Hard-spin mean-field theory: A systematic derivation and exact correlations in one dimension

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Hard-spin mean-field theory is an improved mean-field approach which has proven to give accurate results, especially for frustrated spin systems, with relatively little computational effort. In this work, the previous phenomenological derivation is supplanted by a systematic and generic derivation that opens the possibility for systematic improvements, especially for the calculation of long-range correlation functions. A first level of improvement suffices to recover the exact long-range values of the correlation functions in one dimension.

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I. INTRODUCTION

Hard-spin mean-field theory (HSMFT) [1–11] is a novel ''mean-field'' approach for classical spin models, which correctly gives no finite-temperature phase transition in one dimension, and agrees quantitatively with the existing Monte Carlo data for the finite-field phase diagram of the fully frustrated antiferromagnetic Ising model on a triangular lattice [1,2,8]. The latter has a zero-temperature phase transition in the absence of external field, in contrast to the ferromagnetic version with a finite Curie temperature. All these features attest to its superiority to the standard mean-field methods, which fail in these regards.

In this paper, I present a generic derivation of the HSMFT equations, allowing for systematic improvements of their accuracy, and later argue that the lowest level of approximation is rather inaccurate in predicting $\langle s_i s_j \rangle$. Nevertheless, the next level of approximation within the same framework recovers the exact result in spatial dimension $d=1$. At this level, HSMFT also differentiates between a two-dimensional (2D) triangular and a 3D cubic lattice which is otherwise a typical failure of the mean-field theories.

HSMFT combines the mean-field logic with the hard-spin condition ($s^2=1$) which is in fact a crucial aspect of the frustrated Ising models. Therefore it is particularly successful in the analysis of such systems (for a recent study, see, e.g., [12]). Below is a systematic description of the theory.

II. HARD-SPIN MEAN-FIELD THEORY: A SYSTEMATIC GENERIC DERIVATION

Given a lattice in any dimension, consider the partition in Fig. 1. Consider nearest-neighbor couplings so that there is no direct coupling between the spins in regions S_1 and S_2 (for longer range interactions, the boundary B should be chosen thick enough to ensure this decoupling). Decompose the Hamiltonian into three parts:

$$\mathcal{H}=\mathcal{H}_1+\mathcal{H}_2+\mathcal{H}_B,$$

such that $\mathcal{H}_1$ and $\mathcal{H}_2$ involve interactions within S_1 and S_2 respectively, and $\mathcal{H}_B$ contains the rest of the interactions. Then for a particular spin operator $\mathcal{O}_1$ in S_1,

$$\langle \mathcal{O}_1 \rangle = \frac{\sum_S \mathcal{O}_1 e^{-\beta\mathcal{H}}}{\sum_S e^{-\beta\mathcal{H}}} = \sum_B \frac{\sum_{S\setminus B} \mathcal{O}_1 e^{-\beta(\mathcal{H}_1+\mathcal{H}_2+\mathcal{H}_B)}}{\sum_S e^{-\beta\mathcal{H}}}$$

$$= \sum_B \frac{\sum_{S_2} e^{-\beta(\mathcal{H}_2+\mathcal{H}_B)}}{\sum_S e^{-\beta\mathcal{H}}} \cdot \sum_{S_1} \mathcal{O}_1 e^{-\beta\mathcal{H}_1}$$

$$= \sum_B \frac{\sum_{S\setminus B} e^{-\beta\mathcal{H}}}{\sum_S e^{-\beta\mathcal{H}}} \cdot \frac{\sum_{S_1} \mathcal{O}_1 e^{-\beta\mathcal{H}_1}}{\sum_{S_1} e^{-\beta\mathcal{H}_1}}$$

$$= \sum_B p(B) \langle \mathcal{O}_1 \rangle_1^{(B)}, \quad (1)$$

where $\langle \mathcal{O}_1 \rangle_1^{(B)}$ indicates the average of $\mathcal{O}_1$ over S_1 with a fixed boundary condition (i.e., a frozen configuration of B). Note that above intuitive result is exact. Now, $p(B)$, being a function of spins in B only, can be written as

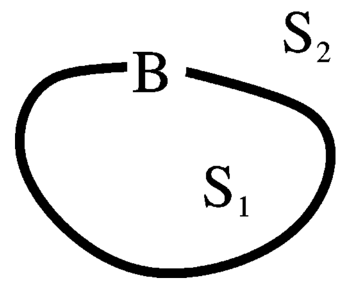

FIG. 1. Decomposition of space into three parts: S_1 (bounded), B (boundary), and S_2 (outside).

