Progress of Theoretical Physics, Vol. 38, No. 1, July 1967

Note on the Critical Behavior of Ising Ferromagnets

Ryuzo ABE

Department of Pure and Applied Sciences
College of General Education
University of Tokyo, Komaba, Meguro-ku, Tokyo

(Received April 3, 1967)

Behavior of Ising ferromagnets near the transition point in the presence of magnetic field is studied by means of the Lee-Yang theorem on the distribution of zeros of partition function. Relations for the critical indices so far obtained by several authors are rederived by the present method, and some discussions are given of the dependence of thermodynamic quantities at the transition point on magnetic field.

§ 1. Introduction

In previous papers[1),2)] [references 1) and 2) will be referred to as I and II, respectively], we discussed a singularity of specific heat C in the second order phase transition. This paper is devoted to a further discussion of singular properties of other physical quantities relevant to magnetic field H, such as the susceptibility χ or the spontaneous magnetization M. The critical behavior of these quantities is usually expressed as

$$C \propto t^{-\alpha}, \qquad \chi \propto t^{-\gamma}, \quad (T>T_c), \tag{1·1a}$$

$$C \propto |t|^{-\alpha'}, \quad M \propto |t|^{\beta}, \quad (T<T_c), \tag{1·1b}$$

$$M \propto H^{1/\delta}, \qquad (T=T_c); \tag{1·1c}$$

where T is the absolute temperature, T_c the transition temperature, and t is a reduced temperature defined by

$$t=(T-T_c)/T_c\,. \tag{1·2}$$

The critical indices α, α', β, γ, δ have been extensively studied[3)] both experimentally and theoretically. These quantities, however, are not always independent. In fact as we have shown in II, an equality $\alpha'=\alpha$ appears to hold for Ising or Heisenberg model with an arbitrary value of spin and arbitrary interaction between spins.

Recently Domb[4)] has analyzed the dependence of M on H and t, and suggested a form

$$M=A_0Ht^{-\gamma}+A_1H^3t^{-\gamma-\Delta}+A_2H^5t^{-\gamma-2\Delta}+\cdots\,. \tag{1·3}$$

Under the assumption that the n-th term in Eq. (1·3) is given by $A_nH^{2n+1}t^{-\gamma-n\Delta}$, he derived an equation

$$H = Mt^{\gamma} G(M^2 t^{2\gamma - \Delta}). \qquad (1\cdot 4)$$

On the basis of these considerations, he discussed the critical behavior of physical quantities and concluded that critical indices can be expressed in terms of two independent parameters, the γ and the high temperature gap index Δ. It should be noted that Suzuki[5] has also derived an expression analogous to Eq. (1·3).

In this paper we will discuss the same problem as Domb's on a more rigorous footing, by using the celebrated Lee-Yang theorem[6] on the distribution of zeros of partition function for Ising ferromagnets. We briefly review in § 2 the Lee-Yang theorem and express physical quantities of our interest in terms of distribution function of zeros. In § 3 we study a condition for the susceptibility to have a singularity given by Eq. (1·1a). By the use of this condition, we discuss the critical behavior of magnetization and specific heat, and derive exactly the same results as Domb's. It is pointed out clearly that Domb's parameter Δ is closely related with the distribution of zeros. Section 4 is devoted to the discussion of the dependence of thermodynamic quantities on magnetic field at the transition temperature. We express the energy E and the specific heat C as

$$E \propto H^{\varepsilon}, \quad C \propto H^{-\sigma}, \quad (T = T_c), \qquad (1\cdot 5)$$

and obtain an expression for parameter ε or σ. It turns out that these indices can be expressed in terms of Δ and γ, in accordance with Domb's conclusion. Numerical values of ε and σ are calculated for two- and three-dimensional Ising models and the results are summarized in Table I. It is shown that the C at $T = T_c$ for two-dimensional Ising model has a logarithmic dependence on H.

§ 2. Partition function in the presence of magnetic field

We consider a crystal composed of N lattice points, each occupied by an Ising spin taking values ± 1. The magnetic moment per spin will be denoted by m, and the interaction between all pairs of spin (not limited to nearest-neighbor pairs) is assumed to be ferromagnetic. The Lee-Yang theorem is then applicable to the system under consideration. Since it is a starting point of our theory, let us review quite briefly the theorem.

