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Universal scaling functions and multi-critical points in the site frustrated Heisenberg model

A. D. Beath and D. H. Ryan
Physics Department and Centre for the Physics of Materials, McGill University, 3600 University Street, Montreal, Quebec H3A 2T8, Canada

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Recently, the ordering scenario of three-dimensional site frustrated Heisenberg models has been challenged. The existence of a decoupled tetracritical point (DTP) where ferromagnetic (FM) and antiferromagnetic (AF) order occur simultaneously has been modified to include a line of multicritical points where both FM and AF occur simultaneously. In addition, numerous studies claim that, within the mixed phase, critical exponents are altered from Heisenberg values. Here we show that within the narrow region of proposed multicritical points, the transition temperatures away from the tetracritical point are indeed distinct, confirming the occurrence of a DTP. In addition, we show a universal scaling collapse of the magnetization both away from, and within, the mixed phase using Heisenberg exponents, demonstrating that the stable fixed points are within the Heisenberg universality class. © *2005 American Institute of Physics*. [DOI: 10.1063/1.1855551]

Multicritical points occur in a wide variety of physical contexts such as superfluidity, superconductivity, and magnetism.[1] The site frustrated Heisenberg model, studied here, is thought to possess a decoupled tetracritical point (DTP) in the concentration-temperature $(x-T)$ phase diagram[2] where ferromagnetic (FM) and antiferromagnetic (AF) phases order simultaneously. As the DTP is approached in concentration, the transitions at T_C and T_N are distinct, with $T_C=T_N$ *only* at the DTP. The upper transition first breaks the O(3) symmetry of the Hamiltonian while the lower transition breaks a reduced O(2) symmetry. The transitions are all second order and the mixed phase is characterized by the coexistence of FM and AF order. The situation is similar to that occurring in superconductors with SO(3) and SO(2) ordered phases,[3] as well as anisotropic antiferromagnets in a uniform external field H which contains,[4] in some cases, a DTP in the $(H-T)$ phase diagram.

The DTP for site frustrated models was first studied 30 years ago by Aharony.[5] The occurrence of the DTP was later questioned by Fishman and Aharony.[6] They concluded that four ordering scenarios were possible although none could be ruled out. The revised conclusion was based on the erroneous assumption that bond and site frustrated models are equivalent and in fact only a bond frustrated model was studied. We have recently determined phase diagrams for the site frustrated Heisenberg model on three different lattices,[2] one of which (simple cubic) is shown in Fig. 1. Our phase diagram is qualitatively similar to those given by others,[7] except in one respect: A recent study[8] has claimed that the DTP at $x=0.5$, where $T_C=T_N$, does not exist and that instead a line of critical points exists for $0.48<x<0.52$ where $T_C=T_N$, and FM and AF order occur simultaneously. In addition, we[2] and others[7,8] have suggested that the ordering within the mixed phase might not be characterized by the Heisenberg universality class of the parent model although a consistent picture has yet to emerge. Here we address both issues, demonstrating that (i) both inside and outside the mixed phase the order is characterized by exponents of the Heisenberg universality class and (ii) both T_C and T_N are not equal within the proposed multicritical phase, strengthening the argument in favor of a DTP at $x=0.5$.

The site frustrated model we consider is a classical Heisenberg model governed by the Hamiltonian

$$\mathcal{H} = -\sum_{\langle ij\rangle} J_{ij}\vec{S}_i \cdot \vec{S}_j, \tag{1}$$

where the sum runs over all nearest neighbor bonds J_{ij} on a simple cubic lattice of linear dimension L with periodic boundary conditions. The distribution of bonds in site frustrated models is expressed as

$$J_{ij} = J_{FF}x_ix_j + J_{AA}(1-x_i)(1-x_j) + J_{FA}[x_i(1-x_j) + x_j(1-x_i)], \tag{2}$$

where $x_i=1$ if site i is occupied by a F (ferromagnetic) site and $x_i=0$ if site i is occupied by an A (antiferromagnetic)

