

## Row Correlation Functions of the Two-Dimensional Ising Model\*

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Expressions for many-site correlation functions of a square-lattice Ising model have been derived for the case in which all sites lie in the same row. The results involve expressions for minors of Toeplitz matrices which are obtained by the Wiener-Hopf technique. We derive an expression for the magnetization at any site in a row if a finite number of defect bonds are distributed at given positions in that row; this expression can be used to study the effect of a dislocation. Some remarks about the decoupling of correlation functions are made.

### 1. INTRODUCTION

IN a recent paper by Pink<sup>1</sup> (hereafter referred to as P) an analytic derivation was given of certain three-site correlation functions of the square-lattice Lenz-Ising model having spins of magnitude  $\frac{1}{2}$ , which are coupled by nearest-neighbor interactions, located at each lattice site. The expressions obtained were used to calculate the magnetization at any site in a row when one of the bonds in that row was a defect bond. It appears to be of interest, however, to derive expressions for many-site correlation functions which can be used to calculate the magnetization at a given site if defect bonds (of possibly unequal strengths), which replace perfect-lattice bonds, are distributed at given positions.

Quite apart from this defect problem, one would wish to know the exact form that many-site correlation functions have because previous use of them<sup>2</sup> has necessitated their approximation, and it is of interest to know to what extent the approximations are valid. This information is especially valuable in the critical region. As far as the defect problem is concerned, much work<sup>3</sup> has been done on calculating the effect upon various bulk properties of the Ising model when defect bonds are distributed at random in the lattice. In contrast to the case of a system described by the Heisenberg Hamiltonian, where some effort has gone into calculating the effect of a single impurity spin upon the magnetization at any site in its neighborhood<sup>4</sup> and upon the elementary excitation spectrum,<sup>5</sup> little work has been done concerning the effect of defects upon microscopic properties of the Ising model.<sup>6</sup>

In this paper we have in mind applications of the Ising model to solid-state problems. For example, Miyazima<sup>7</sup> investigated a decorated square lattice and

found it to have either two or three phase transitions, depending upon the choice of parameters. He suggested that the first case provided a model for Rochelle salt which has a ferroelectric phase between  $-18^{\circ}\text{C}$  and  $25^{\circ}\text{C}$ . In this case impurities can be represented by defect bonds. Thus, in view of the possibility that certain physical systems can be described approximately as an Ising model we can list three cases in which knowledge of the many-site correlation functions is of value.

(i) If we know all three-site correlation functions, we may calculate the magnetization per site at any distance from an isolated impurity or defect bond.

(ii) If there are many impurities present in the crystal, however, we may find it necessary to consider more than one impurity or defect bond in calculating the magnetization per site. In this case, knowledge of higher-order correlation functions is necessary.

(iii) We could consider a line of omitted bonds to represent a simple model of a dislocation. The number of correlation functions needed in this case will depend upon the length of the dislocation.

The object of this paper is to derive relatively simple expressions which are easily applied. The solution of the general problem is, however, no trivial task, and we shall confine ourselves to the presentation of a more modest endeavor.

Here we shall be concerned with deriving an expression for the magnetization at any site in a row if a finite number of defect bonds are distributed at given positions in that row. One would expect that this restriction leaves the third case mentioned relatively unaffected since in that case all the defect bonds lie in the same row. The expressions derived here could, thus, be directly applied to the investigation of the effect of certain kinds of defects (see Sec. 4). The application of the results to the first two cases is considerably restricted but it should shed some light upon the form of the magnetization per site in the general case. The solution will be approached in such a way that it will give expressions for many-site correlation functions when the sites all lie in the same row. The method that will be employed is an extension of that used in P, which was originally

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<sup>1</sup> D. A. Pink, *Can. J. Phys.* **46**, 2399 (1968).

<sup>2</sup> N. Matsudaira, *Can. J. Phys.* **45**, 2091 (1967).

<sup>3</sup> A. A. Lushnikov, *Phys. Letters* **27A**, 158 (1968); M. F. Sykes and J. W. Essam, *Phys. Rev. Letters* **10**, 3 (1963).

