

A Theory of the Second Order Phase Transitions in Spin Systems. II

—Complex Magnetic Field—

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The thermodynamic quantities of the Ising model are analyzed near T_c , using the asymptotic distribution function $g(\theta, t)$ of zeros for the partition function on a unit circle in the plane of the complex magnetic field. The distribution function is derived as $g(\theta, t) = t^\lambda f(\theta/t^{\lambda+\gamma})$, assuming that the susceptibility behaves like $\chi_0^+ \sim t^{-\gamma}$ near T_c where $t = T/T_c - 1$. It is shown that there are two types of the situation: type I, in which a critical angle $\theta_c(t)$ exists such that $g(\theta, t) = 0$ for $0 \leq |\theta| \leq \theta_c$, and type II, in which there is no critical angle. The critical indices are related to one another, using the above $g(\theta, t)$.

The relation between the magnetic equation of state $M = M(h, t)$ and the distribution function is given as follows: $g(\theta, t) = (1/2\pi) \text{Re } M(i\theta, t)$, where $h = 2mH/kT$. $g(\theta, t)$ for an exactly soluble model near T_c is given by the equation $\theta^2 \sim t^3 + a_1 t^2 g^2 + a_2 t g^4 + a_3 g^6$ ($a_i > 0$). This is a good example for the general theory.

§ 1. Introduction

This paper is concerned with the singularities of the thermodynamic quantities near the transition points in spin systems, especially in the Ising model. On this problem, there are several works, such as the present author's semi-phenomenological theory¹⁾ and conjecture,²⁾ Widom's homogeneity assertion,³⁾ Domb and Hunter's conjecture,⁴⁾ Kadanoff's scaling laws⁵⁾ and Patashinsky and Pokrovsky's dimensional analysis.⁶⁾ Kouvel and Rodbell⁷⁾ have studied the magnetic equation of state (1.2) or (1.3) experimentally.

Anyway, in order to explain the singularities of susceptibilities, spontaneous magnetizations, specific heats, etc., the following form of the free energy has been proposed:

$$F(t) = F_0(t) + t^{d-\gamma} f_s(M^2/t^{d-2\gamma}), \quad (1.1)$$

where $t = T/T_c - 1$; (see Eq. (27) in a previous paper by the present author¹⁾). The magnetic equation of state is given in the following,

$$H = - \frac{\partial F}{\partial M} = t^{d'} f_m(M/t^{d'-\gamma}), \quad (1.2)$$

where

$$\Delta' = \Delta/2 \quad \text{and} \quad f_m(x) = -2xf'_s(x^2).$$

If we invert the above equation (1.2) we obtain

$$M = t^{\Delta'-\gamma} \varphi_m(h/t^{\Delta'}) \quad \text{and} \quad h = 2mH/kT. \quad (1.3)$$

Equation (1.3) has been derived above the transition point T_c . Now, we assume that the equation of state (1.3) can be continued analytically beyond T_c . Then, the spontaneous magnetization is given by

$$M_s = |t|^{\Delta'-\gamma} |\varphi_m(0)| \sim |t|^\beta \quad \text{for } t < 0, \quad (1.4)$$

where $\varphi_m(x)$ is such a branch of the solution for Eq. (1.2), as vanishes at $x=0$ above T_c and does not vanish at $x=0$ below T_c . Therefore, the index β is given by

$$\beta = \Delta' - \gamma. \quad (1.5)$$

Above the transition point, the magnetization becomes

$$M \sim ht^{-\gamma} \varphi'_m(h/t^{\Delta'}).$$

Consequently, the susceptibility is, above T_c ,

$$\chi_0^+ \sim t^{-\gamma}. \quad (1.6)$$

Next, the specific heat behaves itself as follows, from Eq. (1.1),

$$C \sim \frac{\partial^2 F(t)}{\partial t^2} \sim t^{\Delta-\gamma-2} \sim t^{-\alpha}. \quad (1.7)$$

Then, we obtain the following relation

$$\alpha = 2 + \gamma - \Delta. \quad (1.8)$$

Thus, we can discuss the relations among the critical indices α , β and γ , in terms of the free energy (1.1) or the magnetic equation of state (1.3).

In § 2, starting from the theorem of Lee and Yang in the Ising model, it is shown that the same relations among the critical indices can be derived, in terms of an asymptotic distribution function. This theory has already been partly reported²⁾ and then Abe has generalized its treatment.⁸⁾ Here, it should be noted that the distribution function of the following form can be derived without assuming the existence of a critical angle $\theta_c(t)$;

$$\theta = t^{\Delta'} \Psi(g/t^{\Delta'-\gamma}) \quad (1.9)$$

or inverting this, we obtain

$$g(\theta, t) = t^{\Delta'-\gamma} f(\theta/t^{\Delta'}). \quad (1.10)$$

In § 3, we discuss the relations between the magnetic equation of state and the distribution function. It is pointed out that Eqs. (1.3) and (1.10) are equivalent each other.

In § 4, the distribution function $g(\theta, t)$ for an exactly soluble model is calculated concretely near the transition point, which is shown to be such a type of distribution functions as discussed in § 2, and which has such a critical angle as $\theta_c(t) \sim t^{3/2}$.