Suppose that the external magnetic field H is applied to the system. Introduce a reduced magnetic field h and the fugacity z defined by

$$h = 2mH/kT, \quad z = e^{-h}, \qquad (2\cdot 1)$$

where k is the Boltzmann constant. The Lee-Yang theorem states: If one considers the partition function $Z(H, T)$ as a function of z, then all the zeros of partition function lie on the unit circle in the complex z-plane. If one introduces a distribution function $g(\theta)$ of zeros so that $Ng(\theta)d\theta$ is the number of zeros with z between $e^{i\theta}$ and $e^{i(\theta+d\theta)}$, one can express the logarithm of partition function as follows:

$$\frac{\ln Z}{N}=\frac{mH}{kT}+\int_0^{2\pi}\ln(z-e^{i\theta})\,g(\theta)\,d\theta\,. \tag{2·2}$$

The $g(\theta)$ is subject to the conditions

$$\int_0^{2\pi}g(\theta)\,d\theta=1,\quad g(-\theta)=g(\theta). \tag{2·3}$$

Note that the $g(\theta)$ depends on the temperature, although we do not write its explicit dependence for a moment. With the aid of Eq. (2·3), we can transform Eq. (2·2) to a form

$$\frac{\ln Z}{N}=\int_0^{\pi}\ln[2(\operatorname{ch}h-\cos\theta)]\,g(\theta)\,d\theta\,. \tag{2·4}$$

From Eq. (2·4) the average magnetization per spin is calculated to be

$$M=2m\operatorname{sh}h\int_0^{\pi}\frac{g(\theta)}{\operatorname{ch}h-\cos\theta}\,d\theta\,. \tag{2·5}$$

So far there have been no any approximations in our expressions. It is, however, possible to simplify Eq. (2·5) when we restrict ourselves to the critical behavior of M. In the vicinity of transition point, it may be expected that the contribution of small θ is the most important. One may therefore expand $\cos\theta$ in Eq. (2·5) and retain the terms up to the order of θ^2. Furthermore, if h is sufficiently small a similar procedure is applicable to $\operatorname{sh}h$ and $\operatorname{ch}h$ in Eq. (2·5). As a result, restoring the dependence of $g(\theta)$ on t, we have

$$M=4mh\int_0^{\pi}\frac{g(\theta,t)}{h^2+\theta^2}\,d\theta\,. \tag{2·6}$$

The susceptibility χ is therefore given by

$$\chi=\frac{8m^2}{kT}\int_0^{\pi}\frac{g(\theta,t)}{\theta^2}\,d\theta\,. \tag{2·7}$$

If we consider the case $T>T_c$, there may be no zeros in the neighborhood of $\theta=0$. Consequently, in this case the distribution function vanishes for θ less than a certain value of θ, i.e.

$$g(\theta,t)=0\quad\text{for }\theta<\theta_c\,. \tag{2·8}$$

It should be noted that the θ_c depends on t, although we do not write its explicit dependence to simplify the notation. It is clear that $\theta_c\to 0$ in the limit

$t \to 0$.*)

§ 3. Singularities of susceptibility, magnetization and specific heat

Let us consider the case above the transition temperature and assume that the susceptibility has a singularity

$$\chi = \Gamma t^{-\gamma} . \tag{3·1}$$

We will derive a condition imposed on $g(\theta, t)$ for the χ to have the singularity of Eq. (3·1), along the line discussed in II.

From what we have mentioned at the end of § 2, it follows that the lower limit of integral in Eq. (2·7) is θ_c. If we introduce a change of variable $\theta = \theta_c x$ and assume that θ_c is sufficiently small, we have

$$\Gamma \frac{kT_c}{8m^2} = \frac{t^\gamma}{\theta_c} \int_1^\infty \frac{g(\theta_c x, t)}{x^2} dx . \tag{3·2}$$

The left-hand side in this equation is independent of t, so should be the right-hand side. If a quantity $t^\gamma g(\theta_c x, t)/\theta_c$ is independent of t, this condition is satisfied. Thus, differentiating it by t and putting again $\theta = \theta_c x$, we get a partial differential equation

$$\frac{\partial g(\theta, t)}{\partial t} + \frac{\theta_c'}{\theta_c} \theta \frac{\partial g(\theta, t)}{\partial \theta} = \left(\frac{\theta_c'}{\theta_c} - \frac{\gamma}{t}\right) g(\theta, t), \tag{3·3}$$

where $\theta_c' = (d/dt)\theta_c(t)$. A general solution of Eq. (3·3) is easily obtained by means of the standard method in the theory of partial differential equation. We are led to

$$g(\theta, t) = t^{-\gamma} \theta_c f(\theta/\theta_c), \tag{3·4}$$

where $f(x)$ is an arbitrary function of x. If one substitutes Eq. (3·4) in Eq. (2·7), one may see that the χ has really the singularity of Eq. (3·1).

