Intercluster coupling in site-frustrated random magnets

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The effects of intercluster coupling strength ($|J_{FA}|$) on the ordering behavior of the site-frustrated Heisenberg model have been investigated. We find that following a weak initial increase, the lower temperature transition is driven to $T=0$ for $|J_{FA}|^{\star}\sim 5.0(5)$, while the upper transition temperature appears to increase without limit. © *2004 American Institute of Physics.*
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A simple, site-frustrated model of a magnetic system with competing interactions can be constructed by randomly decorating a lattice with ferromagnetic (F) and antiferromagnetic (A) sites to create a $F_{1-x}A_x$ solid solution. The sites are then coupled by nearest-neighbor exchange bonds of the form $J_{FF}=-J_{AA}=-J_{FA}=+1$. This model was originally introduced to study tetracritical points in binary magnetic alloys[1] and is directly relevant to the magnetic behavior of alloys containing two magnetic species, such as $a-Fe_{1-x}Mn_xG_y$ (Ref. 2), where G is a mixture of glass-forming metalloids. Four clear results have emerged from a detailed Monte-Carlo study of the three-dimensional (3D) site-frustrated Heisenberg model on cubic lattices:[3] (i) The sign of J_{FA} is irrelevant. A model with $J_{FA}=+1$ can be mapped onto one with $J_{FA}=-1$ by a series of gauge transformations. (ii) The system forms clusters of F and A sites, and all of the frustration resides on the interfaces between these clusters. (iii) As long as the concentration of F (or A) sites exceeds the relevant percolation threshold, ferromagnetic (or antiferromagnetic) order develops in the F (or A) percolating cluster through a conventional phase transition. (iv) Despite significant levels of frustration, the phase diagram (upper panel of Fig. 1) shows *only* ferromagnetic and antiferromagnetic ordering, ruling out the possibility of a conventional spin-glass phase. Ordering in this model therefore consists of largely independent F and A clusters coupled at their boundaries by the J_{FA} bonds. As only J_{FA} is expected to alter the phase diagram in a nontrivial fashion, we examine here the effects of varying J_{FA} from zero to values large enough to establish asymptotic behavior.

It is useful to first consider two simple limiting cases. Setting $J_{FA}=0$ decouples the F and A clusters entirely and the system breaks down into independent clusters of spins. As the lower panel of Fig. 1 shows, decoupling the two types of sites has very little impact: T_C and T_N are reduced slightly, but the overall form of the phase diagram is unchanged.[4] The only feature that is lost when the limited frustration caused by $J_{FA}\neq 0$ is eliminated, is the mutually perpendicular ordering of the ferromagnetic and antiferromagnetic clusters.[3] The similarities between the phase diagrams with $J_{FA}=0$ and $|J_{FA}|=1$ (Fig. 1) serve to emphasize the limited impact of frustration in site-frustrated models. Indeed, it is apparent in Fig. 1 that adding frustration actually leads to an *increase* in both T_C and T_N.

A second case is obtained by setting $J_{FF}=-J_{AA}=0$ and $|J_{FA}|=1$ in order to access the limit $J_{FA}/J_{FF,AA}\rightarrow\infty$. Here, only the F and A sites defining the cluster surfaces are coupled. When either or both of the F and A sites percolate, they form regular D-dimensional volumes with $D-1$-dimensional lattice-spanning surfaces of coupled sites, which could, in principle, order. However, finite-temperature ordering is only possible above a lower critical dimension D_l which, for Heisenberg spins[5] is 2. Thus, for our simplified 3D model with only $J_{FA}\neq 0$, the 2D cluster surface orders at $T=0$. Taking this model with $J_{FF}=-J_{AA}=0$ as a guide to the behavior at large $|J_{FA}|$ (with $J_{FF}=-J_{AA}=+1$), we are led to expect that the initial increase in T_C and T_N with $|J_{FA}|$ eventually ceases, and that both transitions ultimately occur only at zero temperature. This simplified model neglects the role of $J_{FF,AA}$, and as we shall see below, these interactions preserve one of the finite-temperature transitions.