<sup>4</sup> H. P. Van de Braak, *Phys. Letters* **26A**, 569 (1968); D. Hone, H. Callen, and L. R. Walker, *Phys. Rev.* **144**, 283 (1966).

<sup>5</sup> Yu. A. Izyumov and M. V. Medvedev, *Zh. Eksperim. i Teor. Fiz.* **51**, 517 (1966) [English transl.: *Soviet Phys.—JETP* **24**, 347 (1967)]; T. Wolfram, and J. Callaway, *Phys. Rev.* **130**, 2207 (1963).

<sup>6</sup> However, see P. G. Watson, *J. Phys.* **C1**, 575 (1968).

<sup>7</sup> S. Miyazima, *Progr. Theoret. Phys. (Kyoto)* **40**, 462 (1968).

due to Krein.<sup>8</sup> Wu and his collaborators<sup>9</sup> have used this kind of approach in a series of papers.

Each site in the lattice is labeled as  $(k, l)$ , where  $k$  denotes the row and  $l$  the column. The variable  $\sigma_{k,l}$  (which takes on the values  $\pm 1$ ), of the set  $\{\sigma\}$ , is associated with the site  $(k, l)$ , and interactions, which are between nearest-neighbor sites only, are denoted by  $J_1$  (for sites in the same row) and  $J_2$  (for sites in the same column). The number of sites in a row or column is  $N^{1/2}$ , which is allowed to go to infinity, and we shall be concerned with effects far away from the boundary of the lattice. The partition function of the perfect lattice is

$$Z = \sum_{\{\sigma\}} \exp[\beta \sum_{k,l} (J_1 \sigma_{k,l} \sigma_{k,l+1} + J_2 \sigma_{k,l} \sigma_{k+1,l})] = (\cosh \beta J_1 \cosh \beta J_2)^N Z_0, \quad \beta = (k_B T)^{-1} \quad (1.1)$$

where

$$Z_0 = \sum_{\{\sigma\}} S(\alpha), \\ S(\alpha) = \prod_{kl,k'l'} (1 + \alpha_{kl,k'l'} \sigma_{k,l} \sigma_{k',l'}), \\ \alpha_{kl,k'l'} = x_1 \quad \text{for } k'=k, l'=l+1 \\ = x_2 \quad \text{for } k'=k+1, l'=l \\ = 0 \quad \text{otherwise,} \\ x_i = \tanh \beta J_i. \quad (1.2)$$

Each bond has the number  $x_i$  associated with it which we shall call its weight. An  $n$ -site correlation function is defined as

$$\langle \sigma_1 \sigma_2 \cdots \sigma_n \rangle = Z_0^{-1} \sum_{\{\sigma\}} S(\alpha) \sigma_1 \sigma_2 \cdots \sigma_n, \quad (1.3)$$

where  $1, 2, \dots, n$  denote various sites in the lattice. The defect problem will be presented in Sec. 2, and the formal solution to the correlation-function problem given in Sec. 3. In Sec. 4 some simple applications of the results will be presented.

### 2. DEFECT PROBLEM

Let us assume that there are defect bonds lying between the sites labeled  $(1, \lambda_f)$  and  $(1, \lambda_f + 1)$  which have weights  $x_f' = \tanh \beta J_f'$ ,  $f = 1, 2, \dots, n$ . Let us write  $B = \{\lambda_1, \dots, \lambda_n\}$  so that the partition function is

$$Z_B = \sum_{\{\sigma\}} S(\alpha^B), \\ S(\alpha^B) = \prod_{kl,k'l'} (1 + \alpha_{kl,k'l'} \sigma_{k,l} \sigma_{k',l'}), \\ \alpha_{kl,k'l'} = x_f' \quad \text{for } k'=k=1, l'=l+1, l=\lambda_1, \dots, \lambda_n \\ = x_1 \quad \text{for } k'=k, l'=l+1 \\ \quad \text{(excluding first set)} \\ = x_2 \quad \text{for } k'=k+1, l'=l \\ \quad \text{(excluding first set)} \\ = 0 \quad \text{otherwise.} \quad (2.2)$$

<sup>8</sup> M. G. Krein, *Am. Math. Soc. Transl.* **22**, 163 (1962).

