THE BEHAVIOR OF HIGH-ORDER CORRELATION FUNCTIONS NEAR SECOND-ORDER PHASE-TRANSITION POINTS

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The correlation functions for four spins are calculated exactly within the framework of the two-dimensional Ising model. The results of this calculation are compared with the predictions of scaling theory. In all cases the conclusions derived on the basis of scaling laws are confirmed by the exact calculations.

1. The theory of second-order phase transitions developed to date[1,2] allows one to express all the critical indices of the thermodynamic quantities in terms of two independent parameters.

In deriving the relations of scaling theory, Patashinskiĭ and Pokrovskiĭ[2] have utilized the method of correlation functions, and the higher-order correlation (of order 2n) $Q_n = \langle\sigma_1 \ldots \sigma_{2n}\rangle$ were estimated through a multiplicative formula in terms of the second-order correlation functions

$$Q_n \sim Q_1{}^n. \tag{1}$$

The estimate (1) becomes non-obvious when the characteristic distance r between the spins is smaller than the correlation radius r_c, since in that case all the spins which occur in the correlation function are "coupled" to each other. The use of the estimate (1) is obviously legitimate in the case when all spins occurring in (1) can be clustered into pairs, such that the coupling within a pair is stronger than the coupling between the spins belonging to different pairs. It therefore seems interesting to test this assumption (and also the other conclusions of scaling theory, concerning the higher-order correlations) by means of a comparison with exact calculations within the framework of the two-dimensional Ising model. If all characteristic distances between the spins in a correlation function are of the same order of magnitude, the multiplicative (product) estimate (1) turns out to be valid. Other conclusions of scaling theory are also confirmed.

2. Let us estimate by means of scaling theory the correlation function for four spins situated along the same diagonal (the distances between the first two spins and between the last two spins are identical). This function has the form:

$$g(r_1, r_2, \tau) = \langle\sigma_1\ \sigma_{1+r_1}\sigma_{1+r_1+r_2}\sigma_{1+2r_1+r_2}\rangle, \tag{2}$$

where $\tau = (T - T_c)/T_c$ is the reduced temperature, T_c is the critical temperature and T is the temperature of the system; $\sigma_r = \pm 1$ is the spin situated at the lattice site r. On the diagonal the projections of the vector r along the axes are equal to i and we shall characterize the situation of the site by this single index.

Let $r_1, r_2 \gg r_0$ (r_0 is the interatomic distance). We replace the microscopic spins σ_i by the cell angular momenta μ_a where a is the label of a cell with linear dimension L. The Kadanoff transformations[1] have the form

$$r \to r/L, \quad \tau \to \bar{\tau} = \tau L^y, \quad \sigma_r \to L^{x-d}\mu_a, \tag{3}$$

where x and y are the critical indices and d the dimension of the space

$$g(r_1, r_2, \tau) = L^{4(x-d)}\langle\mu_{a_1}\mu_{a_2}\mu_{a_3}\mu_{a_4}\rangle = L^{4(x-d)}g(r_1/L, r_2/L, \tau L^y). \tag{4}$$

A general solution satisfying the equation (4) is

$$g(r_1, r_2, \tau) = \tau^{4(d-x)/y}g(r_1\tau^{1/y}, r_2\tau^{1/y}). \tag{5}$$

We first consider the case $r_1 \ll r_2$. It is convenient to replace the function $g(r_1, r_2, \tau)$ by the quantity $g_1(r_1, r_2, \tau) = g(r_1, r_2, \tau) - \langle\sigma_1\sigma_{1+r_1}\rangle^2$. Taking into account the relation $\langle\sigma_1\sigma_{1+r_1}\rangle^2 = \tau^{4(d-x)/y}f(r_1\tau^{1/y})$ (f is an unknown function) we obtain from (5)

$$g_1(r_1, r_2, \tau) = \tau^{4(d-x)/y}g_1(r_1\tau^{1/y}, r_2\tau^{1/y}), \tag{6}$$

where

$$g_1(r_1\tau^{1/y}, r_2\tau^{1/y}) = g(r_1\tau^{1/y}, r_2\tau^{1/y}) - f(r_1\tau^{1/y}),$$