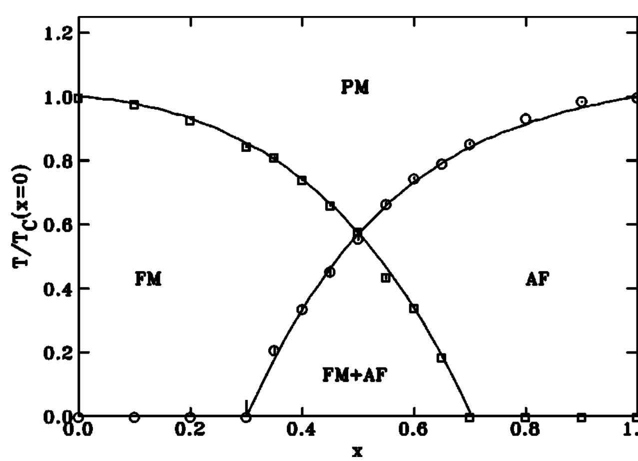

FIG. 1. Phase diagram of site frustrated Heisenberg model on simple cubic lattice. Transition temperatures have been normalized to that of the pure $(x=0)$ model.

site. For random F/A occupancy, the probability of site i being F type $P(x_i=1)=(1-x)$ and the probability of site i being A type $P(x_i=0)=x$. Our site frustrated model corresponds to the choice

$$J_{FF} = -J_{AA} = -J_{FA} = 1. \tag{3}$$

The choice of sign of J_{FA} is irrelevant; phase diagrams with $J_{FA}=+1$ are identical to phase diagrams with $J_{FA}=-1$ via gauge symmetry.[2] We simulate the model using a simple Metropolis algorithm, using a maximum of 10^4 Monte Carlo sweeps prior to averaging over a maximum of 10^5 Monte Carlo sweeps. The number of Monte Carlo sweeps is chosen to be much larger than the measured sample independence time.

We have studied the model previously for many different concentration and lattice types[2] and some of this previously unpublished data are used here. In addition, new data have been taken at nominal concentrations $x=0.49$ and 0.495, within the region where it is proposed that $T_C=T_N$, in conflict with the DTP ordering scenario where $T_C=T_N$ at $x=0.5$ *only*. For these new simulations we have used $L=4$, 6, 8, 10, 12, 16, and 20 averaging over 500 realizations of disorder for the smallest sizes and 100 realizations for the largest. Some new data have also been taken at $x=0.5$, where it can be proved[2] that $T_C=T_N$ for bipartite lattices.

The quantities we measure are various powers of the the magnetization M_f and staggered magnetization M_s. Average values are obtained by averaging first over time $\langle\ \rangle$ and then over disorder [ ] to yield $[\langle M_f^n\rangle]$ and $[\langle M_{st}^n\rangle]$. From $M_{f,s}^n$ we calculate the bond averaged, finite lattice susceptibilities $\chi_{f,s}$,

$$\chi = \beta L^3[\langle M^2\rangle - \langle M\rangle^2] \tag{4}$$

and Binder cumulants $B_{f,s}$,

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

According to finite size scaling the magnetization or staggered magnetization scales according to

$$M_{f,s} \propto L^{-\beta/\nu}\mathcal{M}(atL^{1/\nu}), \tag{6}$$

where β and ν are the usual static critical exponents for second-order phase transitions, a is a metric factor ensuring that the function $\mathcal{M}$ is universal, and $t=(T-T_{C,N})/T_{C,N}$ is the reduced temperature.

We first address the issue of the critical behavior of the site frustrated Heisenberg model. According to the Harris criteria,[9] since the exponent of the free energy α is negative for the pure $(x=0)$ model[10] than the addition of disorder does not affect the leading order critical behavior, and we therefore expect the site frustrated model to remain in the Heisenberg universality class. A good demonstration of this universality can be found by noting that the metric a occurring in Eq. (6) can depend upon the concentration x; a reduced value of $a(x)$ with increasing x implies a reduced critical region dominated by leading scaling exponents. At T_C where $t=0$, $M(x,L,t=0)=bL^{-\beta/\nu}$. The constant b can also depend upon x; a reduced value of $b(x)$ with increasing x implies a decreasing relative volume of the lattice which contributes to the magnetization. Thus, if the Harris criteria is applicable to

