

Correlation function for a plane Ising lattice

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A two-dimensional Ising lattice with interaction between nearest neighbors and without a magnetic field is considered. It is shown that, in the correlation function $\langle S_1 S_{1+r} \rangle$ for spins located in a given row, the terms following the leading term $\langle S_1 S_{1+r} \rangle \sim r^{-1/4}$ are of the order of $r^{-3/4} + r^{-5/4}$

+ $r^{-7/4}$ at the phase transition point $\tau = (T - T_c)/T_c = 0$ for large r . A correction is found to the susceptibility in a weak magnetic field on the assumption that the correlation length is $r_c \sim \tau^{-1}$. The correction is $\Delta\chi \sim \tau^{-1/4} + \tau^{-3/4} + \tau^{-5/4}$.

1. INTRODUCTION

The Ising model, in the form of a plane square array of dipoles, each of which can occupy only one of two positions, is a unique example of a system which undergoes a nontrivial second-order phase transition and admits of an exact solution.^[1] There are good reasons to suppose^[2] that the behavior of real materials such as binary alloys and ferroelectrics of the order-disorder type can be qualitatively described by the Ising model near the critical point.

The behavior of the most important parameters of this model near the phase transition point is known to within terms which are small in the parameter $\tau = (T - T_c)/T_c$. One of these is the correlation function $\langle S_0 S_r \rangle \sim r^{-1/4}$ (correlation radius $r_c \sim \tau^{-1}$). There is also considerable interest in calculations of these parameters (and, particularly, of the correlation function) with a high degree of accuracy. This is connected, firstly, with the possibility of deriving corrections to thermodynamic quantities for the system, such as susceptibility and specific heat. Secondly, the terms following the leading term provide information about the structure of the set of highly fluctuating quantities A_i .^[3] Near the critical point, all the singular quantities, for example, S , can be written in the form of a superposition:^[4]

$$S = \sum_i \alpha_i A_i. \quad (1)$$

Assuming that

$$\langle A_i(r) A_j(r') \rangle \sim \delta_{ij} |r - r'|^{-2\alpha_i},$$

we have

$$\langle S(r) S(r') \rangle = \sum_i \alpha_i^2 |r - r'|^{-2\alpha_i}. \quad (2)$$

The existence of this set forms the basis of the similarity theory developed by Patashinskiĭ and Pokrovskiĭ.^[5]

The aim of this work was to evaluate the row correlation function $\langle S_1 S_{1+r} \rangle$ for a plane Ising lattice to within terms beyond the leading term which is of the order of $r^{-1/4}$. It will be shown that, to within terms which are exponentially small at large distances, these terms are of the form

$$r^{-3/4} + r^{-5/4} + r^{-7/4} + O(r^{-9/4}).$$

It is natural to expect that the correction to the susceptibility in a weak magnetic field, i.e., $\Delta\chi = \chi - \chi_p$ ($\chi_p \sim \tau^{-7/4}$), is of the form

$$\Delta\chi \sim \tau^{-1/4} (1 + \tau^{-1/4} + \tau^{-1}).$$

2. FORMULATION OF THE PROBLEM. MATRIX ELEMENTS

Consider a plane square lattice on which the spin variable $S_{mn} = \pm 1$ ^[1] is assigned to each lattice point n, m . It is well known^[6-8] that the row correlation function $\langle S_1 S_{1+r} \rangle$ is

$$(-1)^r \langle S_1 S_{1+r} \rangle = \Delta_r \operatorname{ch}^2 H^* - \Delta_{-r} \operatorname{sh}^2 H^*, \quad (3)$$

where Δ_r and Δ_{-r} are determinants consisting of the matrix elements Σ_r as follows:

$$\Delta_r = \begin{vmatrix} \Sigma_1 & \Sigma_2 & \dots & \Sigma_r \\ \Sigma_0 & \Sigma_1 & \dots & \Sigma_{r-1} \\ \dots & \dots & \dots & \dots \\ \Sigma_{-r+2} & \dots & \dots & \Sigma_1 \end{vmatrix}, \quad \Delta_{-r} = \begin{vmatrix} \Sigma_{-1} & \dots & \Sigma_{-r} \\ \Sigma_0 & \dots & \Sigma_{-r+1} \\ \dots & \dots & \dots \\ \Sigma_{-r-2} & \dots & \Sigma_{-1} \end{vmatrix}, \quad (4)$$

where

$$\Sigma_r = \frac{1}{\pi} \int_0^\pi \cos[r\omega + \delta(\omega)] d\omega. \quad (5)$$

