Progress of Theoretical Physics, Vol. 38, No. 3, September 1967

Critical Behavior of Pair Correlation Function in Ising Ferromagnets

Ryuzo ABE

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

(Received May 1, 1967)

Behavior of pair correlation function in Ising ferromagnets near the transition point is studied in two different ways. First, it is studied by means of the Lee-Yang theorem on the distribution of zeros of partition function. Secondly, a diagrammatic method is developed and a connection is discussed between the results obtained by these two different methods.

§ 1. Introduction

The purpose of this paper is twofold. First, we would like to extend a discussion given in a previous paper[1] (to be referred to as I) which dealt with singularities of susceptibility, magnetization and specific heat in Ising ferromagnets to that of pair correlation function. As a natural generalization of I, an expression for the pair correlation function is obtained in § 2 by means of the Lee-Yang theorem.[2] We will study in § 3 the critical behavior of pair correlation function in the presence of magnetic field, and compare our results with those of other theories. Throughout §§ 2 and 3 we will use the same notations and definitions as in I, unless otherwise mentioned.

The second purpose of this paper is to discuss the pair correlation function from a diagrammatic point of view. Some time ago, the present author published a paper[3] (to be referred to as D) in which a diagrammatic method is developed for studying the phase transition of Ising model. We were led there to the Curie-Weiss law for the susceptibility, which is not consistent with the singularity $(T-T_c)^{-\gamma}$, $(\gamma>1)$. We will remedy in § 4 this inconsistency and discuss a relevance of the results in § 3 with those obtained by a diagrammatic method.

§ 2. Pair correlation function in Ising ferromagnets

We consider exactly the same system as in I and introduce a pair correlation function defined by

$$\langle\mu_i\mu_j\rangle=\sum_{\mu_1\cdots\mu_N}\mu_i\mu_j\exp\left(\frac{1}{2}\sum_{p,q}K_{pq}\mu_p\mu_q+\frac{mH}{kT}\sum_p\mu_p\right)/Z, \tag{2·1}$$

where μ_i is an Ising spin taking values ±1, $K_{pq}=J_{pq}/kT$ with J_{pq} the exchange interaction between the pth and qth spins, Z is the partition function of the system. It is clear that $\langle\mu_i\mu_j\rangle$ is derived from the Z:

$$\langle\mu_i\,\mu_j\rangle = (\partial/\partial K_{ij})\ln Z. \tag{2·2}$$

From Eq. (2·2) of I we have

$$\langle\mu_i\,\mu_j\rangle = \int_0^{2\pi}\ln(z-e^{i\theta})\,g(\theta,\,ij)\,d\theta, \tag{2·3}$$

where $g(\theta,\,ij)$ is given by

$$g(\theta,\,ij) = (\partial/\partial K_{ij})\,Ng(\theta). \tag{2·4}$$

By the use of Eq. (2·3) of I we find

$$\int_0^{2\pi} g(\theta,\,ij)\,d\theta = 0, \quad g(-\theta,\,ij) = g(\theta,\,ij). \tag{2·5}$$

With the aid of Eq. (2·5), we can write Eq. (2·3) as follows:

$$\langle\mu_i\,\mu_j\rangle = \int_0^{\pi}\ln[2(\mathrm{ch}\,h-\cos\theta)]\,g(\theta,\,ij)\,d\theta. \tag{2·6}$$

It should be noted that the above equation has precisely the same form as Eq. (2·4) of I.

We now restrict ourselves to the case above the transition temperature and note that

$$g(\theta,\,ij) = 0, \qquad \text{for } \theta < \theta_c, \tag{2·7}$$

which follows from Eq. (2·8) of I. It is convenient to define a function $G(\theta,\,ij)$:

$$G(\theta,\,ij) = \int_{\theta_c}^{\theta} g(\theta',\,ij)\,d\theta'. \tag{2·8}$$

Then, using partial integration and Eqs. (2·5) and (2·8), we get from Eq. (2·6)

$$\langle\mu_i\,\mu_j\rangle = -\int_{\theta_c}^{\pi}\frac{\sin\theta}{\mathrm{ch}\,h-\cos\theta}\,G(\theta,\,ij)\,d\theta. \tag{2·9}$$

It is expected that in the neighborhood of transition point the $\langle\mu_i\mu_j\rangle$ depends on the distance $r=|\boldsymbol{r}_i-\boldsymbol{r}_j|$, so that we write it as $g(r)$. (We measure the distance in units of lattice constant.) Furthermore, simplifying Eq. (2·9) as in I, we find

$$g(r) = -\int_{\theta_c}^{\pi}\frac{2\theta}{h^2+\theta^2}\,G(\theta,\,t,\,r)\,d\theta. \tag{2·10}$$

Here we write an explicit dependence of G on t.

