Monte Carlo Mean-Field Theory

In a recent Letter, Netz and Berker [1] proposed a new method combining mean-field theory and Monte Carlo sampling and applied it very successfully to frustrated Ising spin systems in two and three dimensions. The method modified mean-field theory by introducing the hard-spin condition and relied on stochastic sampling to determine the local field acting on a given spin. Specifically, for an Ising spin system with Hamiltonian $\beta H = J\sum_{\langle ij\rangle} S_i S_j$, where the $S_i = \pm 1$ at each lattice site i and the sum is over nearest-neighbor spins, their equations are

$$\langle S_i \rangle = \tanh(H_i) , \qquad (1)$$

$$H_i = -J\sum_j S_j , \qquad (2)$$

with the nearest-neighbor field H_i constructed stochastically with $S_j = \pm 1$, the sign of S_j selected to be equal to $\langle S_i \rangle - r$, where r is a random number in the interval $[-1,1]$. As noted by Netz and Berker, conventional mean-field equations would replace (2) by $H_i = -J\sum_j \langle S_j \rangle$.

We make the following observations:

(1) Equation (2) along with Eq. (1) replaced by $\langle S_i \rangle = \langle \tanh(H_i) \rangle$, where the average is taken with respect to the canonical ensemble, are *exact*. This is readily derived by explicitly tracing out the spin S_i in the exact expression for $\langle S_i \rangle$ followed by simple algebraic manipulations. This is one of the Callen identities [2].

(2) Conventional mean-field theory results on replacing $\langle \tanh(H_i) \rangle$ by $\tanh(\langle H_i \rangle)$.

(3) The approach of Netz and Berker is equivalent to an approximate evaluation of $\langle \tanh(H_i) \rangle$ with a factorized statistical weight $P\{S\} = \prod_i \frac{1}{2}(1 + \langle S_i \rangle S_i)$. This is equivalent to expanding $\tanh(H_i)$ as a sum over all possible products of S_j, taking into account $S_j^2 = +1$. Thus for a triangular lattice with nearest-neighbor exchange and a magnetic field,

$$\tanh H_i = a_0 + \sum_{j=1}^{6} a_1 S_j + \sum_{j \neq k} a_2 S_j S_k + \cdots + a_6 S_1 S_2 S_3 S_4 S_5 S_6 ,$$

where S_j, $j = 1-6$, are nearest-neighbor sites of i. The a's are functions of the magnetic field and coupling. Following the expansion, the averages are factorized, with, e.g., $\langle S_j S_k S_l \rangle = \langle S_j \rangle \langle S_k \rangle \langle S_l \rangle$ $(j \neq k \neq l)$.

(4) Thus, the Netz and Berker method is an improved mean-field theory [3] and does *not* require any Monte Carlo sampling. Indeed, we have been able to rederive the results of Ref. [1], almost trivially, for the nearest-neighbor antiferromagnetic Ising model on a triangular lattice with three coupled equations for the sublattice magnetizations. In practice, for a continuous spin model with no translational symmetry, the Netz-Berker Monte Carlo mean-field idea may be particularly useful.

(5) The improved mean-field theory is exact in one dimension in the absence of an external field. However, it does not distinguish between a ferromagnet on a triangular lattice in two dimensions and on a simple cubic lattice in three dimensions. The improved mean-field theory is exact to $O(1/d^2)$ in a large-d expansion for a nearest-neighbor Ising ferromagnet on a hypercubic lattice.

(6) For an Ising ferromagnet on a square lattice, the improved mean-field theory yields $J_c \simeq 0.3236$ compared with the standard mean-field prediction $J_c \equiv 0.25$ and the Onsager result $J_c \approx 0.4407$. The spectacular agreement of Netz and Berker [1] with conventional Monte Carlo simulations suggests that the factorization approximation is better for fully frustrated systems.

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