§ 2. The critical behavior of the Ising model and the distribution function of zeros

(i) Distribution function of zeros and thermodynamic quantities

The Ising model is represented by the following Hamiltonian,

$$\mathcal{H} = -J \sum S_i S_j - mH \sum S_i, \quad \text{and} \quad S_i = \pm 1. \quad (2.1)$$

The partition function of the system is written as a polynomial of the fugacity z in the following way,

$$\begin{aligned} Z_N(K, h) &= \text{Tr} \exp(-\beta \mathcal{H}) = \text{Tr} \exp\left(K \sum S_i S_j + \frac{h}{2} \sum S_i\right) \\ &= [\exp(h/2)]^N \sum_{k=0}^N a_k z^k, \end{aligned} \quad (2.2)$$

where $z = e^{-h}$, $h = 2mH/kT$, and $a_{N-k} = a_k$. The theorem of Lee and Yang⁹⁾ indicates that the zeros of the partition function lie on the unit circle in the fugacity plane. Therefore, the free energy for infinite N is represented, in terms of the distribution function of zeros,⁹⁾ neglecting a constant term JN_p (N_p : number of pairs),

$$\begin{aligned} -\frac{F}{kT} &= \lim_{N \rightarrow \infty} \frac{1}{N} \log Z_N = \frac{mH}{kT} + \lim_{N \rightarrow \infty} \frac{1}{N} \sum_k \log(z - e^{i\theta_k}) \\ &= \frac{mH}{kT} + \int_0^{2\pi} g(\theta) \log(z - e^{i\theta}) d\theta \\ &= \frac{mH}{kT} + \int_0^\pi g(\theta) \log(z^2 - 2z \cos \theta + 1) d\theta, \end{aligned} \quad (2.3)$$

where $g(\theta, t)$ satisfies the following condition of normalization,

$$\int_0^\pi g(\theta, t) d\theta = \frac{1}{2}.$$

Furthermore, we can rewrite the free energy in the following convenient form,

$$-F/kT = \int_0^\pi g(\theta, t) \log 2 (\cosh h - \cos \theta) d\theta, \quad (2.4)$$

where $t = (T - T_c)/T_c$, and $h = 2mH/kT$. As far as the neighborhood of the transition point and a weak external field are concerned, the integral in the region of small θ and h becomes important, so that we can write as follows,

$$-F/kT \simeq \int_0^\pi g(\theta, t) \log(\theta^2 + h^2) d\theta. \quad (2.5)$$

The magnetization is obtained from Eq. (2.4):

$$\begin{aligned} M &= 2m \sinh h \int_0^\pi \frac{g(\theta, t)}{\cosh h - \cos \theta} d\theta \\ &\simeq 4mh \int_0^\pi \frac{g(\theta, t)}{\theta^2 + h^2} d\theta. \end{aligned} \quad (2.6)$$

The spontaneous magnetization is expressed in terms of $g(0, t)$ as follows,

$$\begin{aligned} M_s &= \lim_{h \rightarrow 0} 4mh \int_0^\pi \frac{g(\theta, t)}{\theta^2 + h^2} d\theta \\ &= 4m \int_0^\pi \pi \delta(\theta) g(\theta, t) d\theta \\ &= 2\pi m g(0, t). \end{aligned} \quad (2.7)$$

Consequently, the susceptibility above T_c is given by the equation

$$\begin{aligned} \chi_0^+ &= (4m^2/kT) \int_0^\pi \frac{g(\theta, t)}{1 - \cos \theta} d\theta \\ &\simeq (8m^2/kT) \int_0^\pi \frac{g(\theta, t)}{\theta^2} d\theta, \end{aligned} \quad (2.8)$$

and below the Curie point, we obtain from Eqs. (2.6) and (2.7)

$$\begin{aligned} \chi_0^- &= \lim_{H \rightarrow 0} \{M(H) - M_s\} / H \\ &= \lim_{H \rightarrow 0} \left\{ \frac{4m^2 H}{kT} \int_0^\pi \frac{g(\theta, t) d\theta}{\cosh h - \cos \theta} - \frac{4m^2 H}{kT} \int_0^\pi \frac{g(0, t) d\theta}{\cosh h - \cos \theta} \right\} \times \frac{1}{H} \\ &= \frac{4m^2}{kT} \int_0^\pi \frac{g(\theta, t) - g(0, t)}{1 - \cos \theta} d\theta \end{aligned} \quad (2.9)$$

$$\simeq \frac{8m^2}{kT} \int_0^\pi \frac{g(\theta, t) - g(0, t)}{\theta^2} d\theta. \quad (2.9')$$

The specific heat is obtained near T_c from the equation

$$C \sim \frac{d^2}{dt^2} \int_0^\pi g(\theta, t) \log \theta d\theta. \quad (2.10)$$

(ii) *Plausible distribution function of zeros*

In the previous paper²⁾, we have shown that the singularities near the transition point can be explained in terms of the following asymptotic distribution function for small θ and t ,

$$g(\theta, t) = a(\theta^\eta - bt^\varepsilon)^\kappa, \quad g(\theta, t) = 0, \quad \text{for } \theta < \theta_c(t), \quad \text{and } \theta_c \sim t^{\varepsilon/\eta}, \quad (2.11)$$

where η is a positive even integer, and ε a positive odd integer. Namely, if we define the critical indices in the following way

$$\begin{aligned} \chi_0^+ &\sim t^{-\gamma}, \quad \chi_0^- \sim |t|^{-\gamma'}, \quad M_s \sim |t|^\beta, \quad M_c \sim H^{1/\delta}, \\ C^+ &\sim t^{-\alpha}(c_1 \log t + c_2) \quad \text{and} \quad C^- \sim |t|^{-\alpha'}(c_1' \log |t| + c_2'), \end{aligned} \quad (2.12)$$

then, from Eqs. (2.6), (2.7), (2.8), (2.9'), (2.10) and (2.11), the six indices are related one another by two independent parameters ε/η and $\varepsilon\kappa$ as follows (Appendix A):

$$\begin{aligned} \gamma &= \gamma' = \varepsilon(1/\eta - \kappa), \quad \beta = \varepsilon\kappa, \\ \alpha &= \alpha' = 2 - \varepsilon(1/\eta + \kappa) \quad \text{and} \quad \delta = 1/\eta\kappa = (\varepsilon/\eta) / (\varepsilon\kappa). \end{aligned} \quad (2.13)$$