<sup>9</sup> T. T. Wu, *Phys. Rev.* **149**, 380 (1966). See also H. Cheng and T. T. Wu, *ibid.* **164**, 719 (1967); B. M. McCoy and T. T. Wu, *ibid.* **174**, 546 (1968).

By making use of  $\sigma_{k,l}^2 = 1$ , we can write

$$Z_B = (1 - x_1^2)^{-n} \prod_{f=1}^n (1 - x_1 x_f') \sum_{\{\sigma\}} \{S(\alpha) \prod_{i=1}^n [1 + (x_i' - x_1) \times (1 - x_1 x_i')^{-1} \sigma_{1,\lambda_i} \sigma_{1,\lambda_i+1}]\}, \quad (2.3)$$

which is an appropriate sum of correlation functions of the form (1.3), each one containing an even number of  $\sigma_p$ .

Here we are interested in calculating the magnetization at the site labeled (1.1) and we shall assume that it is given by

$$\langle \sigma_{1,1} \rangle_B = M^{-1} \lim_{t \rightarrow \infty} \langle \sigma_{1,1} \sigma_{1,1+t} \rangle_B \\ = M^{-1} \lim_{t \rightarrow \infty} Z_B^{-1} \sum_{\{\sigma\}} S(\alpha^B) \sigma_{1,1} \sigma_{1,1+t}, \quad (2.4)$$

where  $M$  is the spontaneous magnetization per site in the perfect lattice. It is understood that  $t \rightarrow \infty$  before any of the  $p \rightarrow \infty$ . Site  $(1, 1+t)$  is thus far away from the defects, which is the reason for the assumption of (2.4). By using the same procedure that led to (2.3), we see that

$$\langle \sigma_{1,1} \rangle_B = M^{-1} (Z_0 Z_B^{-1}) (1 - x_1^2)^{-n} \prod_{f=1}^n (1 - x_1 x_f') \\ \times \lim_{t \rightarrow \infty} Z_0^{-1} \sum_{\{\sigma\}} \{S(\alpha) \prod_{i=1}^n [1 + (x_i' - x_1) (1 - x_1 x_i')^{-1} \times \sigma_{1,\lambda_i} \sigma_{1,\lambda_i+1}] \sigma_{1,1} \sigma_{1,1+t}\}. \quad (2.5)$$

The problem thus reduces to the calculation of correlation functions of the form

$$\lim_{t \rightarrow \infty} \langle \sigma_{1,1} \cdots \sigma_{1,\lambda_i} \sigma_{1,\lambda_i+1} \cdots \sigma_{1,1+t} \rangle.$$

In P it was shown that for the case of  $n = 1$  we had to obtain an expression for a minor which is formed from a Toeplitz matrix<sup>10</sup> by striking out the  $r$ th row and the  $r$ th column (referred to as the corresponding column of the  $r$ th row). In order to display the problem for this case, let us consider

$$\langle \sigma_{1,1} \sigma_{1,\lambda_1} \sigma_{1,\lambda_1+1} \cdots \sigma_{1,\lambda_f} \sigma_{1,\lambda_f+1} \sigma_{1,1+t} \rangle \\ = C(1, \lambda_1, \lambda_1 + 1, \dots, \lambda_f, \lambda_f + 1, t + 1), \\ 1 \leq \lambda_1 \leq \dots \leq \lambda_f \ll t.$$

By inserting factors of  $\sigma_{1,m}^2$ ,  $1 < m < t + 1$ , we can write

$$C(1, \lambda_1, \dots, \lambda_f + 1, t + 1) = x_1^{t-f} \left[ \sum_{\{\sigma\}} S(\beta) \right] / \sum_{\{\sigma\}} S(\alpha), \quad (2.6)$$

$$\beta_{kl,k'l'} = \alpha_{kl,k'l'} + g \Delta_{kl,k'l'}, \quad (2.7) \\ g = 1/x_1 - x_1,$$

$$\Delta_{kl,k'l'} = 1 \quad \text{for } k'=k=1, l'=l+1, l=1, \dots, t, \\ l \neq \lambda_1, \dots, \lambda_f$$

$$= 0 \quad \text{otherwise.} \quad (2.8)$$

<sup>10</sup> V. Grenander and G. Szego, *Toeplitz Forms and Their Applications* (University of California Press, Berkeley, 1958).