Let us go on to a discussion of the magnetization. If we put Eq. (3·4) in Eq. (2·6) and make the same change of variable as before, we find

$$M = 4mht^{-\gamma} \Psi(h/\theta_c), \tag{3·5}$$

where $\Psi(a)$ is defined by

$$\Psi(a) = \int_1^\infty \frac{f(x)}{x^2 + a^2} dx . \tag{3·6}$$

It is clear that $\Psi(a)$ approaches some constant in the limit $a \to 0$. On the other hand, if we take a limit $t \to 0$, i. e. $\theta_c \to 0$, keeping h finite, a goes to infinity.

*) A general tendency of $g(\theta, t)$ as a function of θ and t will be seen in a recent article by Suzuki [M. Suzuki, Prog. Theor. Phys., to be published].

This situation corresponds to Eq. (1·1c) so that we should have

$$\Psi(a) \to a^{(1-\delta)/\delta}, \quad (a \to \infty). \tag{3·7}$$

Equation (3·5) then becomes

$$M \to h^{1/\delta} t^{-\gamma} \theta_c^{(\delta-1)/\delta}, \tag{3·8}$$

except for a constant coefficient. Since the M must be independent of t in this limit, the dependence of θ_c on t is determined as

$$\theta_c \propto t^{\Delta/2}, \quad \Delta = 2\gamma\delta/(\delta-1). \tag{3·9}$$

It will turn out that the Δ introduced here is identical with Domb's parameter.

We now proceed to a study of energy E and specific heat C in the vicinity of transition point. These quantities are expressed as

$$E/N = kT_c(\partial/\partial t)(\ln Z/N), \tag{3·10}$$

$$C/Nk = (\partial^2/\partial t^2)(\ln Z/N). \tag{3·11}$$

In order to calculate E and C, it is convenient to define a function $G(\theta, t)$:

$$G(\theta, t) = \int_{\theta_c}^{\theta} g(\theta', t)\, d\theta'. \tag{3·12}$$

Using partial integration and noting that $G(\pi, t) = 1/2$ and $G(\theta_c, t) = 0$, we have from Eq. (2·4)

$$\frac{\ln Z}{N} = -\int_{\theta_c}^{\pi} \frac{\sin\theta}{\operatorname{ch} h - \cos\theta} G(\theta, t)\, d\theta + \frac{1}{2}\ln[2(\operatorname{ch} h + 1)]. \tag{3·13}$$

The last term in the above equation does not depend on t, so that we will omit it in the following. Furthermore, simplifying the first term as in Eq. (2·6), we get

$$\frac{\ln Z}{N} = -2\int_{\theta_c}^{\pi} \frac{\theta}{h^2 + \theta^2} G(\theta, t)\, d\theta. \tag{3·14}$$

In calculating the E from this equation, we have to note that the lower limit θ_c depends on t. However, since the relation $G(\theta_c, t) = 0$ holds, we can forget the above dependence and take only the derivative of $G(\theta, t)$ with respect to t. Repeating exactly the same procedure, we find

$$\frac{\partial^2}{\partial t^2}\frac{\ln Z}{N} = 2\int_{\theta_c}^{\pi} \frac{h^2 - \theta^2}{(h^2 + \theta^2)^2} P(\theta, t)\, d\theta, \tag{3·15}$$

where

$$P(\theta, t) = \int_{\theta_c}^{\theta} \frac{\partial^2 G(\theta', t)}{\partial t^2}\, d\theta'. \tag{3·16}$$

From Eqs. (3·4) and (3·12), it follows that

$$G(\theta, t) = t^{-\gamma}\theta_c^2 F(\theta/\theta_c), \tag{3·17}$$

where

$$F(x) = \int_1^x f(u)\, du . \tag{3·18}$$

Substituting Eq. (3·17) in Eq. (3·16) and carrying out the necessary differentiation by t, we find

$$P(\theta, t) = t^{(3\Delta/2)-\gamma-2} I(\theta/\theta_c), \tag{3·19}$$

where $I(x)$ is a sum of integrals such as

$$\int_1^x F(u)\, du, \quad \int_1^x uF'(u)\, du, \quad \int_1^x u^2 F''(u)\, du .$$

An explicit form of $I(x)$ is not necessary for our further discussion; an important thing is that it has an argument θ/θ_c in Eq. (3·19).

