

Netz and Berker Reply: The simultaneous implementation [1] of the hard-spin condition and of mean-field theory can indeed be carried out even without using Monte Carlo sampling, as noted by the Comment [2]. In fact, we had also independently come to this conclusion and had proceeded with calculations, some of which will be summarized below. We used the equivalent, compact formulation

$$\langle s_i \rangle \equiv m_i = \sum_{\{s_j\}} \prod_j [(1 + s_j m_j)/2] \tanh \left(\sum_j J_{ij} s_j + H \right), \quad (1)$$

for the spin- $\frac{1}{2}$ Ising model, where $\{s_j\}$ are all spins coupled to s_i , via interactions $\{J_{ij}\}$. Equation (1) constitutes a closed-form approximation to the set of all local magnetizations $\{m_i\}$. This equation can also be generalized to other types of degrees of freedom.

For systems with couplings with translational symmetry, Eq. (1) can be solved with varying degrees of calculational effort. For calculational ease, one can choose to enforce sublatticewise uniformity across the system. For example, this is done in the triangular antiferromagnets by considering solutions in which each of the three sublattices is uniformly magnetized. The phase diagram of the $d=2$ triangular spin- $\frac{1}{2}$ Ising antiferromagnet in a magnetic field is thus obtained quite accurately. However, such uniform solutions are less accurate in frustrated systems that have partially ordered phases, even when the couplings have translational symmetry.

The latter case is illustrated with the $d=3$ stacked-triangular spin- $\frac{1}{2}$ Ising antiferromagnet, with Hamiltonian

$$-\beta\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j + J' \sum'_{\langle ij \rangle} s_i s_j + H \sum_i s_i,$$

where $J > 0$, $s_i = \pm 1$, and the first and second sums are over nearest-neighbor pairs in the x - y planes and along the z direction, respectively. Figure 1(a) shows our calculated magnetizations for $J'=J$ and $H=0$, from solving Eq. (1) for sublatticewise uniform magnetizations. Below the critical temperature $J_c^{-1}=3.40$, two sets of sixfold-degenerate solutions, $(M_a = -M_b, M_c = 0)$ and $(M_a = M_b < -M_c)$ and those related by sublattice interchange and up-down symmetry, appear in addition to the always present zero-magnetization solution. At any temperature, the system is taken to be in the solution that minimizes a free-energy expression [3] that we have derived from Eq. (1). Thus, at the critical temperature, the system undergoes a second-order transition to the $(M_a = -M_b, M_c = 0)$ phase. At a lower temperature, $J_1^{-1}=2.19$, it undergoes a first-order transition to the $(M_a = M_b < -M_c)$ phase.

Figure 1(b) shows the average sublattice magnetizations of the same system, obtained by Monte Carlo implementation of Eq. (1) in which the local magnetization at each site was allowed to vary. Comparing the two figures, it is seen that the restricted (uniform) implementation underestimates the extent of the $(M_a = -M_b, M_c = 0)$ phase. The inset shows the distributions of local magnetizations within each sublattice, in this phase, from

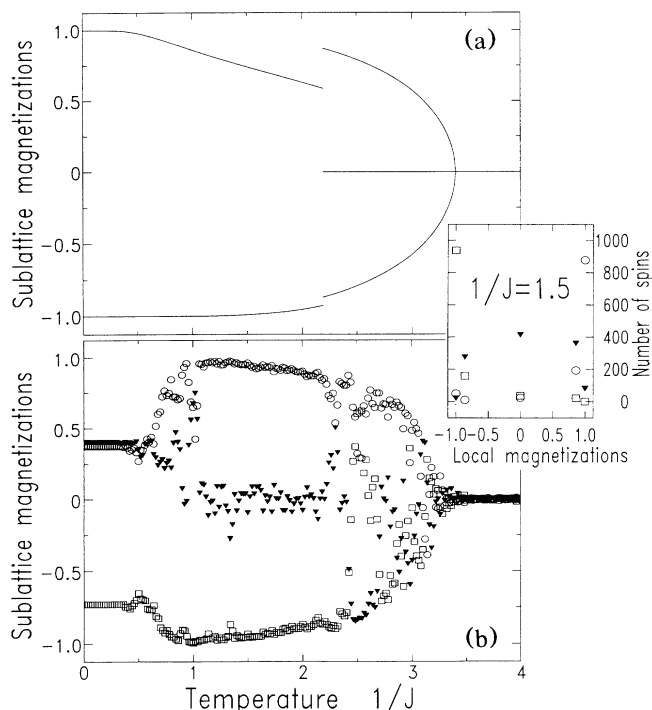


FIG. 1. (a) Uniform sublattice magnetizations of the $d=3$ stacked-triangular spin- $\frac{1}{2}$ Ising antiferromagnet in zero field, obtained from Eq. (1). (b) Average sublattice magnetizations of the same system, obtained from the Monte Carlo implementation of Eq. (1) in which the local magnetization at each site was allowed to vary, using $24 \times 24 \times 12$ spins and 300 MCS after discarding 200 MCS. Both implementations correctly give zero magnetization for the $d=2$ triangular spin- $\frac{1}{2}$ Ising antiferromagnet. Inset: Distributions of local magnetizations within each sublattice (in half of the system), in the intermediate phase of (b).

the calculation of Fig. 1(b). It is seen that the $M_c = 0$ sublattice has a large distribution (64%) of nonzero local magnetizations that average to zero, thus being able to lower considerably its energy. Note that local (nonuniform) solutions of Eq. (1) can also be implemented in closed form without using Monte Carlo sampling [3].

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