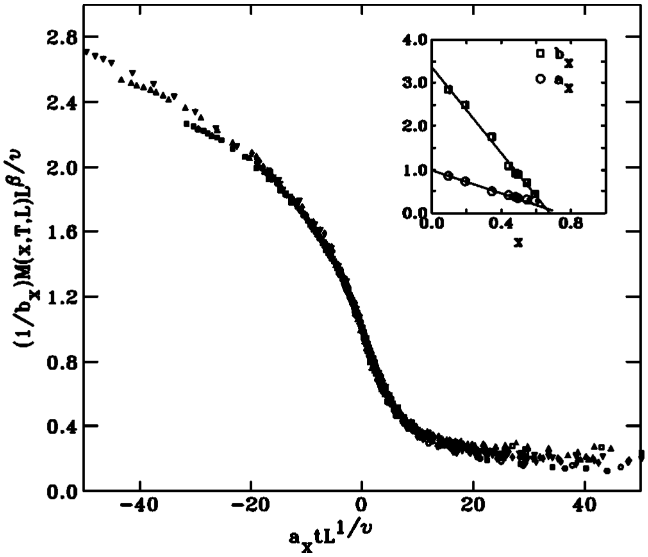

FIG. 2. Finite size scaling collapse of magnetization data for seven concentrations spanning the entire phase diagram. Lattice sizes range from $L_{min}=8$ to $L_{max}=24$. The exponents used are those of the Heisenberg universality class: $\beta/\nu=0.514$ and $\nu=0.705$. Size dependent factors a_x and b_x appear to vanish near the site percolation threshold $x_p=0.31$.

the site frustrated Heisenberg model we should be able to collapse all of the magnetization data according to the universal function

$$\frac{1}{b(x)}M(x,L,T)L^{\beta/\nu} = \mathcal{M}[a(x)tL^{1/\nu}] \tag{7}$$

with $a(x)$ and $b(x)$ being concentration dependent factors and the exponents β and ν those of the Heisenberg universality class.

The fit for the magnetization scaling according to Eq. (7), using concentrations $x=0.1$, 0.2, 0.35, 0.45, 0.49, 0.5, 0.55, and 0.6 and at least three different L for each x ($L_{min}=8$, $L_{max}=24$) totaling 34 different data sets, is shown in Fig. 2. We use as critical exponents[10] $\beta/\nu=0.514$ and $\nu=0.705$. The excellent collapse of the data shows that all transitions are within the Heisenberg universality class. Both $a(x)$ and $b(x)$ (inset Fig. 2) vanish near the critical concentration $x_c=0.69(1)\approx 1-x_p$ where FM order ceases, with x_p being the site percolation threshold. This result is consistent with the picture we have proposed[2] of the site frustrated model as one or two (depending on x) percolating networks of F and/or A sites ordering at finite T_C and/or T_N provided only that a percolating cluster forms.

The second issue concerns the existence of the DTP at $x=0.5$ (Fig. 1). An accurate method for locating transition temperatures is to first locate the extrema of a thermodynamic quantity (here we use both the peak in $\chi_{f,s}$ and the maximum slope in $B_{f,s}$). The extrema occur at system size dependent pseudotransition temperatures $T_{C,N}(L)$ which scale according to

$$T_{C,N}(L) = T_{C,N} + cL^{-1/\nu}. \tag{8}$$

neglecting scaling corrections which are avoided by using large enough L (our previous work[2] shows $L_{min}\sim 8$ for χ and $L_{min}\sim 10$ for B). We fix the exponent ν to that of the Heisen-