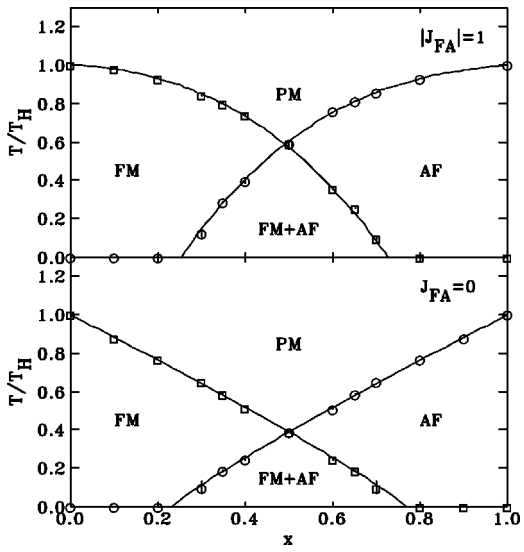

FIG. 1. Phase diagram for site frustrated models with $J_{FA}=1$ (top) and $|J_{FA}|=0$ (bottom) for a bcc lattice. Note that both T_C and T_N increase when $|J_{FA}|=1$ as compared to $J_{FA}=0$, despite frustration.

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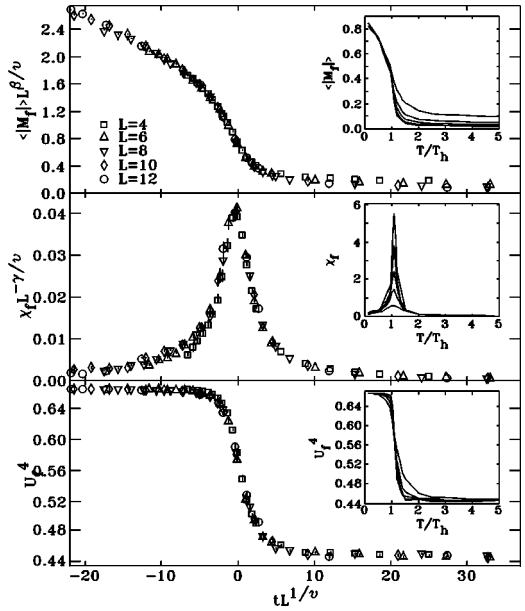

FIG. 2. Scaling plots of the magnetization (top), susceptibility (middle), and Binder cumulant (bottom), for $J_{FA}=2$ using 3D Heisenberg exponents.

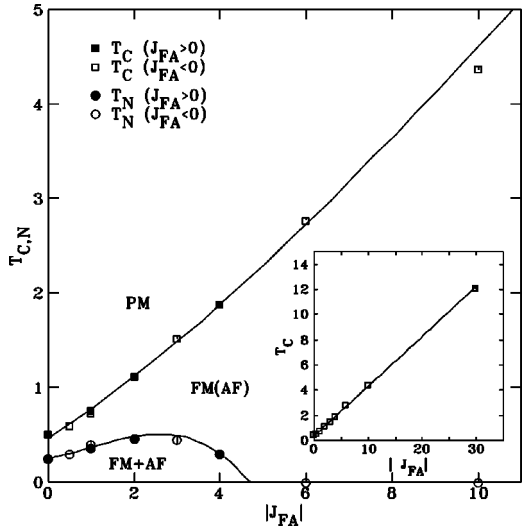

FIG. 3. T_C and T_N vs $|J_{FA}|$ ($J_{FF}=-J_{AA}=+1$) for bcc lattice with $x=0.4$.

