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Ising Metamagnet Under Staggered Field

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We report a Monte Carlo simulation of the layered Ising antiferromagnet under an external magnetic field. We show that under a staggered field, there occurs a phase transition from a metastable state which follows a Vogel–Fulcher law. For a staggered intrasublattice interaction a similar situation occurs.

KEY WORDS: Ising model; staggered field; metastable state.

Interest in the study of layered Ising antiferromagnets is unabated. The meanfield theory (see ref. 1 for review) indicates that in the external field (H)–staggered field (δ)–temperature (T) space, the phase diagram consists of two sheets of antiferromagnetic-to-paramagnetic transition. For a given δ, the transition is of first order for $H > H_c$, $T < T_c$ and of second order elsewhere. The two lines of critical points (H_c, T_c) for $\delta > 0$ and $\delta < 0$ join at a tricritical point. However, the meanfield theory also predicts that if the intrasublattice coupling is much weaker than the intersublattice coupling; then an unusual situation arises and there is a critical endpoint and a double critical endpoint. A recent careful computer simulation[2] has, however failed to identify any double critical endpoint (for $\delta = 0$). Another simulation study[3] (in the context of the precursor magnetization anomaly of $FeBr_2$[4]) was also consistent with the results of ref. 2 and succeeded in reproducing an additional peak [in magnetization (M)–temperature (T) as well as dM/dT–T curve] at $H < H_c$ and $\delta = 0$ by incorporating ten neighbor interactions among spins in adjacent layers. Thus, it seems worthwhile to look for any interesting effect at $\delta \neq 0$. The present note reports a simulation study which finds that for nonzero staggered field (and also for

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staggered intrasublattice interaction) there exists a transition from a metastable state that follows the Vogel–Fulcher law.

We simulated a simple cubic Ising lattice with nearest neighbor ferromagnetic interaction among spins in the same layer (XY plane). The spins in different planes interact by antiferromagnetic nearest neighbor interactions of the same strength. If one starts with an antiferromagnetic initial condition (all spins in layers 1, 2, 3,... are $+1$, -1, $+1$,..., respectively) and applies a homogeneous (positive) field H, then one simply gets an antiferromagnetic-to-paramagnetic phase transition with a smooth magnetization (and sublattice magnetization) versus temperature curve at all $H < H_c$. Something interesting occurs if we switch on an external staggered field which is $-\delta$, $+\delta$, $-\delta$,... for the layers 1, 2, 3,..., respectively ($\delta > 0$). Previously, it did not matter whether the opposite (with respect to H) spins are in layers 1, 3, 5,... or in layers 2, 4, 6,..., but now it does matter, because it costs less energy for them to be in layers 1, 3, 5,... rather than in layers 2, 4, 6,... as the net field is less (namely, $H - \delta$) for the former set of planes. But since the spins were initialized as being opposite to the staggered field, the system becomes metastable and at some stage