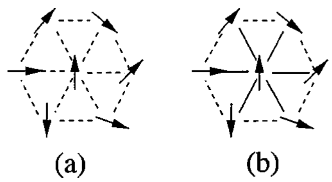

FIG. 2. Standard MFT (a) versus HSMFT (b). Dashed lines indicate the neglected correlations in each case.

$$p(B)=\frac{1}{2^{N_B}}\Bigg(1+\sum_{i\in B} s_i\langle s_i\rangle_S+\sum_{i,j\in B} s_is_j\langle s_is_j\rangle_S+\cdots$$
$$+s_1s_2\ldots s_{N_B}\langle s_1s_2\ldots s_{N_B}\rangle_S\Bigg). \tag{2}$$

HSMFT equations, written down phenomenologically in previous works [1,2], are obtained from this systematic expansion by neglecting the correlations in Eq. (2) for $p(B)$. However, this can be done at different levels. We can neglect all connected graphs by setting

$$\langle s_is_j\cdots s_k\rangle=\langle s_i\rangle\langle s_j\rangle\cdots\langle s_k\rangle. \tag{3}$$

This leads to a set of self-consistent equations for $\langle s_i\rangle$. To contrast with traditional mean-field theory, what we neglect here is the effect of correlations among the boundary spins on the average magnetization of s_0, rather than the correlations of s_0 itself with its neighbors (Fig. 2). We will see below that the above improvement on the traditional mean-field approximation already recovers the exact value of $\langle s\rangle=0$ for the 1D Ising ferromagnet, but predicts the nearest-neighbor correlation $\langle s_is_j\rangle$ incorrectly. Yet the exact values for $\langle s_is_j\rangle$ can be obtained by further including two-point connected graphs in Eq. (2).

III. HSMFT OF THE $d=1$ ISING FERROMAGNET

Consider the one dimensional ferromagnetic Ising model given by the Hamiltonian

$$-\beta\mathcal{H}=J\sum_i s_is_{i+1}.$$

In correspondence with the above partition, define $S_1\equiv\{s_0\},B\equiv\{s_-,s_+\}$ (left and right neighbors of s_0), and S_2 as the rest of the spin chain. Then the self-consistent equation for $\langle s_0\rangle\equiv m$ is

$$m=\sum_{s_-,s_+}\frac{1}{4}(1+s_-m+s_+m+s_-s_+m^2)\tanh[J(s_-+s_+)], \tag{4}$$

which simplifies to

$$m=m\tanh(2J),$$

correctly giving $m=0$ everywhere except at zero temperature. Conventional mean-field theory spuriously yields $m\neq0$ for $J>J_c=0.5$. A similar HSMFT calculation on the square lattice yields

$$\tanh 2J_c=\gamma\simeq0.57\Rightarrow\ \ J_c\simeq0.323,$$

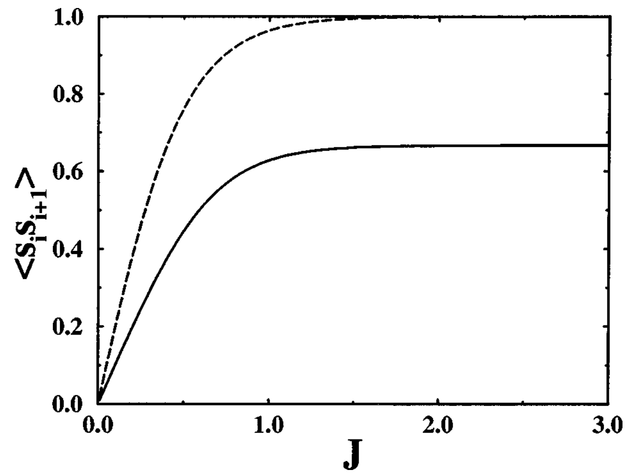

FIG. 3. HSMFT prediction for $\langle s_is_{i+1}\rangle$ (solid) compared with the exact value of $\tanh J$ (dashed), which is recovered at the next level of approximation implemented here.

where γ is the real root of $\gamma^3-2\gamma^2+\gamma-1=0$. This result is to be compared with the exact value $J_c=0.4407$ and the mean-field result $J_c=0.25$.