It is found that

$$\sum_{\{\sigma\}} S(\alpha) = [\det(1-A)]^{1/2},$$

where  $A$  is a matrix obtained from the  $\alpha_{kl,k'l'}$  when they are written in the form of a matrix  $(\alpha_{kl,k'l'})$ .<sup>11</sup> Similarly, it is found that

$$\sum_{\{\sigma\}} S(\beta) = [\det(1-F)]^{1/2}, \tag{2.9}$$

$$F = A + gD.$$

The matrix  $D$  is obtained from  $(\Delta_{kl,k'l'})$  in the same way as  $A$  is obtained from  $(\alpha_{kl,k'l'})$ .<sup>12</sup> Thus, we find

$$C(1, \lambda_1, \dots, \lambda_f + 1, t + 1) = x_1^{t-f} \{ \det[1 - g(1-A)^{-1}D] \}^{1/2}. \tag{2.10}$$

Because of the form of  $D$ , (2.10) is obtained from a  $t \times t$  Toeplitz determinant by striking out the rows labeled  $\lambda_1, \dots, \lambda_f$  and their corresponding columns. We shall refer to it as an  $f$ th minor of a Toeplitz matrix. The matrix elements  $c_{nm} = c_{n-m}$  are given by<sup>13</sup>

$$c_n = (2\pi)^{-1} \int_0^{2\pi} \varphi(\theta) e^{-in\theta} d\theta,$$

$$\varphi(\theta) = [(x_1 x_2^* e^{i\theta} - 1)(x_1 e^{i\theta} - x_2^*) / (e^{i\theta} - x_1 x_2^*)(x_2^* e^{i\theta} - x_1)]^{1/2}$$

$$= \sum_{n=-\infty}^{\infty} c_n e^{in\theta}, \quad x_i^* = (1 - x_i) / (1 + x_i). \tag{2.11}$$

We shall be interested in the limit as  $t \rightarrow \infty$ . Not much effort is required to convince oneself that all correlation functions of the form

$$\lim_{t \rightarrow \infty} \langle \sigma_{1,\lambda_1} \sigma_{1,\lambda_2} \dots \sigma_{1,\lambda_s} \sigma_{1,t} \rangle$$

can be written as (2.6) and so can be expressed as appropriate minors of a Toeplitz matrix.

### 3. FORMAL SOLUTION

Let us consider an  $(f+1)$ st minor,  $V_{(f+1)}$ , of a Toeplitz matrix  $V$ , in which the missing rows are denoted by the set  $(f+1) = \{\lambda_1, \dots, \lambda_f, s\}$ . We write  $(n) = \{\lambda_1, \dots, \lambda_n\}$  with a corresponding definition of  $V_{(n)}$ . Let the matrix elements of  $V$  be  $(V)_{lm} = a_{l-m}$  and write  $(V^{-1})_{lm} = \gamma_{lm}$ ,  $l, m = 0, 1, 2, \dots$ , where  $VV^{-1} = I$ .

<sup>11</sup> N. V. Vdovichenko, Zh. Eksperim. i Teor. Fiz. **47**, 715 (1964) [English transl.: Soviet Phys.—JETP **20**, 477 (1965)].

<sup>12</sup> N. V. Vdovichenko, Zh. Eksperim. i Teor. Fiz. **48**, 526 (1965) [English transl.: Soviet Phys.—JETP **21**, 350 (1965)].

<sup>13</sup> E. W. Montroll, R. B. Potts, and J. C. Ward, J. Math. Phys. **4**, 308 (1963).

