From GM law
to
A powerful mean field scheme

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Abstract

A new and powerful mean field scheme is presented. It maps to a one-dimensional finite closed chain in an external field. The chain size accounts for lattice topologies. Moreover lattice connectivity is rescaled according to the GM law recently obtained in percolation theory. The associated self-consistent mean-field equation of state yields critical temperatures which are within a few percent of exact estimates. Results are obtained for a large variety of lattices and dimensions. The Ising lower critical dimension for the onset of phase transitions is \( d_l = 1 + \frac{2}{q} \). For the Ising hypercube it becomes the Golden number \( d_l = \frac{1+\sqrt{5}}{2} \). The scheme recovers the exact result of no long range order for non-zero temperature Ising triangular antiferromagnets.

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1 Introduction

For many years basic mean-field theory has been applied to a huge variety of problems. It is a very simple way to tackle collective phenomena [1]. Most of the time it yields a correct qualitative description. However, quantitatively the results are very poor. In particular, all aspects of the critical behavior are grossly misrepresented [2]. Moreover some results are even wrong like for instance the existence of long range order for the Ising system at both one dimension for ferromagnets and at two dimensions for the triangular antiferromagnets.

The Bethe scheme [3] was then introduced to extend the Weiss one spin approach [4] to a cluster of fluctuating spins. For decades it has been looked upon as a solid improvement. It yields no long range order at one dimension and even becomes exact for the hypercube at infinite dimensions [1]. However quantitative results are yet rather poor. Moreover it was demonstrated recently that the Bethe scheme violates systematically translational invariance [5]. As such it is forbidden by symmetry.

In this paper we present a new and powerful mean field scheme. It embodies the Bethe idea of including a fluctuating spin cluster yet preserving the overall lattice translational invariance. In addition, the connectivity between fluctuating clusters is rescaled according to the GM law introduced few years ago in percolation theory [6].

Associated critical temperatures are calculated for a large variety of lattices and at several dimensions. Discrepancies with available exact estimates are only within few percent. The lower critical dimension for the onset of phase transitions is found to be $d_l = 1 + \frac{2}{q}$ for Ising systems. It turns to the Golden number $d_l = \frac{1 + \sqrt{5}}{2}$ for hypercubes ($q = 2d$). In the case of the triangular Ising antiferromagnet the exact result of no long range order is reproduced [7].

2 Revisiting the Bethe approximation

Mean-field theory is a one-site approach which first breaks the lattice symmetry by discriminating between fluctuating degrees of freedom and averaged ones [1]. Two interpenetrated lattices are thus defined. Equating the thermal average of fluctuating degree of freedom to the already averaged ones restores
the initial lattice symmetry. Simultaneously a self-consistent equation of state is obtained.

To implement a Bethe scheme [3] on a lattice 3 distinct interpenetrated sublattices (A, B, C) must be introduced. First the fluctuating center (A), then the fluctuating nearest neighbors (B) and last the mean field nearest neighbors (nn) of the nn (B) not including the center (A). From the A-spin plus these B and C shells, a cell is constituted to pave the whole space and reproduce the full lattice topology.

Cluster center (A) has thus all its nn spins (B) which are fluctuating while surface cluster spins (B) have mean-field nn spins (C) and one nn fluctuating spin (A). Simultaneously mean-field spins (C) have all their nn which are fluctuating spins, making their environment identical to the cluster center.

On this basis the Bethe requirement $\langle S_A \rangle = \langle S_B \rangle$ is not compatible with the equality $m_C = \langle S_B \rangle$ which should also hold to ensure translational invariance. The Bethe topology is therefore forbidden by symmetry. It is not the case for one-site Weiss theory. For a detailed demonstration see [5]

Last but not least, it is worth noticing it is indeed this very symmetry problem which makes the Bethe approach exact on the Cayley tree lattice. This lattice does not exhibit translational invariance by construction. This symmetry breaking was overlooked for several decades.

3 A new powerful mean field scheme

From the discovery of a systematic Bethe induced symmetry breaking arises the question of the possibility to indeed extend a mean field treatment to more than one site.

Above analysis of the Bethe scheme emphasizes the role of the cluster center in the irreversible breaking of the symmetry. It hints to avoid such a fluctuating center. One way to achieve this constraint is to use compact closed linear loops within the lattice topology. For instance compact 4-spin squares and 3-spin triangles for respectively square and triangular lattices.

Each one of these plaquettes is then set respectively as A-species (fluctuating) and B-species (mean field) with a staggered-like coverage pattern. A-plaquettes (B-plaquettes) have thus all their nn plaquettes as B-plaquettes (A-plaquettes).

