

## Correlated molecular-field theory for Ising models

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The critical temperature  $T_c$  of Ising models is obtained quite accurately by simple improvements over the standard molecular-field theory. The important physical effect we include is that the effective field of neighboring spins is influenced by the spin state of the central spin. When used in combination with a self-consistency condition, this correlated molecular-field theory leads to estimates of  $T_c$  more accurate than those obtained from the Bethe-Peierls-Weiss approximation.

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### I. INTRODUCTION

Decades have passed since introduction of the Ising model [1] for magnetic phase transitions. The exact solution in one dimension (1D) by Ising [1] exhibits no phase transition at a nonzero temperature. In two dimensions, the exact critical temperature  $T_c$  for the square lattice Ising model was obtained by Kramers and Wannier [2]. In his famous work shortly afterwards, Onsager [3] determined the free energy exactly. Other exact results, including  $T_c$ , have been found for honeycomb and triangular lattices [4–6]. For other lattices and higher dimensions there is no exact calculation of  $T_c$ , however, various forms of molecular field theory [7] have been applied and improved upon. In this work we present a simple, physically motivated modification to molecular-field theory that gives reasonably accurate estimates of  $T_c$ .

In magnetism the molecular or mean-field (MF) approach originally used by Pierre Weiss [8] was very successful at showing the transition to a magnetically ordered state for Heisenberg and Ising models at a nonzero transition temperature  $T_c$ . However, the usual mean-field approach can be shown to be equivalent to having each site interacting equally with all other sites; its prediction of critical temperature is not very accurate. Physically, having a particular spin interacting equally with all others of the system ignores both the presence of a finite correlation length and the strong fluctuations near  $T_c$ . MF theory has other faults; it can predict a phase transition at finite temperature in the 1D Ising model, an impossibility not present in the exact solution. Being a high-temperature and local theory, the MF approach does not produce the correct decay of the magnetization as expected from spinwave theory ( $T^{3/2}$  Bloch law [9]) at very low temperature. The influence of physically important effects near  $T_c$  have been evaluated at length via the renormalization group approach due to Wilson [10], Fisher [11], Kadanoff [12], and others. Despite its known limitations, it is still interesting to consider how to improve the MF approach and see whether it is possible for it to include, at the very least, some local correlation effects.

This is a subject with a long history; here we can mention some of the more notable approaches. The book by Smart

[13] gives an excellent review. Significant improvements to MF theory were achieved by Bethe [14], who developed a procedure to analyze exactly a small cluster of spins near the central one, and then the interaction of the edges of the cluster with the rest of the system is effected by a mean field. Bethe originally developed the procedure for an order-disorder model; it was applied to the Ising model by Peierls [15] and the Heisenberg model by Weiss [16]. The Bethe-Peierls-Weiss (BPW) approach includes *local* spin correlations and fluctuations, and details of the type of lattice, beyond the effects of the coordination number,  $z$ . To obtain a solution, a self-consistency condition is imposed: the mean values of the spins in the cluster (the central spin and some set of neighbors) must all be the same. This condition determines the mean-field due to the spins outside of the cluster. In principle, this cluster approach can be carried out to larger and larger clusters, resulting in a sequence of improved  $T_c$  estimates. In practice, however, it is difficult to calculate exactly beyond a few nearest neighbors.

Oguchi [17] applied a correction originally used by Van Vleck [18], by considering an interacting pair in the mean field of its surrounding sites, however, the method gives little improvement over the MF approach in the estimate of  $T_c$ . A more systematic approach for correcting the MF theory has been developed by Callen [19,20] and co-workers, using a diagrammatic expansion method. The zeroth order approximation in this scheme recovers the MF results, while the first order approximation tends to underestimate  $T_c$  for Ising models. More recently, Mattis [21] considered an Ising model where each spin is subjected to the entire distribution of all allowed values of the molecular field, based on ideas due to Marshall [22] and Klein and Brout [23]. The scheme does not predict  $T_c$  as accurately as the BPW approximation.

Thus we are interested in other MF approximations that include correlation of the neighbors to the central spin and total self-consistency. Here we present a simple improved MF calculation where the molecular field acting on a central spin is allowed to depend on the state of the central spin. While this type of effect *is* included in the BPW approximation, the approximation we present is much simpler and gives estimates of  $T_c$  better than the BPW approximation for most lattices.

For Ising, XY, or Heisenberg models, characterized by the number of spin components  $n = 1, 2, 3$ , respectively, the Onsager reaction field (ORF) theory [24] is another approximate method that includes correlation effects. A clear review of the ORF method is given by White [25].