If $r_1 \to r_0$ then $g(r_1, r_2, \tau)$ becomes proportional to the pair correlation function of the energies $\langle\epsilon_1\epsilon_2\rangle$, where $\epsilon_r = I\sigma_1\sigma_2$ is the exchange energy. According to[3] (p. 405) this correlation function has the form

$$\langle\varepsilon_1\varepsilon_r\rangle - \langle\varepsilon\rangle^2 = \tau^{2(d-y)/y}g_E(r\tau^{1/y}). \tag{7}$$

In the case $a \ll b$, it follows from (6) and (7)

$$g_1(a, b) = a^{4x-2y-2d}g_E(b). \tag{8}$$

It follows from (5), (6), and (8) that

$$g(r_1, r_2, \tau) = \tau^{4(d-x)/y}f(r_1\tau^{1/y}) + \tau^{2(d-y)/y}r_1{}^{4x-2y-2d}g_E(r_2\tau^{1/y}), \quad r_1 \ll r_2. \tag{9}$$

In the region $r_2 \ll r_c \sim \tau^{-1/y}$ the function $g(r_1, r_2, \tau)$ should not depend on τ, hence

$$g(r_1, r_2, \tau) \sim r_1^{-4(d-x)} + O(r_1^{4x-2y-2d}\, r_2^{2(y-d)}). \tag{10}$$

If $r_1 \sim r_2 \sim r$ it follows from (10) that $g(r_1, r_2, \tau) \sim r^{-4(d-x)} \sim \langle\sigma_1\sigma_{1+r_1}\rangle^2$, i.e., the estimate (1) holds.

We now consider the opposite limit $r_2 \ll r_1$. In the limit $r_2 \to r_0$ we have

$$g(r_1, r_2, \tau) \approx \langle\sigma_1\sigma_{1+2r_1}\rangle = \tau^{2(d-x)/y}g_2(2r_1\tau^{1/y}), \tag{11}$$

where g_2 is the function which determines the pair-correlation of spins.

Comparing (11) with (5), we obtain in the case $b \ll a$

$$g(a, b) = b^{-2(d-x)} g_2(a),$$

whence

$$g(r_1, r_2, \tau) \sim \tau^{2(d-x)/y} r_2^{-2(d-x)} g_2(r_1 \tau^{1/y}), \quad r_2 \ll r_1. \tag{12}$$

If $r_1 \ll r_c \sim \tau^{-1/y}$, it follows from (12)

$$g(r_1, r_2, \tau) \sim r_1^{-2(d-x)} r_2^{-2(d-x)}. \tag{13}$$

For $r_1 \sim r_2 \sim r$ the expressions (10) and (13) "join smoothly." Similar correlation functions have been considered in the microscopic theory by Polyakov[4].

3. Within the framework of the two-dimensional Ising model we now compute the correlation function of four spins, as defined by Eq. (2). The simplest way to compute this quantity is to switch on the exchange interaction I_2 along one of the diagonals and making a transition to the model discussed in[5]. Introducing the notation

$$S\{\alpha_{kl|k'l'} | \sigma_{kl}\} = \prod_{kl,k'l'} (1 + \alpha_{kl|k'l'} \sigma_{kl} \sigma_{k'l'})$$

and making use of the identity ($\sigma_{kl}^2 = 1$)

$$\sigma_1 \sigma_{1+r_1} = (\sigma_1 \sigma_2)(\sigma_2 \sigma_3) \ldots (\sigma_{r_1} \sigma_{r_1+1}),$$
$$\sigma_{1+r_1+r_2} \sigma_{1+2r_1+r_2} = (\sigma_{1+r_1+r_2} \sigma_{2+r_1+r_2})(\sigma_{2+r_1+r_2} \sigma_{3+r_1+r_2}) \ldots (\sigma_{2r_1+r_2} \sigma_{1+2r_1+r_2}),$$

