Ordering in the Site Frustrated Heisenberg Ferromagnet Revisited

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Monte Carlo simulations of frustrated and non-frustrated versions of the three dimensional site disordered Heisenberg model have been used to determine the sequence and nature of the magnetic ordering. At sufficiently high concentrations, x, of antiferromagnetic sites for an infinite percolating network to form ($0.31 < x < 0.69$), two ordering events occur: ferromagnetic and antiferromagnetic order co-exist. Coupling the two networks introduces frustration but does not destroy either transition. However, it appears to change the universality class of the antiferromagnetic transition.

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I. INTRODUCTION

A Monte Carlo study of the site frustrated Heisenberg ferromagnet by Neilsen *et al.* [1] yielded behaviour qualitatively similar to that of real materials [2–5]. They observed two ordering events for $0.15 < x < 0.85$, (where x is the concentration of randomly placed antiferromagnetic sites) corresponding to first ferromagnetic (FM) ordering at T_c for $x < 0.5$ (antiferromagnetic $x > 0.5$) followed at a lower temperature (T_{xy}) by antiferromagnetic (AF) ordering for $x < 0.5$ (ferromagnetic $x > 0.5$) perpendicular to the order established at T_c. Only T_c was identified as a true second order thermodynamic phase transition, while T_{xy} was described as likely only a change in short range order and not a phase transition. It was noted however, that a proper finite size scaling analysis would be necessary to determine the actual transition temperatures, and to confirm the nature of the behaviour at T_{xy}.

The inevitability of two co-existing ordered states (FM and AF), can be understood by considering the frustration introduced in the site frustrated Heisenberg ferromagnet as a perturbation of a related non-frustrated model. Sites on a lattice are labeled as either ferro- (F) or antiferro- (A) magnetic. These are then coupled via nearest neighbor exchange interactions (J), with $J_{F-F} = +1$, $J_{A-A} = -1$ and $J_{F-A} = 0$ so that the ferromagnetic sites are completely decoupled from the antiferromagnetic sites. The problem reduces to one of percolation, familiar from the study of dilute magnetism [6], and finite temperature ordering occurs above a critical concentration x_c where the infinite connected cluster emerges. For the simple cubic lattice in three dimensions [7] $x_c \sim 0.31$, and since x_c is less than 0.5 two distinct infinite clusters can co-exist and order independently within the same lattice. There will be two independent second order phase transitions in the concentration regime $0.31 < x < 0.69$ with critical exponents characteristic of the pure system since the exponent α which governs the singular portion of the free energy is negative [8]. Our calculated phase diagram for this model is shown in Fig. 1.

With this simple, non-frustrated model as a starting point, the question of the magnetic ordering in the site frustrated model with $J_{F-A} \neq 0$ can be reduced to the following: does frustration destroy the ordering observed in the non-frustrated case of $J_{F-A} = 0$? Furthermore, if as we show below, the ordering is not destroyed by the frustration, what are the values of the critical exponents, critical temperatures and critical concentrations?

Here we use finite size scaling of three relevant thermodynamic variables to show that both T_c and T_{xy} remain second order phase transitions. Our analysis also demonstrates that the high temperature transition (ferromagnetic for $x < 0.5$), remains in the Heisenberg universality class while the lower temperature transition (transverse antiferromagnetic ordering for $x < 0.5$), belongs to a different universality class when $J_{F-A} \neq 0$.

II. MONTE CARLO METHODS AND CONSIDERATIONS

We have simulated the classical site frustrated Heisenberg model introduced by Neilsen *et al.* [1] using single spin update Metropolis dynamics. Unit 3D vector spins are located on a simple cubic lattice with nearest neighbor interactions, J_{ij}, chosen as described in the introduction. Each Monte Carlo step (MCS) is one attempted update per spin such that one MCS corresponds to $N = L^3$ attempted spin updates where L is the linear size of the lattice comprising N spins. For the results presented here we have chosen an antiferromagnetic site concentration of $x = 0.40$ using lattice sizes $L = 8, 10, 12, 14, 16, 18$ averaged over $128, 96, 64, 32, 16, 16$ realizations of disorder respectively.