These results satisfy the following relations

$$\alpha + 2\beta + \gamma = 2 \quad (2.14)$$

and

$$\alpha + \beta(1 + \delta) = 2. \quad (2.15)$$

Now, the plausible distribution function (2.11) may be also written in the form

$$\theta^\eta = a_1 t^\varepsilon + a_2 g^{1/\kappa}. \quad (2.16)$$

Even if we generalize it in the following form, under the condition of integer ε ,

$$\theta^\eta = \sum_{j=0}^{\varepsilon} a_j t^{\varepsilon-j} (g^{1/\varepsilon\kappa})^j, \quad (2.17)$$

the critical behavior is the same as in the case of Eq. (2.16). In fact, the distribution function of the molecular field theory or its equivalent exactly soluble model is of the form given by substituting $\eta=2$, $\varepsilon=3$ and $\kappa=1/6$ in Eq. (2.17), as shown in § 4.

Extending the plausible distribution function to Eq. (2.17), we notice that there are two types of the situation.

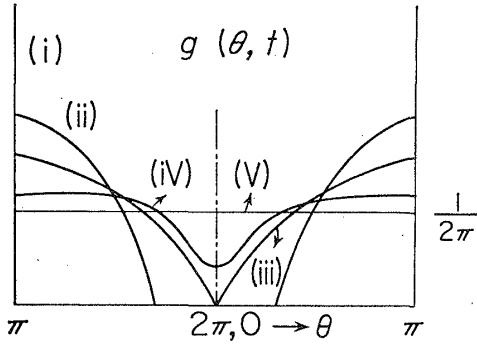


Fig. 1. Schematic distribution function in type I to explain phase transitions.

(i) $T=\infty$, (ii) $T>T_c$, (iii) $T=T_c$,
(iv) $T<T_c$ and (v) $T=0$.

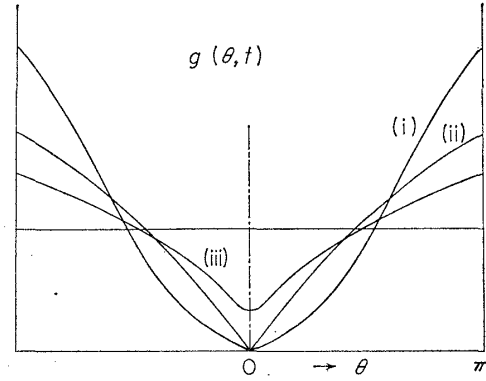


Fig. 2. Schematic distribution function in type II. (i) $T>T_c$, (ii) $T=T_c$ and (iii) $T<T_c$.

<Type I> There exists a critical angle $\theta_c(t)$ in the case $a_0 \neq 0$. In this case, Eqs. (2.16) and (2.17) are essentially the same, and putting $g=0$, we obtain the critical angle, for $t>0$,

$$\theta_c(t) \sim t^{\varepsilon/\eta}, \text{ and } g(\theta, t) = 0 \text{ for } 0 \leq |\theta| \leq \theta_c(t). \quad (2.18)$$

This situation is illustrated schematically in Fig. 1.

<Type II> There exists no critical angle in the case $a_0=0$, because the value $g=0$ corresponds to that $\theta=0$. This situation is shown schematically in Fig. 2.

(iii) *General type of distribution function*

In the above paragraph, we have discussed two types of distribution functions. In any case, the range of $g(\theta, t)$ is

$$0 \leq g \leq g_m(t) \text{ for } t > 0. \quad (2.19)$$

This is expected to hold in general from the condition of continuity for $g(\theta, t)$. Let us investigate a general type of distribution function, using the above property (2.19) and assuming that the susceptibility has the following singularity,

$$\chi_0^+ \sim t^{-\gamma} \text{ for } t > 0. \quad (2.20)$$

Then, we can equate asymptotically in the following way,

$$\int_0^{g_m} \frac{\theta'(g) g dg}{\theta^2(g, t)} \sim t^{-\gamma}, \text{ for } 0 \leq \theta \leq \pi. \quad (2.21)$$

If we make a change of variable

$$g = t^\lambda y \quad (\lambda \text{ is a proper positive constant}),$$

we find that

$$\int_0^{g_m/t^\lambda} \left[\frac{\theta'(t^\lambda y, t) y t^{\gamma+2\lambda}}{\theta^2(t^\lambda y, t)} \right] dy \sim \text{constant}. \quad (2.22)$$

As the upper limit of the integral can be replaced by infinity near T_c , we obtain

$$\int_0^{\infty} \left[\frac{\theta'(t^\lambda y, t) t^{\gamma+2\lambda}}{\theta^2(t^\lambda y, t)} \right] y dy \sim \text{constant}. \quad (2.23)$$

The sufficient condition for the susceptibility to have the singularity of Eq. (2.20) is that, for a proper value of λ ,

$$\frac{\theta'(t^\lambda y, t) t^{\gamma+2\lambda}}{\theta^2(t^\lambda y, t)} = \Phi(y). \quad (2.24)$$

If we return to the former variable

$$g = t^\lambda y,$$

we find the following differential equation

$$\frac{\partial \theta(g, t)}{\partial g} = t^{-\gamma-2\lambda} \theta^2 \Phi(g/t^\lambda). \quad (2.25)$$