To determine T_C and T_N, we use a Monte-Carlo method employing simple Metropolis dynamics. Detailed finite-size-scaling analysis allows extrapolation to the thermodynamic limit (details can be found elsewhere[3]). For the work presented here, we have chosen a concentration $x=0.4$, where $T_N \sim 0.5 T_C$. We use a bcc lattice containing $N=2L^3$ spins with several system sizes $L=4,6,8,10$, and 12, which appear to be very close to the limit of asymptotic scaling ($L_{\min} \sim 6$–8). Typical scaling plots in the vicinity of T_C, including unscaled data presented as insets, are shown in Fig. 2 for the magnetization M_f, susceptibility χ_f, as well as the Binder cumulant U_f^4. For the scaled data we have used exponents from the 3D Heisenberg universality class:[6–8] $\beta=0.364$, $\gamma=1.386$, and $\nu=0.705$. The values of T_C and T_N found using the extrema of several thermodynamic quantities,[3] are used to construct the plot of $T_{C,N}$ vs $|J_{FA}|$, shown in Fig. 3. Clearly, the lower temperature transition (T_N for $x<0.5$) vanishes for $|J_{FA}|>5.0(5)$, while for all $|J_{FA}|$ the upper temperature transition (T_C for $x<0.5$) is found to increase indefinitely and approximately linearly, beyond the point where T_N is observed to collapse. This linear increase simply reflects the linear dependence of the available exchange energy while increasing J_{FA}.

Our finding that T_N vanishes for $|J_{FA}|>5.0(5)$ is supported by: (i) a lack of a finite-temperature peak in the staggered susceptibility which increases with L; (ii) a lack of a crossing of the Binder cumulant which remains at the high temperature limit $\frac{4}{9}$, except near $T=0$; and (iii) a scaling of the staggered magnetization $M_{\rm st}$, which is found to scale, at both high and low T, as

$$M_{\rm st}(T,L) \propto L^{-3/2} \mathcal{M}(T). \tag{1}$$

The third observation is most significant, as Eq. (1) implies that in the thermodynamic limit $M_{\rm st}=0$, this normally describes the behavior well above any ordering temperature. If finite T ordering occurred, $M_{\rm st}$ could not possibly scale according to Eq. (1). Explicitly, for $J_{FA}=-10$, we find that $M_{\rm st} \propto L^{-\alpha}$ with $\alpha=1.503(3)$ at $T=15T_H$, and $\alpha=1.45(10)$ at $T=0.1T_H$. Together, these observations strongly suggest that for $|J_{FA}|>5.0(5)$, the antiferromagnetic transition no longer occurs at any finite temperature.

To understand the initial rise and subsequent collapse of T_N with increasing $|J_{FA}|$, we turn to a simpler site-frustrated model for which exact ground states can be identified: Ising spins on 2D square nets. To determine the ground state, plaquettes (the smallest closed loop of connected spins) which are frustrated (only those plaquettes which contain two neighboring A sites and two neighboring F sites are frustrated in this model) are joined together with a line called a dual string. Bonds traversed by the dual string are unsatisfied while all remaining bonds are satisfied. For symmetric couplings ($|J|=1$), the ground state is that configuration which minimizes the total length of dual strings.[9] When the couplings are asymmetric ($|J_{FA}| \neq 1$), the contribution to the total length of the dual string by each element is weighted according to the magnitude of the bonds traversed: A dual string traversing one $|J|=3$ bond is energetically equivalent to a dual string traversing three $|J|=1$ bonds.

The model with $J_{FA}=0$ is equivalent to the model with $|J_{FA}|=1$ [Fig. 4(a)], provided that (i) the dual strings are confined to the surfaces of F/A clusters and (ii) the total length of the dual strings encircling a cluster is exactly half of the cluster perimeter. With both of these criteria satisfied, a cluster of F or A sites can be flipped with no energy cost, as in the case where $J_{FA}=0$. In general, this perfect cancellation does not take place, and finite clusters of A or F sites embedded within a percolating cluster of F or A sites will couple rigidly to the surrounding cluster [Fig. 4(b)]. This rigid coupling of an embedded cluster to the percolating cluster will effectively increase the total number of connected spins within the percolating cluster, as compared to the case with $J_{FA}=0$. This is equivalent to an increase in available exchange energy, and so both T_C and T_N initially increase with $|J_{FA}|$. However, when $|J_{FA}|$ increases beyond