The primary quantities of interest are the magnetisation (M_f) and staggered magnetisation (M_{st}), the instantaneous values of which are given at time t by:

$$M_f(t) = N^{-1}\sqrt{(\sum_i S_i^x)^2 + (\sum_i S_i^y)^2 + (\sum_i S_i^z)^2} \quad (1)$$

$$M_{st}(t) = N^{-1}\sqrt{(\sum_i L_i S_i^x)^2 + (\sum_i L_i S_i^y)^2 + (\sum_i L_i S_i^z)^2} \quad (2)$$

where x, y, z denote Cartesian components and L_i is an operator with the symmetry of the antiferromagnetic state. Average values are obtained by averaging first over time $< >$ and then over disorder [ ] to yield $[< M_f >]$ and $[< M_{st} >]$. The ferromagnetic and staggered susceptibilities are given by:

$$\chi_{f,st} = N\beta[< M_{f,st}^2 > - < M_{f,st} >^2], \quad (3)$$

where $\beta = 1/k_B T$, T is the temperature and $k_B = 1$.

We have used the autocorrelation functions:

$$A_{M_{f,st}}(t) = [< M_{f,st}(0) M_{f,st}(t) > - < M_{f,st}(0) >< M_{f,st}(t) >] \quad (4)$$

to check that equilibrium has indeed been obtained, by requiring that the autocorrelation functions should not depend on the absolute origin of time [9]. We begin each simulation from the high temperature paramagnetic phase at $T = 5T_h$ [10] and cool in small temperature steps $0.5T_h \geq \Delta T \geq 0.025T_h$ depending on the temperature regime of interest. At each temperature we first discard between a tens to thousands of correlation times of the slowest mode obtained from the autocorrelation functions prior to calculating the averages used in our analysis.

III. RESULTS AND DISCUSSION

Autocorrelation functions generated from stochastic discrete time Metropolis dynamics can be written in general as a sum of exponentials [11]: $A(t) = \sum_i a_i e^{-\frac{t}{\tau_i}}$. The correlation time τ of either M_f or M_{st} is the slowest τ_i in the corresponding $A_M(t)$ and is related to the appropriate correlation length ξ by a dynamical exponent z such that [12] $\tau \sim \xi^z$. The correlation times show the critical slowing down associated with second order phase transitions because the correlation length diverges as $\xi \sim (T - T_c)^{-\nu}$ near a second order phase transition.

To extract the transition temperatures and critical exponents we make finite size scaling plots of $M_{f,st}$, $\chi_{f,st}$ and $\tau_{f,st}$. These quantities should scale in the critical region as

$$M = L^{-\beta/\nu} M(tL^{1/\nu}) \quad (5)$$

$$\chi = L^{\gamma/\nu} \chi(tL^{1/\nu}) \quad (6)$$

$$\tau = L^z \tau(tL^{1/\nu}) \quad (7)$$

where the reduced temperature $t = (T - T_c)/T_c$. In our scaling plots we have use the currently accepted values of the static critical exponents of the Heisenberg model [13]: $\beta = 0.364$, $\gamma = 1.387$ and $\nu = 0.705$. The dynamical exponent used is $z = 1.98$ as found by Brown *et al.* [14] for the pure Heisenberg model ($x = 0$). The scaling around the ferromagnetic transition at $x = 0.4$ for the frustrated (Fig. 2) and unfrustrated cases yields an excellent collapse, implying that T_c remains in the Heisenberg universality class despite the presence of frustration. We have found that this is also true for the antiferromagnetic transition in the unfrustrated model, as expected, for concentrations $x = 0.35, 0.40$ and 0.45 while no transition occurs for $x = 0.30$ as this is below the percolation threshold.

By contrast, scaling of the antiferromagnetic transition for the frustrated case with $x = 0.40$ demanded the use of different exponents (Fig. 3). The ratios β/ν and γ/ν, as well as the dynamic exponent z can be estimated by fitting $M_{st} \propto L^{-\beta/\nu}$, $\chi \propto L^{\gamma/\nu}$ and $\tau \propto L^z$ respectively, valid for $T = T_{xy}$. We have found $\frac{\beta}{\nu} \sim 0.35$ and $\frac{\gamma}{\nu} \sim 2.5$, in reasonable agreement with the hyperscaling relation $d = 2\frac{\beta}{\nu} + \frac{\gamma}{\nu}$ while $z \sim 3.5$. Using these values with $\nu = 0.7$ produces the best collapse. This analysis results in a critical temperature $T_{xy} = 0.34T_h$. These same exponents are found to produce good collapse of the data for the frustrated model at $x = 0.35$ and $x = 0.45$. No transition was observed at $x = 0.30$. While it is possible that the deviations from the Heisenberg exponents arise from either corrections to scaling which may be important for the small lattice sizes studied, or from the fits for to M_{st}, χ and τ being carried out too far from T_{xy}, the differences are large and consistent strongly suggesting that while transverse spin freezing remains a phase transition, frustration changes its universality class.