The solution is given by

$$\theta(g, t) = t^{\lambda+\gamma} \Psi(g/t^\lambda), \quad (2.26)$$

where

$$\Psi(x) = - \left[\int \Phi(x) dx \right]^{-1}.$$

In the case $\Psi(0) \neq 0$, the following critical angle is derived, by putting $g=0$ in Eq. (2.26):

$$\theta_c(t) = \Psi(0) t^{\lambda+\gamma} \quad \text{for } t > 0. \quad (2.27)$$

This is the case of type I. For $\Psi(0) = 0$, the case of type II is obtained. If we invert Eq. (2.26), the distribution function becomes of the form

$$g(\theta, t) = t^\lambda f(\theta/t^{\lambda+\gamma}). \quad (2.28)$$

In the case of type I, this is written in the following way, using the critical angle θ_c in Eq. (2.27),

$$g(\theta, t) = t^{-\gamma} \theta_c f_2(\theta/\theta_c) \quad \text{for } t > 0, \quad (2.29)$$

which agrees with the form derived by Abe.⁸⁾

It is clear that Eqs. (2.11) and (2.17) yield simple examples of the general form (2.26) or (2.28), taking that $\lambda = \varepsilon\kappa$, and that $\lambda + \gamma = \varepsilon/\eta$.

Now, if we assume that the function (2.28) can be continued analytically below T_c , the critical indices are expressed as follows, from Eqs. (2.6), (2.7), (2.8), (2.9') and (2.10),

$$\begin{aligned} \alpha &= \alpha' = 2 - 2\lambda - \gamma, \quad \beta = \lambda, \\ \gamma' &= \gamma \quad \text{and} \quad \delta = (\lambda + \gamma)/\lambda. \end{aligned} \quad (2.30)$$

Consequently, the relations (2.14) and (2.15) hold.

In the case of type II, the distribution function of the form (2.28) can be derived more simply (Appendix B). Here, it should be emphasized that the distribution function (2.28) has been derived without assuming the existence of a critical angle.

§ 3. The relation between the magnetic equation of state and $g(\theta, t)$

(i) *General relation* Let us assume that the magnetic equation of state is given by

$$M = \varphi_M(h, t) \quad \text{and} \quad h = 2mH/kT. \quad (3.1)$$

Then, what relation exists between the distribution function and the equation of state? If we invert Eq. (3.1) as a power series in M , we obtain

$$h = \sum_{k=0}^{\infty} a_k(t) M^{2k+1}, \quad (3.2)$$

where the coefficients $\{a_k(t)\}$ may be singular at $t=0$.¹⁾ In principle, according to the theory of Lee and Yang,⁹⁾ the distribution function can be obtained from the complex value of the magnetization on a unit circle of the fugacity plane. Therefore, putting

$$h = i\theta \quad \text{and} \quad M = Re^{i\varphi}, \quad (3.3)$$

and substituting them into (3.2), we obtain

$$\left. \begin{aligned} \sum_{k=0}^{\infty} a_k R^{2k+1} \cos(2k+1)\varphi &= 0 \\ \sum_{k=0}^{\infty} a_k R^{2k+1} \sin(2k+1)\varphi &= \theta \end{aligned} \right\} \quad (3.4)$$

and

It can easily be found that if $M_1 = Re^{i\varphi}$ is a solution of Eq. (3.4), then

$$M_2 = Re^{i(\pi-\varphi)} = -Re^{-i\varphi}, \quad (3.5)$$

is another branch of the solution for Eq. (3.4), and consequently for Eq. (3.2). Therefore, the distribution function is obtained as follows,

$$g(\theta, t) = \frac{1}{4\pi} (M_1 - M_2) = \frac{1}{2\pi} R \cos \varphi = \frac{1}{2\pi} \hat{g}, \quad (3.6)$$

where

$$\hat{g} = R \cos \varphi = \text{Re } M(i\theta, t). \quad (3.7)$$

Hence we get the following theorem.

Theorem I. If the magnetic equation of state is given by (3.1), then the distribution function is

$$g(\theta, t) = \frac{1}{2\pi} \operatorname{Re} \varphi_M(i\theta, t). \quad (3.8)$$

(ii) In particular, for the magnetic equation of state of the following form,

$$M = t^\beta \varphi_m(h/t^{d'}), \quad (3.9)$$

which has been discussed in § 1, we find that

$$g(\theta, t) = t^\beta f(\theta/t^{d'}), \quad (3.10)$$

where

$$f(x) = \frac{1}{2\pi} \operatorname{Re} \varphi_m(ix). \quad (3.11)$$

The distribution function of the form (3.10) has been derived in § 2, under the assumption of the singularity (2.20) of the susceptibility.

(iii) Inversely, it can be shown that if the distribution function is given by Eq. (3.10), then, the magnetic equation of state obeys the relation (3.9) near T_c . The magnetization is, from Eqs. (2.6) and (3.10),

$$M \simeq 4mh \int_0^\pi \frac{t^\beta}{\theta^2 + h^2} f\left(\frac{\theta}{t^{d'}}\right) d\theta. \quad (3.12)$$

If we make a change of variable

$$x = \theta/t^{d'}$$

in Eq. (3.12), and replace the upper limit of the transformed integral by infinity, then we find that

$$M \simeq t^\beta \varphi_m(h/t^{d'}), \quad (3.13)$$

where

$$\varphi_m(y) = 4m \int_0^\infty \frac{yf(x)}{x^2 + y^2} dx. \quad (3.14)$$

Thus, it follows that the homogeneity assertion for the magnetic equation of state is equivalent to that for the distribution function.

§ 4. $g(\theta, t)$ for an exactly soluble model

In this section, the situation for the distribution function discussed in the previous sections is exemplified in the molecular field theory or its equivalent exactly soluble model near the transition point.