Combining Eq. (3·19) with Eq. (3·15), we obtain

$$\frac{C}{Nk} = 2t^{\Delta-\gamma-2} \int_1^\infty \frac{(h/\theta_c)^2 - x^2}{[(h/\theta_c)^2 + x^2]^2} I(x)\, dx . \tag{3·20}$$

Putting $h=0$, one may see that the critical index α is given by

$$\alpha = 2 + \gamma - \Delta , \tag{3·21}$$

which is exactly the same as the one derived by Domb. Therefore, the Δ introduced here is shown to be identical with Domb's. As is clear from Eq. (3·9), the Δ is a parameter which describes how fast the zeros of partition function approach the point $\theta=0$ as t goes to zero. From Eqs. (3·9) and (3·21), the α is also expressed as

$$\alpha = 2 - \gamma(\delta+1)/(\delta-1). \tag{3·22}$$

Returning now to the discussion of magnetization, we note that Eq. (3·5) can be rewritten as Eq. (1·4), if we solve h in terms of M and t. Repeating Domb's procedure,[4] we find

$$\beta = (\Delta/2) - \gamma \quad \text{or} \quad \beta = \gamma/(\delta-1). \tag{3·23}$$

It is easily verified that Eqs. (3·21) and (2·23) lead to

$$\alpha + 2\beta + \gamma = 2, \quad \alpha + \beta(1+\delta) = 2. \tag{3·24}$$

These relations were first given by Essam and Fisher.[7] Also, one would obtain them if one replaces Rushbrooke's[8] or Griffiths'[9] inequality by equality.

We have so far assumed that θ_c is not identically zero. However, a possibility $\theta_c \equiv 0$ for $t>0$ may not be excluded from the general discussion. If this happens, introduce a transformation $\theta = tx$ in Eq. (2·7). Then we have $g(\theta, t) = t^{-\gamma+1}f(\theta/t)$, by using the same procedure as to derive Eq. (3·4). This equation leads to $1/\delta = 1-\gamma$, which is not consistent with the exact results for two-dimensional case or the numerical results for three-dimensional case ($\gamma > 1$, $\delta > 0$). This is the reason why we discarded the possibility $\theta_c = 0$.

§ 4. Discussion

We are now in a position to discuss the behavior of thermodynamic functions at the transition point. From Eqs. (3·14) and (3·17), we get

$$\ln Z/N = t^{-\gamma}\theta_c^{\,2}\Phi(h/\theta_c), \tag{4·1}$$

where

$$\Phi(a) = -2\int_1^\infty \frac{x}{x^2+a^2} F(x)\,dx. \tag{4·2}$$

We note that there should occur no phase transition in the presence of magnetic field. In other words, the right-hand side in Eq. (4·1) is a power series of t if $h \neq 0$. Now suppose that $\Phi(h/\theta_c)$ involves a term $(\theta_c/h)^m$. Then the right-hand side in Eq. (4·1) is expressed as $t^{\Delta-\gamma+m\Delta/2}h^{-m}$. From what we have mentioned above, it follows that $\Delta-\gamma+m\Delta/2 = n$, $(n = 0, 1, 2, \cdots)$. Thus solving m in terms of n, we obtain

$$\frac{\ln Z}{N} = \sum_{n=0}^{\infty} a_n t^n h^{2(\Delta-\gamma-n)/\Delta}. \tag{4·3}$$

Therefore the ε and σ defined in Eq. (1·5) are given by

$$\varepsilon = 2(\Delta-\gamma-1)/\Delta, \quad \sigma = 2(2-\Delta+\gamma)/\Delta. \tag{4·4}$$

The fact that these parameters are expressed in terms of γ and Δ is in accordance with Domb's conclusion. It should be noted that Eq. (4·1) is consistent with the results of Widom,[10] Kadanoff[11] and Suzuki.[5]

We have calculated ε and σ for two- and three-dimensional Ising models and the results are summarized in Table I, together with other critical indices.

Table I. Numerical values for the critical indices. $2I$, $3I$ and C indicate two-dimensional Ising model, three-dimensional Ising model and classical theory, respectively.