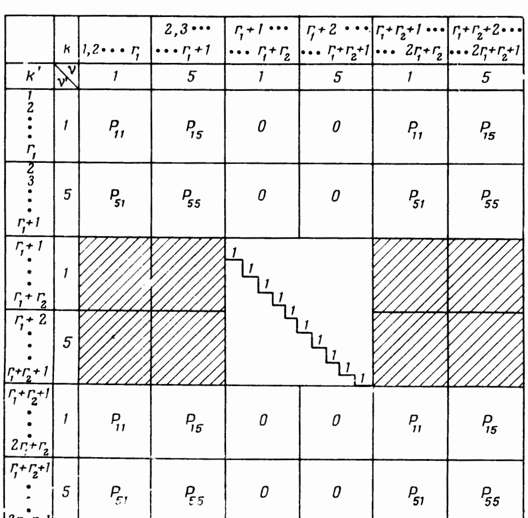
we obtain

$$g(r_1, r_2, \tau) = \langle (\sigma_1 \sigma_2) \ldots (\sigma_{r_1} \sigma_{r_1+1})(\sigma_{1+r_1+r_2} \sigma_{2+r_1+r_2}) \ldots (\sigma_{2r_1+r_2} \sigma_{1+2r_1+r_2}) S \rangle / \langle S \rangle. \tag{14}$$

Following the method of[5-7], we are led to the formula

$$g(r_1, r_2, \tau) = \det{}^{1/2} P_{\nu\nu'}(kl | k'l'), \tag{15}$$

where the matrix $P_{\nu\nu'}(kk|k'k')$ has the form represented in the figure. The other off-diagonal matrix elements are zero, whereas the diagonal ones are equal to one. The shaded part of the matrix contains nonvanishing matrix elements, but they do not contribute to the determinant.



Similarly we obtain[5]

$$P_{15} = P_{51} = 0, \quad P_{11} = P_{55} = P(k-k') = \int_0^{2\pi} \frac{d\omega}{2\pi} e^{i(k-k')\omega} \bar{f}(\omega), \tag{16}$$

where

$$\bar{f}(\omega) = \left[\frac{(e^{i\omega}\alpha_1 - 1)(e^{i\omega}\alpha_2 - 1)}{(e^{i\omega} - \alpha_1)(e^{i\omega} - \alpha_2)} \right]^{1/2},$$

$$\alpha_1 = \frac{1+z_2}{1-z_2} \frac{(z_1^2+1)^2 z_2 + 4z_1^2}{(1-z_1^2)^2}, \quad \alpha_2 = z_2 \frac{1-z_2}{1+z_2} \frac{(1-z_1^2)^2}{(z_1^2+1)^2 + 4z_1^2 z_2},$$

$$z_1 = \operatorname{th} \frac{I_1}{T}, \quad z_2 = \operatorname{th} \frac{I_2}{T}.$$

We now pass to the usual Ising model by setting in (16) $I_2 = 0$. We shall consider the case $r_1 \tau \ll 1$ and $r_2 \tau \ll 1$ and set in (16) $\tau = 0$. As a result we shall have

$$P(k-k') = 2/\pi[2(k-k')+1]. \tag{17}$$

Taking this into account, the determinant discussed here above has the value

$$B = \det \begin{vmatrix} P_{11} & 0 & P_{11} & 0 \\ 0 & P_{55} & 0 & P_{55} \\ P_{11} & 0 & P_{11} & 0 \\ 0 & P_{55} & 0 & P_{55} \end{vmatrix}. \tag{18}$$

Permuting the last two rows in (18) and then the last two columns we obtain

$$B = C^2, \quad C = \det \begin{vmatrix} p^{11} & p^{12} \\ p^{21} & p^{22} \end{vmatrix}, \tag{19}$$

where p^{ij} is the matrix formed with the elements (17) with the index $i = 1$ ($j = 1$) corresponding to the values $1 \le k \le r_1$ ($1 \le k' \le r_1$) and the index $i = 2$ ($j = 2$) to $r_1 + r_2 + 1 \le k \le 2r_1 + r_2$ ($r_1 + r_2 + 1 \le k' \le 2r_1 + r_2$). It follows from (15) and (19) that

$$g(r_1, r_2, \tau) = C. \tag{20}$$

4. In order to compute the determinant (19) we consider the minor of the matrix $P_{ij} - P_{ij,p}$ situated along the principal diagonal, and obtained by crossing out the last $r_1 - p$ rows and columns, so that in the last row (column) of this minor stands the matrix element (17) with $k(k') = r_1 + r_2 + p$.