In order to find a possible form of $G(\theta, t, r)$, we assume as in Fisher's theory[4] that the $g(r)$ in the absence of magnetic field is written as

$$g(r) = r^{-\lambda} F(rt^{\nu}). \tag{2·11}$$

From this equation the temperature dependence of correlation length L in the vicinity of transition point is expressed as

$$L \propto t^{-\nu}. \tag{2·12}$$

Furthermore, assuming that $F(0) = \text{const}$ we find

$$g(r) \propto r^{-\lambda}, \quad (r \to \infty) \tag{2·13}$$

at the transition point. A parameter λ is related with a more conventional η as

$$\lambda = d - 2 + \eta, \tag{2·14}$$

where d is the dimensionality of the system. Since the susceptibility χ is given by

$$\chi = \frac{m^2}{kT} \sum_j \langle \mu_0 \, \mu_j \rangle, \tag{2·15}$$

repeating Fisher's procedure[4] we have

$$\gamma = \nu (d - \lambda). \tag{2·16}$$

Absorbing a factor -2 in Eq. (2·10) in the definition of G and carrying out a change of variable $\theta = \theta_c x$, we obtain in the case $h = 0$

$$\frac{F(rt^{\nu})}{r^{\lambda}} = \int_1^{\infty} \frac{G(\theta_c x, t, r)}{x} dx. \tag{2·17}$$

This equation yields some condition to be imposed on G. From Eq. (3·9) of I we have $\theta_c \propto t^{\Delta/2}$, and therefore if we introduce a transformation

$$r \to ar, \; t \to a^{-1/\nu} t, \; \theta_c \to a^{-\Delta/2\nu} \theta_c,$$

where a is an arbitrary constant, we find

$$\frac{F(rt^{\nu})}{r^{\lambda}} = \int_1^{\infty} \frac{a^{\lambda} G(a^{-\Delta/2\nu} \theta_c x, a^{-1/\nu} t, ar)}{x} dx. \tag{2·18}$$

This equation should hold for any value of a. Since the left-hand side is independent of a, it follows that a quantity

$$a^{\lambda} G(a^{-\Delta/2\nu} \theta_c x, a^{-1/\nu} t, ar)$$

is also independent of a. Thus differentiating it by a, we have

$$\left(\frac{\Delta}{2\nu}\theta\frac{\partial}{\partial\theta}+\frac{t}{\nu}\frac{\partial}{\partial t}-r\frac{\partial}{\partial r}\right)G(\theta,t,r)=\lambda G(\theta,t,r). \tag{2·19}$$

A general solution of this equation is shown to be

$$G(\theta,t,r)=r^{-\lambda}P(rt^{\nu},r\theta^{2\nu/\Delta}), \tag{2·20}$$

where $P(x,y)$ is an arbitrary function of x and y.

§ 3. Pair correlation function in magnetic field

We are going to discuss in this section the pair correlation function in the presence of magnetic field. Putting Eq. (2·20) in Eq. (2·10), we obtain

$$g(r)=\frac{1}{r^{\lambda}}\int_1^{\infty}\frac{xdx}{(h/\theta_c)^2+x^2}P(rt^{\nu},rt^{\nu}x^{2\nu/\Delta}). \tag{3·1}$$

Therefore, the $g(r)$ is expressed as

$$g(r)=\frac{1}{r^{\lambda}}F\left(rt^{\nu},\frac{h}{\theta_c}\right). \tag{3·2}$$

We notice that the $g(r)$ should approach M^2 in the limit $r\to\infty$. Consequently, a factor r in the F in Eq. (3·2) should cancel out with r^{λ} in this limit. As a result, a limiting form of $g(r)$ is given by

$$\lim_{r\to\infty}g(r)=t^{\lambda\nu}\frac{h^2}{\theta_c^{\,2}}\varphi\left(\frac{h}{\theta_c}\right)=M^2. \tag{3·3}$$

Comparing this equation with Eq. (3·5) of I, we find

$$2\gamma=\Delta-\lambda\nu. \tag{3·4}$$

Combining Eq. (2·16) with Eq. (3·4), we get

$$\nu d=\Delta-\gamma. \tag{3·5}$$

This result is consistent with previous suggestions of Widom,[5] Patashinsky and Pokrovsky,[6] and Kadanoff.[7] In the two-dimensional Ising model, the exact values $\Delta=15/4$, $\lambda=1/4$, $\nu=1$, $\gamma=7/4$ satisfy Eqs. (2·16) and (3·5). In the three-dimensional case, if we adopt[8] $\Delta=25/8$, $\gamma=5/4$, we have

$$\nu=5/8,\ \lambda=1. \tag{3·6}$$

It should be noted that these values have already been suggested by Domb.[8]