Before presenting our modified molecular-field approach, we summarize the procedures and results of the BPW and ORF methods, for later comparison of results.

## II. THE BETHE-PEIERLS-WEISS APPROXIMATION

The Ising Hamiltonian under consideration is

$$H = -J \sum_{(i,j)} \sigma_i \sigma_j, \quad (1)$$

where the sum is over near-neighbor pairs on some lattice,  $J$  is the bond coupling strength, and each  $\sigma_i$  takes values  $\pm 1$ . In the lowest approximation due to BPW, the  $z$  nearest neighbors  $\sigma'_i$  of a site  $\sigma_i$  do not take on the mean-field values. Instead, the second nearest neighbors  $\sigma''_i$  have the mean-field values, the nearest neighbors are allowed to take on the values  $\pm 1$  and are treated exactly. The constraint that the averages  $\langle \sigma_i \rangle$  and  $\langle \sigma'_i \rangle$  must both give the same value leads to the prediction for the critical coupling  $\beta_c \equiv J/(k_B T_c)$ ,

$$\coth \beta_c = z - 1. \quad (2)$$

The result is only a function of the coordination number and is a surprising improvement over the mean-field result,  $\beta_c = z^{-1}$ . For the 2D square lattice Eq. (2) gives  $k_B T_c/J = 2.885$ , compared with the mean-field result,  $k_B T_c/J = 4$ , and the exact result  $k_B T_c/J = 2.269 \dots$  from Onsager's equation [3]  $\sinh 2\beta_c = 1$ . There are corresponding (lesser) improvements for other lattices with higher coordination number, these are summarized below after we discuss our improvements to the standard mean-field approach.

## III. ONSAGER REACTION FIELD CORRECTION

In the ORF calculation (see Ref. [25] for more details), the spin at a chosen site interacts with the mean-field reduced by a "reaction field" that depends on the spin at that site [24]. The idea is that the mean-field is strongly determined by the polarization of the central spin being considered, so in essence one should subtract this reaction part to avoid counting a self-interaction part. The reaction field is determined self-consistently, with the calculation realized in wave vector space. The ORF procedure depends on a Fourier transform of the spin field  $\sigma_i$  into the reciprocal space quantity,  $\sigma_{\mathbf{q}}$ . As such it includes effects dependent on the coordination number  $z$ , the number of spin components  $n$ , and the actual lattice structure. For reference, the ORF theory predicts the critical temperature  $T_c$  as

$$\frac{k_B T_c}{J} = \frac{z}{nI}, \quad (3)$$

where the constant  $I$  is given from a q-space sum for  $N$  sites,

$$I = \frac{1}{N} \sum_{\mathbf{q}} \frac{1}{1 - J(\mathbf{q})/J(\mathbf{0})}, \quad (4)$$

and  $J(\mathbf{q}) = \sum_j J e^{-i\mathbf{q} \cdot \mathbf{a}_j}$  is the Fourier-transformed exchange interaction (sum over displacements to nearest neighbors,  $\mathbf{a}_j$ ). From sums over the appropriate Brillouin zones, the values of  $I$  are 1.516, 1.393, and 1.345 for sc, bcc, and fcc lattices, respectively. When applied to the Ising model ( $n = 1$ ) in three dimensions, one gets  $k_B T_c/J = 3.957, 5.742, 8.924$  for sc, bcc, and fcc lattices. The ORF procedure, however, does not work in one or two dimensions, where the sum  $I$  diverges. Also, there are modifications necessary to apply ORF to lattices with a basis [26]. For the diamond lattice, using the underlying fcc lattice with a basis, one gets  $I = 1.79288$  and  $k_B T_c/J = 2.2310$ .

## IV. CORRELATED MOLECULAR-FIELD THEORY: NEIGHBOR CORRELATIONS

Here we consider an even simpler idea to modify and improve the standard MF theory for Ising models, that we refer to as "correlated field" (CF) approximation. The calculation is carried out in real space. A central spin directly influences the mean-value of its nearest neighbors, which then act back on the central spin, similar in spirit to the Onsager reaction field. Thus, it is reasonable to set the molecular field of the nearest neighbors to be two *different* values, say,  $m^+$  and  $m^-$ , depending on whether the central site has values  $+1$  or  $-1$ , respectively. With this "correlated neighbor field," the correlated-MF Hamiltonian for a given spin  $\sigma_i$  can be written

$$H_{\text{MMF}} = -\sigma_i h_{\text{eff}}, \quad (5)$$

where the effective field due to its  $z$  nearest neighbors is taken as

$$h_{\text{eff}} = zJ(\delta_{\sigma_i, 1} m^+ + \delta_{\sigma_i, -1} m^-). \quad (6)$$