Then if we apply Jacobi's theorem,<sup>14</sup>

$$V_{(f+1)} = \begin{vmatrix} \gamma_{\lambda_1 \lambda_1} & \gamma_{\lambda_2 \lambda_1} & \dots & \gamma_{s \lambda_1} \\ \vdots & \vdots & \vdots & \vdots \\ \gamma_{\lambda_1 s} & \dots & \dots & \gamma_{ss} \end{vmatrix} \det(V). \tag{3.1}$$

Jacobi's theorem, however, must be used with care when dealing with infinite matrices<sup>15</sup> and we shall present a derivation of (3.1) which is valid when  $f$  is finite. There we shall see the problem that occurs when  $f$  is not finite, but we shall not take up that solution in this paper. The derivation of (3.1) will also serve to display expressions for the  $\gamma_{lm}$ .

Consider the set of equations

$$\sum_{k=0}^{\infty} a_{j-k} \xi_k^{(f)} - \sum_{i=1}^f a_{j-\lambda_i} \xi_{\lambda_i}^{(f)} = \eta_j^{(f)},$$

$$j = 0, 1, \dots, \quad j \neq \lambda_1, \dots, \lambda_f, \tag{3.2}$$

$$\xi_j^{(f)} = \eta_j^{(f)}, \quad j = \lambda_1, \dots, \lambda_f.$$

If we multiply each equation by  $\zeta^j$  and sum over  $j$ , we get

$$\sum_{j=0}^{\infty} \sum_{k=0}^{\infty} a_{j-k} \zeta^{j-k} \xi_k^{(f)} \zeta^k - \sum_{j=0}^{\infty} \sum_{i=1}^f a_{j-\lambda_i} \zeta^{j-\lambda_i} \xi_{\lambda_i}^{(f)} \zeta^{\lambda_i}$$

$$= \sum_{i=1}^f \left[ \sum_{k=0}^{\infty} a_{\lambda_i-k} \xi_k^{(f)} - \sum_{m=1}^f (\delta_{im} + a_{\lambda_i-\lambda_m}) \xi_{\lambda_m}^{(f)} \right] \zeta^{\lambda_i}$$

$$= \sum_{j=0}^{\infty} \eta_j^{(f)} \zeta^j. \tag{3.3}$$

Then, if  $f$  is finite,

$$a(\zeta) \left[ \xi^{(f)}(\zeta) - \sum_{i=1}^f \xi_{\lambda_i}^{(f)} \zeta^{\lambda_i} \right] = \eta^{(f)}(\zeta) + \sum_{i=1}^f [A_{\lambda_i}^{(f)}(\xi) - \sum_{m=1}^f (\delta_{im} + a_{\lambda_i-\lambda_m}) \xi_{\lambda_m}^{(f)}] \zeta^{\lambda_i} + b^{(f)}(\zeta), \tag{3.4}$$

where

$$a(\zeta) = \sum_{k=-\infty}^{\infty} a_k \zeta^k, \quad \xi^{(f)}(\zeta) = \sum_{k=0}^{\infty} \xi_k^{(f)} \zeta^k,$$

$$\eta^{(f)}(\zeta) = \sum_{k=0}^{\infty} \eta_k^{(f)} \zeta^k, \quad A_{\lambda_i}^{(f)}(\xi) = \sum_{k=0}^{\infty} a_{\lambda_i-k} \xi_k^{(f)},$$

$$b^{(f)}(\zeta) = \sum_{j=-\infty}^{-1} \zeta^j \left[ \sum_{k=0}^{\infty} a_{j-k} \xi_k^{(f)} - \sum_{i=1}^f a_{j-\lambda_i} \xi_{\lambda_i}^{(f)} \right]. \tag{3.5}$$

We shall assume that

$$\sum_{k=-\infty}^{\infty} |a_k| < \infty, \quad a(\zeta) \neq 0, \quad |\zeta| = 1, \tag{3.6}$$

<sup>14</sup> A. C. Aitken, *Determinants and Matrices* (Oliver and Boyd Ltd., Edinburgh, 1959), Sec. 42.