Let us turn our attention to a discussion of how the correlation length at the transition point depends on h. For this purpose, we define a net correlation function $g_1(r)$ as

$$g_1(r)=g(r)-M^2. \tag{3·7}$$

It is clear from Eqs. (3·2) and (3·3) that

$$g_1(r)=r^{-\lambda}F_1(rt^{\nu},\ ht^{-\Delta/2}). \tag{3·8}$$

Or, if we choose another set of independent variables, we can write $g_1(r)$ as

$$g_1(r)=r^{-\lambda}\Psi_1(rh^{2\nu/\Delta},\ h^{-2/\Delta}t). \tag{3·9}$$

The convenience of this choice lies in the fact that $g_1(r)$ is a regular function of t if $h\neq 0$. Thus, putting $t=0$ in Eq. (3·9), we find

$$L\propto h^{-2\nu/\Delta}. \tag{3·10}$$

In the two-dimensional case $L\propto h^{-8/15}$ and in the three-dimensional one $L\propto h^{-2/5}$.

§ 4. Diagrammatic discussion

One of the ways of studying the phase transition is to employ a diagrammatic technique.[9] This section is devoted to a discussion of how the results obtained in previous sections are reflected in such a method. We will use the same definitions and notations as in D, except that we write here explicitly the t dependence of $I(q)$. Before going into details, we denote the Fourier transform of $g(r)$ by $g[q]$ and study its t dependence. With the aid of Eq. (2·11), the $g[q]$ is expressed as

$$g[q]=\int_0^\infty g(r)\,r^{d-1}S(qr)\,dr=q^{\lambda-d}\,Q\left(\frac{q}{t^{\nu}}\right). \tag{4·1}$$

We write this equation as

$$\begin{aligned} g[q]&=q^{\lambda-d}/[a_1(q/t^{\nu})^{\lambda-d}+a_2(q/t^{\nu})^{\lambda-d+2}+a_3(q/t^{\nu})^{\lambda-d+4}+\cdots] \\ &=1/(a_1t^{\gamma}+a_2t^{\gamma}q^2t^{-2\nu}+a_3t^{\gamma}q^4t^{-4\nu}+\cdots), \end{aligned}$$

where use is made of Eq. (2·16). In this way, we are led to

$$g[q]=1/t^{\gamma}f(q^2t^{-2\nu}). \tag{4·2}$$

As was shown in D, the $g[q]$ is written as

$$g[q]=I(q,t)/[1-K(q)I(q,t)]. \tag{4·3}$$

Therefore it follows that

$$1-I(0,t)K(0)\propto t^{\gamma}. \tag{4·4}$$

We will study in the following how the $I(0,t)$ depends on t, assuming for the time being that the $g[q]$ is given by Eq. (4·2).

The function I_{ij} is expressed in terms of diagrams as illustrated in Fig. 5 of D. Let us first study the t dependence of M_2. If we define a square part as is shown in Fig. 1, its contribution to $I(0,t)$ is proportional to

$$\int K^2(q) g[q] d\boldsymbol{q} \propto \int K^2(q) \frac{q^{d-1}dq}{t^\gamma f(q^2 t^{-2\nu})}. \tag{4·5}$$

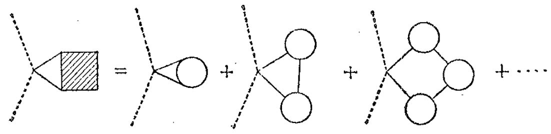

Fig. 1. Diagrammatic representation of square part. A circle in the figure means I function.

Introducing a change of variable $q=t^\nu x$, we find that Eq. (4·5) yields a contribution of the order of $t^{\nu d-\gamma}$. Therefore, if n square parts are connected to a given point, its contribution to $I(0, t)$ is proportional to $t^{n(\nu d-\gamma)}$. Next, we consider the second diagram in Fig. 5 of D. Its contribution to $I(0, t)$ is proportional to

$$\int \frac{d\boldsymbol{k}_1 d\boldsymbol{k}_2}{t^{3\gamma} f(k_1^2 t^{-2\nu}) f(k_2^2 t^{-2\nu}) f(|\boldsymbol{k}_1+\boldsymbol{k}_2|^2 t^{-2\nu})} \propto t^{2\nu d-3\gamma}. \tag{4·6}$$

This result is easily generalized to a more complicated diagram. As in D, let the number of points and of lines in a given diagram be p and l, respectively. Since each line yields a factor $t^{-\gamma}$, the contribution of lines is proportional to $t^{-l\gamma}$. Also, note that the number of independent integral variables is $l-(p-1)$ and that each variable yields a factor $t^{\nu d}$ after the change of variables mentioned above. Therefore, if a given diagram involves n square parts, the total contribution to $I(0, t)$ is proportional to

$$t^{(l-p+1)\nu d-l\gamma+n(\nu d-\gamma)} = t^{(l+n)(\nu d-\gamma)-(p-1)\nu d}. \tag{4·7}$$