Let us consider the following Hamiltonian with a long-range interaction,

$$\mathcal{H} = -J \sum_{i,j}^{\text{all}} S_i S_j - mH \sum_i S_i; \quad S_i = \pm 1 \quad \text{and} \quad J > 0. \quad (4.1)$$

The same kind of models have been investigated by several authors,^{10)-13), 21)} but there have been no explicit expression for the distribution function.

If we define the intensity of the magnetization as $M = \langle S_i \rangle$, and put

$$\lim_{N \rightarrow \infty} (NJ) = a \text{ (finite)}, \quad (4.2)$$

then, the magnetic equation of state in the limit of infinite N is given by¹³⁾

$$M = \tanh(a\beta M + \beta mH), \quad (4.3)$$

where $\beta = 1/kT$. This agrees with the results in the molecular field theory. Namely, the Curie point is determined by

$$a\beta = 1, \quad \text{or} \quad T_c = a/k. \quad (4.4)$$

The susceptibility is

$$\chi_0 \sim 1/(T - T_c), \quad (4.5)$$

and the spontaneous magnetization takes the form

$$M_s \sim (T_c - T)^{1/2}. \quad (4.6)$$

Now, the magnetic equation of state (4.3) is rewritten as follows,

$$M = \tanh\{(1-t)M + \beta mH\}, \quad (4.7)$$

where

$$t = 1 - T_c/T = (T - T_c)/T_c + (\text{higher order}). \quad (4.8)$$

Equation (4.7) can be inverted to give⁴⁾

$$\frac{\hat{h}}{2} = \frac{M - \tanh\{(1-t)M\}}{1 - M \tanh\{(1-t)M\}}, \quad (\hat{h} = 2 \tanh(\beta mH)). \quad (4.9)$$

Near T_c , the expansion of this equation up to the third order of M gives

$$\frac{\hat{h}}{2} = Mt + \frac{1}{3}M^3. \quad (4.10)$$

As we have discussed in the previous sections, the distribution function can be obtained from the value of M for the pure imaginary magnetic field $\hat{h} = i\theta$. Then, putting

$$\hat{h} = i\theta, \quad M = Re^{i\varphi} \quad \text{and} \quad \hat{g} = Re M(i\theta, t),$$

and substituting them into (4.10), we obtain the following simultaneous equations,

$$\begin{cases} tR \cos \varphi + \frac{1}{3}R^3 \cos 3\varphi = 0, & (4.11) \\ tR \sin \varphi + \frac{1}{3}R^3 \sin 3\varphi = \frac{1}{2}\theta, & (4.12) \\ R \cos \varphi = \hat{g}. & (4.13) \end{cases}$$

Eliminating the parameters R and φ from the above equations (4.11), (4.12) and (4.13), we can derive a relation between \hat{g} and θ near T_c as follows,

$$\theta^2 = \left(\frac{4}{3}\right)^2 \left(t + \frac{1}{3}\hat{g}^2\right) \left(t + \frac{4}{3}\hat{g}^2\right)^2, \quad (4.14)$$

where we have used the following trigonometric formulae

$$\left. \begin{aligned} \cos 3\varphi &= 4 \cos^3 \varphi - 3 \cos \varphi \\ \sin 3\varphi &= \sin \varphi (4 \cos^2 \varphi - 1). \end{aligned} \right\} \quad (4.15)$$

The distribution function $g(\theta, t)$ is given by

$$g(\theta, t) = \hat{g}/2\pi. \quad (4.16)$$

Equation (4.14) is just of the form (2.17) with the parameters $\eta=2$, $\varepsilon=3$ and $\kappa=1/6$, and consequently it satisfies the general relation (2.28). Putting $g=0$ in Eq. (4.14), the critical angle is obtained as follows,

$$\theta_c(t) = \frac{4}{3}t^{3/2}. \quad (4.17)$$

The distribution function at the critical point is also given by

$$g(\theta, 0) = \{3^{5/6}/(2^{7/3}\pi)\}\theta^{1/3}. \quad (4.18)$$

Therefore, the distribution function is essentially the same as that given by the relation*)

$$\theta^2 = a_1 t^3 + a_2 g^6 \quad \text{for } g^2/t > 1, \quad (4.19)$$

which can be rewritten as

$$g(\theta, t) = a(\theta^2 - bt^3)^{1/6}. \quad (4.20)$$

This is just a nice example for the general theory discussed in the previous sections. It can be easily shown from Eq. (4.14) or consequently from Eq. (4.20), that

i) for $t > 0$, we obtain

$$g(\theta, t) = \begin{cases} = 0 & \dots 0 \leq |\theta| \leq \theta_c \\ \neq 0 & \dots \theta_c < |\theta|, \end{cases} \quad (4.21)$$

and

$$g_\theta(\theta_c, t) = \infty \quad \left(g_\theta \equiv \frac{\partial}{\partial \theta} g(\theta, t)\right),$$

*) S. Katsura kindly pointed out to the author that for $\hat{g}^2/t < 1$, $\hat{g} \simeq (1/\sqrt{2})t^{-1/4}(\theta - \theta_c(t))^{1/2}$ in terms of Eq. (4.14).

and

ii) for $t < 0$, we get

$$g(0, t) \neq 0 \quad \text{and} \quad g_\theta(0, t) = 0.$$

These features are schematically illustrated in Fig. 1. The same results are obtained from Katsura's implicit relations for the Husimi-Temperley model.¹⁰⁾