<sup>15</sup> I am indebted to E. Schuegraf for some comments on this point.

and that the expressions appearing in (3.4) converge absolutely inside the closed unit disk at the origin. Then, if the index of  $a(\zeta)$ ,  $\text{inda}(\zeta)$ , which is the increase in the argument of  $a(\zeta)/2\pi$  as  $\zeta$  moves around the unit circle at the origin in the positive direction, satisfies  $\text{inda}(\zeta)=0$ , we have

$$a^{-1}(\zeta) = g_+(\zeta)g_-(\zeta), \quad |\zeta| = 1, \quad (3.7)$$

where  $g_+(\zeta)$  and  $g_-(\zeta^{-1})$  are analytic inside the unit circle at the origin and are continuous on the unit circle, so that

$$g_\mu(\zeta) = \sum_{n=0}^{\infty} \gamma_n^{(\mu)} \zeta^{\mu n}, \quad \mu = +, -. \quad (3.8)$$

We can then write

$$g_+(\zeta)^{-1}(\xi^{(f)}(\zeta) - \sum_{i=1}^f \xi_{\lambda_i}^{(f)} \zeta^{\lambda_i}) - P_+(g_-(\zeta).N^{(f)}(\zeta)) = g_-(\zeta)b^{(f)}(\zeta) + (1 - P_+)(g_-(\zeta).N^{(f)}(\zeta)), \quad (3.9)$$

where

$$N^{(f)}(\zeta) = \eta^{(f)}(\zeta) + \sum_{i=1}^f [A_{\lambda_i}^{(f)}(\xi) - \sum_{m=1}^f (\delta_{im} + a_{\lambda_i - \lambda_m}) \xi_{\lambda_m}^{(f)}] \zeta^{\lambda_i}, \quad (3.10)$$

$$P_+(\sum_{j=-\infty}^{\infty} d_j \zeta^j) = \sum_{j=0}^{\infty} d_j \zeta^j.$$

The left- (right-) hand side of (3.9) is analytic inside (outside) the unit circle, and the right-hand side goes to zero as  $\zeta \rightarrow \infty$ . Thus,

$$\xi^{(f)}(\zeta) - \sum_{i=1}^f \xi_{\lambda_i}^{(f)} \zeta^{\lambda_i} = g_+(\zeta)P_+(g_-(\zeta).N^{(f)}(\zeta)). \quad (3.11)$$

By equating coefficients of  $\zeta^k$  we find

$$\xi_k^{(f)} - \sum_{i=1}^f \xi_{\lambda_i}^{(f)} \delta_{k\lambda_i} = \sum_{n=0}^{\infty} \gamma_{kn} \eta_n^{(f)} + \sum_{i=1}^f [A_{\lambda_i}^{(f)}(\xi) - \sum_{m=1}^f (\delta_{im} + a_{\lambda_i - \lambda_m}) \eta_{\lambda_m}^{(f)}] \gamma_{k\lambda_i}, \quad (3.12)$$

where

$$\gamma_{kn} = \sum_{m=0}^{\infty} \gamma_{k-m}^{(+)} \gamma_{n-m}^{(-)}. \quad (3.13)$$

The  $\gamma_{kn}$  are the matrix elements of  $V^{-1}$  given previously. By putting  $k = \lambda_i$  in turn,  $i = 1, \dots, f$ , we obtain a set of equations for the  $A_{\lambda_i}^{(f)}(\xi)$ . We are interested in solving for  $\xi_s^{(f)}$  when  $\eta_s^{(f)} = 1$  and  $\eta_j^{(f)} = 0$  for  $j \neq s$ ,  $s \geq \lambda_f$ . The condition  $s \geq \lambda_f$  is one imposed merely by our

choice of  $\lambda_1, \dots, \lambda_f$ , and  $s$ . We find that

$$\xi_s^{(f)} = \gamma_{ss} + \sum_{i=1}^f A_{\lambda_i}^{(f)}(\xi) \gamma_{s\lambda_i}, \quad (3.14)$$

$$\sum_{i=1}^f A_{\lambda_i}^{(f)}(\xi) \gamma_{\lambda_m \lambda_i} = -\gamma_{\lambda_m s}. \quad (3.15)$$

