Critical temperature of $(d+1)$-dimensional Ising films

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(Received 25 February 1992)

An alternative approach is proposed to treat the critical point for general Ising spin systems. From the analytic properties of the free energy, we are in principle able to calculate analytically the critical temperature $T_c(l)$ for $(d+1)$-dimensional Ising films to any order cumulant as a function of the number l of hyperlayers in the hyperfilm. Explicit expressions up to the fourth order are given. It is shown from the general expression for $T_c^{(m)}(l)$ that $[T_c(l)-T_c]/T_c=b/(l+a)$ in the limit $l\to\infty$. Comparisons with existing results for $d=2$ are discussed.

PACS number(s): 05.50.+q, 05.70.Jk, 75.10.Hk, 75.40.Cx

The physics of phase transitions and critical phenomena covers a wide variety of subjects in many different fields of science. It turns out that common features are observed near critical points of various types in all different systems. The study of critical points has been and still is one of the most interesting topics of research. The simplest approximation is the mean-field theory. Substantial improvement of the mean-field theory may require a great deal of effort or the almost exact solution. Thus Onsager's historical work [1] on the two-dimensional Ising model represents a great leap forward in the theoretical development. In fact, the Ising model is the only example of a phase transition that can be worked out with mathematical rigor.

While general properties of phase transitions were rigorously treated by Yang and Lee [2], a totally different approach of exploiting symmetries was later developed from scaling laws of Fisher [3], Kadanoff [4], Griffiths [5], and others to the renormalization group of Wilson [6]. On the other hand, the method of high-temperature series-expansion extrapolation (HTSEE) for locating singularities and singular structures has proved the most powerful one and the critical temperature and various critical exponents for Ising model were determined with fantastic accuracy [7].

The method of series expansion of a physical quantity is based on the fact that the quantity diverges at the critical point which is then determined approximately by the extrapolation procedure [7–10]. The question is, however, the following: Is it really necessary to expand a thermodynamic quantity that is divergent at the critical point instead of the free energy itself for the determination of the critical temperature?

We propose, in this paper, an alternative approach to the problem and demonstrate that analytic expressions for T_c can be obtained formally for hyperfilms of dimension $d+1$ to an arbitrary order of accuracy. We start with the variational cumulant expansion (VCE) developed in recent years in discussions of lattice gauge-field models [11]. It has been shown very recently [12] that in the high-temperature limit, the VCE is identical to the well-known linked-cluster expansion (LCE). Following the notation of Ref. [12], we consider the Hamiltonian

$$H=\frac{1}{s^2}\sum_{\langle i,j\rangle}J_{ij}s_i^z s_j^z-\frac{\mu}{s}\sum_i H_i s_i^z\ , \tag{1}$$

where $s^z=-s,-s+1,\ldots,s$, J_{ij} stands for the exchange energy between the spin pair i and j, μ represents the magnetic moment of a spin, and H_i is the inhomogeneous external field in the z direction. The variational cumulant expansion of the free energy up to the order m is given by

$$W\approx W_0-\sum_{n=1}^{m}\frac{1}{n!}\langle(S-S_0)^n\rangle_c=W_{\mathrm{eff},m}\ , \tag{2}$$

where W_0 is the free energy for the corresponding noninteracting system with the action

$$\tilde{S}=\frac{1}{s}\sum_i\left[\xi_i+\frac{\mu H_i}{k_BT}\right]s_i^z\ , \tag{3}$$

where we have introduced the variational parameters ξ_i. W_0 is exactly known [12]. The symbol $\langle\ \rangle_c$ represents the cumulant averaged over the Boltzmann weight $e^{\tilde{S}}$. The action S is defined by

$$S=-\frac{1}{s^2}\sum_{\langle i,j\rangle}\frac{J_{ij}}{k_BT}s_i^z s_j^z=\frac{1}{k_BT}X\ , \tag{4}$$

and the corresponding trial action S_0 is simply $\tilde{S}$ in the absence of the external field H_i.