§ 5. Discussion

The concept of complex magnetic field can be applied to the Heisenberg model. In general, let us consider the following Hamiltonian,

$$\mathcal{H} = \mathcal{H}_0 - mH \sum_i S_i^z, \quad S_i^z = \pm 1, \quad \text{and} \quad [\mathcal{H}_0, \sum_i S_i^z] = 0, \quad (5.1)$$

where

$$\mathcal{H}_0 = - \sum J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j, \quad \text{etc.} \quad (5.2)$$

Then, the partition function can be expressed by the following polynomial of the "fugacity" z ,

$$\begin{aligned} Z &= \text{Tr} \exp(-\beta \mathcal{H}_0) \exp(h' \sum_i S_i^z) \\ &= (e^{h'})^N \text{Tr} \exp(-\beta \mathcal{H}_0) \prod_i \left(\frac{1+z}{2} + S_i^z \frac{1-z}{2} \right) \\ &= (e^{h'})^N \sum_{k=0}^N a_k z^k \end{aligned} \quad (5.3)$$

$$\equiv (e^{h'})^N f_N(z, \beta), \quad (5.3')$$

where $z = e^{-2h'}$ and $h' = \beta mH$. It may be expected that the zeros of the partition function in the ferromagnetic Heisenberg model lie on a unit circle of the "fugacity" plane as in the Ising model. This conjectured theorem can be easily shown in the case of small finite lattices. For example, in the case $N=2$, we obtain

$$f_2(z, K) = z^2 + z(1 + e^{-4K}) + 1, \quad (5.4)$$

where $K = J/kT$. The zeros of Eq. (5.4) lie on a unit circle of the z -plane. In the same way, we have found that the theorem holds for $N=3$ and $N=4$. For $N \geq 5$, numerical calculations will be needed. The validity of the conjectured theorem in the case $N=6$ has been proved by Katsura.¹⁴⁾

Anyway, even if the theorem does not hold in general, the zeros of the partition function in the Heisenberg model are, at least, expected to lie asymptotically on a unit circle near the positive real axis in the vicinity of the Curie point. Therefore, the theory described in § 2 may be applied to the Heisenberg model, asymptotically.

Next, what properties are there on the distribution of the zeros in the case of the antiferromagnetic Ising model? It is easily shown in the one-dimensional

antiferromagnetic Ising model that the zeros of the partition function for the ring of number N is given by

$$(\tanh h')_k = \pm \left\{ \frac{\exp(-4K) + \tan^2[\pi(K+1/2)/N]}{\exp(-4K) - 1} \right\}^{1/2}, \quad (5.5)$$

where $K=J/kT$, and $k=0, 1, 2, \dots, N-1$. For $J<0$, we get, from Eq. (5.5),

$$(\tanh h')_k > 1, \text{ or } (\tanh h')_k < -1,$$

and consequently, the zeros on z -plane are given by

$$z_k = e^{-2h'} = \frac{1 - \tanh h'}{1 + \tanh h'} < 0. \quad (5.6)$$

That is, all the zeros lie on the *negative real* axis. At a glance, the same situation may also be expected in the two- and three-dimensional antiferromagnetic Ising models. However, we have found a counter example in such a small finite model, as is shown in Fig. 3. The existence of complex roots is proved analytically, using the following theorems (Appendix C).

Theorem II. Let us consider the following equation

$$a_n x^n + a_{n-1} x^{n-1} + \dots + a_0 = 0, \quad a_n \neq 0 \text{ and } a_k = \text{real}. \quad (5.7)$$

The conditions necessary for all the roots of Eq. (5.7) to lie on a unit circle are:

$$(i) \quad \text{Eq. (5.7) should be a reciprocal equation: } a_{n-k} = a_k \quad (5.8)$$

and

$$(ii) \quad |a_k| \leq C_k |a_0|. \quad (5.9)$$

Theorem III. If all the coefficients of Eq. (5.7) are positive ($a_k > 0$), the condition necessary and sufficient for all the roots of Eq. (5.7) to lie on the negative real axis is that all the roots of the following equation should lie on a unit circle,

$$\sum_{k=0}^n a_{n-k} (1+x)^{2(n-k)} (1-x)^{2k} = 0. \quad (5.10)$$

The existence of complex roots may be also proved analytically in the same way for a finite lattice (4×4) as is shown in Fig. 4, the numerical solution of which will be reported elsewhere.^{15), 16), 20)}

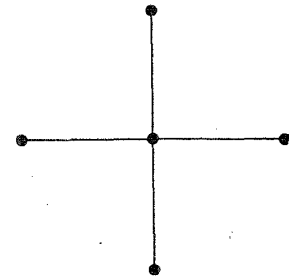


Fig. 3. A counter example which has complex roots in the antiferromagnetic case.

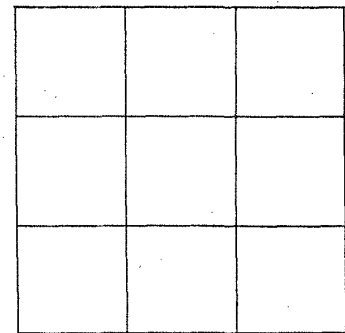


Fig. 4. A small lattice which may have complex roots in the antiferromagnetic case.