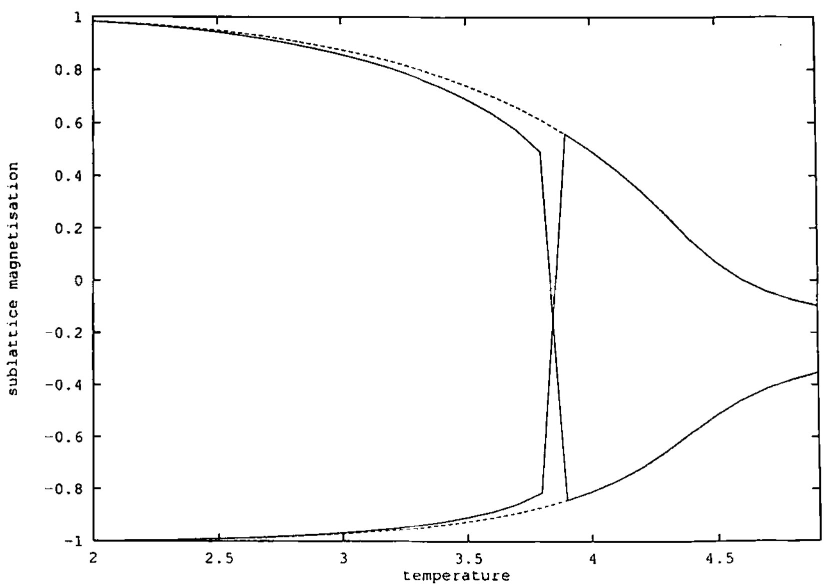

Fig. 1. Transition from a metastable state for a staggered field. The dashed and continuous lines correspond to $\delta = -0.05$ and 0.05, respectively. We performed 20,000 iterations with a $30 * 30 * 30$ system with periodic boundaries. The data plotted are averages over the last 10,000 iterations at $H = 1$. The curve for a stagerred intrasublattice interaction looks similar.

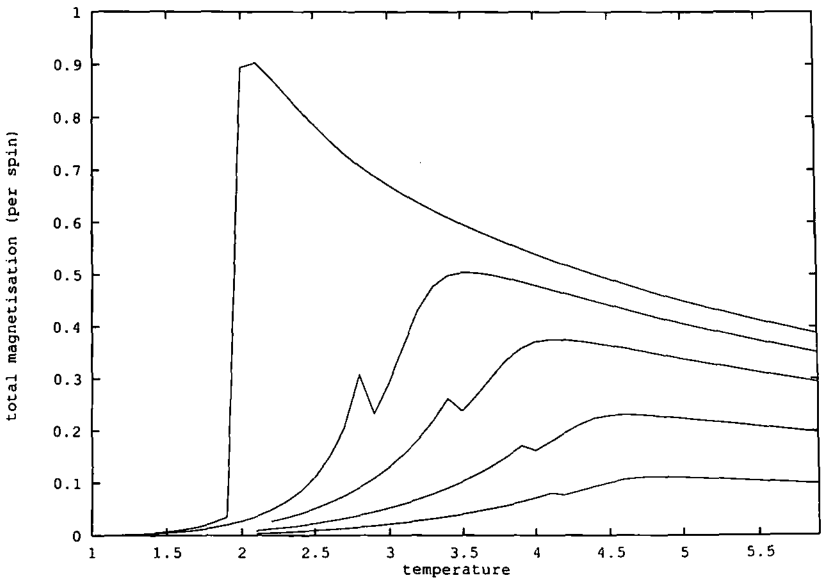

Fig. 2. Same as Fig. 1, but for $\delta = 0.03$, and $H = 2.0$, 1.8, 1.5, 1.0, 0.5 (top to bottom).