The temperature parameters are: $2H^* = \ln \coth H$, $H = (kT)^{-1} J$, $H' = (kT)^{-1} J'$ (J and J' are, respectively, the interaction energies between neighboring spins in a given column and a given row). The phase transition occurs at the temperature $H' = H^*$. The function $\delta(\omega)$ is the internal angle of the hyperbolic triangle and can be expressed in terms of the sides $2H^*$ and $2H'$ by the formulas of hyperbolic trigonometry.^[6,8]

The simplest form of $\delta(\omega)$ is found at the phase transition points^[6,8,9] for the correlation spins located in a row:

$$\cos \delta(\omega) = \frac{\sqrt{2} \sin(\omega/2)}{[1 + \sin^2(\omega/2)]^{1/2}}, \quad \sin \delta(\omega) = \frac{\cos(\omega/2)}{[1 + \sin^2(\omega/2)]^{1/2}}, \quad (6)$$

and, on the diagonal

$$\cos \delta(\omega) = \sin \frac{\omega}{2}, \quad \sin \delta(\omega) = \cos \frac{\omega}{2}. \quad (7)$$

Accordingly, the matrix elements are given by

$$\Sigma_r = \frac{2}{\pi} \int_0^{\pi/2} \frac{d\omega}{[1 + \sin^2(\omega/2)]^{1/2}} (\sqrt{2} \cos 2r\omega \sin \omega - \sin 2r\omega \cos \omega), \quad (8)$$

$$\Sigma_r = -2\pi^{-1} (2r-1)^{-1}. \quad (9)$$

Onsager and Kaufman^[6] evaluate the determinant (4) with the elements given by (9) and show that the correlation along the diagonal at the transition point decreases with distance r in accordance with a power law:

$$\langle S_1 S_{1+r} \rangle = \frac{2}{\pi} \prod_{s=1}^r \frac{\Gamma^2(s+1)}{\Gamma(s+1/2)\Gamma(s+3/2)} \sim r^{-1/4}. \quad (10)$$

The next term in r in (10) is of the order of $r^{-9/4}$ ^[10] and can be neglected. However, the evaluation of the

matrix elements (8) corresponding to row correlation is carried out in [16] only for $|r| \leq 3$. It was subsequently shown, [11] using the expansion of (8) for large values of r ,

$$\Sigma_r \sim \frac{1}{\pi r} \left(1 - \frac{\sqrt{2}}{2r} + \frac{1}{2r^2} - \frac{\sqrt{2}}{2r^3} + \dots \right), \quad (11)$$

that the row correlation decays at the phase transition point, again in accordance with the law $r^{-1/4} + r^{-9/4}$. On the other hand, (4) contains both large and small r , for which the expression given by (11) is unsuitable. It will be shown below that this approximation can be regarded as reasonable only to the extent to which it leads to the smallest term $\sim r^{-1/4}$ in the asymptotic expression for the row correlation function.

To evaluate (8), let us expand $(1 + \sin^2 \omega)^{-1/2}$ into a series in powers of $\sin^2 \omega$, and use the reduction formula given in [12]. The result is

$$\Sigma_r = \frac{1}{\pi} \left(\frac{\beta_0}{2r-1} + \frac{\alpha_0}{2r+1} + \sum_{i=1}^{\infty} \left(\frac{\beta_i}{2r-2l-1} + \frac{\alpha_i}{2r+2l+1} \right) \right) \quad (12)$$

where the coefficients α_i, β_i are given by

$$\alpha_0 = (\sqrt{2}-1) \left(1 + \sum_k A(k, 0, 0) \right) - (\sqrt{2}+1) \sum_k A(k, 0, 1),$$

$$\beta_0 = (\sqrt{2}-1) \sum_k A(k, 0, 1) - (\sqrt{2}+1) \left(1 + \sum_k A(k, 0, 0) \right),$$

$$\alpha_i = (\sqrt{2}+1) \sum_k A(k, l, 1) - (\sqrt{2}-1) \sum_k A(k, l-1, 1), \quad (13)$$

$$\beta_i = (\sqrt{2}+1) \sum_k A(k, l-1, 1) - (\sqrt{2}-1) \sum_k A(k, l, 1)$$

and

$$(-1)^k \frac{(2k+2l-1)!! C_{2k+2l}^{k-m}}{(2k+2l)!! 2^{2k+2l-1}} = A(k, l, m). \quad (14)$$

