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Damage spreading in two-dimensional geometrically frustrated lattices: the triangular and kagome anisotropic Heisenberg model

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Abstract
The technique of damage spreading is used to study the phase diagram of the easy axis anisotropic Heisenberg antiferromagnet on two geometrically frustrated lattices. The triangular and kagome systems are built up from triangular units that either share edges or corners, respectively. The triangular lattice undergoes two sequential Kosterlitz–Thouless transitions while the kagome lattice undergoes a glassy transition. In both cases, the phase boundaries obtained using damage spreading are in good agreement with those obtained from equilibrium Monte Carlo simulations.

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1. Introduction

Frustrated antiferromagnets are particularly interesting because they allow novel kinds of low-temperature magnetic states to develop [1, 2] which are quite different from those observed in conventional magnets [3]. When the frustration is due entirely to the geometry of the lattice, exact results for the $S = 1/2$ Ising model on the triangular [4] and kagome [5] lattices have shown that there is no long-range order at any temperature and the system has a macroscopic ground-state degeneracy. In the triangular case, the spin–spin correlation function decays with a power law [6] whereas, in the kagome geometry, it decays exponentially at zero temperature [7, 8]. For isotropic vector spin models (XY or Heisenberg) on a triangular lattice [9–11] where the elementary triangles share edges, the frustration is partially relieved and a noncollinear planar ground-state forms with neighbouring spins making angles of 120°. Finite temperature transitions are evident in both cases (XY and Heisenberg) but are topological in nature. However, for the kagome lattice, the cornering sharing geometry leads to a disordered ground state for the Heisenberg model with the phenomenon of order by disorder occurring in the limit $T \to 0$ with fluctuations favouring coplanar spin configurations [12].

In order to explore the Heisenberg model on these geometrically frustrated lattices, various types of perturbations have been applied and have shown a strong effect on the ground-state manifold [13]. We consider the following anisotropic Hamiltonian

$$H = J \sum_{i<j} (S_{ix}S_{jx} + S_{iy}S_{jy} + AS_{iz}S_{jz}) \tag{1}$$

where ($S_{i\alpha}$, $\alpha = x, y, z$) represents a classical three-component spin of unit magnitude located at each site i of a (triangular/kagome) lattice and the exchange interactions are restricted to nearest-neighbour pairs of sites. The parameter A describes the strength of the exchange anisotropy. We restrict our attention to the case where $A > 1$ represents an easy-axis anisotropy and we measure temperature and energy in units of $J = 1$. The limit $A \to 1$ corresponds to the isotropic Heisenberg model whereas the limit $A \to \infty$ corresponds to an infinite spin Ising model.

Monte Carlo studies have shown for the triangular lattice the existence of two distinct KT types of defect-mediated phase transitions at finite temperature [14, 15] for $A > 1$. By examining the limit $A \to 1$, the transition at the Heisenberg point also appears to be purely topological in character [16] but with exponentially decaying spin correlations in the low-temperature phase. Studies of the same model on the kagome lattice [17, 18] indicate the existence of a finite, but very low, temperature ferromagnetic transition for intermediate values of A. Static results for the magnetization, susceptibility and specific heat indicate an Ising-like transition but with a nonuniversal critical behaviour [18] in which the values of the exponents vary with the strength of the anisotropy A. The individual spins do not exhibit any long-ranged spatial order and resemble a glassy phase. An analysis of the time evolution of the double time spin auto-correlation function following a quench of the system from infinite temperature into a non-equilibrium state at low temperature displays the phenomenon of aging which is a characteristic of many glassy systems. Additional evidence for the glassy nature of this low-temperature state has also recently been found in a study of relationship of the spin auto-correlation function to the response of the system to an external magnetic field [19]. A violation of the fluctuation dissipation theorem is observed with properties similar to both structural glasses and spin glasses.

