Ferromagnetic phase boundary in the bond frustrated Heisenberg model

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We determine the ferromagnetic phase boundary for the short range $\pm J$ bond frustrated Heisenberg model in three dimensions using a very efficient Monte Carlo algorithm which eliminates the critical slowing down usually experienced at a second order phase transition. The phase boundary is identified by measuring the correlation length directly, a method which we show to be superior to more conventional methods such as the crossing of the Binder cumulant. The critical concentration of antiferromagnetic bonds beyond which ferromagnetism is lost is $x_c=0.208(2)$. © *2005 American Institute of Physics*. [DOI: 10.1063/1.1851916]

The addition of antiferromagnetic bonds with concentration x to an otherwise ferromagnetic matrix introduces exchange frustration which leads to the eventual loss of ferromagnetic order at a critical concentration x_c. The mean field phase diagram[1] for the bond frustrated Heisenberg model is typical of the effect of exchange frustration, as demonstrated by the similarity with experimental phase diagrams.[2] Despite this agreement, little is known regarding the phase diagram of the bond frustrated Heisenberg model in three dimensions. Only a few Monte Carlo studies have addressed the existence of the various phases, and disagreement exists even for the ferromagnetic phase boundary. While Thomson *et al.*[3] found $x_c=0.25$, finite size effects were not taken into account. Matsubara *et al.*[4] have claimed that the actual value is much smaller ($x_c=0.21$) based upon poor scaling of the magnetization using Heisenberg exponents at $x=0.22$. However, this criteria is not the best one can think of considering that corrections to scaling are probably quite important for the small lattice sizes studied, especially as x_c is approached. Here we measure the correlation length directly for various x using a hybrid Monte Carlo method, demonstrating that this quantity is very good for locating phase transitions, and we present the ferromagnetic phase boundary.

The short range $\pm J$ bond frustrated Heisenberg model is described by the Hamiltonian

$$\mathcal{H}=-\sum_{\langle i,j\rangle} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j=-\sum_i \mathbf{S}_i\cdot\mathbf{B}_i, \tag{1}$$

where the sum $\langle i,j\rangle$ runs over all nearest neighbor bonds $J_{ij}=\pm 1$ on a three-dimensional simple cubic lattice and $\mathbf{B}_i$ is an effective local field experienced at site i due to coupling with nearest neighbor, three dimensional, unit vector spins $\mathbf{S}_j$. The J_{ij} are chosen to be quenched random variables with probabilities $P(J_{ij}=+1)=1-x$ and $P(J_{ij}=-1)=x$. We measure several thermodynamic quantities with a Monte Carlo algorithm utilizing a mixture of Metropolis and over-relaxation[5] techniques, found elsewhere to produce a very efficient algorithm for frustrated Heisenberg models.[6] Following every Metropolis update (one hit per lattice site) we use five over-relaxation steps which evolve the spins according to

$$\mathbf{S}_i\rightarrow 2\frac{\mathbf{S}_i\cdot\mathbf{B}_i}{\mathbf{B}_i\cdot\mathbf{B}_i}\mathbf{B}_i-\mathbf{S}_i. \tag{2}$$

The efficiency of this algorithm is determined by measuring the time decay of a suitably normalized autocorrelation function of the magnetization M:

$$A_M(t)=[\langle M(t)M(0)\rangle]-[\langle M(0)\rangle][\langle M(0)\rangle], \tag{3}$$

where $\langle\ \rangle$ represents a thermal average and $[\ ]$ represents an average over disorder. The A_M decays are discrete sums of exponential decays, $\Sigma_i a_i e^{-t/\tau_i}$, and the largest τ_i is the asymptotic correlation time τ_A. The correlation times are shown for various lattice sizes L in Fig. 1. Using conventional Metropolis dynamics a critical slowing down is experienced as we approach T_C, with a power law size dependence of the form $\tau_i\sim L^z$. Considering the magnetization to be either a vector or scalar quantity, Metropolis dynamics at temperature T yields $z=0,2$ and 3 for $T>T_C, T\sim T_C$, and $T<T_C$, respectively. The hybrid algorithm by contrast yields $z\sim 0$ at all but the lowest temperatures and is thus very efficient for this particular model. Using this algorithm we have