From the topological structure of our diagrams, it is clear that

$$l=2p-1,\ 2p+1,\ 2p+3,\ \cdots. \tag{4·8}$$

If we set $l+n$ by l again, we find from Eqs. (4·7) and (4·8) that a general term of $I(0, t)$ is of the order of

$$t^{l(\nu d-\gamma)-(p-1)\nu d}, \tag{4·9}$$

where

$$l=2p-1+m,\quad (m=0,\ 1,\ 2,\ \cdots). \tag{4·10}$$

It may happen that the proportionality constants in Eq. (4·9) are zero for $l<l'$, i.e. $m<m'$ with fixed p, but is not for $l=l'$. Then comparing Eq. (4·9) with Eq. (4·4), we have

$$\gamma=l'(\nu d-\gamma)-(p-1)\nu d, \tag{4·11}$$

where

$$l'=2p-1+m'. \tag{4·12}$$

Solving γ from Eq. (4·11) and writing m' by m, we get

$$\gamma/\nu d = (p+m)/(2p+m), \tag{4·13}$$

where

$$p=2, 3, 4, \cdots \text{ and } m=0, 1, 2, \cdots. \tag{4·14}$$

Equation (4·13) implies that the ratio $\gamma/\nu d$ should be equal to some rational number subject to the condition (4·14). In the two-dimensional Ising model, we know that $\nu d=2$ and $\gamma=7/4$, so that we find $m=6p$ from Eq. (4·13). If we put $p=2$, we have $m=12$ or $l'=15$ from Eq. (4·12). This result means that in the present case the diagrams with two points yield no contributions to $I(0, t)$ if $l\leq 14$. When l reaches 15, the diagram at first gives rise to a contribution to $I(0, t)$. It is quite speculative that the result $\delta=15$ leads to the above value of l.

So far we have assumed that the $g[q]$ is given by Eq. (4·2). However, under the assumption that a similar vanishing of diagrams occurs also for the case $q\neq 0$, it is seen that Eq. (4·2) is self-consistent if one considers the q dependence of $I(q, t)$ along the line conjectured above.

One may be tempted to extend the above-mentioned speculation to the three-dimensional case. In this case, we have $\delta=5$.[5] Thus, putting $p=2$ and $l'=5$ in Eq. (4·12), we find $m'=2$ and therefore $\gamma=2\nu$ from Eq. (4·13). If the value $\gamma=5/4$ is substituted we get $\nu=5/8$, which is consistent with Eq. (3·6). It is not clear at present, however, why the value of l which leads to a nonzero contribution to $I(0, t)$ coincides with that of δ. This problem seems to need a further investigation.

In closing we would like to mention some remarks on the recent calculations[10] by Fisher and Burford. They have obtained from series expansions numerical values which are consistent with $\eta=1/18$ and $\nu=9/14$. When this value of ν and $\gamma=5/4$, $d=3$ are substituted in Eq. (4·13), we find

$$p=19m/16. \tag{4·15}$$

The minimum value of p satisfying both Eq. (4·14) and Eq. (4·15) is 19. Thus, the Fisher-Burford result implies an extraordinary cancellation of diagrams; all the diagrams with $p\leq 18$ should yield no contributions to $I(0, t)$. It is an open question, however, which is true, the former case ($p=2$) or the latter case ($p=19$) or another possibility different from these two cases.

References

1) R. Abe, Prog. Theor. Phys. **38** (1967), 72.
2) T. D. Lee and C. N. Yang, Phys. Rev. **87** (1952), 410.
3) R. Abe, Prog. Theor. Phys. **33** (1965), 600.
4) M. E. Fisher, Physica **28** (1962), 172.
5) B. Widom, J. Chem. Phys. **43** (1965), 3892, 3898.

6) A. Z. Patashinsky and V. L. Pokrovsky, Soviet Phys.-JETP **23** (1966), 292.
7) L. P. Kadanoff, Physics **2** (1966), 263.
8) C. Domb, *Proceedings of the* 1966 *Low Temperature Calorimetry Conference*, edited by O. V. Lounasmaa, Ann. Acad. Sci. Fennicæ **A VI** (1966), 167.
9) G. Horwitz and H. B. Callen, Phys. Rev. **124** (1961), 1757.
F. Englert, Phys. Rev. **129** (1963), 567.
A. Z. Patashinsky and V. L. Pokrovsky, Soviet Phys.-JETP **19** (1964), 677.
F. H. Stillinger, Jr., Phys. Rev. **146** (1966), 209.
10) M. E. Fisher, *Proceedings of the Conference on Phenomena in the Neighborhood of Critical Points* (National Bureau of Standards, Washington, D. C., 1965), p. 108.
R. J. Burford, Thesis, University of London.
M. E. Fisher and R. J. Burford, Phys. Rev. **156** (1967), 583.