Intercluster coupling in site-frustrated random magnets

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Presented on 8 January 2004

The effects of intercluster coupling strength (|JFA|) 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 TC = 0 for |JFA| ≈ 5.0(5), while the upper transition temperature appears to increase without limit. © 2004 American Institute of Physics.

[DOI: 10.1063/1.1676111]

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 F1−xAx solid solution. The sites are then coupled by nearest-neighbor exchange bonds of the form JF = −JAA = −JFA = +1. This model was originally introduced to study tetrahedral points in binary magnetic alloys and is directly relevant to the magnetic behavior of alloys containing two magnetic species, such as Fe1−xMnxG2 (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: (i) The sign of JFA is irrelevant. A model with JFA = +1 can be mapped onto one with JFA = −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 JFA bonds. As only JFA is expected to alter the phase diagram in a nontrivial fashion, we examine here the effects of varying JFA from zero to values large enough to establish asymptotic behavior.

It is useful to first consider two simple limiting cases. Setting JFA = 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: TC and TN are reduced slightly, but the overall form of the phase diagram is unchanged. The only feature that is lost when the limited frustration caused by JFA ≠ 0 is eliminated, is the mutually perpendicular ordering of the ferromagnetic and antiferromagnetic clusters. The similarities between the phase diagrams with JFA = 0 and |JFA| = 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 TC and TN. A second case is obtained by setting JFF = −JAA = 0 and |JFA| = 1 in order to access the limit JFA/JFF,AA → ∞. 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 Dl which, for Heisenberg spins is 2. Thus, for our simplified 3D model with only JFA ≠ 0, the 2D cluster surface orders at T = 0. Taking this model with JFF = −JAA = 0 as a guide to the behavior at large |JFA| (with JFF = −JAA = +1), we are led to expect that the initial increase in TC and TN with |JFA| eventually ceases, and that both transitions ultimately occur only at zero temperature. This simplified model neglects the role of JFF,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 JFA = 1 (top) and |JFA| = 0 (bottom) for a bcc lattice. Note that both TC and TN increase when |JFA| = 1 as compared to JFA = 0, despite frustration.](image-url)
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). For the work presented here, we have chosen a concentration $x = 0.4$, where $T_N \approx 0.5T_C$. We use a bcc lattice containing $N = 2L^3$ spins with several system sizes $L = 4, 6, 8, 10, 12$, which appear to be very close to the limit of asymptotic scaling ($L_{\text{min}} \approx 6–8$). 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 $\chi_f$, as well as the Binder cumulant $U_f$. For the scaled data we have used exponents from the 3D Heisenberg universality class: $\beta = 0.364$, $\gamma = 1.386$, and $\nu = 0.705$. The values of $T_C$ and $T_N$ found using the extrema of several thermodynamic quantities, 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 $\frac{1}{2}$, except near $T = 0$; and (iii) a scaling of the staggered magnetization $M_a$, which is found to scale, at both high and low $T$, as

$$M_a(T, L) \propto L^{-3/2} \mathcal{A}(T).$$

The third observation is most significant, as Eq. (1) implies that in the thermodynamic limit $M_a = 0$, this normally describes the behavior well above any ordering temperature. If finite $T$ ordering occurred, $M_a$ could not possibly scale according to Eq. (1). Explicitly, for $J_{FA} = -10$, we find that $M_a \propto L^{-\alpha}$ 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. 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...
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 of the otherwise ordered 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 $M_{F, st}$, which scales according to Eq. (1) at $T=0$. The critical value of $|J_{FA}|^c$, 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 $J_{FA}=0$.\(^\text{10}\)

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 $|J_{FA}| < J_{FA}^c$, the transition temperatures of both types of percolating clusters initially increase due to an increase in effective cluster size from embedded finite clusters. As $J_{FA}^c$ 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 $x = \frac{3}{4}$ 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.

This work was supported by grants from the Natural Sciences and Engineering Research Council of Canada, and Fonds pour la formation de chercheurs et l’aide à la recherche, Québec.

\[^1\] A. Aharony, Phys. Rev. Lett. 34, 590 (1975).


\[^4\] We normalize all transition temperatures to $T_C$ of the pure $(x = 0)$ ferromagnet which for bcc lattices is $T_C = 2.054$.


