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COMPARISON OF CROSS-OVER EFFECTS FOR WEAKLY DILUTED ISING ANTIFERROMAGNETS AND FERROMAGNETS

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Abstract. – We present a Monte Carlo calculation of the effect of small site or bond dilution in a nn/nnn Ising model in two dimensions. Whereas the Harris criterion for the cross-over exponent, $\phi = \alpha$, is satisfied by the ferromagnetic system, the calculated value of $\phi$ for the antiferromagnet is consistent with $\phi = \gamma - 2\beta$.

It has been predicted by Harris [1] that the critical behaviour of ferromagnetic systems is unaffected by the presence of small amounts of non-magnetic impurities if the specific heat exponent $\alpha$ is less than zero. If $\alpha$ is greater than zero, a cross-over from the regime free of impurity effects is expected, such that $t_c$, the cross-over value of the reduced temperature, satisfies,

$$ t_c \sim (\delta J)^{1/\phi}, $$

where $\delta J$ is the random variation in the exchange constant. It has been predicted that $\phi = \alpha$ for these systems.

The purpose of this communication is to present numerical results which exhibit the drastically different cross-over behaviour of Ising antiferromagnets (AF) with $n$-fold degenerate ground states ($n \geq 2$), from that of Ising ferromagnets (F).

We introduce a small perturbation in an Ising model such that

$$ H = H_0 + \sum_{(nn)} \delta J_{ij} S_i S_j, $$

where $H_0$ stands for the Ising model with nearest neighbour ((nn)) and next-nearest neighbour ((nnn)) interactions [2],

$$ H_0 = -J_1 \sum_{(nn)} S_i S_j - J_2 \sum_{(nnn)} S_i S_j $$

and $\delta J_{ij}$ is an independent random variable.

We consider here two cases: (i) $J_1 = J_2 > 0$, and (ii) $J_1 = J_2 < 0$. The ordered state is ferromagnetic in case (i) and antiferromagnetic in case (ii). As it is well known [3], the ground state of this AF can be pictured as two interpenetrating sublattices coupled by $J_1$. There is an AF on each sublattice, and reversal of all spins on any of the two sublattices leaves the ground state energy invariant, since half of the $J_1$ bonds are fulfilled and half of them are broken. Hence, the ground state is $n = 2$ fold degenerate. Removal of a single bond removes the degeneracy, and random removal of bonds or sites has been shown [4, 5] to generate a spatially random bias for one of the two ground states. This mechanism is akin to a random field (or a random anisotropy) and operates with no need of an external field. It is not at all like the Harris mechanism and has been shown to lead to [5]:

$$ \phi = \gamma - 2\beta $$

for an $n \geq 2$ AF (in two or more spatial dimensions), instead of $\phi = \alpha$, which holds for ferromagnets. The purpose of this note is to contrast these two different critical behaviours.

We perform a Monte Carlo simulation of a two dimensional Ising model with nearest and next-nearest neighbor interactions. The Metropolis algorithm [6] was applied to systems with periodic boundary conditions. At least $10^4$ sweeps were made in equilibrium and 1500 sweeps to equilibrate.

The values of $T_c$, $\gamma / \nu$ and $\alpha / \nu$ were calculated for the pure system in the following way. Defining a quantity $S$ such that,

$$ S = N^{-1} \left[ \left( \sum_i \eta_i S_i \right)^2 + \left( \sum_j S_j \right)^2 \right] $$

where $\sum_i \left( \sum_j \right)$ is a sum over all $i$ and $j$ on the one (the other sublattice), $\eta_i = 1$ for the F and takes alternatively the values of $\pm 1$ when summing over the lattice sites of the AF. As $L \to \infty$, for $T < T_c$, $S \to L^d$ ($d$ is the dimensionality of the system, and $L$ its linear size), whereas for $T > T_c$, as $L \to \infty$, $S \to \text{constant}$.

From finite size scaling [7] we know that at $T = T_c$, $S \sim L^{\alpha / \nu}$. In figure 1 we show $\ln \left( \frac{S}{L} \right)$ versus $\ln \left( \frac{L}{\epsilon} \right)$, for several values of $T$. From these results we get, $kT_c = (2.08 \pm 0.01)$ for the AF, and $kT_c = (5.25 \pm 0.01)$ for the F. The errors are obtained from a statistical analysis of the Monte Carlo results.

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Now, if we define a quantity $R$, such that

$$R = \frac{1}{N} \left( \frac{\partial^2 F}{\partial g^2} \right)_{g \to 0} = \sum_i \left[ \frac{\langle S_i S_{i+\delta} \rangle^2}{N} - \frac{\langle S_i \rangle^2}{N} \right]$$

(12)

combining (12) with (8) and (11) we get, $R(T_c) \sim \frac{v}{\varepsilon}$.

Figure 2 shows values of $\ln (R)$ versus $\ln (L)$ at $T = T_c$. From this figure we get the value of $\phi / \nu = 1.63 \pm 0.05$ for the AF, and $\phi / \nu = [-0.1, 0.1]$ for the ferromagnet.

From finite size scaling we know that the specific heat behaves as $C \sim L^{\alpha / \nu}$, at $T = T_c$. A plot of $\ln (C)$ versus $\ln (L)$, at $T = T_c$ (Fig. 2), gives the values, $\alpha / \nu = 0.46 \pm 0.02$ for the AF, and $\alpha / \nu = 0.2 \pm 0.1$ for the F.

We obtain the value of $\phi$ as follows. Consider a pure system with Hamiltonian

$$H \rightarrow H_0 - g \sum_i S_i S_{i+\delta},$$

where $\sum_i$ stand for a sum over all the sites in the lattice, and $i + \delta$ is a (nn) to a site $i$, no sum over $\delta$ is performed. Then, by translational invariance

$$\frac{1}{N} \left( \frac{\partial F}{\partial g} \right)_{g \to 0} = -\langle S_i S_{i+\delta} \rangle$$

(7)

where $F$ is the free energy. From scaling $F \sim t^{2-\alpha} f_\alpha (g / t^\gamma, \xi / L)$ then

$$\langle S_i S_{i+\delta} \rangle \sim t^{2-\alpha-\gamma} f_\gamma (\xi / L).$$

(8)

On the other hand, going back to the impure system given by (2), and expansion of the free energy ($F$) in powers of $\delta J^2$ gives,

$$-\beta F = -\beta F_0 + \frac{\delta^2 J^2}{2} \sum \left[ \langle (S_i S_j)^2 \rangle - \langle (S_i S_j) \rangle^2 \right]$$

(9)

and, assuming scaling,

$$F \sim t^{2-\alpha} f \left( \frac{\delta J^2}{t^\delta} \right).$$

(10)

Comparing (9) with (10), we get,

$$t^{2-\alpha-\phi} \sim \langle S_i S_{i+\delta} \rangle^2$$

(11)

where, $i$ and $i + \delta$ are nearest neighbours.

Fig. 1. - $\ln S$ are shown versus $\ln (L)$, at different temperatures, for an nn/nnn Ising ferromagnet (F) ($J_1 = J_2 > 0$), and for an nn/nnn Ising antiferromagnet (AF) ($J_1 = J_2 < 0$), both with $L \times L$ spins. The slope of the straight line at $kT = 2.08$, is 1.79. The slope of the straight line at $kT = 5.25$ is 1.77.

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