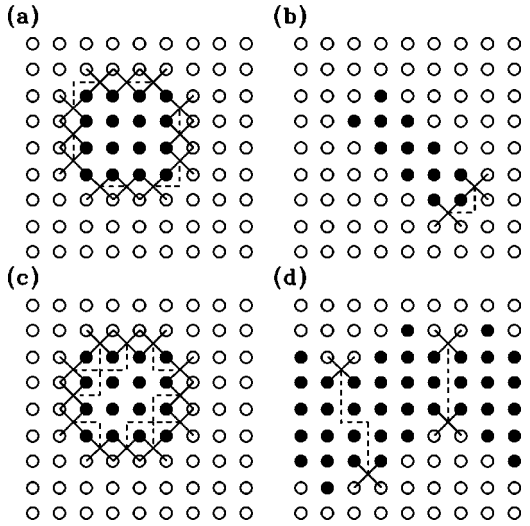

FIG. 4. Two-dimensional square nets of F (○) and A (●) sites. Frustrated plaquettes are denoted by a cross, while dual strings connecting frustrated plaquettes are denoted by a dashed line.

1, the optimal dual strings begin to migrate away from the cluster interfaces in order to avoid traversing the larger J_{FA} bonds, as depicted in Fig. 4(c). The linking of frustrated plaquettes now involves longer dual strings, which alters the effective volume of rigidly connected spins within a percolating cluster [compare Figs. 4(a) and 4(c)]. As $|J_{FA}|$ continues to increase, dual strings will eventually traverse the volume a percolating cluster, as depicted in Fig. 4(d), breaking the $J_{FA}=0$ ground-state order into domains. This fragmentation causes the percolating cluster to exhibit an order parameter $M_{f,\mathrm{st}}$, which scales according to Eq. (1) at $T=0$. The critical value of $|J_{FA}|^{\star}$, where the transition temperature vanishes, corresponds to the value of $|J_{FA}|$, where the effective volume of the ordered cluster becomes zero. Domain formation, driven by dual strings passing through the volume of the otherwise $(J_{FA}=0)$-ordered percolating cluster, causes the transition temperature to vanish at large $|J_{FA}|$. Indeed, 2D site-frustrated models with Ising spins show that with $|J_{FA}|=1$ the value of x_c where T_C vanishes is increased, compared to the value of x_c when $J_{FA}=0$.[10]

Domain formation might be expected to cause the upper transition (T_C here) to decline as well. To explain the continued increase we note that for 3D models in the regime $x_c<x<1-x_c$, the 2D lattice-spanning surface of the percolating F cluster is defined by the 2D lattice-spanning surface of the percolating A cluster. Since frustrated plaquettes, which act as sources and sinks of defect energy, are *shared* by A and F clusters, the least energetic (shortest, J_{FA} avoiding) path between frustrated plaquettes at the boundary of percolating A and F clusters is found through the smaller cluster. Only the smaller percolating cluster is expected to break into domains at large $|J_{FA}|$.

Our observations show that for values of $|J_{FA}|<J_{FA}^{\star}$, the transition temperatures of both types of percolating clusters initially increase due to an increase in effective cluster size from embedded finite clusters. As $J_{FA}^{\star}$ is approached, domain formation leads to the destruction of the finite T transition for the smaller percolating cluster. Thus, in the limit $|J_{FA}|\to\infty$ the tetracritical point observed at $x=\frac{1}{2}$ evolves into a bicritical point where both T_N and T_C vanish simultaneously at $x=0.5$ and $T=0$. Alternatively, if *both* T_C and T_N vanish in the limit $|J_{FA}|\to\infty$ (this is not observed, but cannot be ruled out yet), then a gap will open in the center of the phase diagram where periodic ordering does not occur and spin-glass ordering might be possible.

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