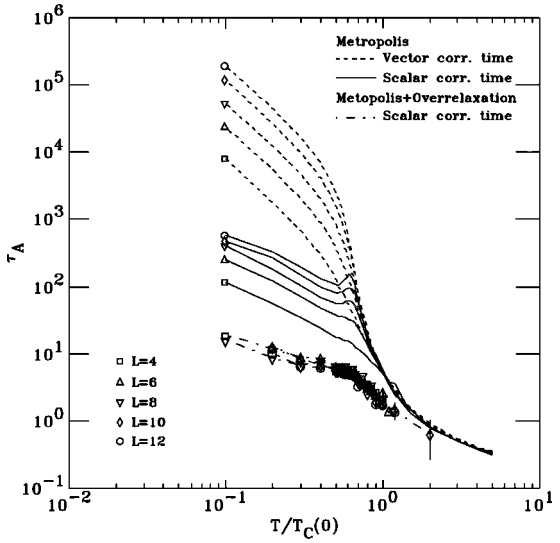

FIG. 1. Asymptotic correlation times vs temperature for various small system sizes using both the Metropolis algorithm and a hybrid algorithm as discussed in the text for the bond frustrated Heisenberg model at $x=0.15$.

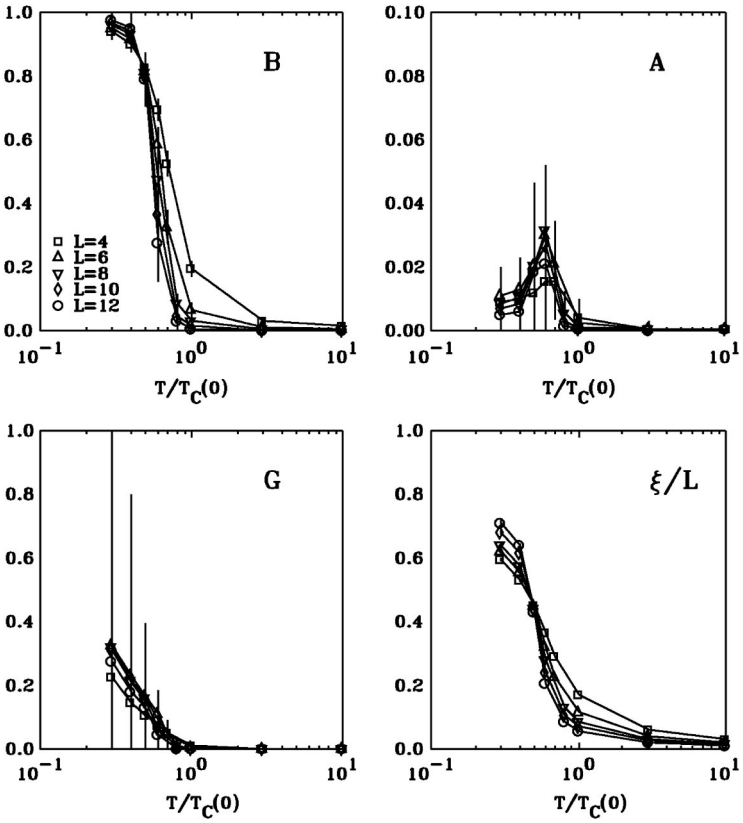

FIG. 2. Dimensionless ratios B, A, G, and ξ/L vs temperature at $x=0.18$.

simulated the model for lattice sizes $L=4$, 6, 8, 10, and 12 for several x and T using 500 independent [ ] samples and a minimum of 500 independent $\langle\ \rangle$ samples ($\sim 4\times 10^4$ Monte Carlo updates).

