Magnetic ordering in the three-dimensional site frustrated Heisenberg model

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We study transverse spin freezing in the site frustrated three-dimensional classical Heisenberg model using Monte Carlo simulations. For small values of the site randomness, there is no transverse spin freezing in the ferromagnetic state. As the fraction of the antiferromagnetic sites is increased beyond 16%, we observed that the transverse component of the spins freeze in random directions at temperatures below some value T_{xy}. Similar behavior is observed in the antiferromagnetic state. We compare results of this model to those of the bond frustrated model. Finally an approximate phase diagram of this model is presented.

I. INTRODUCTION

Recent experimental studies[1–3] of partially frustrated magnetic systems have demonstrated the existence of a transverse spin freezing phenomenon below the ferromagnetic transition. Such a freezing is characterized by the sudden increase of the local spin length, as measured by Mössbauer spectroscopy, when the temperature is lowered below some value T_{xy}. This behavior is found for a range of frustrations in systems such as a-Fe_xZr_{1-x} and $Au_{1-x}Fe_x$.[1] In a recent paper,[4] we examined theoretically the spin freezing phenomenon and the critical behavior of a bond frustrated three-dimensional Heisenberg model. Our Monte Carlo calculations gave results in qualitative agreement with the experimental findings. In particular, we found that at a low temperature T_{xy} below the Curie temperature T_c, the transverse spin component freezes out, leading to an increase in the total spin length.[4]

The bond-frustrated model seems to describe the transverse spin freezing in systems such as a-Fe_xZr_{1-x}, where there is only one magnetic compound, and the magnetic interaction are determined from nearest-neighbor distances. However, there are other magnetic systems for which this model is not appropriate. An example is $Eu_{1-x}Gd_xS$ in which the spin glass phase is induced by site frustration.[5] Theoretically, site randomness can be introduced by replacing a fraction f of ferromagnetic sites by antiferromagnetic sites. If f is small then no frustration is expected. However, at larger values of f when the antiferromagnetic sites start to form a percolating network, the randomness will lead to frustration and change the magnetic behavior of the system. Thus, we expect that site frustration will give rise to a somewhat different phase diagram compared with the bond frustration model, especially for transverse spin freezing which crucially depends on the degree of frustration. It is the purpose of this work to investigate the behavior of the site frustrated Heisenberg model using Monte Carlo simulations.

II. MODEL

We consider a system of classical Heisenberg spins $\mathbf{S}_i$ on a simple cubic lattice in zero magnetic field. The Hamiltonian is given by $H=-\Sigma_{n.n.}J_{ij}\mathbf{S}_i\mathbf{S}_j$. Here, J_{ij} is the exchange interaction between nearest-neighbor spins on lattice sites i and j, respectively. We introduce site randomness into the system by replacing a fraction f of ferromagnetic sites by antiferromagnetic sites. The values for the Curie temperature of the ferromagnetic Heisenberg model ($f=0$) and the Néel temperature of the antiferromagnetic Heisenberg model ($f=1$) are identical, $T_H=1.44J$.

The model with site frustration was investigated using the standard Metropolis Monte Carlo method. A three-dimensional system of 8^3 spins on a simple cubic lattice was initiated with high-temperature configurations.[6] The system was then annealed via 25 temperature intervals to a low temperature of $0.0005T_H$. At each temperature, statistical averages of relevant physical quantities were taken. A calculation of the relaxation time for temperatures away from T_H revealed that about 2000 Monte Carlo steps per spin (MCSs) were needed to reach equilibrium at such temperatures, and a larger number of MCSs were needed close to T_H where critical slowing down becomes important. After the system reached equilibrium, statistical averages of physical quantities were collected over 4000 MCSs. We found that fluctuations in the energy were indeed Gaussian distributed for 4000 MCSs thus our choice of the number of steps was reasonable. Finally, results for ten different realizations of the site randomness for a given f were averaged. The values of f used in the simulations ranged from 0 to 1 and we were thus able to calculate the entire magnetic phase diagram for the system.

