# Molecular-field theory method for evaluating critical points of the Ising model

K. K. Zhuravlev
*Los Alamos Natonal Laboratory, Los Alamos, New Mexico 87545, USA*
(Received 20 June 2005; revised manuscript received 29 August 2005; published 3 November 2005)

The molecular-field theory is one of the most common approximations used to calculate properties of materials with the Ising model. A generalization, improving the previous results of molecular-field theory, is proposed. It has also been shown that this method distinguishes between two lattices with different geometries but equal numbers of nearest neighbors, such as square, diamond, triangular, and simple cubic lattices, a result that is missing from most other mean-field approaches.

DOI: 10.1103/PhysRevE.72.056104 PACS number(s): 64.60.Cn

## I. INTRODUCTION

The Ising model is the simplest model of ferromagnetism and it is probably the most studied since its introduction by Ising [1]. It has been solved by Ising for the one-dimensional case and by Onsager in the case of the two-dimensional square lattice [2]. Some other two-dimensional cases, like honeycomb and triangular lattice Ising models, have also been solved [3]. Various other solutions have been obtained after Onsager's one, including the method of Kac and Ward [4], which involved a combinatorial argument, the Kasteleyn solution [5], and the Vdovichenko method [6]. Baxter and Enting [7] obtained yet another solution to the Ising model, using only the star-triangle relation [8]. The Ising model has also been applied to a variety of other problems, so a general method of solution is valuable. Reviews of the theory of Ising model and critical phenomena are in papers by Newell and Montroll [9], Kadanoff *et al.* [10], and Fisher [11].

Up to now no solution or exact value of $T_c$, the critical temperature, has been obtained for three-dimensional lattices. Various approximate methods have been applied, the most obvious being the molecular-field approach. A review of those methods can be found in Ref. [12]. Molecular-field theory gives a qualitatively correct picture of the phase transition, but fails to predict values of various important quantities, such as the critical point and critical exponents. Therefore it is always of interest to introduce modifications to the mean-field approach, which will be able to predict critical parameters with better accuracy. Recently, the correlated molecular-field theory has been proposed by Wysin and Kaplan [13]. In their work they allowed the value of magnetization of nearest neighbors in the Ising model to take two different values $m^+$ or $m^-$, depending on the orientation of the central spin. They also let the second-nearest neighbors have analogous values for the magnetization, which led them to results for the values of critical points improved compared to the other molecular-field methods. This method was called the "self-consistent" correlated field (SCCF) approximation. The central equation in their method used only the number of nearest neighbors as a variable parameter. Thus the values for critical points for triangular and simple cubic lattices, for example, are the same in the SCCF approximation.

Here we introduce an idea, which further improves the result of the SCCF method and allows one to obtain critical points for all lattices with better accuracy. Also this approach naturally makes a distinction between various lattices with equal numbers of nearest neighbors, but different geometrical structures. This paper is organized as follows. In the next section we describe SCCF theory and its limitations, then the original molecular-field theory is described, and the central idea of our method is introduced. Later we discuss the results obtained in the framework of our method. The final section contains discussion about corrections to our method and is followed by conclusion.

## II. CORRELATED MOLECULAR-FIELD THEORY

In the correlated molecular-field theory the Hamiltonian for a given spin $\sigma_i$, is written as follows:

$$H_{MFT} = -\sigma_i h_{eff}, \tag{1}$$

where the value of the effective field $h_{eff}$ is determined by

$$h_{eff} = zK(m^+ \delta_{\sigma_i,1} + m^- \delta_{\sigma_i,-1}). \tag{2}$$

Here $z$ is the number of nearest neighbors and $K$ is a dimensionless coupling. Values of the neighbor field depend on the value of the central spin. Those values are determined self-consistently. The details are described in Ref. [13], here we give only final result:

$$\Delta = \frac{m^+ + m^-}{2},$$

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

$$m^- = \tanh K[(z-1)\Delta - 1]. \tag{3}$$

The system of equations (3) determines $\Delta$. Expansion around $\Delta = 0$ gives the central equation of the SCCF approximation, which determines the critical point:

$$\cosh^2 K_c = (z-1)K_c. \tag{4}$$

The correlated molecular-field theory gives a significant improvement over other mean-field methods, such as the Bethe-Peierls-Weiss (BPW) approximation [14–16] or the Onsager reaction field (ORF) correction [17], for the values of critical points for various lattices. Nonetheless, in this theory only the nearest-neighbor spins correlate with the cen-

 

tral spin. This insensitivity to the geometrical structure of the lattice has been already mentioned.

In the next section we introduce an alternative idea for improving the molecular-field theory and evaluate critical points for various lattices.

## III. THEORY

For the Ising model in the absence of external magnetic field the Hamiltonian can be written as

$$H = -J\sum_{\langle ij\rangle} \sigma_i\sigma_j \tag{5}$$

where $J$ is the coupling between spins and symbol $\langle\ \rangle$ denotes the sum over all nearest neighbors. Before we describe our approach, we will briefly review the mean-field approach to the problem.

In the mean-field theory the central spin is considered to be subject to some effective magnetic field, which is given by

$$h_{eff} = Jzm. \tag{6}$$

Here $z$ is the number of nearest neighbors and $m$ is the magnetization. Since the magnetization is the average value of spin at a given site, it can be written as follows:

$$m = \frac{e^{Kzm} - e^{-Kzm}}{e^{Kzm} + e^{-Kzm}} = \tanh(Kzm). \tag{7}$$

In Eq. (7) $K=J/k_BT$ is a dimensionless coupling constant. Equation (7) is then solved for $m$ and one finds that a nontrivial solution appears at

$$\beta_c = \frac{k_BT_c}{J} = z, \tag{8}$$

where $\beta_c$ is the critical temperature.

Now we are ready to introduce our approach. Our approach generalizes ordinary molecular-field theory by distinguishing contributions from various spins in the lattice, whereas in the original theory, as well as in SCCF theory, those contributions were the same from all spins. We start with the simple square lattice for the purpose of clarity. Let us consider the central spin and suppose that it interacts with all other spins. It is obvious that in order to keep the model consistent the interaction should decrease very quickly with the distance between the spins. Therefore, the field due to any spin, which is seen by a central spin, should vanish very fast with the increase of the distance from it to the central spin. This is equivalent to the screening effect that takes place in plasma or electrolytes. Therefore, we refer to this approach as "screened magnetic field" (SMF) approximation. Here we use the function that decreases fastest with distance, i.e., $f(r)=\exp(-r^2/a_0^2)$, $a_0$ being the characteristic distance over which the field goes to zero. The only characteristic length parameter in the problem is the lattice constant. The effective field seen by a central spin can be represented as follows:

$$h_{eff} = Jm\sum_{\{\sigma\}} e^{-r_\sigma^2/a_0^2} \tag{9}$$

where the sum is taken over all spins on the lattice. Thus, for the simple square lattice we have

$$h_{eff} = J\left(\sum_{i=-\infty}^{\infty}\sum_{k=-\infty}^{\infty} e^{-(i^2+k^2)} - 1\right)m = J[\vartheta_3^2(0,e^{-1}) - 1]m. \tag{10}$$