Since

$$\sum_{k=1}^{\infty} A(k, l, 1) = -\frac{2\Gamma^2(l+1/2)}{\pi\Gamma(2l+3)} F\left(l + \frac{3}{2}, l + \frac{3}{2}, 2l+3, -1\right) = -B(l), \quad (15)$$

$$\sum_{k=1}^{\infty} A(k, l-1, 1) = -\frac{2\Gamma^2(l+1/2)}{\pi\Gamma(2l+1)} F\left(l + \frac{1}{2}, l + \frac{1}{2}, 2l+1, -1\right) = -E(l),$$

where $F(a, b, c, x)$ is the hypergeometric function, [12] we obtain the final expression for the matrix element in the form

$$\Sigma_r = \sum_{i=0}^{\infty} \left(\frac{\beta_i}{2r-2l-1} + \frac{\alpha_i}{2r+2l+1} \right); \quad (16)$$

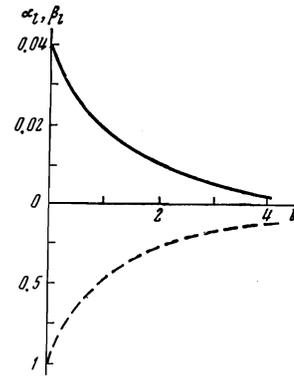
$$\alpha_i = \pi^{-1} [(\sqrt{2}-1)E(l) - (\sqrt{2}+1)B(l)], \quad (17)$$

$$\beta_i = \pi^{-1} [(\sqrt{2}-1)B(l) - (\sqrt{2}+1)E(l)].$$

The figure shows the values of α_l and β_l for $l=0, 1, 2, 3, \dots$ (the discrete set of points is joined by the solid curve for α_l and by the broken curve for β_l). It is clear from the figure that $\beta_l < 0, \alpha_l > 0, \alpha_l < 1$ for all values of l .

3. EVALUATION OF THE DETERMINANTS Δ_r AND Δ_{-r}

To evaluate Δ_r and Δ_{-r} , which determine the row correlation function $\langle S_1 S_{1+r} \rangle$, we shall substitute (16) in (4). If we represent this determinant as a sum of determinants, [13] and take out the common factors α_l, β_l



from each row, we obtain (the expression for Δ_{-r} is obtained by substituting $r \rightarrow -r$)

$$\Delta_r = [(\beta_0)^r |c_{2r-1}| + (\beta_1)^r |c_{2r-3}| + \dots + (\alpha_0)^r |c_{2r-1}| + (\alpha_1)^r |c_{2r+3}| + \dots] + \left\{ \alpha_0 (\beta_0)^{r-1} \begin{vmatrix} c_{2r+1} \\ c_{2r-1} \end{vmatrix} + (\alpha_0)^2 (\beta_1)^{r-2} \begin{vmatrix} c_{2r+1} \\ c_{2r-3} \end{vmatrix} \dots + (\alpha_0)^{r-2} (\beta_0)^2 \begin{vmatrix} c_{2r-1} \\ c_{2r+1} \end{vmatrix} + \dots \right\}, \quad (18)$$

where the symbol $|\dots|$ represents a determinant. In (18), we use the notation

$$[2r \pm (2l+1)]^{-1} = c_{2r \pm (2l+1)}, \quad l=0, 1, 2, \dots \quad (19)$$

The expression in square brackets in (18) contains the Toeplitz determinants [14]

$$|c_{2r \pm (2l+1)}| = \begin{vmatrix} \frac{1}{2 \pm (2l+1)} & \dots & \frac{1}{2r \pm (2l+1)} \\ \frac{1}{\pm (2l+1)} & \dots & \frac{1}{2(r-1) \pm (2l+1)} \\ \dots & \dots & \dots \\ \frac{1}{2(-r+2) \pm (2l+1)} & \dots & \frac{1}{2 \pm (2l+1)} \end{vmatrix}. \quad (20)$$

The determinants in the braces form all the possible combinations of determinants of the form given by (20). For example, the first term in the braces in (18) is constructed as follows: the first row of the determinant $|c_{2r-1}|$ is replaced by the first row of $|c_{2r+1}|$ and the remaining $r-1$ rows are left without change. In the second term, the first and second rows of $|c_{2r-3}|$ are replaced by the first and second rows of $|c_{2r+1}|$ and the remaining $r-2$ rows are left unaltered, and so on. We shall use m to label the row and n the column of a determinant, where $m, n=1, 2, 3, \dots, r$. The Toeplitz determinants (20) can then be rewritten in the form

$$|c_{2r-2l-1}| = |c_{2(m-n)-(2l-1)}|, \quad |c_{2r+2l+1}| = |c_{2(n-m)+2l+3}|. \quad (21)$$

Determinants of this type can be evaluated with the aid of the following formula: [15, 16]

$$|c_{mn}^{-1}| = \prod_{1 \leq m < n \leq r} (a_n - a_m) (b_n - b_m) / \prod_{m, n=1}^r (a_n + b_m), \quad (22)$$

where $|c_{mn}^{-1}|$ vanishes if $a_n = a_m$ or $b_n = b_m$ for $m \neq n$.