The delta functions constrain the neighbor-field to the different values  $m^+$  and  $m^-$  according to the value of the central spin  $\sigma_i$ . The neighbor fields  $m^+$  and  $m^-$  are determined self-consistently in this theory, below. Averaging over the values  $\pm 1$  of site  $i$ , with this Hamiltonian, gives

$$m \equiv \langle \sigma_i \rangle = \frac{e^{\beta z m^+} - e^{-\beta z m^-}}{e^{\beta z m^+} + e^{-\beta z m^-}}, \quad (7)$$

where  $\beta \equiv J/(k_B T)$  is the inverse temperature.

Now suppose the average value of one of the nearest neighbors ( $\sigma_j$ ) of site  $i$  is evaluated, separately for the two cases,  $\sigma_i = +1$  and  $\sigma_i = -1$ . There are  $(z-1)$  near neighbors of site  $j$  which are second nearest neighbors to site  $i$ , and we can suppose in a first approximation that they take some mean magnetization value,  $m$ . This is reminiscent of the BPW approximation. The average values of  $\sigma_j$ , depending on whether site  $i$  is  $+1$  or  $-1$ , are

$$m^+ = \langle \sigma_j \rangle_{\sigma_i = +1} = \tanh \beta[(z-1)m + 1], \quad (8)$$

$$m^- = \langle \sigma_j \rangle_{\sigma_i = -1} = \tanh \beta[(z-1)m - 1]. \quad (9)$$

Substitution of Eqs. (8) and (9) into Eq. (7), followed by expansion for  $m \ll 1$ , which is the limit  $T \rightarrow T_c$  from below, leads to

$$\cosh \beta_c = \sqrt{z(z-1)} \beta_c. \quad (10)$$

The equation gives a modest improvement over the standard mean-field approach. For example, applied to the 2D square lattice,  $z=4$ , this predicts  $k_B T_c/J = 3.312$ , less accurate than the BPW approximation, but simpler to obtain. However, this correlated-field approximation contains an interesting physical effect—the local neighbor fields  $m^+$  and  $m^-$  as determined by Eqs. (8) and (9) do not go to zero even for  $T > T_c$ , although the average magnetization  $m$  does. Thus the theory in some sense includes fluctuations away from the mean magnetization.

### V. SELF-CONSISTENT CORRELATED FIELD APPROXIMATION

As described above, the correlated field approximation, and Eqs. (8) and (9), do not fully implement the idea that the neighbor fields should depend on the central spin. That is, the  $(z-1)$  neighbors of site  $j$  that were given values  $m$  should really also be allowed to have values  $m^+$  or  $m^-$ , corresponding to when  $\sigma_j$  has values  $+1$  or  $-1$ , respectively. This further improvement we refer to as “self-consistent correlated field” approximation (SCCF). Then averaging over  $\sigma_j = \pm 1$ , with  $\sigma_i$  held fixed at the values  $+1$  or  $-1$ , Eqs. (8) and (9) are replaced by

$$m^+ = \langle \sigma_j \rangle |_{\sigma_i = +1} = \frac{e^{\beta[(z-1)m^+ + 1]} - e^{-\beta[(z-1)m^- + 1]}}{e^{\beta[(z-1)m^+ + 1]} + e^{-\beta[(z-1)m^- + 1]}}, \quad (11)$$

$$m^- = \langle \sigma_j \rangle |_{\sigma_i = -1} = \frac{e^{\beta[(z-1)m^+ - 1]} - e^{-\beta[(z-1)m^- - 1]}}{e^{\beta[(z-1)m^+ - 1]} + e^{-\beta[(z-1)m^- - 1]}}. \quad (12)$$