It is not difficult to see that these equations give

$$\xi_s^{(f)} = \begin{vmatrix} \gamma_{\lambda_1 \lambda_1} & \dots & \gamma_{s \lambda_1} \\ \vdots & & \vdots \\ \gamma_{\lambda_1 s} & \dots & \gamma_{ss} \end{vmatrix} \bigg/ \begin{vmatrix} \gamma_{\lambda_1 \lambda_1} & \dots & \gamma_{\lambda_f \lambda_1} \\ \vdots & & \vdots \\ \gamma_{\lambda_1 \lambda_f} & \dots & \gamma_{\lambda_f \lambda_f} \end{vmatrix}. \quad (3.16)$$

What we want is  $\xi_s^{(f)} \det(V_{(f)})$ , which is given by

$$\xi_s^{(f)} \det(V_{(f)}) = \xi_s^{(f)} \xi_{\lambda_f}^{(f-1)} \dots \xi_{\lambda_1}^{(0)} \det(V), \quad (3.17)$$

where  $\xi_n^{(k)}$  is evaluated with  $\eta_n^{(k)} = 1$ ,  $\eta_j^{(k)} = 0$  if  $j \neq n$ . By combining (3.17) and (3.16) we obtain (3.1).

At this point we should refer back to (3.3) and note that if  $f = \infty$ , then (3.4) does not follow. In order to deal with this case, we should consider a set of equations like (3.2) where  $k$  and  $j$  run over  $0, 1, \dots, K$ , solve them for  $K$  finite, but much larger than  $\lambda_f$ , and then let  $K$  and  $f$  go to infinity together. We shall not take up this problem here.

For  $T < T_c$ , the critical temperature, we identify, as Wu<sup>9</sup> first pointed out,

$$a(\zeta) = [(1 - \alpha_1 \zeta)(1 - \alpha_2 \zeta^{-1}) / (1 - \alpha_2 \zeta)(1 - \alpha_1 \zeta^{-1})]^{1/2}, \quad \alpha_1 = x_1 x_2^*, \quad \alpha_2 = x_2^* / x_1. \quad (3.18)$$

In this case  $\alpha_1 < \alpha_2 < 1$ , so that  $\text{inda}(\zeta) = 0$ . Then  $a_{j-k} = c_{j-k}$  and

$$g_+(\zeta) = [(1 - \alpha_2 \zeta) / (1 - \alpha_1 \zeta)]^{1/2}, \quad g_-(\zeta) = [(1 - \alpha_1 \zeta^{-1}) / (1 - \alpha_2 \zeta^{-1})]^{1/2}. \quad (3.19)$$

It is easy to show (see the Appendix) that

$$\gamma_{kn} = c_{n-k} - \Omega_{k-n}^{n+1}, \quad (3.20)$$

$$\begin{aligned} \Omega_{k-n}^{n+1} &= \sum_{l=n+1}^{\infty} \gamma_{l+k-n}^{(+)} \gamma_l^{(-)} \quad \text{if } k \geq n \\ &= \sum_{l=k+1}^{\infty} \gamma_l^{(+)} \gamma_{l+n-k}^{(-)} \quad \text{if } k \leq n. \end{aligned} \quad (3.21)$$

When  $l$  is very large, it was shown in P that

$$\begin{aligned} \gamma_l^{(+)} &\sim -[\alpha_2 / 4\pi(\alpha_2 - \alpha_1)]^{1/2} \alpha_2 l^{-3/2}, \\ \gamma_l^{(-)} &\sim [(\alpha_2 - \alpha_1) / \pi \alpha_2]^{1/2} \alpha_2 l^{-1/2}, \end{aligned} \quad (3.22)$$

so that

$$\begin{aligned} \Omega_{k-n}^{n+1} &\sim -(2\pi)^{-1} \sum_{l=n+1}^{\infty} \alpha_2^{2l+k-n} (l+k-n)^{-3/2} l^{-1/2}, \\ &\quad k \geq n \\ &\sim -(2\pi)^{-1} \sum_{l=k+1}^{\infty} \alpha_2^{2l+n-k} l^{-3/2} (l+n-k)^{-1/2}, \\ &\quad k \leq n. \end{aligned} \quad (3.23)$$