In Eq. (10) $\vartheta_3(0,e^{-1})$ is the theta function [18] and 1 is subtracted in order to avoid self-interaction. The rest is easy: Eq. (10) resembles Eq. (6) with $z=\vartheta_3^2(0,e^{-1})-1$. Thus the critical point for the simple square lattice is given by the expression

$$\beta_c^{(sq)} = \vartheta_3^2(0,e^{-1}) - 1. \tag{11}$$

The same procedure can be repeated for the simple cubic lattice. The calculation gives the value of critical temperature as

$$\beta_c^{(sc)} = \vartheta_3^3(0,e^{-1}) - 1. \tag{12}$$

Using the same ideas, we calculated the critical points for other types of lattices:

$$\beta_c^{(bcc)} = \vartheta_2^3(0,e-4/3) + \vartheta_3^3(0,e-4/3) - 1 \quad \text{(bcc lattice)}, \tag{13}$$

$$\beta_c^{(fcc)} = \vartheta_3(0,e^{-2})[3\vartheta_2^2(0,e^{-2}) + \vartheta_3^2(0,e^{-2})] - 1 \quad \text{(fcc lattice)}. \tag{14}$$

For the triangular, honeycomb, and diamond lattices there is no closed analytical expression for the critical point. The critical points for those lattices had to be computed approximately, by evaluating the sum, analogous to the one in Eq. (10). The formulas look as follows:

$$\beta_c^{(tr)} = \sum_{i=-\infty}^{\infty}\sum_{k=-\infty}^{\infty} e^{-[(i+k)^2+i^2+k^2]/2} - 1, \tag{15}$$

$$\beta_c^{(hc)} = \sum_{i=-\infty}^{\infty}\sum_{k=-\infty}^{\infty} (e^{-[(i+k)^2+i^2+k^2]/2} + e^{-[(i+k)^2+i^2+k^2]/2-3/4-3(i+k)/2}) - 1, \tag{16}$$

$$\begin{aligned}\beta_c^{(diam)} = -1 + \sum_{i=-\infty}^{\infty}\sum_{j=-\infty}^{\infty}\sum_{k=-\infty}^{\infty} (&e^{-16[(i+1/2)^2+j^2+k^2]/3} + e^{-16[i^2+(j+1/2)^2+k^2]/3} + e^{-16[i^2+j^2+(k+1/2)^2]/3} \\ &+ e^{-(16/3)(i^2+j^2+k^2)} + e^{-(16/3)[(i+1/4)^2+(j+1/4)^2+(k+1/4)^2]} \\ &+ e^{-(16/3)[(i+3/4)^2+(j+1/4)^2+(k+3/4)^2]} \\ &+ e^{-(16/3)[(i+3/4)^2+(j+3/4)^2+(k+1/4)^2]} \\ &+ e^{-(16/3)[(i+1/4)^2+(j+3/4)^2+(k+31/4)^2]}).\end{aligned} \tag{17}$$

The formulas (11)–(17) give significant improvement in the

TABLE I. Critical temperatures for various types of lattices from different approximations and exact or series values. Dashes indicate the absence of results.

| Lattice | Exact or series | BPW | ORF | SCCF | SMF | Corrected SMF |
|---|---|---|---|---|---|---|
| Honeycomb | 1.51865… | 1.820 | — | — | 1.464 | — |
| Triangular | 3.64095… | 4.933 | — | 4.788 | 2.628 | 3.543 |
| Square | 2.26918… | 2.885 | — | 2.595 | 2.142 | — |
| Diamond | 2.7040… | 2.885 | 2.231 | 2.595 | 2.670 | — |
| sc | 4.5103… | 4.933 | 3.955 | 4.788 | 4.570 | — |
| bcc | 6.3508… | 6.952 | 5.743 | 6.853 | 6.234 | — |
| fcc | 9.794… | 10.97 | 8.932 | 10.91 | 6.875 | 10.005 |
| hcp | ≈10 | 10.97 | 8.934 | 10.91 | 6.875 | 10.005 |
| Hexagonal | — | 6.952 | — | 6.853 | 5.43 | — |

values of critical points compared to the previous methods, with exception of fcc lattice. We also calculated critical points for a hcp and a simple hexagonal lattice. Those can be calculated according to the formulas

$$\beta_c^{(hcp)} = \sum_{i=-\infty}^{\infty}\sum_{k=-\infty}^{\infty}\sum_{j=-\infty}^{\infty}\left[e^{-[(2i-k)^2+3k^2]/4-8j^2/3} + e^{[(2i-k)^2+3(k+2/3)^2]/4-8(j+1/2)^2/3}\right]-1, \quad (18)$$

$$\beta_c^{(hex)} = \sum_{i=-\infty}^{\infty}\sum_{k=-\infty}^{\infty}\sum_{j=-\infty}^{\infty} e^{-[(2i-k)^2+3k^2]/4-j^2}-1. \quad (19)$$