2. Method and results

In the present work we present a numerical study of the model described by Hamiltonian (1) for both lattices using a damage spreading algorithm. In the damage spreading method [21], the damage distance between two different initial spin configurations is measured as they evolve with the same thermal noise. The distance between two configurations is defined in the following way: if $\mathbf{S}_i^{(A)}$ and $\mathbf{S}_i^{(B)}$ are the spins of the two different replicas, then the distance between them at time t is defined as

$$D^{AB}(t) = \frac{1}{4N} \sum_{i=1}^{N} \left|\mathbf{S}_i^{(A)} - \mathbf{S}_i^{(B)}\right|^2 = \frac{1}{2N} \sum_{i=1}^{N} \left(1 - \mathbf{S}_i^{(A)}.\mathbf{S}_i^{(B)}\right) \tag{2}$$

where N is the total number of spins and $0 \leqslant D^{AB}(t) \leqslant 1$. The procedure of the spreading of damage is as follows: for a given value of the anisotropy A and temperature T we first initialize the system $\mathbf{S}_i^{(A)}$ in a random configuration and then let it evolve to a steady state. Then we make two additional copies of the system, $\mathbf{S}_i^{(B)}$ and $\mathbf{S}_i^{(C)}$. We introduce damage in both systems B and C by inverting a fraction of the spins. The two copies B and C correspond to cases where (1) a randomly chosen spin is flipped with $D^{AB}(0) = 1/N$ and (2) all the spins are flipped with $D^{AC}(0) = 1$. Given these different initial conditions we let all the

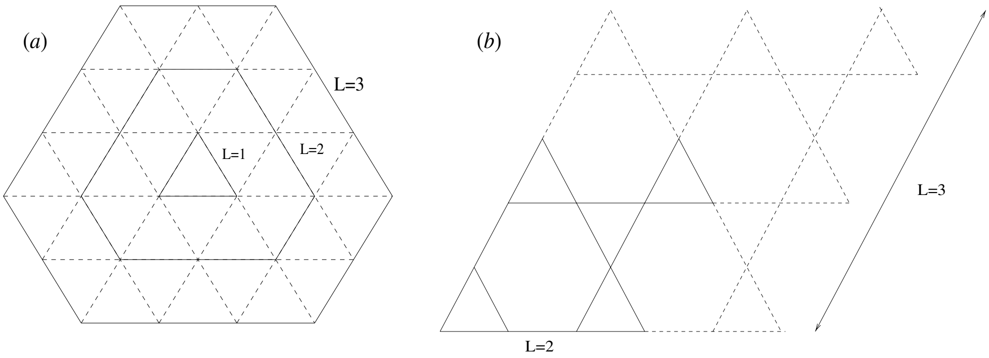

Figure 1. The two geometrically frustrated lattices: (*a*) the triangular and (*b*) the kagome lattices.

configurations evolve in time according to the same dynamics, i.e, the same rule and the same random number sequence in the Monte Carlo procedure. After a relaxation time needed for the damaged copies to be thermalized, we monitor the damage in order to calculate the time average $\langle D(t)\rangle$ of the distance (2). This procedure is repeated for many different samples (initial configurations A and damaged configurations B and C). At high temperatures, the averages $\langle D^{AB}\rangle$ and $\langle D^{AC}\rangle$ are equal but at low temperatures they approach different values. We interpret this result as indicating that the free energy landscape has a single valley at high temperature and that a transition to a more complicated multi-valley landscape occurs as the temperature is lowered.

Figure 1 shows the geometry of the two lattices for different sizes L. In both cases the number of sites $N = 3L^2$ and periodic boundary conditions are applied. Our simulations have been performed for sizes ranging from $L = 12$ to $L = 60$, but all of the results are presented with $L = 24$ where finite size effects are sufficiently small and a larger number of Monte Carlo sweeps (MCS) are possible. For each temperature we calculate the time average of the damage using 10 000 MCS and typically 200 samples were used to compute the averages.