Thermodynamic quantity	Index	$2I$	$3I$	C
High temperature susceptibility	γ	7/4	5/4	1
High temperature gap index	Δ	15/4	25/8	3
High temperature specific heat	$\alpha = 2+\gamma-\Delta$	0	1/8	0
Spontaneous magnetization	$\beta = (\Delta/2)-\gamma$	1/8	5/16	1/2
Magnetization vs field at T_c	$\delta = \Delta/(\Delta-2\gamma)$	15	5	3
Energy vs field at T_c	$\varepsilon = 2(\Delta-\gamma-1)/\Delta$	8/15	14/25	2/3
Specific heat vs field at T_c	$\sigma = 2(2+\gamma-\Delta)/\Delta$	0	2/25	0

We also list their values obtained in the classical theory of phase transition (e. g. in the molecular field approximation). In dealing with the three-dimensional model, we used $\gamma=5/4$ and $\Delta=25/8$ as in Domb's theory.[4)]

The result $\sigma=0$ in the two-dimensional Ising model strongly suggests that the specific heat has a logarithmic dependence on magnetic field. That this is really the case will be shown as follows. If we consider the case $h=0$ and assume that $I(x)\simeq -I_0 x$ for large x, we find from Eq. (3·20)

$$\frac{C}{Nk}\simeq 2I_0\int_1^{1/\theta_c}\frac{dx}{x}=2I_0\ln\frac{1}{\theta_c}=I_0\Delta\ln\frac{1}{t}\,, \tag{4·5}$$

where we have taken the upper limit of integral to be $1/\theta_c$ which has so far been assumed to be ∞. In the same way, if we put $t=0$ keeping h finite, we get

$$C/Nk\simeq 2I_0\ln(1/h)\,,\quad (T=T_c)\,. \tag{4·6}$$

Therefore if we write

$$C\simeq -A_T\ln|T-T_c|,\ (H=0),\ C\simeq -A_H\ln H,\ (T=T_c),$$

the ratio A_T/A_H depends only on a single parameter Δ:

$$A_T/A_H=\Delta/2\,. \tag{4·7}$$

Although the present results are obtained for Ising ferromagnets, it may be tempting to apply them to Heisenberg ferromagnets. Since the relation $\sigma=2\alpha/\Delta$ is derived and the result $\alpha=0$ is believed to be valid, we find $\sigma=0$ in Heisenberg ferromagnets. So that it would be expected that the specific heat at $T=T_c$ has also a logarithmic dependence on H in this case.

Finally we would like to discuss the critical index α. The result $\alpha=1/8$ in the three-dimensional Ising model is not consistent with our conjecture given in I. Nevertheless, a part of the results obtained in I is useful in estimating the ratio of the coefficients appearing in the expression for the specific heat. If we write

$$C=C_\pm|T-T_c|^{-\alpha},\quad (T\gtrless T_c),$$

we have from Eq. (3·11) in II that $C_+/C_-=\cos[(2-\alpha)\varphi]/\cos[(2-\alpha)\varphi+\alpha\pi]$. Putting $\alpha=1/8$ and a value of φ discussed in I, we find $C_+/C_-\simeq 0.8$ for the case of simple cubic lattice. Thus the low temperature specific heat has a slightly larger coefficient than the high temperature one.

Acknowledgements

The author would like to express his sincere thanks to Professor C. Domb for sending him reprints on the critical behavior of ferromagnets. He is also indebted to Professor M. E. Fisher for a number of critical comments.

References

1) R. Abe, Prog. Theor. Phys. **37** (1967), 1070.
2) R. Abe, Prog. Theor. Phys., to be published.
3) See, for example, M. E. Fisher, *Lectures in Theoretical Physics* (University of Colorado Press, Boulder, 1964), Vol. **7c**, p. 1.
4) C. Domb and D. L. Hunter, Proc. Phys. Soc. **86** (1965), 1147.
C. Domb, *Proceedings of the 1966 Low Temperature Calorimetry Conference*, edited by O. V. Lounasmaa, Ann. Acad. Sci. Fennicae **A VI** (1966), 167.
5) M. Suzuki, J. Phys. Soc. Japan **22** (1967), 757.
6) T. D. Lee and C. N. Yang, Phys. Rev. **87** (1952), 410.
7) J. W. Essam and M. E. Fisher, J. Chem. Phys. **38** (1963), 802.
8) G. S. Rushbrooke, J. Chem. Phys. **39** (1963), 842.
9) R. B. Griffiths, J. Chem. Phys. **43** (1965), 1958.
10) B. Widom, J. Chem. Phys. **43** (1965), 3898.
11) L. P. Kadanoff, Physics **2** (1966), 263.