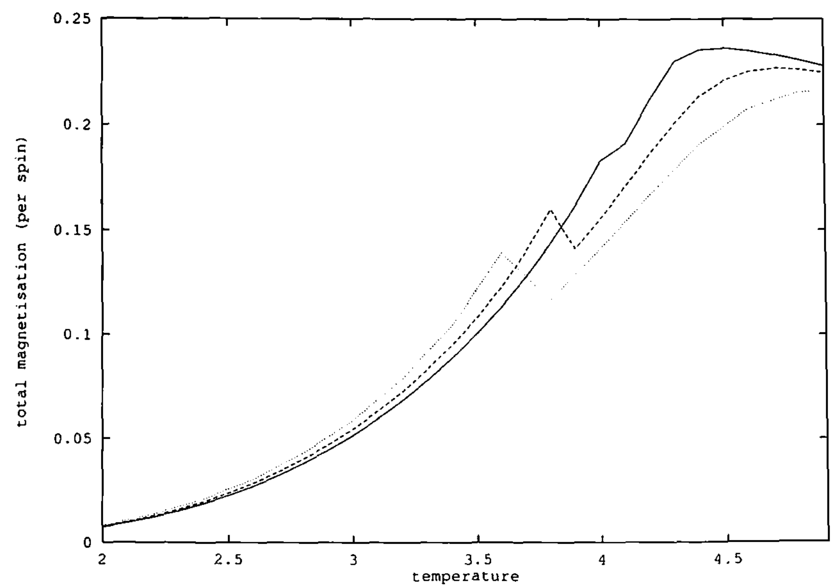

Fig. 3. Same as Fig. 1, but for $H = 1$ and $\delta = 0.01$ (continuous), 0.05 (dashed), 0.1 (dotted).

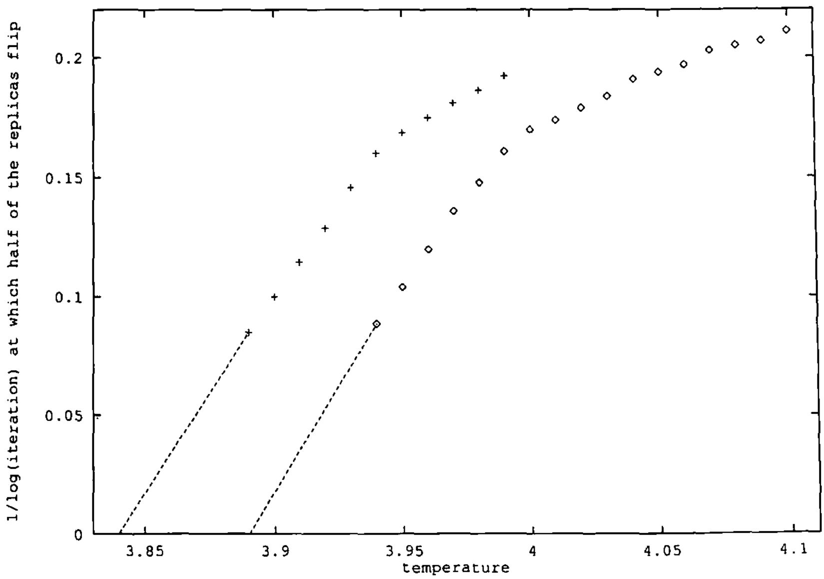

Fig. 4. Variation of the transition temperature with number of iterations. We started with 136 replicas of a 30 * 30 * 30 system (with periodic boundaries) at $H=1$ and noted the iteration at which half of the replicas underwent transition. The diamonds correspond to staggered field and $\delta=0.03$, and the crosses to staggered intralayer interaction and $\delta=0.1$. The dashed line is a guide to the eye and meets the X axis at $T_0=3.89$ (for diamonds) and 3.84 (for crosses).

(depending on the temperature, magnitude of δ, the number of iterations, etc.) there occurs a global flipping (Fig. 1) so that the spins in the layers 1, 2, 3,... become -1, $+1$, -1,..., respectively. The system maintains the antiferromagnetic order and a small peak appears in the M–T curve (Figs. 2 and 3). The transition to the paramagnetic phase occurs in the usual way at a higher temperature (for a given H) leading to a second peak in the M–T curve. As a result, the dM/dT–T curve also shows two peaks. The temperature T_m at which the transition from the metastable state takes place is found to decrease with increase of H, δ, and the number of iterations. However, as the number t of iterations tends to infinity, the value of T_m seems to approach a nonzero value $T_0=3.89$ (Fig. 4), suggesting that the transition cannot occur at a temperature below T_0. Thus the transition at T_m seems to follow the Vogel–Fulcher law

$$t \propto \exp[\text{const}/(T_m - T_0)]$$

better than the Arrhenius law

$$t \propto \exp[\text{const}/T_m]$$

Here t is the time after which the transition occurs at a temperature T_m. In order to measure t, we started with several replicas of the sample (each with a different seed for the random number generator) and took t as the iteration at which half of the replicas have flipped. Before concluding our discussion on the staggered field, we should mention that for $\delta < 0$, the initial condition (all spins in layers; 1, 2, 3,... are $+1$, -1, $+1$,..., respectively) does correspond to the global energy minimum and thus no metastable transition takes place (as confirmed by our simulations). The situation is similar for ferromagnetic initialization.

