Monte Carlo study of the local-field distribution in the dilute antiferromagnetic Ising model on the triangular lattice

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Monte Carlo studies of spin glasses universally exhibit a "zero-field hole" in the distribution of local fields, $P(h)$. There is some dispute in the literature as to whether the dilute antiferromagnetic Ising model on the triangular lattice has a spin-glass phase; in this paper we present Monte Carlo results for $P(h)$ which further support the hypothesis that indeed this system does exhibit a spin-glass phase.

I. INTRODUCTION

It is widely accepted that frustration and disorder are the two essential ingredients for a system to be a spin glass (SG). In the canonical Ruderman-Kittel-Kasuya-Yosida (RKKY) -type spin glass,[1] frustration and disorder are introduced through the rapid spatial variation of the long-range exchange forces. Over a period of years, attention has been focused on the question of whether insulators, in which the exchange interactions are short ranged, can also be spin glasses.[2–9] Experimentally, spinels[9,10] are known to exhibit spin-glass behavior, and several other insulating alloys with dominant antiferromagnetic (AF) nearest-neighbor interactions have been studied.[11–14]

If the interactions are strictly nearest neighbor, then frustration can be introduced through the geometry of the lattice as in the (close-packed) triangular ($d=2$) and fcc ($d=3$) lattices. Disorder is introduced through random quenched impurities, which, in the model considered here, are taken to be fixed vacancies.

Monte Carlo calculations[15] of the standard Edwards-Anderson[1] order parameter q_0 for the triangular lattice indicated a spin-glass phase for concentrations of spins, x, in the range

$$0.5 \le x < 1 \tag{1}$$

and for temperatures $T/J \lesssim 0.9$ (with units in which $k_B=1$). One of the difficulties in evaluating q_0 by Monte Carlo methods is that one must extend the calculation to very long times,

$$q_0 = \lim_{t\to\infty} q(t) \; . \tag{2}$$

The characteristic time τ for the decay of $q(t)$ is expected to be given by[16]

$$\tau \sim \exp[A/(T-T_{SG})^c] \; , \tag{3}$$

where A and c are of order unity and T_{SG} is the spin-glass freezing temperature. Anderico *et al.*[16] find a value for T_{SG} consistent with zero; i.e., no spin-glass transition at a finite temperature. In addition, Blackman *et al.*[17] argue that for a small amount of dilution the ground state exhibits sufficient entropy so that long-range order is not possible. Direct calculation of the entropy by the transfer-matrix method[16] as a function of concentration, however, does show a very slight minimum in the neighborhood of $x=0.9$ at $T/J=0.3$.

II. MONTE CARLO RESULTS

The technical difficulties involved in calculating the SG order parameter q_0 can be circumvented if one is willing to accept the existence of a zero-field hole in $P(h)$, the distribution of local magnetic fields h, as a signal for the existence of a spin glass. Of course, systems which exhibit ordinary ferromagnetic or antiferromagnetic order will also exhibit such a zero-field hole,[18] but in the model under consideration here such long-range order is not possible. Previous numerical studies have universally observed such a local minimum in $P(h)$ at $h=0$.[19–23] In addition, an exact calculation of $P(h)$ for the perfect antiferromagnetic Ising model on the triangular lattice by Choy and Sherrington[24] indicates the $P(h)$ exhibits only a weak maximum at $h=0$.

Using standard Monte Carlo methods we have calculated $P(h)$ for a triangular lattice over a range of temperatures and concentrations. The results presented were calculated for lattices of size 50×50 with periodic boundary conditions. Equilibrium was established by running 1500 MCS/spin (Monte Carlo steps per spin), and thermal averages were then taken over the following 1000 MCS/spin. In addition, to check for finite-size effects, $P(h)$ was calculated for perfect lattices ($x=1.0$) of size up to 100×100 (Fig. 1) at low temperature. The absence of any strong variation in $P(h)$ with lattice size, and the excellent agreement of the Monte Carlo results with the exact results for $P(h)$ at $T=0$ (Ref. 24) lend confidence to our Monte Carlo results. Monte Carlo results for $P(h)$ for the perfect lattice ($x=1$) at $T/J=1.0$ and $T/J=0.25$ are shown in Fig. 2. In addition, in order to verify spin-glass behavior we have calculated the order parameter Ψ described by Binder.[20] This order parameter, which is given by

$$\Psi = \lim_{t\to\infty} \left| \frac{1}{N} \sum_i \phi_i S_i(t) \right| , \tag{4}$$