For a uniform spin-$\frac{1}{2}$ Ising system in the absence of external fields $J_{ij}=J$, $\xi_i=\xi$, and $H_i=0$, the first-order free energy $W_{\mathrm{eff},1}$ in the VCE is given by

$$\frac{1}{N}W_{\mathrm{eff},1}=-\ln(2\cosh\xi)-\frac{d}{\Theta}Y^2+\xi Y\ , \tag{5a}$$

$$Y=\tanh\xi \ . \tag{5b}$$

The dimensionality is denoted by d, and $\Theta=k_BT/J$ represents the reduced temperature. By setting to zero the first variation of the function $W_{\text{eff},1}$, one finds

$$\xi=\frac{2d}{\Theta}\tanh\xi \ . \tag{6}$$

The solutions of Eq. (6) depend on d and Θ. Their qualitative behavior is shown schematically in Fig. 1. For $\Theta>\Theta_c=2d$, Eq. (6) has only one solution $\xi_0=0$ which corresponds to the minimum of the first-order free energy. For $\Theta<\Theta_c$, there are three solutions for every given Θ value. $\xi_\pm$ correspond to the minimum of $W_{\text{eff},1}$ and ξ_0 the maximum of $W_{\text{eff},1}$. The situation is completely analogous to Landau's theory of the second-order phase transition [13]. In this analogy, ξ plays the role of the order parameter $\langle M_z\rangle$ which is determined by minimizing the free energy in Landau theory.

Since all the bonds are decoupled in the first-order cumulant, the results are those of the mean-field theory. Thus, at the bifurcation point or the mean-field critical point,

$$\Theta_c=\frac{k_BT_c}{J}=2d \ . \tag{7}$$

$\xi=0$ represents the point of inflection of the function $W_{\text{eff},1}$, that is, Θ_c satisfies the condition

$$\left.\frac{\delta^2W_{\text{eff},1}}{\delta\xi^2}\right|_{\xi=0}=0 \ . \tag{8}$$

Equation (8) identifies the critical temperature T_c, in the first-order approximation, for a uniform bulk spin-$\frac{1}{2}$ Ising system in the absence of the external field. It is not difficult to see that the argument is valid for Ising systems of arbitrary spin s.

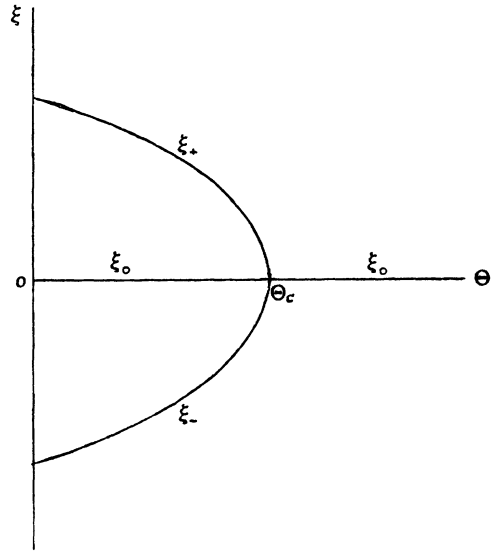

FIG. 1. Schematic diagram of solutions to Eq. (6). When $\Theta>\Theta_c$ ($=2d$), there is only one solution. When $\Theta<\Theta_c$, there are three solutions.

This provides us with the insight that the critical temperature may be determined to any order $W_{\text{eff},m}$ by locating the bifurcation point. As has been proved in Ref. [12], the VCE yields identical free energy to every order in the high-temperature limit ($\xi=0$) to the well-established LCE in the same limit. It is therefore reasonable to expect that $\xi=0$ corresponds to an extremum of the function $W_{\text{eff},m}$ for any higher-order m at high temperatures and that for the mth-order cumulant, $\xi=0$ remains the solution as the temperature decreases until the critical point. Consequently we conjecture that for systems homogeneous throughout the bulk in the absence of external fields, the critical temperature to the mth-order cumulant approximation is determined by the condition

$$\left.\frac{\delta^2}{\delta\xi^2}W_{\text{eff},m}(\Theta_c,\xi)\right|_{\xi=0}=0 \ . \tag{9}$$

It corresponds to the bifurcation point. This means that we have assumed ξ to be the order parameter of the system to any order of accuracy. The temperature dependence of the parameter is not of concern to us.