## IV. DISCUSSION OF RESULTS

In Table I we summarize the results obtained by the SMF method and other approximate methods. We also compared our calculations to the exact results or approximate values from the series expansion methods. For example, for a square lattice our calculation yields numerical value of $\beta_c^{(sq)} \approx 2.1422$. The exact value of $\beta_c^{(sq)}$ is $\beta_c^{(sq)} = 2/\mathrm{Arc\ sinh}(1) \approx 2.2692$. Our result is very close to the exact result, in fact, it gives a better estimate for the critical point than SCCF theory, which gives $\beta_c^{(sq)} \approx 2.5952$.

Unfortunately, our approach does not result in significant improvement in critical point determination for the fcc lattice. Also the critical point is not very accurately estimated for the triangular lattice. The reason for the discrepancies is that this method overestimates screening effect in both cases. Later we propose a correction, which will partially compensate this overestimate. Also we must mention that our approach predicts a phase transition for the one-dimensional case, whereas it does not exist.

In our approach we used a Hamiltonian in the regular molecular-field theory form,

$$H = -h_{eff}\sum_i \sigma_i \quad (20)$$

with $h_{eff}$ given by Eq. (9). We, therefore, expect that the critical exponents will be the same as mean-field ones. Here the critical exponent $\beta$ (not to be confused with temperature), which describes the behavior of magnetization near the critical point, will be obtained. Other critical exponents can be derived in the same fashion.

The magnetization is given by

$$\langle m\rangle = \frac{\sum_{\sigma_i=\pm 1}\sigma_i \exp(\sigma_i h_{eff}/kT)}{Z} \quad (21)$$

where $Z$ appears as follows:

$$Z = \sum_{\sigma_i=\pm 1}\exp(\sigma_i h_{eff}/kT). \quad (22)$$

After substituting Eq. (22) into Eq. (21) and summing over two values of spin $\sigma_i$, one obtains

$$\langle m\rangle = \tanh\left(\frac{h_{eff}}{kT}\right) = \tanh\left(\frac{\langle m\rangle J\sum_{\{\sigma\}} e^{-r_\sigma^2/a_0^2}}{kT}\right) = \tanh\left(\frac{\langle m\rangle T_c}{T}\right). \quad (23)$$

Here the expressions for $h_{eff}$ from Eq. (9) and for critical temperature from Eqs. (8) and (10) were used. In the vicinity of the critical point the argument of hyperbolic tangent is small and, therefore, $\tanh(x) \approx x - x^3/3$. Then it immediately follows that

$$\langle m\rangle = \frac{\sqrt{3}T}{T_c}\sqrt{1-\frac{T}{T_c}} \quad (24)$$

when $T_c - T \ll T_c$. Thus $\langle m\rangle \propto (T_c - T)^{1/2}$ and critical exponent $\beta = \frac{1}{2}$, as in mean-field theory.

## V. CORRECTION FOR fcc, hcp, AND TRIANGULAR LATTICES

It is apparent that the SMF method predicts critical points for all but fcc and hcp lattices with a precision far better than that of other available methods. The discrepancy in the fcc and hcp cases, as well as for the triangular lattice, can be explained in the following way. We assumed that the screening length equals the lattice constant. In the case of triangular, hexagonal close-packed, and face-centered cubic lattices,

TABLE II. Correction to the screening length $\alpha$ [Eq. (25)] for various lattices.

| Lattice | Correction coefficient $\alpha$ | Coordination number |
|---|---|---|
| Honeycomb | 0.97 | 3 |
| Square | 0.96 | 4 |
| Triangular | 0.78 | 6 |
| Diamond | 0.99 | 4 |
| Simple cubic | 1.01 | 6 |
| bcc | 0.99 | 8 |
| fcc | 0.81 | 12 |
| hcp | 0.81 | 12 |

the screening length is larger than the lattice constant.