We compute a time average of the spin components and of the square of the transverse spin components at each site, i.e.,

$$\mathbf{m}_i=\frac{1}{\tau}\sum_{\tau'=1}^{\tau}\mathbf{S}_i(\tau')$$

and

$$m_{\perp i}^2=\frac{1}{\tau}\sum_{\tau'=1}^{\tau}[S_{ix}(\tau')^2+S_{iy}(\tau')^2]$$

where, as mentioned above, $\tau=4000$ MC steps. From these local quantities we calculate the following spatially averaged quantities: (1) the root-mean-square spin length $S_{\rm rms}=1/N\Sigma_{i=1}^{N}(\mathbf{m}_i\cdot\mathbf{m}_i)^{1/2}$, (2) the bulk magnetization $M_f=1/N|\Sigma_{i=1}^{N}\mathbf{m}_i|$, (3) the staggered magnetization

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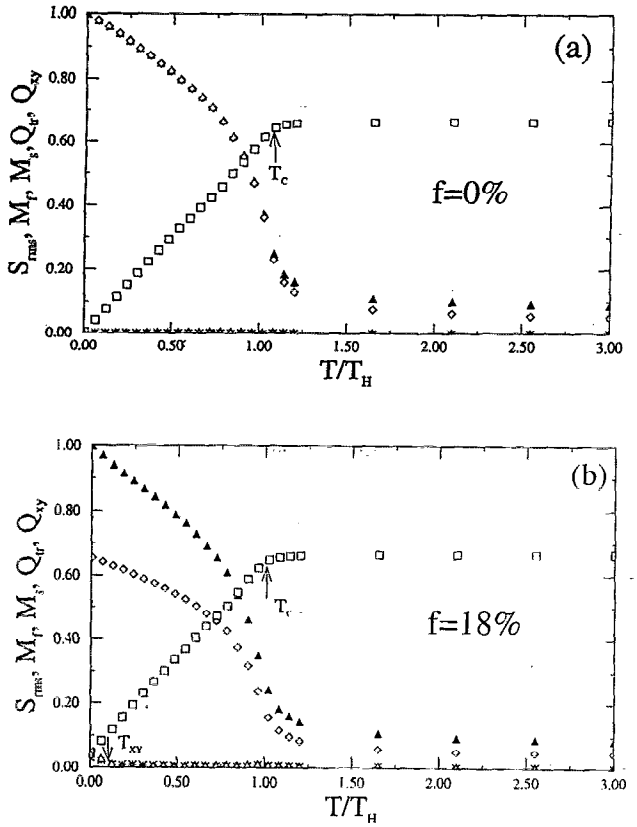

FIG. 1. Temperature dependence of the different spin averages. (▲) $S_{\rm rms}$, (◇) M_f, (*) M_s, (□) $Q_\perp$, and (△) Q_{xy}. T_c is the temperature where $Q_\perp$ starts to decrease from 2/3. (a) $f=0$; (b) $f=18\%$. T_{xy} in (b) is the temperature where Q_{xy} becomes nonzero.

$M_s=1/N|\Sigma_{i=1}^N \mathscr{S}\mathbf{m}_i|$, where $\mathscr{S}$ is a matrix with the symmetry of the antiferromagnetic structure of the lattice, (4) the mean square of the spin projection on the x-y plane $Q_\perp=1/N\Sigma_{i=1}^N m_{\perp i}^2$; (5) the x-y projection of the time-averaged spin components $Q_{xy}=1/N\Sigma_{i=1}^N(m_{ix}^2+m_{iy}^2)$. The last two quantities take into account ordering in the x-y plane and may therefore exhibit the onset of anisotropy and spin freezing in the system.