To calculate the critical temperature, we first derive the recursion formulas for the moments

$$\langle A(p,q)\rangle_0=\langle S^pS_0^q\rangle_0 \ , \tag{10}$$

where p,q are positive integers. The symbol $\langle\ \rangle_0$ stands for the Boltzmann average of the enclosed quantity with the weight $e^{\tilde{S}}$. It is easily shown that the moments satisfy the following relations:

$$\langle A(p,q+1)\rangle_0=\sum_i\xi_i\left[\frac{\delta}{\delta x_i}\ln Z_0+\frac{\delta}{\delta x_i}\right]\langle A(p,q)\rangle_0 \ , \tag{11}$$

$$\langle A(p+1,q)\rangle_0=\sum_{\langle i,j\rangle}\beta_{ij}\left[\frac{\delta^2}{\delta x_i\delta x_j}+2\frac{\delta\ln Z_0}{\delta x_i}\frac{\delta}{\delta x_j}+\frac{\delta\ln Z_0}{\delta x_i}\frac{\delta\ln Z_0}{\delta x_j}+\frac{\delta^2\ln Z_0}{\delta x_i\delta x_j}\right]\times\langle A(p,q)\rangle_0 \ , \tag{12}$$

where $x_i=\xi_i+mH_i/k_BT$, β_{ij} measures the exchange integral J_{ij} in the unit of k_BT, and $Z_0=e^{-W_0}$ is the partition function for the corresponding free energy W_0 of the noninteracting system. For a system of N spins, the moments are polynomials of N and are related to cumulants of the same order by the well-known relation

$$\langle S^pS_0^q\rangle_c=\text{the linear term of }\langle S^pS_0^q\rangle_0 \ . \tag{13}$$

Next, we note that

$$\left.\frac{\delta^2}{\delta\xi^2}\langle S^mS_0^n\rangle_c\right|_{\xi=0}=0, \quad n\geq 3,\ m=0,1,2,\ldots \ , \tag{14a}$$

$$\frac{\delta^2}{\delta\xi^2}\langle S_0^n\rangle_c\bigg|_{\xi=0}=0,\quad n\geq 3\ , \tag{14b}$$

because S_0^n involves ξ^n only when $n\geq 3$. From the relations (11) and (13) one finds

$$\langle S^n S_0\rangle_c=\xi\frac{\delta}{\delta\xi}\langle S^n\rangle_c\ , \tag{15}$$

which leads to

$$\frac{\delta^2}{\delta\xi^2}\langle S^n S_0^2\rangle_c\bigg|_{\xi=0}=\frac{\delta^2}{\delta\xi^2}\langle S^n S_0\rangle_c\bigg|_{\xi=0}=2\frac{\delta^2}{\delta\xi^2}\langle S^n\rangle_c\bigg|_{\xi=0}\ . \tag{16a}$$

Similarly, one can show that

$$\frac{\delta^2}{\delta\xi^2}\langle S_0^2\rangle_c\bigg|_{\xi=0}=-2\frac{\delta^2 W_0}{\delta\xi^2}\bigg|_{\xi=0}\ . \tag{16b}$$

Starting from the first-order cumulant in Eq. (5a) and making use of Eqs. (14) and (16), one can prove by the mathematical induction that Eq. (9) reduces to

$$\left[\frac{\delta^2}{\delta\xi^2}\langle S^{m-1}\rangle_c-\frac{1}{m}\frac{\delta^2}{\delta\xi^2}\langle S^m\rangle_c\right]_{\xi=0}=0 \tag{17}$$

up to any order m. Equation (17) implies immediately that the critical temperature $T_c^{(m)}$ calculated to mth order in the VCE is given by

$$k_B T_c^{(m)}=\frac{1}{m}\frac{\delta^2}{\delta\xi^2}\langle X^m\rangle_c\Big/\frac{\delta^2}{\delta\xi^2}\langle X^{m-1}\rangle_c\bigg|_{\xi=0}\ , \tag{18a}$$

where $X=k_B TS$ as defined in Eq. (4). Therefore we find the critical temperature for the system simply by extending m to infinity, namely,

$$T_c=\lim_{m\to\infty}T_c^{(m)}\ . \tag{18b}$$

Before the result is applied to any model system, a few remarks about the implications of Eqs. (18) are in order. Since we have not specified the spin statistics, the lattice structure, the dimensionality, and the range of exchange interactions in our formalism, the method can be generalized without much difficulty to other systems which exhibit second-order phase transitions. Since the ratio $(\delta^2/\delta\xi^2)\langle X^m\rangle_c/(\delta^2/\delta\xi^2)\langle X^{m-1}\rangle_c$ diverges linearly with increasing m around the critical point, and the proportionality constant is $k_B T_c^{(m)}$ according to Eq. (18a), the critical temperature is somehow related to the infinitely long-range interactions and the size of the system. This means that T_c is related to all infinitely connected coupled bonds or to some kind of scaling of this coupling. All the finite characteristic lengths become ineffective and the correlation length at this point becomes infinite. The critical temperature depends upon the dimension of the system rather than its detailed character.