Since

$$|c_{2n-2m+2l+1}| = (-1)^r |c_{2n-2m-2l-1}|, \quad (23)$$

we find the contribution of the Toeplitz determinants (20) to the row correlation function:

$$\langle S_1 S_{1+r} \rangle = \epsilon_0 |c_{2n-2m+1}| + \epsilon_1 |c_{2n-2m+3}| + \epsilon_2 |c_{2n-2m+5}| + \dots \quad (24)$$

where

$$2\epsilon_0 = (\sqrt{2}+1)\beta_0^r - (\sqrt{2}-1)\alpha_0^r + (-1)^r [(\sqrt{2}+1)\beta_1^r - (\sqrt{2}-1)\alpha_1^r], \quad (25)$$

$$2\epsilon_i = (-1)^r [(\sqrt{2}-1)\alpha_{i-1}^r - (\sqrt{2}-1)\beta_{i-1}^r + (\sqrt{2}+1)\beta_{i+1}^r - (\sqrt{2}-1)\alpha_{i+1}^r].$$

In the last two expressions, we have taken into account the fact that $(\alpha_l)^r = \alpha_l^r$, $(\beta_l)^r = (-1)^r \beta_l^r$.

If we evaluate the determinants in (24) with the aid of (20) (see Appendix), we find that each of them is equal to the product of the corresponding gamma functions $\Gamma(r)$ and the function

$$G(r) = 1^{r-1} 2^{r-2} 3^{r-3} \dots (r-2)^2 (r-1). \quad (26)$$

Using the asymptotic expansion for $G(r)$ for large r [10]

$$\ln G(r) \sim \frac{1}{12} - \ln A + \frac{1}{2} \ln 2\pi + \left(\frac{1}{2} r^2 - \frac{1}{12}\right) \ln r - \frac{3}{4} r^2 + \sum_n (-1)^n \frac{B_{n+1}}{2n(2n+2)} r^{-2n}, \quad (27)$$

where B_n is the Bernoulli numbers and $A \sim 1.282$, we find that

$$|c_{2n-2m+1}| \sim r^{-n/4}, \quad |c_{2n-2m+3}| \sim r^{-n/4}. \quad (28)$$

Since, moreover, $\alpha_l \ll 1$, $\beta_l \sim 0.4$, and therefore terms of the order of $\alpha_l^r = \exp(-r/r_c)$, $r_c \ll 1$, can be neglected, we finally obtain

$$\langle S_i S_{i+r} \rangle = [C_0^0 - C_1(-1)^r \exp(-r \ln 2.25)] r^{-n/4} + O(r^{-n/4}), \quad (29)$$

$$C_0^0 = 1/2 (\sqrt{2} + 1) e^{1/2} 2^{1/2} A^{-3}.$$

The formula given by (29) is identical with the Onsager-Kaufman result [6] to within the exponentially small term.

We must now evaluate the determinants in the braces in (18). These determinants form all the possible combinations made up of the rows of the Toeplitz determinants in (20). Their contribution to Δ_r is

$$\Delta_r = (\beta_0)^r f_r^1 + (\beta_0)^{r-2} f_r^2 + \dots + (\beta_1)^{r-1} \varphi_r^1 + \dots + (\alpha_0)^{r-1} \omega_r^1 + \dots, \quad (30)$$

where f_r^1 is obtained by replacing one row in $|c_{2R-1}|$ by any row in $|c_{2R \pm (2l+1)}|$, f_r^2 is obtained by replacing two rows from $|c_{2R-1}|$ by $|c_{2R \pm (2l+1)}|$, φ_r^1 by replacing one of the rows in $|c_{2R-3}|$, and so on. For example, consider f_r^1 :

$$f_r^1 = \alpha_0 \Delta_{r0} + \alpha_1 (\Delta_{r1} + \Delta_{r1}') + \alpha_2 (\Delta_{r2} + \Delta_{r2}' + \Delta_{r2}'') + \dots \quad (31)$$

Thus, it is clear from (31) that Δ_{r0} consists of $r-1$ rows of $|c_{2R-1}|$ and the first row of $|c_{2R+1}|$, Δ_{r1} , Δ_{r1}' , consist of $r-1$ rows of $|c_{2R-1}|$ and the first and second rows taken from $|c_{2R+3}|$, and so on. In setting up (31), we used the fact that the determinant is zero when two rows are identical.