In the case of the triangular lattice, recent Monte Carlo simulations [16] have shown the existence of two finite temperature KT transitions. The upper transition T_{c2} corresponds to the onset of power law correlations for the spin components parallel to the easy axis $A > 1$ and the lower transition T_{c1} corresponds to the onset of power law correlations for the perpendicular components. In both cases there is a corresponding spin stiffness coefficient which vanishes. In order to identify both transitions, we also compute the following measure of the damage distance associated with the transverse (xy) components of the spins in the two replicas

$$D_{xy}^{AB} = \frac{1}{2N}\sum_{i=1}^{N}\left(1 - S_{ix}^{(A)}S_{ix}^{(B)} - S_{iy}^{(A)}S_{iy}^{(B)}\right). \tag{3}$$

As shown in figure 2(a) for the isotropic Heisenberg case ($A = 1$) both distances are independent of the initial damage at high temperature but become dependent on it below the same temperature $T_c \sim 0.31$ which agrees quite well with previous estimates of the transition temperature using equilibrium methods [9, 10]. However, for values of $A > 1$, three different temperature regions are observed as shown in figure 2(b) for the case $A = 2$: (i) $T < T_{c1}$, both distances depend on the initial damage, (ii) $T_{c1} < T < T_{c2}$, $\langle D_{xy}\rangle$ is independent of the initial damage whereas $\langle D\rangle$ still depends on the initial damage and (iii) $T > T_{c2}$, both distances become independent of the initial damage. The damage spreading approach is able

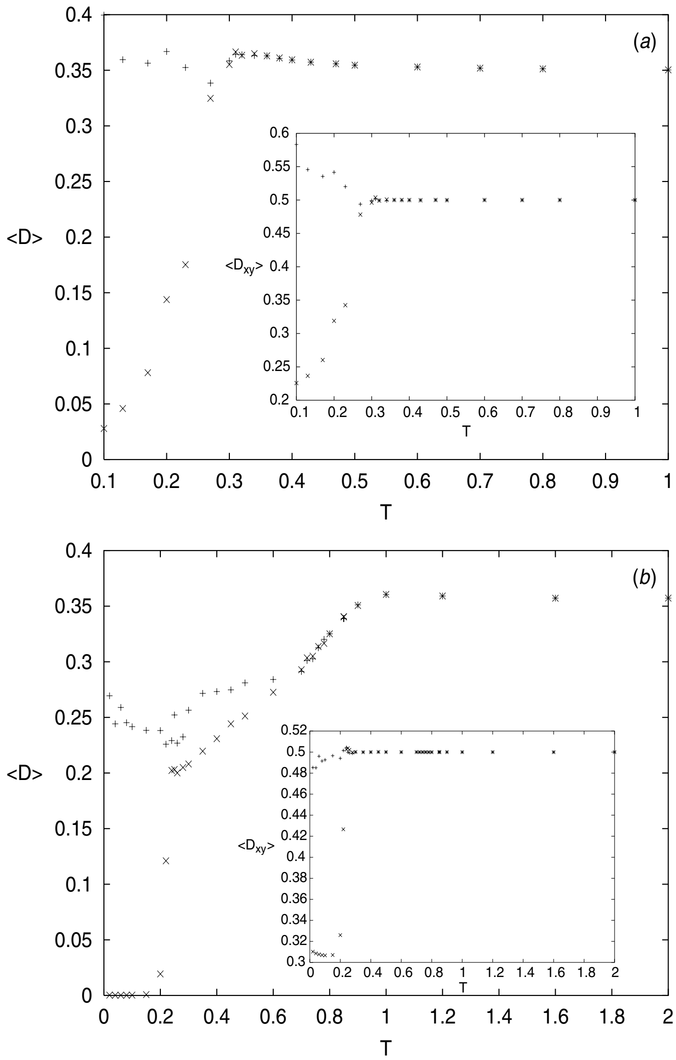

Figure 2. Average distance $\langle D \rangle$ versus temperature for the triangular lattice with $L = 24$ and two different values of the anisotropy (*a*) $A = 1$ and (*b*) $A = 2$ for different initial damage: $D(0) = 1.0$ (plus) and $D(0) = 1/N$ (crosses). The insets show the average distance associated with the transverse components.

to identify both transitions which, in this case, correspond to defect unbinding transitions and it also predicts a finite-temperature transition in the Heisenberg limit.

Our results for the Kagome lattice are shown in figure 3. In this case there are only two phases: a low-temperature phase $T < T_c$ where the value of $\langle D \rangle$ is dependent on the initial value of D and a high-temperature phase $T > T_c$ where $\langle D \rangle$ is independent of the initial damage. The transverse distance D_{xy} does not indicate any transition at all. The value of T_c depends on the value of the anisotropy A and approaches zero in both the $A \rightarrow 1$ and $A \rightarrow \infty$ limits. In figure 4, we show the phase diagrams obtained using this damage spreading approach for both lattices. Both phase diagrams are in remarkably good agreement with those obtained from equilibrium studies [14, 15, 17, 19] within errorbars.