III. RESULTS

Figures 1(a) and 1(b) show data for quantities M_f, $S_{\rm rms}$, M_s, $Q_\perp$, and Q_{xy} as functions of temperature, for several values of site frustration f. In Fig. 1(a) the pure ferromagnetic case ($f=0$) is shown. This shows, as expected, that the order parameter M_f and the local spin length $S_{\rm rms}$ are identical below the critical temperature T_c (which is equal to T_H in this case), as the system orders to a collinear configuration. Above T_c, $Q_\perp$ takes the value 2/3 since the spins are randomly rotating in three dimensions thus spending 2/3 of the time in the transverse plane where $Q_\perp$ is computed. Below T_c, $Q_\perp$ decreases to zero at $T=0$ as expected for $f=0$. Naturally the quantity Q_{xy} is zero for all T when $f=0$ since there is no spin freezing.

Up to $f\approx 0.16$, the behavior is similar to the $f=0$ case. As we further increase the site randomness f, interesting features start to show. Figure 1(b) are the data for $f=0.18$. Here, we can see that Q_{xy} becomes nonzero at a low temperature T_{xy}. Since Q_{xy} measures the time-averaged length of the spin components in the transverse plane, a nonzero value of Q_{xy} signals the freezing out of that component. In this situation $Q_\perp$, the mean square of the spin projection on the x-y plane, remains nonzero as T approaches 0. For a simple cubic lattice there are six neighboring spins per site, thus we expect that, on average, all the spins will be affected when the site randomness reaches 16%–17%. Indeed, spin freezing is observed around this value of frustration. This is very different from the behavior of the bond-frustrated system. There, any finite f gives rise to the transverse freezing.[4] In the bond frustrated system, frustration is induced by just replacing one ferromagnetic bond by an antiferromagnetic bond. In the site frustrated model, however, the replacement of a single ferromagnetic site by an antiferromagnetic site only decreases the bulk magnetization and has no other effect. Frustration for the site frustrated model can only occur when there are at least two neighboring antiferromagnetic sites. This occurs on average at a value given by $f=q^{-1}$ where q is the coordination number of the lattice. For our case, $q=6$ at $f=0.167$. Finally we notice the different values of M_f and $S_{\rm rms}$ below T_c: part of the difference is now contributed by the transverse spin freezing as $S_{\rm rms}$ is the vector sum of the z as well as the transverse components of the spins. For higher values of f, all features are similar to those of Fig. 1(b). Due to more frustration in the system with higher f, it is easier to freeze out the transverse spin components, thus T_{xy} has increased to higher values.

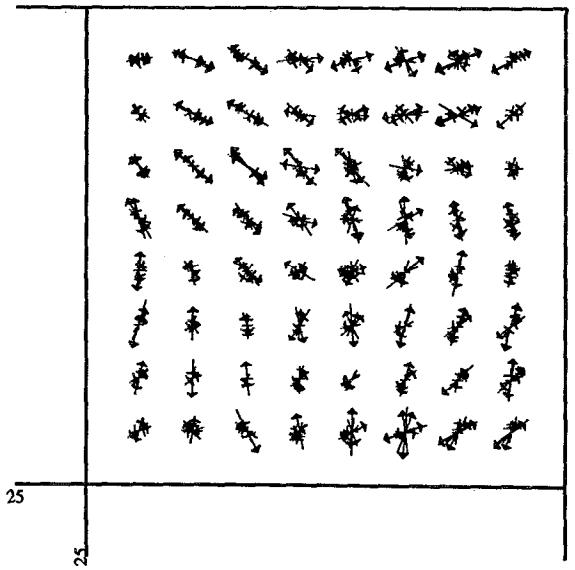

FIG. 2. Time averaged spin configuration for $f=36\%$ and $T=0.12T_H$ of a 8^3 system projected onto the x-y plane. Each point therefore is a stack containing eight spins.