Similarly, by choosing S_1 to be a cluster of two spins, one can write down self-consistent equations for m and $\Gamma_1\equiv\langle s_0s_1\rangle$ and solve simultaneously. Let now $S_1\equiv\{s_1,s_2\}$ (a nearest-neighbor pair), $B\equiv\{s_-,s_+\}$ (left and right neighbors of the S_1 cluster), and S_2 the rest of the spin chain. As before, $m=0$ is obtained from Eq. (1) and we calculate Γ_1 similarly as

$$\Gamma_1=\sum_{s_-,s_+}\frac{1}{4}[1+m\,(s_-+s_+)+m^2s_-s_+]$$
$$\times\frac{\sum_{s_1,s_2}s_1s_2e^{J(s_-s_1+s_1s_2+s_2s_+)}}{\sum_{s_1,s_2}e^{J(s_-s_1+s_1s_2+s_2s_+)}}, \tag{5}$$

which simplifies to give

$$\Gamma_1=\frac{1}{2}\left(\frac{e^{2J}\cosh 2J-1}{e^{2J}\cosh 2J+1}+\frac{e^{2J}-\cosh 2J}{e^{2J}+\cosh 2J}\right). \tag{6}$$

Figure 3 provides a comparison of Eq. (6) and the exact value, $\Gamma_1=\tanh J$. In the low temperature limit ($J\rightarrow\infty$), we incorrectly obtain $\Gamma_1\rightarrow2/3$ rather than 1. Yet, note that we obtain a nonzero correlation in spite of the fact that *all* connected graphs are neglected in Eq. (2). Without including any connected graphs, this result can be improved by considering a larger S_1 cluster, as was suggested in Ref. [2]. For example, for a cluster of three spins, one gets $\Gamma_1=3/4$ and $\Gamma_2=\langle s_0s_2\rangle=1/2$. A nonzero value for $\langle s_is_j\rangle$ is inaccessible for $m=0$ with standard mean-field theory.

In this paper, we suggest, as an alternative approach, to take into account two-point connected graphs while calculating $\Gamma_r\equiv\langle s_0s_r\rangle$, so that Eq. (2) is now approximated using

$$\langle s_1 s_2 \cdots s_n \rangle = m^n + m^{n-2} \sum_{i>j} \langle s_i s_j \rangle_c + m^{n-3} \sum_i \sum_{j>k}{}' \langle s_i s_j \rangle_c \langle s_i s_k \rangle_c + \frac{1}{2} m^{n-4} \sum_{i>j} \sum_{k>l}{}' \langle s_i s_j \rangle_c \langle s_k s_l \rangle_c + \cdots, \tag{7}$$

where ''primed'' sums exclude the index (indices) fixed by the preceeding sum, and $\langle \cdot \rangle_c$ refers to the connected part, i.e., $\langle s_i s_j \rangle_c = \langle s_i s_j \rangle - m^2$. This improvement in the HSMFT is qualitatively different from what is suggested in Ref. [2]. The latter relies on considering larger S_1 clusters so that the boundary effects become less important, whereas the former takes into account the correlations of boundary spins for a chosen S_1 cluster. In one dimension, where the boundary consists of only two spins independent of the size of the cluster S_1, we expect to get the exact result $\langle s_0 s_r \rangle = (\tanh J)^r$ after including the second term on the LHS of Eq. (7), since there are no higher order connected graphs left out. HSMFT equations in this case reduce to hierarchical equations relating Γ_{2n-1} to Γ_{2n+1}:

$$\Gamma_{2n-1} = \frac{1}{2} f^+_{2n-1} + \frac{\Gamma_{2n+1}}{2} f^-_{2n-1}, \tag{8}$$

where

$$f^\pm_{2n-1} = \frac{\beta_{2n-1}\cosh 2J - 1}{\beta_{2n-1}\cosh 2J + 1} \pm \frac{\beta_{2n-1} - \cosh 2J}{\beta_{2n-1} + \cosh 2J},$$

and

$$\beta_{2n+1} = \frac{\beta_{2n-1}\cosh 2J + 1}{\beta_{2n-1} + \cosh 2J}, \quad \beta_1 = e^{2J}.$$

Therefore by substitution,

$$\Gamma_{2n+1} = \frac{1}{2} f^+_{2n+1} + \frac{1}{4} f^-_{2n+1} f^+_{2n+3} + \frac{1}{8} f^-_{2n+1} f^-_{2n+3} f^+_{2n+5} + \cdots. \tag{9}$$

It was confirmed numerically that Eq. (9) converges to

$$\Gamma_{2n+1} = (\tanh J)^{2n+1},$$

which is the exact value. The correlations for spins separated with an even lattice spacing can be calculated in exactly the same manner by the initial choice of three nearest-neighbor spins for S_1. Also note that using Eq. (7) in two and three dimensions allows for *different* sets of coupled equations similar to Eq. (8) (yet certainly more cumbersome), even though the coordination number may be the same. The solutions of such equations in higher dimensions may require further approximations since the problem gets intrinsically difficult, yet still easier than an exact solution due to the neglecting of all but two-point connected graphs. In contrast with the standard mean-field equations, they will be dimension-sensitive since the boundary of a cluster grows as L^{d-1}. It can be interesting to see if the power-law decay of the critical correlations in high dimensions is accessible within HSMFT. Study in this direction is in progress.

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