It can be shown that T_c as given by Eq. (18b) coincides with that derived from the high-temperature LCE of the susceptibility χ by the ratio method [8]. The idea of the ratio method is based on the fact that χ diverges at the critical temperature. The point is that our method is developed on the basis of the analytic properties of the free energy as a function of ξ and Θ. That χ diverges at T_c is a consequence rather than an assumed knowledge on which the high-temperature series approach is based. Thus we have provided, in certain sense, a justification for the ratio method. It should be emphasized that the trial action in the VCE can in principle take a variety of forms. Hence other order parameters can also be identified and Eq. (9) will then lead to different expansions for the determination of T_c.

Since there has been considerable experimental interest in the finite-size effect on the phase transition in magnetic thin films in recent years [14,15] and since highly accurate numerical results for the critical temperature of Ising films [9,10] are available for comparison, we calculate T_c for a $(d+1)$-dimensional Ising films of spin $\frac{1}{2}$ with free surfaces. For definiteness, the lattice structure is taken to be hypercubic, although the method applies equally well to other structures. From the recursion formula (12) and Eq. (13), we calculate the cumulants $\langle S^m\rangle_c$ up to the desired order m. The results obtained at this point are perfectly general because the cumulants are expressed in terms of average spins at different lattice sites with exchange integral J_{ij} between any pair. Assuming nearest-neighbor interactions, topologically equivalent terms are summed according to the geometry specified in the problem. Various graph methods may be devised for this purpose. For instance, in our fourth-order calculation six topologically distinct connected graphs are involved. The second-order variation of the results thus obtained are then substituted in Eq. (18a) for the critical temperature. The procedure is nontrivial and the calculation is tedious. We present in the following, up to the fourth-order cumulant, the critical temperature as a function of the dimension d and the number l of hyperlayers in the hyperfilm:

For $m=1$,

$$T_c^{(1)}(l)=\frac{J}{k_B}\frac{(2d+2)l-1}{l},\quad l\geq 2\ . \tag{19}$$

For $m=2$,

$$T_c^{(2)}(l)=\frac{J}{k_B}\frac{(2d^2+3d+1)l-36d^2-3d-8}{(d+1)l-1},\quad l\geq 2\ . \tag{20}$$

For $m=3$,

$$T_c^{(3)}(l)=\frac{J}{k_B}\frac{(12d^3+24d^2+14d+2)l-36d^2-30d-8}{3[2d^2+3d+1)l-4d-2]},\quad l\geq 3\ , \tag{21a}$$

$$T_c^{(3)}(2)=\frac{J}{k_B}\frac{24d^3+12d^2-2d-1}{6(2d^2+d)}\ . \tag{21b}$$

For $m=4$,

$$T_c^{(4)}(l)=\frac{J}{k_B}\frac{(48d^4+120d^3+88d^2+18d+3)l-192d^3-216d^2-92d-28}{(24d^3+48d^2+28d+4)l-72d^2-60d-16},\quad l\geq 4\ , \tag{22a}$$

$$T_c^{(4)}(3)=\frac{J}{k_B}\frac{72d^4+84d^3+24d^2-19d-2}{36d^3+36d^2+12d-2}\ , \tag{22b}$$

$$T_c^{(4)}(2)=\frac{J}{k_B}\frac{48d^4+24d^3-20d^2-4d-3}{24d^3+12d^2-2d-2}\ . \tag{22c}$$

The corresponding T_c for a $(d+1)$-dimensional bulk is readily obtained by letting $l\to\infty$. It is obvious that the first-order result (19) is exactly the mean-field result [9]. In principle, the calculation can be extended to arbitrary order of accuracy. In practice, computer codes can be developed to generate all graphs needed in higher-order calculations for various lattice structures. Work along this line is being carried out and results will be reported elsewhere.

Numerical results for $d=2$ from Eqs. (19)–(22) are plotted in Fig. 2. For comparison purpose, we have also drawn the Bethe approximation [9] by the dashed line and the numerical result of Capehart and Fisher [10] by the dash-dotted line which represents HTSEE results up to 12th order for films up to seven spin layers. It is observed that the convergence rate up to the fourth order is pretty fast. It is also noted that Bethe's approximation is as accurate as our third-order results for $l=1,2$ and starts to deviate for $l=3$. A simple calculation reveals that it yields good results again in the limit $l\to\infty$. This is understandable because in Bethe's approximation the geometry of a film of l layers is simply represented by the mean coordination number $[6(l-2)+10]/l$ which yields the exact coordination number for $l=1,2$ and $l\to\infty$. Therefore it gives correct results only in these cases.