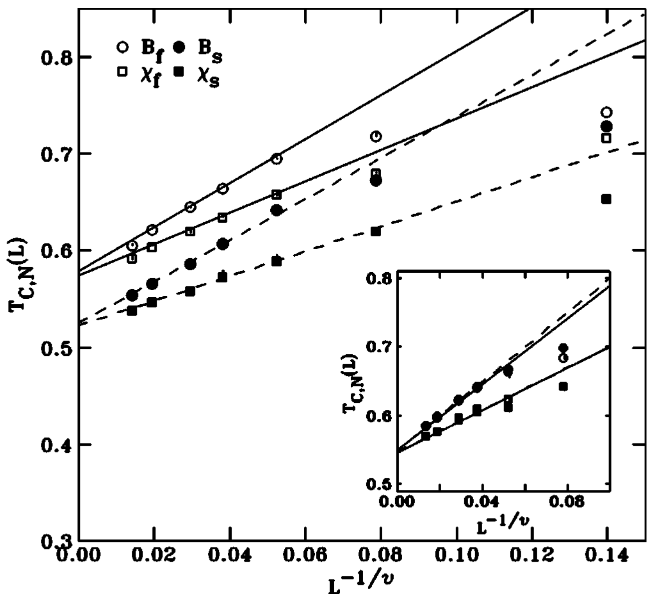

FIG. 3. Scaling plots of pseudotransition temperatures $T_C(L)$ at $x=0.49$, within the region of the phase diagram where it is proposed (Ref. 8) that $T_C=T_N$. The data clearly disagrees with this ordering scenario. Inset shows the same plot for $x=0.5$, where it can be proved that $T_C=T_N$, a claim which is supported by the data.

berg universality class, which Fig. 2 demonstrated to be correct. All of the transition temperatures are normalized to that of the pure $(x=0)$ model which we take as $T_C(x=0)=1.443\ J/k_B$. The data and fits according to Eq. (8) are shown in Fig. 3. Good agreement is found for both T_C and T_N using the independent measures provided by the extrema of $\chi_{f,s}$ and $B_{f,s}$, the difference in measures being less than one σ, yet clearly both transitions are distinct; the difference between $T_C=0.5737(10)$ and $T_N=0.5217(11)$ is more than 50σ. It is unlikely therefore that the ordering scenario proposed in Ref. 8 is correct. Instead, the data supports the existence of a DTP at $x=0.5$.

Further support is provided by repeating the calculation at $x=0.495$ (not shown) and 0.5 (inset of Fig. 3). At $x=0.495$ we get $T_C=0.5664(35)$ and $T_N=0.5356(23)$ and at $x=0.5$ we get $T_C=0.5481(19)$ and $T_N=0.5495(29)$. In addition, gauge symmetry requires that $T_C=T_N$ at $x=0.5$ for bipartite lattices,[2] a symmetry which applies also for finite lattices with periodic boundary conditions provided that L is even. Thus we must have $T_C(L)=T_N(L)$ for all L as shown in the inset of Fig. 3. We remark here that use of odd L by

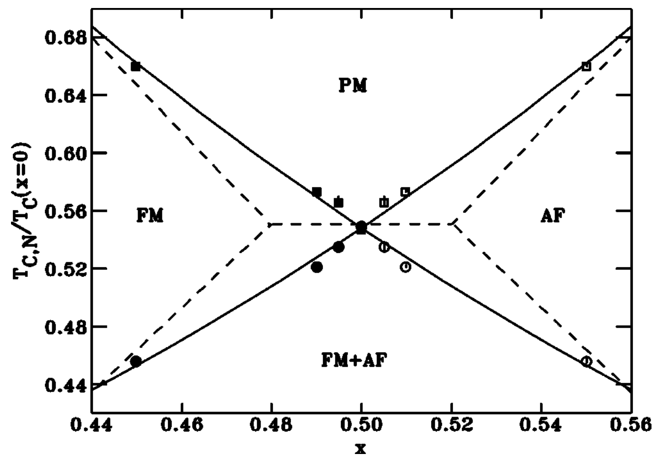

FIG. 4. Phase diagram of short range $\pm J$ Heisenberg site frustrated model in the vicinity of the DTP at $x=0.5$. Solid lines represent the DTP ordering scenario while dashed line is a representation of the ordering scenario given in Ref. 8. Filled points are measured transitions while open points are given by symmetry.

Matsubara[7] results in an exchange strain, producing a twist of the AF order which is not inherent to the model. This will give critical behavior different then the pure $(x=1)$ AF, and is probably why Heisenberg universality was not found in that study.[7]

In summary, our data confirms the DTP ordering scenario for the site frustrated Heisenberg model. The phase diagram in the immediate vicinity of the DTP is summarized in Fig. 4. In addition, we have demonstrated that the order parameters scale with Heisenberg exponents both inside and outside the mixed phase.

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