As  $T \rightarrow T_c$  from below, the mean magnetization  $m$  given in Eq. (7) goes to zero, while the local molecular fields  $m^+$  and  $m^-$  remain nonzero. Their algebraic average,

$$\Delta \equiv \frac{m^+ + m^-}{2}, \quad (13)$$

however, by symmetry, must go to zero at  $T_c$ . Thus it is advantageous to express  $m$ ,  $m^+$  and  $m^-$  in terms of  $\Delta$ , and make an expansion for  $\Delta \ll 1$  to determine  $T_c$ . One has

$$m = \tanh z\beta\Delta, \quad (14)$$

$$m^+ = \tanh \beta[(z-1)\Delta + 1], \quad (15)$$

$$m^- = \tanh \beta[(z-1)\Delta - 1]. \quad (16)$$

Equations (13), (15) and (16) result in an equation that determines  $\Delta$ :

$$2\Delta = \tanh \beta[1 + (z-1)\Delta] - \tanh \beta[1 - (z-1)\Delta]. \quad (17)$$

Expansion around  $\Delta = 0$  gives leading terms,

$$\Delta = x \operatorname{sech}^2 \beta \left\{ \Delta + \left( \frac{2}{3} - \operatorname{sech}^2 \beta \right) x^2 \Delta^3 + \dots \right\}, \quad (18)$$

TABLE I.  $k_B T_c/J$  from various approximations and exact/series [27,28] values. Dashes indicate where a theory fails.

Lattice	$z$	Exact/Series	BPW	ORF	CF	SCCF
honeycomb	3	1.51865 ...	1.820	-	2.220	-
square	4	2.26918 ...	2.885	-	3.312	2.595
triangular	6	3.64095 ...	4.933	-	5.384	4.788
diamond	4	2.7040 ...	2.885	2.231	3.312	2.595
sc	6	4.5103 ...	4.933	3.955	5.384	4.788
bcc	8	6.3508 ...	6.952	5.743	7.416	6.853
fcc	12	9.794 ...	10.97	8.932	11.44	10.91

where

$$x \equiv (z-1)\beta. \quad (19)$$

The critical temperature occurs where the linear order terms cancel, and only a  $\Delta = 0$  solution remains, leading to

$$\cosh^2 \beta_c = (z-1)\beta_c. \quad (20)$$

This equation gives a further improved estimate of  $T_c$ , except for the lowest values of  $z$ .

### VI. DISCUSSION OF RESULTS

In Table I we display  $T_c$  from SCCF, Eq. (20), and from CF, Eq. (10), as well as the ORF and mean-field results, together with either exact or approximate values from series estimates [27], for various lattices. Our CF and SCCF calculations almost always overestimate  $T_c$ , just as the simple mean-field prediction. In particular, for the 2D square lattice Ising model Eq. (20) gives  $k_B T_c/J = 2.595$ , closer to the exact result than the BPW approximation. We could also compare with the Mattis [21] approach, which gives  $k_B T_c/J = 3.090$  for  $z=4$  and  $k_B T_c/J = 5.073$  for  $z=6$ , both somewhat higher than the BPW results. The ORF calculation does not work in 2D or 1D, however, in 3D, where it is applicable, it consistently underestimates the true value of  $T_c$ , and gives results quite close to the diagrammatic expansion of Horwitz and Callen [19]. Both Eqs. (10) and (20) do not give a phase transition at the 1D limit,  $z=2$ , just as in the BPW approximation.

Note, however, that at  $z=4$ , the transition temperature from the SCCF estimate is *below* the exact  $T_c$  for the diamond lattice, as determined from series. For this unusual case SCCF somehow is overestimating the fluctuation effects and thus underestimating  $T_c$ , although not by very much. However, we realize this accuracy seen for the SCCF prediction of the diamond lattice  $T_c$  is at odds with the corresponding higher error for the 2D square lattice. As SCCF uses only the coordination number  $z$  as input, it certainly cannot accurately predict  $T_c$  for both of these lattices simultaneously. For the 3D lattices considered, however, it is interesting to note that the ORF calculation of  $T_c$  also is most inaccurate for the diamond lattice; it seems to be a difficult case for the ORF approach. (The ORF procedure *does* take into account the specific lattice structure, beyond the coordination number, but unfortunately does not work in 2D.)

