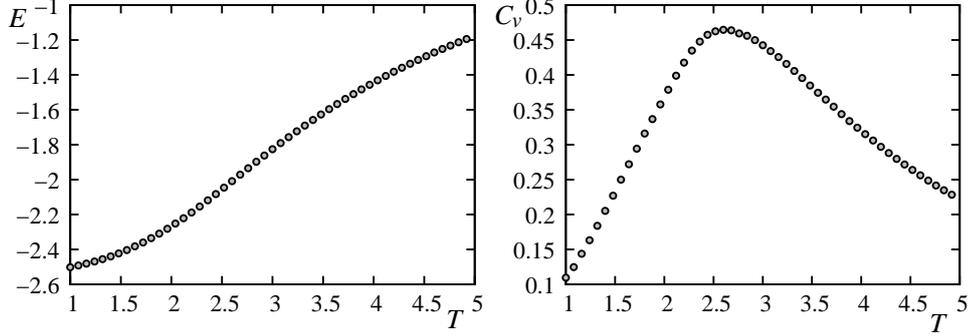


Fig. 6. Energy (left) and specific heat (right) vs temperature for $p = 0.5$ and $L = 12$.

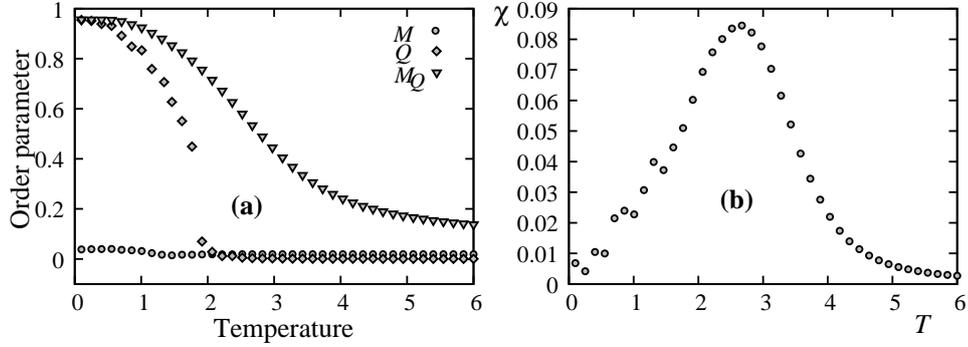


Fig. 7. (a) Magnetization M , order parameter Q , and $M_Q = M(Q_{\Delta t})$ with $\Delta t = 30000$ vs temperature for $p = 0.5$. (b) $\chi = N(\langle M(Q_{\Delta t})^2 \rangle - \langle M(Q_{\Delta t}) \rangle^2)/T$ vs temperature for $p = 0.5$ and $L = 12$.

In a strong bond disorder, the magnetization M tends to zero at any T so that it cannot distinguish a frozen phase from the paramagnetic phase. We show now the result for $p = 0.5$ where the bond disorder is strongest. We plot in Fig. 6 the energy and the specific heat versus temperature for $p = 0.5$.

To study the phase transition in the "equilibrated" regime, let us define the following quantities

$$Q_{\Delta t}(t) = \sum_i^N \left| \sum_t^{t+\Delta t} S_i(t) \right|, \quad (10)$$

$$M(Q_{\Delta t}) = \sum_t Q_{\Delta t}(t). \quad (11)$$

where $\sum_t^{\Delta t}$ indicates a sum over Δt MC steps starting from t and \sum_i^N indicates a sum over the system sites. In Eq. 11, $M(Q_{\Delta t})$ is the average of $Q_{\Delta t}$ calculated over all successive intervals of Δt steps until the end of the total run time t_a . $M(Q_{\Delta t})$ is thus averaged with $t_a/\Delta t = 2 \times 10^5$ intervals (taking $\Delta t = 20$ for instance). Note that Δt is nothing but the

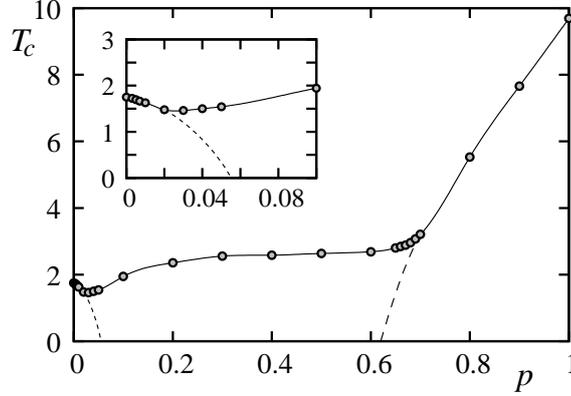


Fig. 8. The phase diagram (T_C, p) for $L = 12$.

so-called "waiting time" when measuring the magnetization. In the case of $\Delta t = 1$ we obtain $M(Q_{\Delta t}) \equiv M$, and when $\Delta t = t_a$ we have $M(Q_{\Delta t}) \equiv Q$. As shown in Fig. 7(a), the magnetization is zero at any temperature for $p = 0.5$. Therefore, it is impossible to obtain the susceptibility defined by the variance of M or Q . However, we can do that for $M(Q_{\Delta t})$: $\chi = N(\langle M(Q_{\Delta t})^2 \rangle - \langle M(Q_{\Delta t}) \rangle^2)/T$. Of course, the result of χ will depend on Δt . We show an example of χ for $\Delta t = 30000$ in Fig. 7(b).

The phase diagram (T_C, p) , where T_C is obtained at the maximum of specific heat is shown in Fig. 8. The inset enlarges the small p region. Discontinued lines are extrapolations from the antiferromagnetic-paramagnetic (AF-P) and ferromagnetic-paramagnetic (F-P) transition lines. The region below each discontinued line has a reentrant shape. This should be further clarified before a firm conclusion can be said. This is not the purpose of this work.

IV. CONCLUSIONS

We studied in this work the phase transition behaviors of Ising spins on the FCC lattice. We found that the first-order transition has been destroyed with a tiny amount of ferromagnetic bond $p \sim 0.01$.

Using the new quantity $M(Q_{\Delta t})$, we can obtain the susceptibility χ as a function of temperature which defined by the variance of $M(Q_{\Delta t})$, but not by the variance of M or Q . Therefore, the transition temperature T_C is obtained at the maximum of χ .

The phase diagram (PD) shows that the antiferromagnetic phase changes into a spin glass and then to ferromagnetic phase, then this PD suggests that the spin-glass phase exists in the range $0.055 < p < 0.62$. The PD is not symmetric with respect to p . This is due to the fact that the FCC lattice is highly frustrated at $p = 0$ (antiferromagnetic) and non frustrated at $p = 1$. It is not therefore surprising that the introduction of even very small amount of ferromagnetic bonds breaks immediately the long-range order. Note that the case where the pure system is non frustrated such as the simple cubic ferro- or antiferromagnets, the phase diagram (T_C, p) is symmetric because the system is invariant with respect to the local transformation of every spin pair ($J_{ij} \rightarrow -J_{ij}; S_j \rightarrow -S_j$).

ACKNOWLEDGMENTS

This work was supported by the Nafosted (Vietnam National Foundation for Science and Technology Development), Grant No. 103.02-2011.55.

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