For a given plaquette, each spin has two nn spins of the same species
within the plaquette itself and \((q - 2)\) nn spins of the other species belonging to nn plaquettes. At this stage we have a series of fluctuating one-dimensional closed chains in an external field \(h\). The number of spins \(N\) in each chain is determined from lattice topology. It is \(N = 4\), \(N = 3\), \(N = 3\) and \(N = 6\) for respectively square, triangular, Kagomé and Honeycomb lattices.

It is the interactions with nn mean-field spin plaquettes which produce the field \(h\). We have \(h = \delta Jm\) where \(\delta\) accounts for connectivity to B-sublattices, \(J\) is the nn coupling constant and \(m\) the averaged magnetization on the B-sublattice. The problem can now be solved exactly. In particular, the chain site magnetization is [1],

\[
<S_i> = \beta \exp 2K \left\{ \frac{(1 - \tanh(K)^N)}{(1 + \tanh(K)^N)} \right\} h ,
\]

at order one in \(h\). Here \(i \in A\)-plaquettes. \(K \equiv \frac{J}{k_B T}\) where \(k_B\) is the Boltzmann constant and \(T\) the temperature.

Putting \(<S_i> = m\) restores the initial lattice symmetry. It is indeed possible since only two sublattices were involved which was not the case for the 3 sublattice Bethe scheme. The self-consistent equation of state is,

\[
m = \delta K \exp 2K \left\{ \frac{(1 - \tanh(K)^N)}{(1 + \tanh(K)^N)} \right\} m + ... ,
\]

at order one in \(m\) and using \(h = \delta Jm\). To solve Eq. (2) needs to determine the value of \(\delta\).

It is then worth to evoke a recent work on percolation thresholds, the GM law [6]. It shows that relevant connectivity variables for site and bond dilution are respectively \((d - 1)(q - 1)\) and \((d - 1)(d - 1)\). In other words, for site percolation, the number of possible directions \((q - 1)\) from a given site, has to be multiplied by \((d - 1)\). For bond percolation this effective number of site directions has to be divided by dimension \(d\). Using these variables, the GM law was found to yield all percolation thresholds for all Bravais lattices at all dimensions [6].

This percolation finding suggests to consider here a rescaled connectivity between closed loops instead of \(\delta = q - 2\). Using above counting, we first start with \(q\) instead of \((q - 1)\) since now dealing with pair exchange interactions and not percolation. Second we renormalize \(q\) by \((d - 1)\) giving \(q(d - 1)\). However the 2 neighboring sites which are treated exactly within the closed loop have
to be substracted from the effective number of sites which gives \( q(d - 1) - 2 \).
Moreover, interactions being related to bonds, we divide this number by \( d \) as for bond percolation. These considerations lead to a connectivity,
\[
\delta = \frac{q(d - 1) - 2}{d}.
\] (3)

4 Results

We can now check the validity of our simple symmetry preserving model with respect to critical temperatures. From Eq. (2) we get,
\[
\delta K_c^G \exp 2K_c^G \left\{ \frac{(1 - \tanh(K_c^G)N)}{(1 + \tanh(K_c^G)N)} \right\} = 1.
\] (4)
The trivial connectivity counting \( \delta = q - 2 \) already improves Weiss model. For instance \( K_c^G = 0.29 \) in the square case and \( T_c = 0 \) at \( d = 1 \). We now proceed using Eq. (3) for connectivity.

For the square case (\( q = 4, N = 4 \)), \( \delta = 1 \) which gives \( K_c^G = 0.4399 \). Exact result is \( K_c^G = 0.4407 \). In the case of triangular lattice (\( q = 6, N = 3 \)), \( K_c^G = 0.2919 \) with \( \delta = 2 \) while the exact estimate is \( K_c^G = 0.2746 \). For Kagomé (\( q = 4, N = 3 \)) \( \delta = 1 \) yielding \( K_c^G = 0.4649 \) for an exact estimate of \( K_c^G = 0.4666 \). And \( K_c^G = 0.6160 \) for the honeycomb lattice (\( q = 3, N = 6 \)) where \( \delta = \frac{1}{2} \) for an exact estimate of \( K_c^G = 0.6585 \) (see Table I).

Going to \( d = 3 \) imposes to restrict the plaquette size to \( N = 4 \) since a one-dimensional loop cannot embody a three-dimensional topology. However there exits a \( d \)-dependence through Eq. (3). We get \( \delta = \frac{10}{3}, \delta = \frac{14}{3} \) and \( \delta = \frac{22}{3} \) for respectively cubic, fcc and bcc lattices. Corresponding critical temperatures are given by \( K_c^G = 0.2012, 0.1568, 0.1096 \) respectively for exact estimates of 0.2217, 0.1575, and 0.1021 (see Table I).

Critical temperature estimates [8, 9] are available for the hypercube at \( d = 5, 6, 7 \). These are \( K_c^e = 0.1139, 0.0923, 0.0777 \) respectively.