We determine several quantities used to study phase transitions in disordered models.[7] Those discussed here are the following:

$$B=\frac{1}{2}\left(5-3\frac{[\langle M^4\rangle]}{[\langle M^2\rangle]^2}\right), \tag{4}$$

$$A=\frac{[\langle M^2\rangle^2]-[\langle M^2\rangle]^2}{[\langle M^2\rangle]^2}, \tag{5}$$

$$G=\frac{[\langle M^2\rangle^2]-[\langle M^2\rangle]^2}{[\langle M^4\rangle]-[\langle M^2\rangle]^2}, \tag{6}$$

as well as the ratio ξ/L, where ξ is the correlation length to be defined below. The four quantities $X=B$, A, G, and ξ/L are dimensionless and so are expected to scale according to

$$X=\mathcal{X}(tL^{1/\nu}), \tag{7}$$

where ν is the exponent of the correlation length ξ and $t=(T-T_C)/T_C$ is the reduced temperature. Equation (7) implies that at T_C, $X=B$, A, G, and ξ/L take universal, L independent, values $X^\star$ such that a plot of $X(L)$ vs T exhibits a crossing at T_C for different L.

B is the commonly studied Binder cumulant,[8] normalized for the pure Heisenberg model. In the pure, disorder free, model ($x=0$) the uniqueness of the ground state is enough to ensure that B scales according to Eq. (7). However, for disordered models B may *not* cross even though a phase transition occurs due to a lack of a uniquely ordered ground state (replica symmetry breaking or RSB) which causes $B(T=0)$ to take nontrivial L dependent values, as found in Heisenberg spin glasses.[9,10] The parameter A is introduced to study the so-called lack of self averaging[11] whose cause, among other reasons, can be the occurrence of RSB. When self averaging is found A is zero in the thermodynamic limit. In the absence of self averaging A is finite in the thermodynamic limit and B may not exhibit a crossing. G, on the other hand, is sensitive to the pattern of RSB which occurs and may be finite even though A is zero.[7] A lack of self-averaging has been found in mean field models of spin glasses,[7] at T_C in dilute Ising models[11] and has been discussed in the case of the present model.[12] A detailed discussion here is, however, beyond the scope of the present work.

The parameters A, B, and G are shown in Fig. 2 at a concentration $x=0.18$. It is clear that although A, B, and G show hints of a crossing at finite T_C, the data is far too noisy to be conclusive. The large statistical noise in the data is due to the fact that (i) B is essentially a four-point correlation function and so is inherently noisy; (ii) A measures small sample to sample fluctuation which may very well be zero in the thermodynamic limit; and (iii) G is the ratio of two small quantities, which may be zero in the thermodynamic limit, but whose ratio is in all probability finite. That A, B, and G can be noisy has been reported in the context of spin glasses.[7]

A far less noisy quantity is the ratio ξ/L, which we calculate using the following definition:[9]

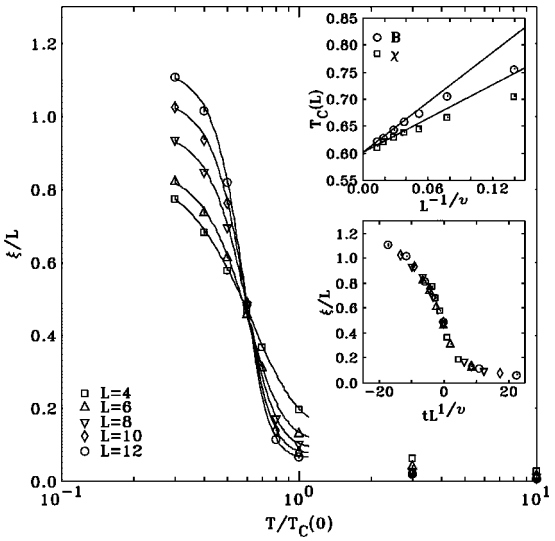

FIG. 3. The crossing of ξ/L for $x=0.15$ using very small system sizes. Inset (a) shows the transition temperature determined from the extrema of several thermodynamic quantities using larger systems, which is $T_C=0.601(3)$ in agreement with the crossing of ξ/L. Inset (b) shows the scaling collapse of ξ/L using the Heisenberg exponent $\nu=0.705$.

