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STUDIES OF FCC HEISENBERG ANTIFERROMAGNETS BY MONTE CARLO SIMULATION ON LARGE SPIN ARRAYS

W. Minor (1) and T. M. Giebultowicz (2)

(1) Purdue University, West Lafayette, IN 47907, U.S.A.
(2) University of Notre Dame, Notre Dame, IN 46556, and National Bureau of Standards, Gaithersburg, MD 20899, U.S.A.

Abstract. We report Monte Carlo studies of fcc Heisenberg antiferromagnets carried out on arrays with 108,000 spins. A lattice with only $J_{NN} \neq 0$ was found to exhibit a Type I AF order despite the disordered nature of its ground state. Contrary to previous reports, our data indicate in this case a first order phase transition.

So far, all reported Monte Carlo (MC) studies of fcc Heisenberg antiferromagnets [1-3] have been done on relatively small samples (up to 4,000 spins). In order to examine the role of finite size effects in such calculations, we have carried out a series of simulations on decidedly larger arrays, with 108,000 fcc sites (i.e., $30 \times 30 \times 30$ cubic cells). In this paper, we report some results obtained for fully occupied lattices. The calculations have been done for classical vector spins, assuming periodic boundary conditions, and using the conventional MC simulation technique [4]. However, for time economy reasons, instead of the commonly used Metropolis algorithm we have applied the heat bath algorithm developed by Walker and Walded which offers a decidedly faster convergence [5]. The calculations have been run on a CYBER 205 supercomputer using a partially vectorized program, and on two VAXes (8820 and 780).

The fcc antiferromagnetic (AF) lattice exhibits a variety of magnetic structures depending on the relative magnitudes of the NN and NNN exchange interactions. We have investigated two such cases, (i) a lattice with both AF $J_{NN}$ and $J_{NNN}$ (i.e., positive in our notation), taking $J_{NNN} = 0.1 J_{NN}$, and (ii) a lattice with only $J_{NN} \neq 0$. In the first case, the system represents a model of a Type III structure antiferromagnet (such as, e.g., $\beta$-MnS), for which the equilibrium condition is $0 < J_{NNN} < 0.5 J_{NN}$. This type of order has been, indeed, obtained in the simulated systems at low $T$. In agreement with theoretical considerations and with the results of experiments on $\beta$-MnS [6], the system exhibits a first-order phase transition, as is clearly indicated by the discontinuity and hysteresis in the internal energy $U$ vs. $T$ (see Fig. 2a). Quite surprisingly,

![Diagram](https://example.com/diagram1.png)  
**Fig. 1.** - The arrangement of spins in Type III (a) and Type I (b) antiferromagnetic order on fcc lattice.

![Diagram](https://example.com/diagram2.png)  
**Fig. 2.** - Magnetic energy vs. $T$ in the vicinity of the phase transition points for a system with $J_{NNN} = 0.1 J_{NN}$ (a), and with only $J_{NN} \neq 0$ (b). The lines are guides for the eye.
The transition temperatures $T_0(1)$ and $T_0(1')$, as well as sublattice magnetization vs. $T$ differ only slightly from the results obtained previously [3] for a sample with 4 000 spins, showing that these system characteristics are not particularly sensitive to finite size effects.

As is illustrated in figure 1a, the Type III AF ground state configuration consists of (100)-type planes of antiferromagnetically coupled spins, with the planes stacked along the [001] direction with an $ABABAB$ sequence (where the bars denote spin reversal). Since all interactions between the spins in $A-B$ planes sum up to zero, the only interplanar coupling in this structure is maintained by the AF NNN interactions, leading to an antiparallel orientation of spin in the $A-A$, $B-B$ planes. On the other hand, if the NNN interaction is ferromagnetic ($J_{NN} > 0$, $J_{NNN} < 0$), the system chooses the Type I structure (Fig. 1b) in which the orientation of spins in the $A-A$, $B-B$ planes is parallel (i.e., the stacking sequence is $ABABAB$). A particularly interesting special case is a lattice with zero NNN interactions. Since the interplanar coupling vanishes, the system may break up into independent planes, with spin orientation changing randomly from plane to plane. Because of the analogy with a planar Heisenberg antiferromagnet, it has been suggested [7] that this model may not exhibit a phase transition for $T > 0$. In contrast, Monte Carlo studies performed by Fernandez et al. [1] clearly indicated a transition (identified as a second order process) at $T_0 \approx 0.4 J_{NN}/k_B$, leading to the conclusion that some kind of magnetic coupling develops between the planes at $T > 0$ due to thermal excitations. However, this mechanism was not studied in detail. In order to obtain a new insight into this problem, we have investigated ordering effects in the samples by calculating the structure factor $S(q)$ defined by the equation:

$$S(q) = N^{-1} \left[ \sum_n S_n \exp(iq \cdot r_n) \right] \times \left[ \sum_n S_n \exp(-iq \cdot r_n) \right]$$

where $r_n$ denotes the position of the $n^{th}$ spin, $S_n$, and the sum is over all $N$ spins in the sample. If there is a periodic spin structure in the system, $S(q)$ exhibits maxima at characteristic reciprocal space points $q_0$. For example, in the case of Type I and Type III order such points are $(2\pi/\alpha)(1,0,0)$ and $(1,0,\frac{1}{2})$, respectively. The $S(q)$ data we have obtained for a lattice with $J_{NN} \neq 0$ only fully confirm the conclusions of Fernandez et al. [1], showing that the system indeed forms a three-dimensional AF order below $T_0$. After a sufficiently large number of MC steps/spin, we have repeatedly observed an onset of the Type I structure in the samples. The ordering process is extremely slow and passes through many metastable phases; nonetheless, in some runs we have obtained $S(q_0)$ values as high as 50% of the value for a fully ordered lattice (after $\sim 50,000$ MC steps/spin). It is not clear why the system prefers the Type I structure, considering that both Type I and Type III order are ground state configurations for this lattice. It should be noted that also the Ising lattice favors the Type I structure [8]. As has been demonstrated by several studies, the phase transition in the Ising lattice is of the first order [8, 9]. Contrary to the results of Fernandez et al. [1], our data indicate that this is also the case in the Heisenberg lattice. However, the discontinuity in energy, and the hysteresis (see Fig. 2b) is decidedly weaker in this transition than for the Type III lattice. It might be therefore difficult to notice these effects in a system with only 2 048 spins studied by these authors because of large statistical fluctuations which usually occur in Heisenberg systems of that size.

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