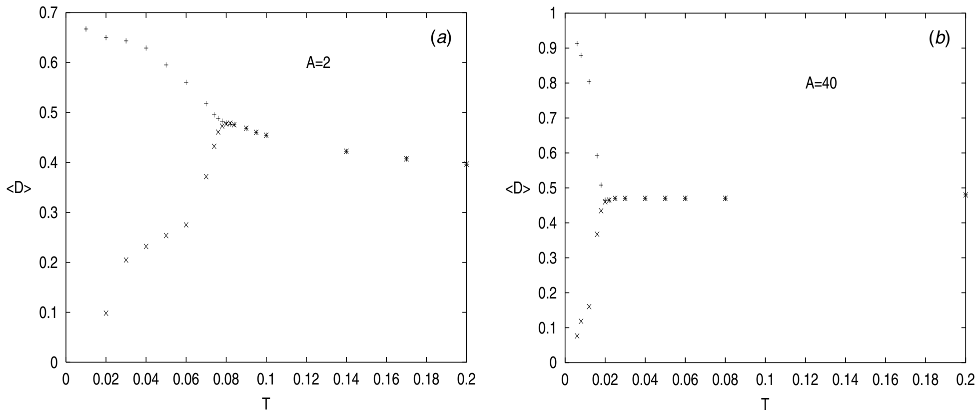

Figure 3. Averaged distance $\langle D \rangle$ versus temperature for the kagome lattice with $L = 24$ and two different values of the anisotropy (*a*) $A = 2$ and (*b*) $A = 40$ for the initial damage $D(0) = 1.0$ (plus) and $D(0) = 1/N$ (crosses).

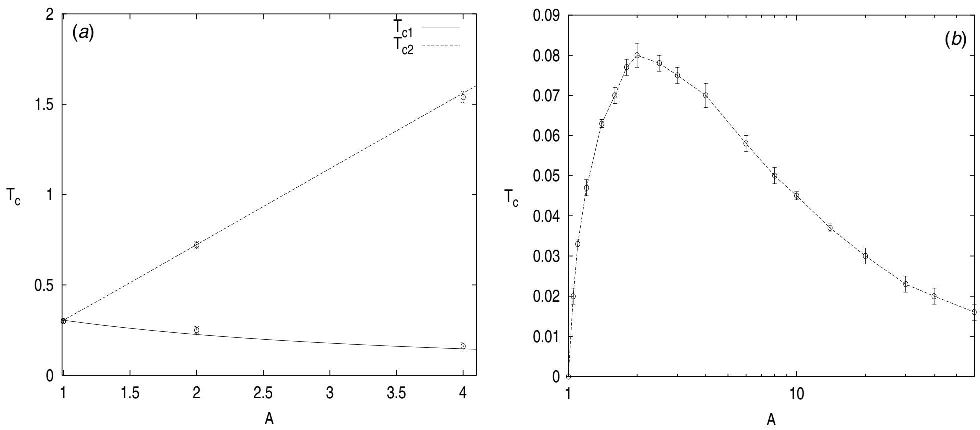

Figure 4. Phase diagrams obtained from the damage spreading method for (*a*) the triangular and (*b*) the kagome lattices, respectively. The two lines in (*a*) correspond to the equations $T_{c1} = T_c \frac{4(2A+1)}{3(1+A)^2}$ and $T_{c2} = T_c \frac{4A^2(A+2)}{3(1+A)^2}$ with $T_c = (0.305 \pm 0.005)$ [15].

3. Conclusion

In summary, we have shown that the technique of damage spreading can be applied successfully to models where analytical solutions are lacking and where the low-temperature phase displays novel behaviour associated with geometrical frustration. We can clearly identify the damage transitions with those obtained previously using conventional Monte Carlo simulations. Both defect-mediated and glass-like transitions are detected by the method. Further work is needed to extract more detailed information about the critical properties using this approach.

Acknowledgments

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