The screening length is larger because the six nearest neighbors for the triangular lattice are screened by 12 next-nearest neighbors, six of which are at $a_0\sqrt{3}$ and the other six at $2a_0$ distance from the central spin, respectively, therefore the field due to nearest neighbor spins is less screened by other spins than in the case of the square lattice. Analogously for the fcc lattice, as well as for the hcp lattice, the 12 nearest neighbors are screened by just six next-nearest neighbors at $a_0\sqrt{2}$ distance from the central spin. Therefore, a correction to the screening length is necessary. This can be expressed as follows:

$$h_{eff} = J\sum_{\sigma} e^{-(r_\sigma^2/a_0^2)\alpha}, \tag{25}$$

where $\alpha$ is the correction coefficient.

The correction factor in this case is $\alpha=0.78$ for the triangular lattice and $\alpha=0.81$ for fcc and hcp lattices. The resulting critical points are $\beta_c^{(tr)} \approx 3.6508$ for triangular and $\beta_c^{(fcc)} = \beta_c^{(hcp)} \approx 9.8022$ for fcc and hcp lattices, respectively, which is a significant improvement. It should also be mentioned that both triangular and fcc lattices have one feature in common, namely, they are both so-called close-packed structures.

A natural question that arises is whether such a correction should be applied to every lattice. One, in fact, can find the necessary corrections for other lattices; the results are summarized in Table II.

The correction to a screening length is the simplest way to make the results coincide with correct critical points. There could be other methods, including different functional forms of screening, e.g., a Yukawa potential instead of a Gaussian one. One can imagine the use of cubic or quartic terms in distance, along with quadratic terms, i.e., writing an effective field in the form $h_{eff} \propto \exp(-r^2/a^2 - r^3/b^3 - r^4/c^4 - \cdots)$. It is immediately apparent that there is a connection between the geometrical structure of the lattice and the correction coefficient introduced. But the exact nature of this connection still remains an open question. Attempts to link this correction to either the relative contribution from nearest and next-nearest neighbors or successive terms in series from Eq. (9) found no obvious connection in either case.

From Table II it is clear that, while for most lattices the correction coefficient is close to 1, it is significantly smaller than one for close-packed lattices. The reason, as it was indicated earlier, is in the smaller screening effect for those lattices, due to their structure. Therefore, for the purpose of keeping this method as simple as possible, it suffices to introduce the "universal" correction coefficient for the close-packed structures to be equal to 0.8. The corrected critical points, calculated for this value of correction coefficient $\alpha$, are also listed in Table I.

In the Appendix we give approximate analytical formulas, which allow calculations of critical points for honeycomb, hexagonal, triangular, diamond, and hcp lattices.

## VI. CONCLUSION

An mean-field approach to the Ising model has been proposed. It is called the screened magnetic field method. It was shown that the summation over all spins with screening taken into consideration results in a relatively simple analytical formula for the effective number of nearest neighbors, which, in turn, gives the critical point for the system and it happens to be in very good agreement with the exact results or series expansion data. The advantage of this method is that it allows one to obtain the critical temperature for the Ising model with great precision and relatively little effort.

For the triangular, face-centered cubic, and hexagonal close-packed lattices the correction to the screening length was introduced in order to account for the extra number of the nearest neighbors. The correction coefficient $\alpha=0.8$ achieves very good agreement with exact and series expansion results. Finally, such a method might prove to be useful in estimating critical points for other lattices and other statistical mechanics problems.