One also observes a metastable transition if the external magnetic field is homogeneous but the intralayer (ferromagnetic) interaction strength is $(J-\delta)$, $(J+\delta)$, $(J-\delta)$,... $(\delta > 0)$ for the layers 1, 2, 3,..., respectively. (The antiferromagnetic interlayer interaction is always $-J$). With the same initialization as before, a transition occurs at a temperature T_m when all the spins are flipped. The reason for this transition is, however, slightly

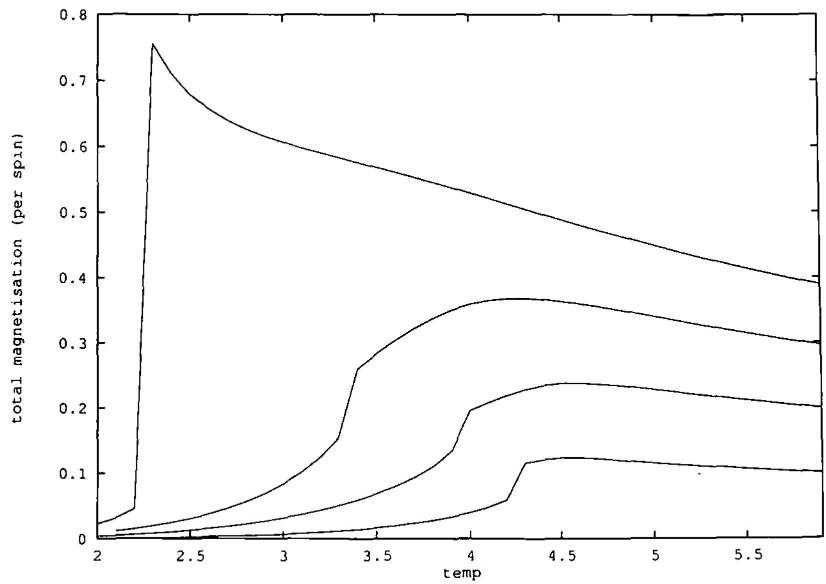

Fig. 5. Transition from a metastable state for staggered intralayer interaction. We performed 20,000 iterations with a $30 * 30 * 30$ system with periodic boundaries. The data plotted are averages over the last 10,000 iterations at $\delta = 0.1$, and $H = 2.0$, 1.5, 1.0, 0.5 (top to bottom).

more complicated. In order to understand the transition, let us denote by n the number of nearest neighboring pairs of antiparallel spins in a particular layer. Now, in the initial condition, $n = 0$ in each layer, but with time, n increases. In layers 1, 3, 5,... the majority of spins are aligned parallel to the external field and the number of down spins (and hence n) is small, whereas in the layers 2, 4, 6,... the majority of spins are aligned opposite to the field and n is larger. It costs less energy if the layers with large n have less intralayer interaction and so a transition occurs at some temperature T_m, when all the spins are flipped. (Again, this transition would not occur if $\delta < 0$ or if one starts with ferromagnetic initialization.) As in the previous case, the temperature T_m decreases with increase of H, δ and the number of iterations (Fig. 5) and this transition is also found to be compatible with the Vogel–Fulcher law with $T_0 = 3.84$ (Fig. 4). Also, at the temperature T_m, there is indeed a kink in the M–T curve (Fig. 5), but in contrast to the previous case, there is only one peak in the dM/dT–T curve.

In summary, we find that an Ising metamagnet shows a phase transition (following the Vogel–Fulcher law) if one switches on a staggered magnetic field or a staggered intrasublattice interaction.

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