IV. ACKNOWLEDGEMENTS

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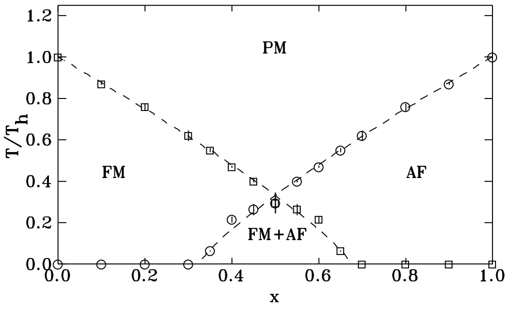

FIG. 1. Phase Diagram for the non-frustrated Site disordered model on a simple cubic lattice in three dimensions. Solid lines represent second order phase transitions between paramagnetic (PM), ferromagnetic (FM) and antiferromagnetic (AF) states respectively. Results obtained using system sizes $L = 6, 8, 10, 12, 14$ averaged over 16 configurations of disorder.

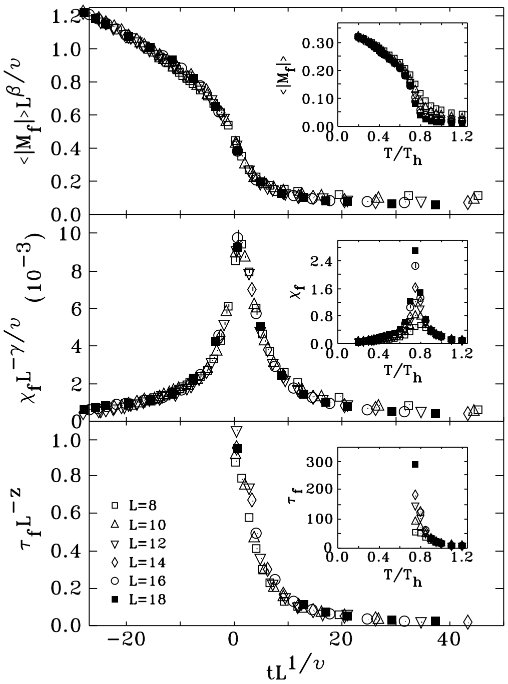

FIG. 2. Finite size scaling of the magnetisation (top), susceptibility (middle) and correlation time (bottom) for $x = 0.4$ in the frustrated case. The raw unscaled data is plotted in the insets. $T_c = 0.74T_h$. The exponents used are given in the text.

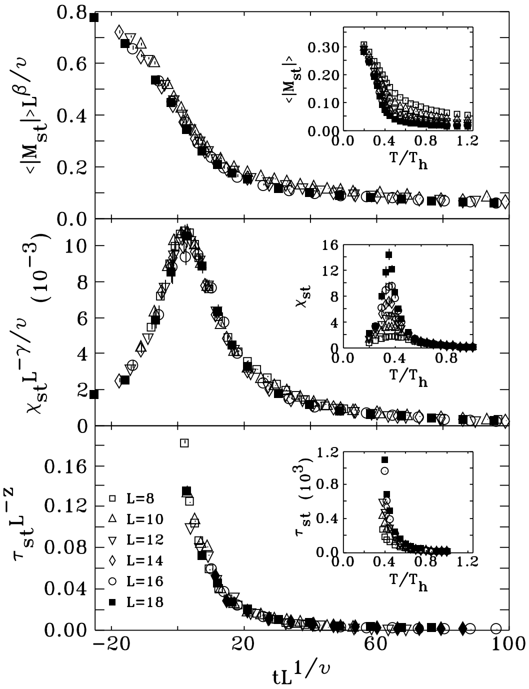

FIG. 3. Finite size scaling of the staggered magnetisation (top), susceptibility (middle) and correlation time (bottom) for $x = 0.4$ in the frustrated case. The raw unscaled data is plotted in the insets. $T_N = 0.34T_h$. The exponents used are given in the text.