$$\xi = \frac{1}{2\sin(|\mathbf{k}_{\min}|/2)}\left(\frac{\chi(0)}{\chi(\mathbf{k}_{\min})}-1\right)^{1/2} \tag{8}$$

with $\chi(\mathbf{k})$ the wave vector dependent susceptibility, and $\mathbf{k}_{\min}$ the minimum wave vector allowed by the choice of boundary conditions which in our case is $\mathbf{k}_{\min}=(2\pi/L)(1,0,0)$. For a ferromagnet $\chi(\mathbf{k})$ is given by

$$\chi(\mathbf{k}) = \beta L^{-3}\sum_i \sum_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{S}_i\cdot\mathbf{S}_{i+\mathbf{r}} \tag{9}$$

and $\beta=1/k_BT$, with $k_B=1$. For a second order phase transition a plot of the ratio ξ/L *will* cross at T_C, independent of the complexity within the ordered state unlike the quantities A, B, and G which, as we have seen, depend upon details such as self averaging and the pattern of RSB. As observed in Fig. 2, the ratio ξ/L shows a very clear crossing at a well defined transition temperature $T_C(x=0.18)=0.495(2)$ in stark contrast to A, B, and G.

The transition temperature determined from the crossing of ξ/L might include significant finite size effects, and so we compare the crossing temperature for these small lattices with a different method which contain large, resolvable, finite size corrections. According to finite size scaling theory, the extrema of a thermodynamic quantity occurs at a pseudotransition temperature $T_C(L)$ which scales according to[13]

$$T_C(L) = T_C + aL^{-1/\nu} \tag{10}$$

neglecting scaling corrections, which can be avoided by using large enough L. In Fig. 3 we show the crossing of ξ/L for $L=4$, 6, 8, 10, and 12 along with the extrema of B and $\chi(0)$ used to obtain T_C with Eq. (10) for $L=4$, 6, 8, 10, 12, 16, and 20. For the scaling plot we use the Heisenberg exponent[13] $\nu=0.705$, which a collapse of the ξ/L data, also shown in Fig. 3, demonstrates to be valid. Excluding the data for $L<10$ a weighted average yields $T_C(x=0.15)=0.601(3)T_C(x=0)$, where we have taken $T_C(x=0)=1.443J/k_B$ (Ref. 13). The ξ/L data for even the very small lattice sizes shows an almost perfect crossing at $T_C(x=0.15)=0.608(5)T_C(x=0)$, showing that finite size effects in the ξ/L plot are negligible.

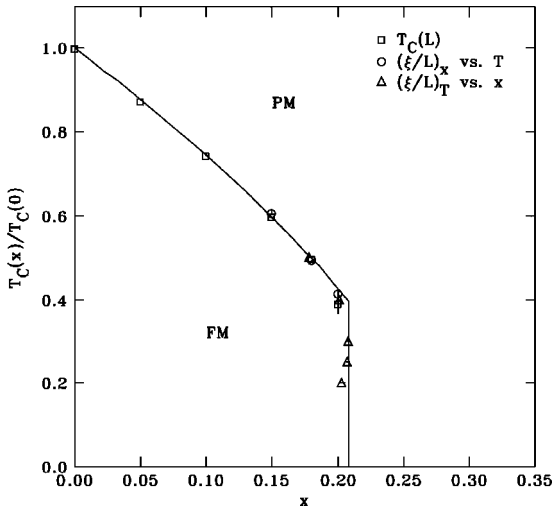

FIG. 4. The ferromagnetic phase boundary for the short range $\pm J$ bond frustrated Heisenberg model. All transitions have been normalized to the transition temperature of the pure ($x=0$) model which we take here (Ref. 13) as $T_C(x=0)=1.443J/k_B$.

Finally, we construct the ferromagnetic phase boundary from the transition temperatures found in this study, shown in Fig. 4. If we allow for a continuous decrease of $T_C(x)$ for increasing x such as a power law, then $x_c=0.276(9)$, a value inconsistent with our finding that the curves of ξ/L fail to cross at any temperature at or beyond $x=0.22$. Rather, a vertical phase boundary at x_c is drawn, as found in both the mean field phase diagram[1] as well as experiments.[2] Evidence for a phase boundary at $x_c=0.208(2)$ in this model is found by constructing plots of ξ/L at constant T for various x. A crossing is found near the same x for three different T's below $T_C(x_c)$ (see Fig. 4), consistent with a vertical phase boundary although we are unable to prove it. Assuming a vertical phase boundary we quote $x_c=0.208(2)$.

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