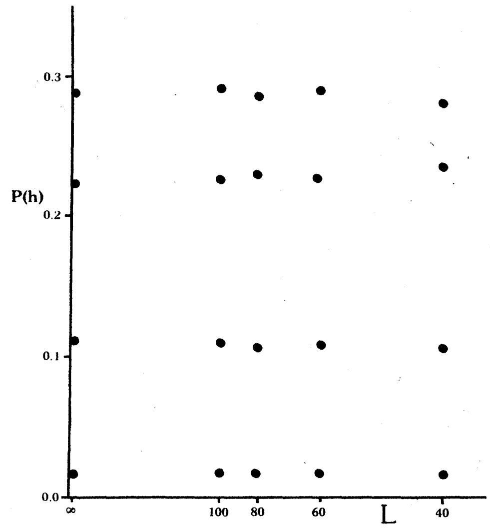

FIG. 1. $P(h)$ for $x=1.0$ and $T/J=0.25$ for lattices of increasing size. The points at $L=\infty$ are the exact results of Choy and Sherrington for $T=0$ (Ref. 24).

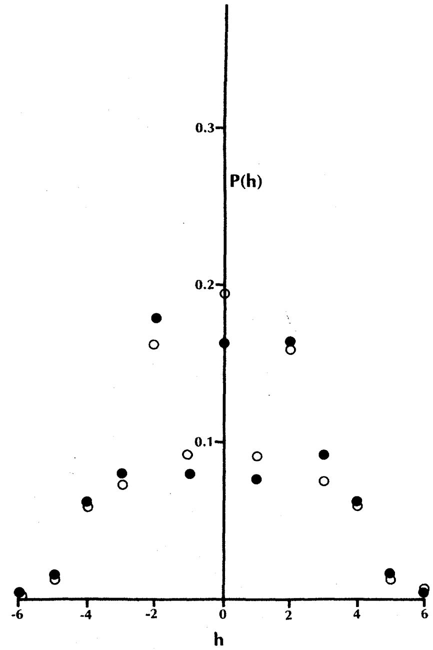

FIG. 3. $P(h)$ for $x=0.9$ at $T/J=1.0$ (○) and $T/J=0.25$ (●).

where ϕ_i is a particular ground-state configuration of the system, is identical to the usual Edwards-Anderson[1] order parameter in the limit of low temperatures.

The Monte Carlo results for $P(h)$ for diluted lattices ($x=0.9$ and 0.75) are shown in Figs. 3 and 4, respectively, for the same two temperatures as in Fig. 2. The most prominent feature of Figs. 3 and 4 is the local minimum of $P(h)$ at $h=0$. This "zero-field hole," which becomes more prominent as the concentration x decreases, indicates the presence of a spin-glass state. Further evidence is provided by the behavior of the Binder order parameter

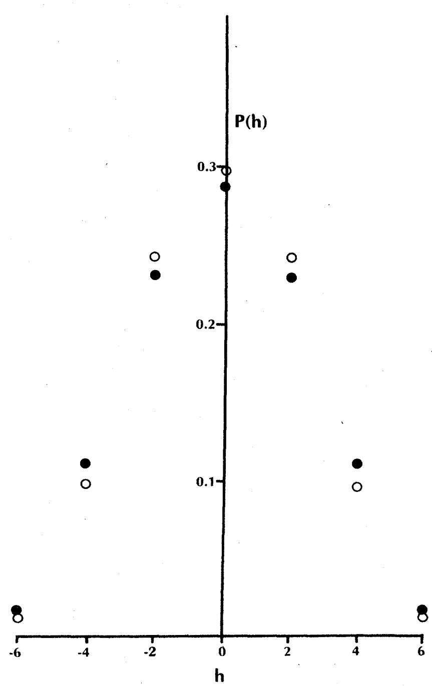

FIG. 2. $P(h)$ for $x=1.0$ at $T/J=1.0$ (○) and $T/J=0.25$ (●).

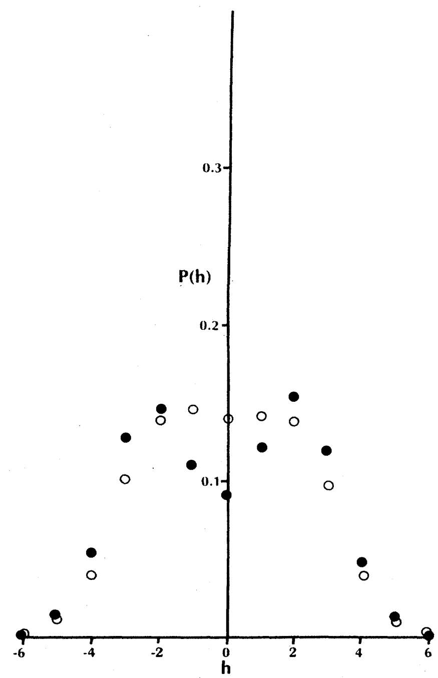

FIG. 4. $P(h)$ for $x=0.75$ at $T/J=1.0$ (○) and $T/J=0.25$ (●).