Let us compute $C_p = \det P_{ij,p}$. For this purpose we factor out from each row a common factor $2/\pi$ and then multiply the last row of the minor by $1/[2(s - r_1 - r_2 - p) + 1]$ and subtract it from the s-th row. As a result all matrix elements in the last column vanish, with the exception of the one on the principal diagonal. After this procedure the matrix element at the intersection of the s-th row and t-th column has the form

$$c_{st} = \frac{4(r_1+r_2+p-s)(r_1+r_2+p-t)}{[2(s-t)+1][2(r_1+r_2+p-s)-1][2(r_1+r_2+p-t)+1]}.$$

After factoring out in front of the determinant all common factors we are led to the relation

$$C_p = \left(\frac{\Gamma(r_1+r_2+p)\Gamma(p)}{\Gamma(r_2+p)} \right)^2 \frac{\Gamma(r_2+p-1/2)}{\Gamma(r_1+r_2+p-1/2)\Gamma(p-1/2)} \times \frac{\Gamma(r_2+p+1/2)}{\Gamma(r_1+r_2+p+1/2)\Gamma(p+1/2)} C_{p-1}, \tag{21}$$

where $\Gamma(x)$ is the gamma-function.

Taking into account the expression for the pair-correlation function in the region $r_1 \tau \ll 1$[8]

$$\langle \sigma_1 \sigma_{1+r_1} \rangle = \prod_{p=1}^{r_1} \frac{\Gamma^2(p)}{\Gamma(p+1/2)\Gamma(p-1/2)},$$

we obtain from (20) and (21) the required formula:

$$g(r_1, r_2, \tau) = \langle \sigma_1 \sigma_{1+r_1} \sigma_{1+r_1+r_2} \sigma_{1+2r_1+r_2} \rangle = \langle \sigma_1 \sigma_{1+r_1} \rangle^2 \zeta(r_2) \zeta^{-1}(r_1 + r_2), \tag{22}$$

where

$$\zeta(x) = \prod_{p=1}^{r_1} \frac{\Gamma(x+p-{}^1/_2)\Gamma(x+p+{}^1/_2)}{\Gamma^2(x+p)}.$$

Making use of the Stirling formula for the gamma function, we obtain

$$\zeta(x) \sim \left(\frac{x+r_1}{x}\right)^{1/4},$$

whence

$$g(r_1, r_2, \tau) \sim r_1^{-1/2} \left(\frac{r_1+r_2}{r_2}\right)^{1/4} \left(\frac{r_1+r_2}{2r_1+r_2}\right)^{1/4}. \tag{23}$$

In the region $r_1 \sim r_2 \sim r$ we have $g(r_1, r_2, \tau) \sim r^{-1/2}$, i.e., we are led to the multiplicative approximation (1).

In the two limiting cases we obtain from (23)

$$g(r_1, r_2, \tau) \sim \begin{cases} r_1^{-1/2}(1 + r_1^2/r_2^2), & \text{when } r_1 \ll r_2 \\ r_1^{-1/4} r_2^{-1/4}, & \text{when } r_1 \gg r_2 \end{cases}. \tag{24}$$

In the two-dimensional case ($d = 2$, $x = 15/8$, $y = 1$) for $r_1 \ll r_2$ the expression (24) coincides with (10), and for $r_1 \gg r_2$ it coincides with (13).

Thus, the exact calculation of the correlation functions for four spins confirms in all cases the estimates of scaling theory. One can consider in a similar manner the correlation functions of an arbitrary even (2n) number of spins, situated along one diagonal. Generalizing the method exposed above, we obtain in the region $n(r_1 + r_2)\tau \ll 1$

$$g_{2n}(r_1, r_2, \tau) = \langle \sigma_1 \sigma_{1+r_1} \sigma_{1+r_1+r_2} \sigma_{1+2r_1+r_2} \sigma_{1+2r_1+2r_2} \ldots \sigma_{1+(n-1)r_1+(n-2)r_2} \sigma_{1+nr_1+(n-1)r_2} \rangle = \langle \sigma_1 \sigma_{1+r_1} \rangle^n \prod_{j=2}^{n} \prod_{i=2}^{j} \zeta((i-2)r_1 + (i-1)r_2) \times \zeta^{-1}((i-1)r_1 + (i-1)r_2). \tag{25}$$

If all characteristic distances between spins are of the same order of magnitude, the multiplicative approximation (1) holds in the two-dimensional case.

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