Unfortunately, at  $z=3$  (2D honeycomb lattice) the situa-

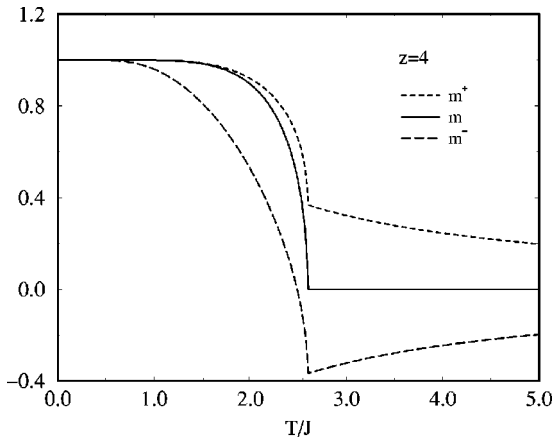


FIG. 1. The mean and nearest-neighbor magnetizations versus temperature from the improved mean-field theory (SCCF) for  $z=4$ , using  $\Delta$  obtained by iterating Eq. (17).

tion is worse: Eq. (20) has no solution and this SCCF approximation wrongly predicts a disordered phase for all temperatures, whereas the CF and BPW approximations are better and still overestimate  $T_c$ . For comparison, the Mattis approach [21] gives  $k_B T_c / J = 2.10373$ , slightly better than CF but not as good as the BPW result. Nevertheless, with the exception of these most open lattices, the SCCF approximation makes notably good estimates for  $T_c$ .

As expected for a mean-field theory, the magnetization near  $T_c$  behaves as  $m \sim (T_c - T)^{1/2}$  just below the transition. It is interesting to note, however, that the local neighbor-fields  $m^+$  and  $m^-$  do not go to zero, even above  $T_c$ . Only the sum  $\Delta$  becomes zero in the disordered phase. In Fig. 1 we show this effect for  $z=4$ , which was obtained by solving Eq. (17) iteratively for  $\Delta$ . For higher values of  $z$ , similar curves are obtained, but with smaller differences between  $m^+$  and  $m^-$  for all temperatures.

We can use the nearest neighbor pair correlation function  $\langle \sigma_i \sigma_j \rangle$ , to calculate the internal energy  $U$  and specific heat  $C$ , from

$$U = -\frac{1}{2} z N J \langle \sigma_i \sigma_j \rangle, \quad C = \frac{dU}{dT}. \quad (21)$$

The needed average value is

$$\langle \sigma_i \sigma_j \rangle = \frac{m^+ e^{\beta z m^+} - m^- e^{-\beta z m^-}}{e^{\beta z m^+} + e^{-\beta z m^-}}, \quad (22)$$

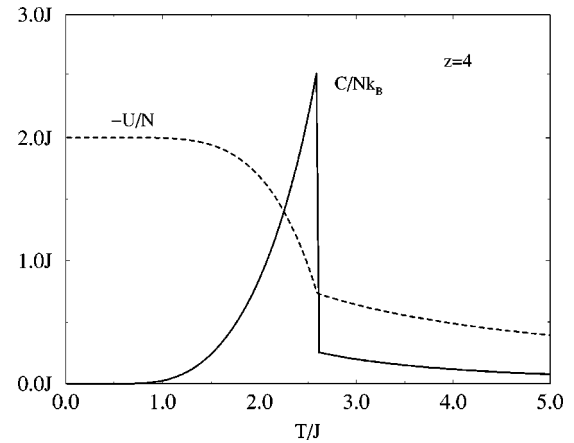


FIG. 2. The internal energy and specific heat per site, from the improved mean-field theory (SCCF) for  $z=4$ .

where we averaged over the two possibilities,  $\sigma_i = +1$  with  $\sigma_j = m^+$  and  $\sigma_i = -1$  with  $\sigma_j = m^-$ . Using Eq. (13) this becomes

$$\langle \sigma_i \sigma_j \rangle = \Delta \tanh z \beta \Delta + \frac{1}{2} (m^+ - m^-). \quad (23)$$

The internal energy and specific heat, for  $z=4$ , are shown in Fig. 2. For larger values of  $z$ , the specific heat peak becomes weaker. Note that the first term of Eq. (23) vanishes above  $T_c$ , while the second vanishes only at  $T=0$ , which leads to a discontinuity in the slope of the internal energy at  $T_c$ . Thus there is a discontinuity in the specific heat at  $T_c$ , which maintains a nonzero value above  $T_c$ , like the BPW results but unlike the usual MF results.

In conclusion, this correlated-field approximation, that includes the correlation of the local neighbor-fields to the central spin, contains a simple physical picture of local spin fluctuations near  $T_c$ , and is able to give fairly good predictions of  $T_c$  for the Ising model, except for  $z < 4$ . It gives values for  $T_c$  quite accurately, because both the site being considered and its neighbors interact with a self-consistently determined fluctuating molecular field, represented by  $m^+$  and  $m^-$ , rather than a single-valued mean field. Because of its simplicity and accuracy, in the future it will be interesting to consider whether such a picture can be applied with any success to other discrete-valued lattice models.

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