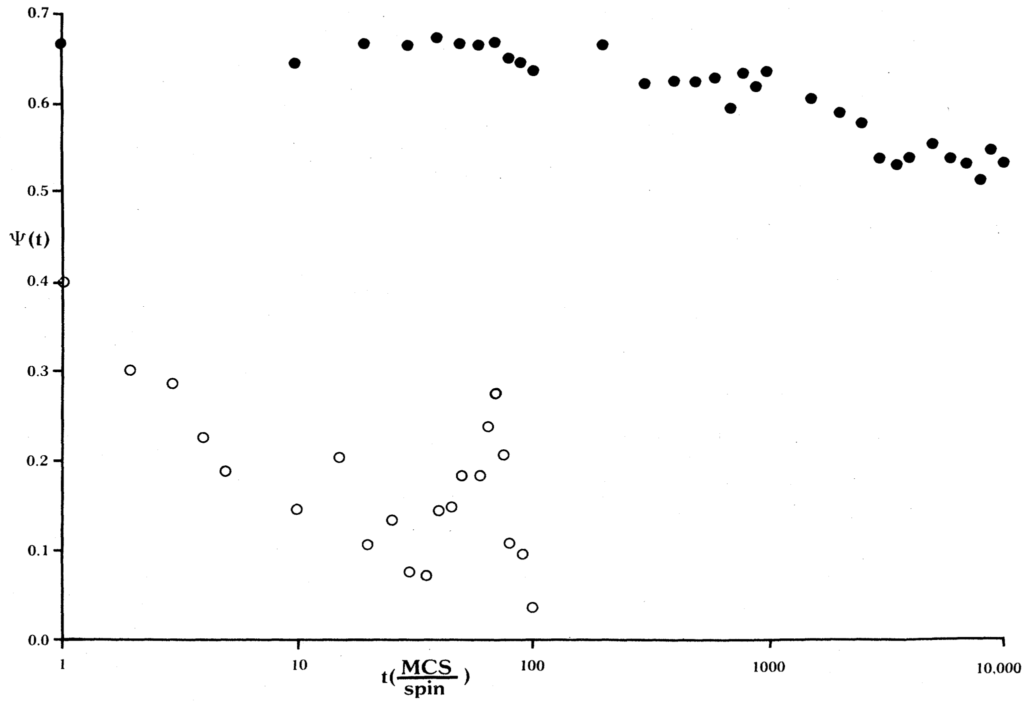

FIG. 5. $\psi(t)$ for $x=1.0$ (○) and $x=0.9$ (●) for $T/J=0.25$.

ψ which is shown in Fig. 5 for $T/J=0.25$ and $x=1.0$ and 0.9. We see from the figure that for $x=0.9$, ψ remains quite large for very long times, namely 10^4 MCS/spin, as would be expected for a spin glass.

In contrast, for $x=1.0$ the system is known to be paramagnetic for all temperatures. As shown in Fig. 5, $\psi(t)$ exhibits large fluctuations that nevertheless decrease rapidly to zero at low temperatures.

III. DISCUSSION

It is clear from the results for $P(h)$ at $x=0.9$ that for small dilution $P(h)$ will vary continuously with the concentration and therefore cannot be a sensitive indicator of the spin-glass phase. However, at lower concentrations the change in $P(h)$ with temperature is more pronounced as shown in Fig. 4 for $x=0.75$. It is also interesting to note that at this concentration the disparity between even and odd local fields is gone.

We cannot, however, rule out the possibility that this behavior is due to the system being trapped for long periods of time in metastable states. Recent work by Bhatt and Young[25] suggests the lower critical dimension for spin-glass behavior is $d_c=3$, although the results of Ogielski and Morgenstern[26] on larger lattices are consistent with $d_c<3$.

IV. CONCLUSION

Our Monte Carlo results have shown that the dilute antiferromagnetic Ising model on the triangular lattice does indeed exhibit the characteristic zero-field hole in the spin-glass regime of Grest and Gabl.[15] However, because only nearest-neighbor interactions are considered in this model, the local field assumes integer values in the range $-6\leq h\leq 6$, and a large number of sites do experience zero local field. Since spins at these sites are free to flip, the maximum value of the spin-glass order parameter is necessarily less than unity.

Although our results strongly favor the conclusion that indeed a spin-glass phase exists, the exact nature of the critical behavior (if any) remains to be established. This issue and the effect of isolated clusters of spins are currently under study.

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