It is instructive to write out the full expression for Δ_{r1}' :

$$\Delta_{r1}' = \begin{vmatrix} \frac{1}{1} & \frac{1}{3} & \frac{1}{5} & \dots & \frac{1}{2r-1} \\ \frac{1}{3} & \frac{1}{5} & \frac{1}{7} & \dots & \frac{1}{2r+1} \\ -\frac{1}{3} & -\frac{1}{1} & \frac{1}{1} & \dots & \frac{1}{2r-5} \\ \dots & \dots & \dots & \dots & \dots \\ \frac{1}{-2r+3} & \frac{1}{-2r+5} & \dots & \dots & \frac{1}{1} \end{vmatrix}. \quad (32)$$

Determinants of this kind can be expressed in terms of the general element $c_{mn} = a_m + b_m$. However, following Akhiezer, [15] we can obtain a formula analogous to (22) for each particular determinant. For example, let us consider the contribution to (31) of determinants in which only the first row from $|c_{2n-2m+1}|$ is replaced by the rows $|c_{2n-2m+2l+1}|$, $l=1, 2, 3, \dots$. We have

$$f_r^l = \sum_{i=0}^r \alpha_i \Delta_{ri}. \quad (33)$$

Formula (22) for Δ_{rl} assumes the following form:

$$\prod_{n=2}^r (a_n - d_1^l) \prod_{2 \leq m < n \leq r} (a_n - a_m) \prod_{1 \leq m < n \leq r} (b_n - b_m) \times \left[\prod_{n=2}^r \prod_{m=1}^r (a_m + b_n) \prod_{m=1}^r (b_m + d_1^l) \right]^{-1}, \quad (34)$$

where $d_1^l = a_1 + 2l$, $a_n = -2n + 1$, $b_m = 2m$.

We now evaluate (34) for each determinant Δ_{rl} , use the asymptotic value for the function $G(r)$ given by (27), and substitute the resulting Δ_{rl} in (33). Evaluation of this sum yields

$$f_r^l \sim C_1^0 r^{-l/4} + C_1^1 r^{-l/4} + C_1^2 r^{-l/4}. \quad (35)$$

The coefficients C_k^l are given in the table.

Proceeding in the same way for all the other determinants in which only one row is replaced, we can show that each depends on r as in (35). The coefficients in front of equal powers of r in each term are positive and of the same order. We note that the number of such terms is $2r$ (r terms from $|c_{2n-2m+2l+1}|$ and r from $|c_{2n-2m-2l-1}|$), so that

$$1/2 f_r^l \sim C_1^0 r^{-l/4} + C_1^1 r^{-l/4} + C_1^2 r^{-l/4}. \quad (36)$$

We now carry out similar steps for determinants in which two rows are replaced

$$f_r^2 \sim C_2^0 r^{-l/4} + C_2^1 r^{-l/4}, \quad (37)$$

three rows are replaced

$$f_r^3 \sim C_3^0 r^{-l/4} + C_3^1 r^{-l/4} \quad (38)$$

and so on, so that we obtain the final contribution of determinants of the mixed type (30) to the row correlation function

$$\langle S_i S_{i+r} \rangle \sim C_0^1 r^{-l/4} + C_0^2 r^{-l/4} + C_0^3 r^{-l/4} + O(r^{-l/4}). \quad (39)$$

We note that (35) and (39) do not include terms of the order of

$$(-1)^r \exp(-r/r_c) [r^{-l/4} + r^{-l/4} + r^{-l/4}], \quad r_c \sim 1,$$

which can be neglected for $r \gg r_c$. Combining (29) and (39), and using the expression for Δ_{-r} given by (4), we have

$$\langle S_i S_{i+r} \rangle \sim C_0^0 r^{-n/4} + C_0^1 r^{-n/4} + C_0^2 r^{-n/4} + C_0^3 r^{-n/4} + O(r^{-n/4}). \quad (40)$$

Thus, the row correlation function given by (40) differs from the diagonal correlation [6] by the presence of the intermediate terms of the order of $r^{-3/4}$, $r^{-5/4}$, $r^{-7/4}$.

As already noted, the additional terms in the diagonal correlation begin only with $r^{-9/4}$. Therefore, the next terms after the leading term $r^{-1/4}$ in the Ising model are anisotropic. This can be seen in the fact that the coefficients C_k^l in (40) depend on the polar angle θ : on a diagonal $C_k^l(\theta) = 0$, whilst along a row or column

Table of coefficients C_k^l

k	l			
	0	1	2	3
0	0.8	0.28	0.22	0.012
1	0.23	0.003	0.002	
2	0.09	0.004		
3	0.007	0.0006		