In this paper, the singularities of the thermodynamic quantities of the Ising model near the Curie point are analyzed in terms of the concept of complex magnetic field. The concept of complex temperature may be also useful for the purpose of investigating the singularities (Appendix D).^{15)-19), 22)}

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Appendix A

The susceptibility χ_0^+ in terms of Eqs. (2.8) and (2.11) is

$$\chi_0^+ \simeq \frac{8m^2}{kT} \int_{\theta_c}^{\pi} \frac{a(\theta^\eta - bt^\epsilon)^\kappa}{\theta^2} d\theta. \quad (\text{A} \cdot 1)$$

If we make a change of variable

$$\theta = \theta_c y; \quad \theta_c^\eta = bt^\epsilon, \quad (\text{A} \cdot 2)$$

we find

$$\chi_0^+ \simeq \frac{8am^2}{kT} \cdot \theta_c^{\eta\kappa-1} \cdot \int_1^{\pi/\theta_c} \frac{(y^\eta - 1)^\kappa}{y^2} dy. \quad (\text{A} \cdot 3)$$

As the upper limit of the integral can be replaced by infinity near T_c , we obtain

$$\chi_0^+ \simeq \frac{8am^2}{kT} \cdot I(\eta, \kappa) \cdot [\theta_c(t)]^{\eta\kappa-1}, \quad (\text{A} \cdot 4)$$

where

$$I(\eta, \kappa) = \int_1^\infty \frac{(y^\eta - 1)^\kappa}{y^2} dy. \quad (\text{A} \cdot 5)$$

This integral is convergent for $\eta\kappa < 1$. Therefore, the susceptibility above the Curie point takes the form

$$\chi_0^+ \sim t^{\epsilon\kappa - \epsilon/\eta}. \quad (\text{A} \cdot 6)$$

Below the Curie point, the susceptibility in terms of Eqs. (2.9') and (2.11) is

$$\chi_0^- \simeq \frac{8m^2}{kT} \int_0^\pi \frac{a(\theta^\eta + b|t|^\epsilon)^\kappa - ab^\kappa|t|^{\epsilon\kappa}}{\theta^2} d\theta. \quad (\text{A} \cdot 7)$$

If we make a change of variable

$$\theta = \hat{\theta}_c y; \quad \hat{\theta}_c = (b|t|^\epsilon)^{1/\eta}, \quad (\text{A} \cdot 8)$$

we find

$$\chi_0^- \simeq \frac{8am^2}{kT} \cdot \hat{\theta}_c^{\eta\kappa-1} \cdot \int_0^{\pi/\hat{\theta}_c} \frac{(1+y^\eta)^\kappa - 1}{y^2} dy. \quad (\text{A} \cdot 9)$$

As the upper limit of the integral can be replaced by infinity near T_c , we obtain

$$\chi_0^- \simeq \frac{8am^2}{kT} \cdot \hat{I}(\eta, \kappa) [\hat{\theta}_c(t)]^{\eta\kappa-1}, \quad (\text{A} \cdot 10)$$

where

$$\hat{I}(\eta, \kappa) = \int_0^\infty \frac{(1+y^\eta)^\kappa - 1}{y^2} dy. \quad (\text{A} \cdot 11)$$

This integral is convergent for $\eta > 1$ and $\eta\kappa < 1$. Therefore the susceptibility below the Curie point also takes the form

$$\chi_0^- \sim |t|^{\epsilon\kappa - \epsilon/\eta}. \quad (\text{A} \cdot 12)$$

Appendix B

In the case of type II, the condition for the susceptibility to have the singularity of Eq. (2.20) is

$$\int_0^\pi \frac{g(\theta, t)}{\theta^2} d\theta \sim t^{-\gamma}. \quad (\text{B} \cdot 1)$$

If we make a change of variable

$$\theta = t^\mu y \quad (\mu \text{ is a proper positive constant}),$$

we find, in the same way as before,

$$\int_0^\infty \frac{g(t^\mu y, t)}{t^{\mu-\gamma} y^2} dy \sim \text{constant}. \quad (\text{B} \cdot 2)$$

As a sufficient condition, we obtain

$$g(t^\mu y, t) / t^{\mu-\gamma} = \Psi(y). \quad (\text{B} \cdot 3)$$

Therefore, the distribution function takes the form

$$g(\theta, t) = t^{\mu-\gamma} \Psi(\theta/t^\mu). \quad (\text{B} \cdot 4)$$

This agrees with Eq. (2.28).

Appendix C

Theorem II can be easily shown, using the fact that if all the zeros of a

polynomial (5.7) lie on a unit circle, the polynomial should be decomposed as follows,

$$\begin{aligned} & a_n z^n + a_{n-1} z^{n-1} + \cdots + a_0 \\ &= a_n (z+1)^p \prod_k (z - e^{i\theta_k}) (z - e^{-i\theta_k}) \\ &= a_n (z+1)^p \prod_k (z^2 - 2z \cos \theta_k + 1), \end{aligned} \quad (\text{C} \cdot 1)$$

where $p=0$ or 1 , for n even or odd, respectively. Then, we find theorem II, from the expression for the coefficients $\{a_k\}$ in terms of $\{\cos \theta_k\}$.

Theorem III is evident from the following transformation,

$$x = \frac{1 - \sqrt{z}}{1 + \sqrt{z}} \quad \text{or} \quad z = \left(\frac{1-x}{1+x} \right)^2. \quad (\text{C} \cdot 2)$$

In terms of the transformation (C.2), negative z corresponds to a point on a unit circle of the x -plane.