## ACKNOWLEDGMENTS

The author would like to thank R. K. Sander for carefully reading this paper and suggesting some improvements. This work was supported by the U.S. Department of Energy under Contract No. W-7405-ENG-36.

## APPENDIX

Here we present simple analytical formulas, which approximate exact sums in Eqs. (15)–(19). These formulas are

$$\beta_c^{(tr)} = v_3(0,e^{-1})v_3(0,e^{-3/4}) - 1, \tag{A1}$$

TABLE III. Critical temperatures for various lattices by approximate analytical formulas and direct summation of series from Eq. (9).

| Lattice | $\beta_c$ by direct summation/corrected | Approximate analytical value |
|---|---|---|
| Triangular | 2.628/3.534 | 2.628/3.534 |
| Honeycomb | 1.464 | 1.423 |
| Diamond | 2.670 | 2.742 |
| Simple hexagonal | 5.43 | 5.431 |
| hcp | 6.875/10.005 | 6.876/10.006 |

$$\beta_c^{(hc)} = v_3(0,e^{-9/4})v_3(0,e^{-3}) + v_2(0,e^{-9/4})v_2(0,e^{-3}) - 1, \tag{A2}$$

$$\beta_c^{(diam)} = 6v_2^2(0,e^{-16/3})v_3(0,e^{-16/3}) + 2v_3^3(0,e^{-16/3}) - 1, \tag{A3}$$

$$\beta_c^{(hex)} = v_3^2(0,e^{-1})v_3(0,e^{-3/4}) - 1, \tag{A4}$$

$$\beta_c^{(hcp)} = v_3(0,e^{-1})v_3(0,e^{-3/4})[v_3(0,e^{-8/3}) + v_2(0,e^{-8/3})] - 1. \tag{A5}$$

The numerical values are very close to actual results obtained by direct summation of the series and are summarized in Table III. The corrected results for triangular and hcp lattices were obtained for $\alpha=0.8$.

Thus the approximate formulas give results very close to actual theory and can be used in estimating critical points for the lattices, where no exact analytical expression exists.


[1] E. Ising, Z. Phys. **31**, 253 (1925).
[2] L. Onsager, Phys. Rev. **65** 117 (1944).
[3] R. J. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic Press, San Diego, 1982), Chap. 6.
[4] M. Kac and J. C. Ward, Phys. Rev. **76**, 1232 (1952).
[5] P. W. Kasteleyn, J. Math. Phys. **4**, 287 (1963).
[6] N. V. Vdovichenko, Sov. Phys. JETP **21**, 350 (1965).
[7] R. J. Baxter and I. G. Enting, J. Phys. A **11**, 2463 (1978).
[8] G. H. Wannier, Rev. Mod. Phys. **17**, 50 (1945).
[9] G. F. Newell and E. W. Montroll, Rev. Mod. Phys. **25**, 353 (1953).
[10] L. P. Kadanoff, W. Gotze, D. Hamblen, R. Hecht, E. A. S. Lewis, V. V. Palciauskas, M. Rayl, and J. Swift, Rev. Mod. Phys. **39** 395 (1967).
[11] M. E. Fisher, Rep. Prog. Phys. **30**, 615 (1967).
[12] J. S. Smart, *Effective Field Theories of Magnetism* (W. B. Saunders Co., Philadelphia, 1966).
[13] G. M. Wysin and J. Kaplan, Phys. Rev. E **61**, 6399 (2000).
[14] H. A. Bethe, Proc. R. Soc. London, Ser. A **150**, 552 (1935).
[15] R. E. Peierls, Proc. Cambridge Philos. Soc. **32**, 477 (1936).
[16] P. R. Weiss, Phys. Rev. **74**, 1493 (1948).
[17] L. Onsager, J. Chem. Phys. **58**, 1486 (1936).
[18] I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series and Products* (Academic Press, New York, 1965), p. 921.