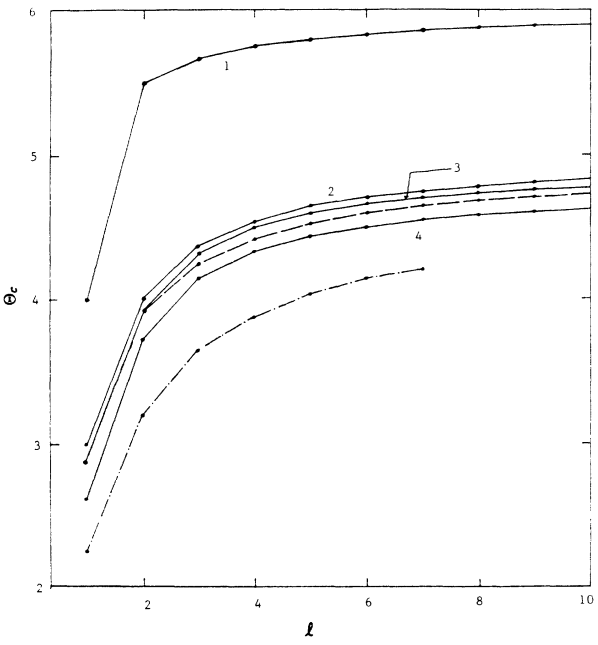

FIG. 2. Dimensionless critical temperature Θ_c vs the number of layers. Lines are drawn just to guide the eye. Results calculated in this work to various orders of approximation are indicated by numerals. Bethe's approximation is connected by the dashed line and the accurate results of Capehart and Fisher by the dash-dotted line.

It is found from Eq. (18a) that to any order m, the critical temperature for a $(d+1)$-dimensional l-layer hyperfilm can be written as

$$T_c^{(m)}(l)=\frac{J}{k_B}\frac{a_m l+b_m}{a_{m-1}l+b_{m-1}},\quad l\geq m \tag{23}$$

where a's and b's are polynomials in d. This is so because two types of graphs contribute to the free energy. Those connected to the surfaces are l independent and those not connected to surfaces result in a term linear in $(l-2)$. In the limit $l\to\infty$, $m\to\infty$ but $l>m$, we find

$$\lim_{\substack{l\to\infty\\ m\to\infty}}\frac{T_c^{(m)}(l)-T_c^{(m)}}{T_c^{(m)}}=\frac{b}{l+a}\ , \tag{24}$$

where the constants are defined by the limiting values $a=\lim_{m\to\infty}(b_{m-1}/a_{m-1})$ and $b=\lim_{m\to\infty}(b_m/a_m-b_{m-1}/a_{m-1})$. That $l>m$ is required in Eq. (24) appears to have restricted our discussions to clusters of size typically smaller than the film thickness. This of course introduces the major error in the calculation of $T_c^{(m)}(l)$ for small l. As l increases, however, the contribution from clusters of size larger than the film thickness to $T_c^{(m)}(l)$ decreases because the surface effect on the critical temperature decreases monotonically with increasing l. In the limit $l\to\infty$, then the analytic expression of $T_c^{(m)}(l)$ is expected to approach the true T_c when $m\to\infty$ even if $m<l$.

Compared to the general equation that defines the crit-

ical exponent for finite systems, Eq. (24) implies that $\lambda=1$, in contrast to $a=0$, $\lambda=1.56$ predicted by the HTSEE method [10]. While experimental data [14] seem to support $\lambda=1.56$, it has been observed by Allan [9] that Eq. (24) also fits the high-temperature extrapolation data. Furthermore, Domb [16] and Binder [17] also predicted $\lambda=1$. It is important to point out that λ is *derived* even though the convergence in the limit $m \to \infty$ to the true T_c remains to be proven.

As a final remark we note that, for hyperfilms with periodic boundary condition, all spins on the torus are equivalent. Equation (18a) always leads to the bulk critical temperature for $m < l$, since there is no graph which goes around the torus and connects to the initial point. The situation is exactly the same in the high-temperature extrapolation [10]. Therefore the critical exponent cannot be derived for this case in the present theory because there is no general formula for T_c when $m \leq l$.

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