Next, let us consider an example as shown in Fig. 3. The partition function of this cluster is given by

$$\begin{aligned} Z &= \text{Tr} \exp \{ K S_1 \sum_2^5 S_i + h \sum_1^5 S_i \} \\ &= e^h \{ 2 \cosh(K+h) \}^4 + e^{-h} \{ 2 \cosh(K-h) \}^4. \end{aligned} \quad (\text{C} \cdot 3)$$

If we put $Z=0$, we obtain the equation

$$a^4 (z^5 + 1) + (4a^3 + 1) (z^4 + z) + (6a^2 + 4a) (z^3 + z^2) = 0, \quad (\text{C} \cdot 4)$$

where

$$z = e^{-2h}, \quad a = e^{2K}, \quad K = J/kT \text{ and } J < 0.$$

By the transformation (C.2), we obtain

$$\begin{aligned} & (x^2)^5 (a+1)^4 + (x^2)^4 (45a^4 + 52a^3 - 18a^2 - 12a + 13) \\ & + \cdots = 0. \end{aligned} \quad (\text{C} \cdot 5)$$

It is clear that the condition (5.9) does not hold for small a :

$$|a_4/a_0| \sim 13 >_5 C_4 \quad \text{for } a \sim 0. \quad (\text{C} \cdot 6)$$

This means that complex roots in the fugacity plane appear at low temperature, at least. In the above case, the existence of complex roots can be also shown directly from Eq. (C.4) in the following way. The solution of Eq. (C.4) is given by

$$z = -1, \quad z = -\frac{1}{2} [f_i(a) \pm \{f_i^2(a) - 4\}^{1/2}], \quad (i=1, 2) \quad (\text{C} \cdot 7)$$

where

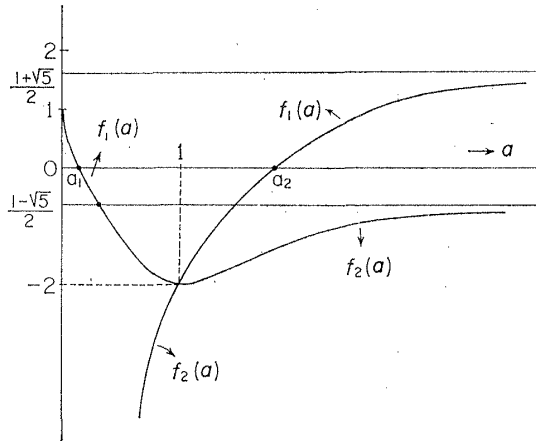


Fig. 5. The functions $f_1(a)$ and $f_2(a)$, where $a_1 = (4 + 2\sqrt{2})^{1/2} - (1 + \sqrt{2})$ and $a_2 = (4 - 2\sqrt{2})^{1/2} + (\sqrt{2} - 1)$.

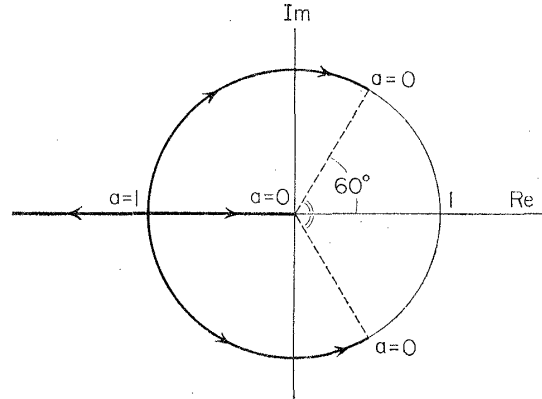


Fig. 6. Loci of zeros for the counter example, where $a = e^{2K}$.

$$f_{1,2}(a) = (a^4 - 4a^3 - 1 \pm \sqrt{D}) / (2a^4) \quad (\text{C} \cdot 8)$$

and

$$D = (a-1)^2 (5a^6 + 18a^5 + 23a^4 + 12a^3 + 3a^2 + 2a + 1).$$

The features of the functions $\{f_i(a)\}$ are illustrated in Fig. 5. Therefore, we obtain the loci of zeros shown in Fig. 6. In the whole region of temperature, a pair of complex roots appear on a unit circle of the fugacity plane.

Appendix D

For brevity, distribution of zeros of the one-dimensional Ising model is investigated in the complex temperature plane. The zeros of the partition function for the ring of number N is given as follows, from Eq. (5.5),

$$z = \tanh K = \frac{1 - i\sqrt{D}}{1 + i\sqrt{D}}, \quad (\text{D} \cdot 1)$$

where

$$D = \sinh^2 h' + \cosh^2 h' \tan^2 \left[\pi \left(k + \frac{1}{2} \right) / N \right]. \quad (\text{D} \cdot 2)$$

This means that the zeros of the one-dimensional model lie on a unit circle of the complex temperature plane, even in the presence of the external field. If we put

$$z = e^{i\theta}, \quad (\text{D} \cdot 3)$$

then the distribution function on $\tanh K$ plane for N infinite takes the form

$$g(\theta, h') = \frac{1}{2\pi} \frac{\sin(\theta/2)}{[\sin^2(\theta/2) - \tanh^2 h']^{1/2}}. \quad (\text{D} \cdot 4)$$

The critical angle is, consequently, given by

$$\theta_c = 2 \sin^{-1}(\tanh h'), \quad (\text{D}\cdot 5)$$

and $g(\theta, h') = 0$ for $|\theta| < \theta_c(h')$. The loci of zeros cut the positive real axis in the complex temperature plane, only in the absence of the magnetic field. That point on the positive real axis which the loci of zeros approach corresponds to the transition point (in the present case, $z_c = 1$ or $T_c = 0$).

Equation (5.5) or Eq. (D.1) is derived from the equation

$$\begin{aligned} & \tanh^2 h' + (e^{-2K})^2 - (\tanh h' \cdot e^{-2K})^2 \\ &= -\tan^2 \left[\pi \left(k + \frac{1}{2} \right) / N \right]. \end{aligned} \quad (\text{D}\cdot 6)$$

This shows the duality of magnetic field and temperature in the following way,

$$\tanh h' \longleftrightarrow e^{-2K}$$

or

$$e^{-2h'} \longleftrightarrow \tanh K. \quad (\text{D}\cdot 7)$$

This duality seems to be due to the special features of the one-dimensional model.

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