To get the \( d \rightarrow \infty \) asymptotic limit of our model we take both \( q \rightarrow \infty \) and \( J \rightarrow 0 \) under the constraint \( qJ = \text{cst} \). From Eq. (3) connectivity limit is \( \delta \rightarrow q(1 - \frac{1}{d}) \) which gives always,
\[
\delta \rightarrow q \quad \text{(5)}
\]
at leading order. Indeed $q$ diverges always quicker than $\frac{2}{d}$ even for $fcc$-lattices where $q = 2d(d - 1)$. In turn Eq. (4) becomes,

$$K^G_c = \frac{1}{q} ,$$

which is the mean-field result [1] as expected in the $d \to \infty$ limit.

To evaluate the sensibility on the loop size, it is fruitful to expand Eq. (4) in powers of $K$. It gives

$$K^G_c (1 + 2K^G_c + \ldots + \frac{(2K^G_c)^N}{N!})(1 - (K^G_c)^N + \ldots)(1 - (K^G_c)^N + \ldots) = \frac{1}{\delta} .$$

Since $N \geq 3$, a simple analytic expression is obtained only at order one,

$$K^G_c = \frac{1}{\delta} .$$

At two dimensions Eq. (8) gives $K^G_c = 1, \frac{1}{2}, 1, 2$ for respectively the square, triangular, Kagomé and for honeycomb lattices. These results are rather poor and shows the importance of the finite value of $N$ which embodies part of the lattice topology.

5 Conclusion

We have presented a very simple self-consistent model which yields rather good values for critical temperatures within a few percent of exact results. Besides a rescaled lattice connectivity, the finite length of the loops is also taken into account. This new scheme represents a substantial improvement over existing mean-field cluster approximations.

We can also determine from our model a lower critical dimension for phase transitions. It comes from the condition $h = 0$ for which we have a one-dimensional finite system. Such a system has no long range order at $T \neq 0$. Phase transitions are thus obtained only in the range $h \neq 0$ which gives $q(d - 1) > 2$ leading to,

$$d_l = 1 + \frac{2}{q} .$$
For the Ising hypercube ($q = 2d$) it becomes the Golden number $d_l = \frac{1 + \sqrt{5}}{2}$, which excludes the $d = 1$ case and contains $d = 2$ as it should be. Last but not least, applying our scheme to the Ising triangular antiferromagnet[7] we do recover the exact result of no long range order at non-zero temperatures; contrary to usual mean field approaches.
References

1. R. K. Pathria, Statistical Mechanics, Pergamon Press (1972)
2. Sh-k Ma, Modern Theory of Critical Phenomena, The Benjamin Inc.: Reading MA (1976)
3. H. A. Bethe, Proc. Roy. Soc. London A150, 552 (1935)
4. P. Weiss, J. Phys. Radium, Paris 6, 667 (1907)
5. S. Galam, Phys. Rev. B54, 1599 (1996)
6. S. Galam and A. Mauger, Phys. Rev. B53, 2171 (1996)
7. S. Galam and P. V. Koseleff, to be published (2000)
8. M. E. Fisher, Repts. Prog. Phys. VXXX (II), 671 (1967)
9. J. Adler, in “Recent developments in computer simulation studies in Condensed matter physics”, VIII, edited by D. P. Landau, Springer (1995)
| Dimension | Lattice   | $q$ | $\delta$ | $K_e^c$ | $K_G^c$ |
|-----------|-----------|-----|--------|--------|--------|
| $d = 2$   | Square    | 4   | 1      | 0.4407 | 0.4399 |
|           | Honeycomb | 3   | $\frac{1}{2}$ | 0.6585 | 0.6160 |
|           | Triangular| 6   | 2      | 0.2746 | 0.2837 |
| $d = 2$   | Kagome*   | 4   | 1      | 0.4666 | 0.4649 |
| $d = 3$   | Diamond   | 4   | 2      | 0.3698 | 0.2857 |
|           | sc        | 6   | $\frac{10}{3}$ | 0.2216 | 0.2012 |
|           | bcc       | 8   | $\frac{14}{3}$ | 0.1574 | 0.1568 |
|           | fcc       | 12  | $\frac{22}{3}$ | 0.1021 | 0.1096 |
| $d = 4$   | sc        | 8   | $\frac{21}{4}$ | 0.1497 | 0.1380 |
|           | fcc       | 24  | $\frac{23}{2}$ | 0.0749 |        |
| $d = 5$   | sc        | 10  | $\frac{24}{5}$ | 0.1139 | 0.1064 |
|           | fcc       | 40  | $\frac{158}{5}$ | 0.0298 |        |
| $d = 6$   | sc        | 12  | $\frac{29}{3}$ | 0.0923 | 0.0869 |
| $d = 7$   | sc        | 14  | $\frac{34}{7}$ | 0.0777 | 0.0737 |

Table 1: $K_G^c$ from this work compared to “exact estimates” $K_e^c$ taken from [8, 9].