An interesting result is the behavior of the staggered magnetization as f is increased from zero. We found that M_{st} starts to have nonzero values at the same temperature as T_{xy}. This seems to indicate that in the x-y plane the spin components freezes antiferromagnetically. To see this, we plot a typical configuration of the spin components in the x-y plane in Fig. 2 for $f=0.36$ at $T=0.12T_H$. Indeed, we see that the

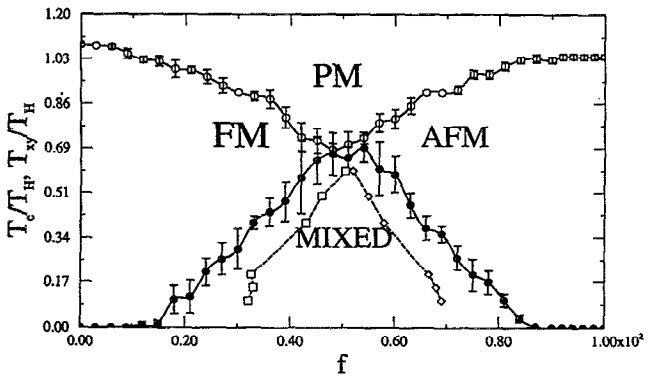

FIG. 3. An approximate phase diagram of the model. Open circles are temperatures T_c. Solid circles are temperatures T_{xy}. The dashed line with open boxes and diamonds roughly separates the mixed phase from the FM and AFM regions. The line is determined from the peak position in the susceptibility as we sweep f at fixed temperature. The error bars are determined as standard deviation from ten realizations of site randomness for each value of f.

transverse components try to order antiferromagnetically.

In Fig. 3 we present an estimate of the phase diagram for this model. The phase transition lines from the paramagnetic state (PM) to the ferromagnetic (FM) and antiferromagnetic (AFM) states were determined by calculating the susceptibility of the system. We took the peak position of the susceptibility as the transition point.[7] The T_{xy} line was determined as the temperature where $Q_\perp$ just became nonzero. We note that there is no phase transition across the line of T_{xy} and it represents the short-range behavior of the transverse spin freezing. The onset of the freezing occurs at frustration $f\sim16\%$ in the ferromagnetic state, and $f\sim84\%$ in the antiferromagnetic state. At these values of f, the phase transition temperature T_c starts to decrease. In the region between $f=45\%$ and $f=55\%$, T_c and T_{xy} merge together.

Apart from the usual states, at the middle region of the phase diagram there is a state we termed "mixed phase." We found that in the mixed phase $Q_\perp$ remains nonzero down to zero temperature and, in fact, it has rather substantial values at low temperatures. For instance with $f=51\%$, $Q_\perp\approx0.45$ at $T=0$. We have checked from the spin configurations that this large value of $Q_\perp$ was due to the fact that many spins lie almost completely in the transverse plane in the mixed phase, and that they actually form antiferromagnetic configurations (Fig. 2). Thus this part of the phase diagram is characterized by ferromagnetic domains pointing in the z direction mixed with antiferromagnetic domains pointing in the transverse plane. We have performed simulations to compute the susceptibility at fixed temperatures by sweeping f. A peak occurred in the susceptibility at the broken line in the phase diagram which separates the FM and AFM from the mixed phase. Unfortunately, we were not able to determine the nature of the region near this line as extremely large simulations are needed to determine whether there is a true phase transition from the FM or AFM states to the mixed phase as f or T is varied. We hope to report such a study in the future.

IV. CONCLUSIONS

Our Monte Carlo simulations on the site frustrated Heisenberg model give qualitatively similar results to those of the bond frustrated model. In particular the transverse spin freezing phenomena are observed which lead to an increase of the local spin length. However, the frustration does not set in until the site randomness reaches ~16%. Thus, the transverse spin freezing temperature T_{xy} remains zero until f reaches that value. We have observed a mixed phase for large values of the site randomness at low temperatures. Such a disordered phase is characterized by the configurations of mixed ferromagnetic and antiferromagnetic domains. Finally we have estimated the phase diagram of this model and it is in qualitative agreement with experimental findings.[5]

ACKNOWLEDGMENTS

This work was supported by the Natural Sciences and Engineering Research Council of Canada and le Fonds pour la Formation de Chercheurs et l'Aide à la Recherche de la Province du Québec.

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[6] To check finite size effects some simulations were performed using 20^3 spins and qualitatively the same results were obtained.
[7] To accurately determine the transition points a proper finite size scaling analysis should be performed, as was done in Ref. 4. However, here we are only interested in the general phase behavior, thus we simply took the peak position of the susceptibility as the transition temperature.