If, in addition,  $J_1=J_2=J$ ,  $\epsilon=J(T_c-T)/k_B T T_c$  is very small, and  $\epsilon(k+n)$  is very large, we have

$$\begin{aligned} \Omega_{k-n}^{n+1} &\sim -4\epsilon\pi^{-1} \int_{4\epsilon(k+n+2)}^{\infty} e^{-y} dy [y+4\epsilon(k-n)]^{-3/2} \\ &\quad \times [y-4\epsilon(k-n)]^{-1/2}, \quad k \geq n \\ &\sim -4\epsilon\pi^{-1} \int_{4\epsilon(k+n+2)}^{\infty} e^{-y} dy [y-4\epsilon(n-k)]^{-3/2} \\ &\quad \times [y+4\epsilon(n-k)]^{-1/2}, \quad k \leq n \end{aligned} \quad (3.24)$$

wherein one should note the correction to the asymptotic form [28] in P which corresponds to the case  $k=n$ .

4. APPLICATIONS

(i) First we see that

$$\begin{aligned} \lim_{l \rightarrow \infty} C(1, \lambda_1+1, \lambda_1+2, \dots, \lambda_f+1, \lambda_f+2, l+1) \\ = M^2 \begin{vmatrix} \gamma_{\lambda_1 \lambda_1} & \dots & \gamma_{\lambda_f \lambda_1} \\ \vdots & & \vdots \\ \gamma_{\lambda_1 \lambda_f} & \dots & \gamma_{\lambda_f \lambda_f} \end{vmatrix}. \end{aligned} \quad (4.1)$$

When only a few sites are involved, this expression is quite simple to evaluate. Even when a large number of sites appear, there are obvious advantages over the infinite determinant with which we started. From (4.1) we can obtain an expression for any correlation function involving a finite number of sites in row 1. For example, by letting  $\lambda_1, \dots, \lambda_f \rightarrow \infty$  keeping all  $\lambda_i - \lambda_m$  fixed, we find

$$\begin{aligned} \langle \sigma_{1, \lambda_1+1} \sigma_{1, \lambda_1+2} \dots \sigma_{1, \lambda_f+1} \sigma_{1, \lambda_f+2} \rangle \\ = \begin{vmatrix} c_0 & c_{\lambda_1-\lambda_2} & \dots & c_{\lambda_1-\lambda_f} \\ \vdots & & & \vdots \\ c_{\lambda_f-\lambda_1} & \dots & & c_0 \end{vmatrix}, \end{aligned} \quad (4.2)$$

which reduces to the expression given by Stephenson<sup>16</sup> when  $f=2$ . In this case we have

$$\begin{aligned} \langle \sigma_{1,1} \sigma_{1,1+r} \sigma_{1,2+r} \sigma_{1,1+s} \sigma_{1,2+s} \rangle \\ - \langle \sigma_{1,1} \rangle \langle \sigma_{1,1+r} \sigma_{1,2+r} \sigma_{1,1+s} \sigma_{1,2+s} \rangle \\ = M [ -c_0(\Omega_0^{r+1} + \Omega_0^{s+1}) + c_{s-r} \Omega_{s-r}^{r+1} + c_{r-s} \Omega_{r-s}^{s+1} \\ + \Omega_0^{r+1} \Omega_0^{s+1} - \Omega_{s-r}^{r+1} \Omega_{r-s}^{s+1} ], \end{aligned} \quad (4.3)$$

which vanishes as  $(T_c - T)^{9/8}$ .

When  $T > T_c$ ,  $\alpha_1 < 1 < \alpha_2$ , so that  $\text{ind} a(\zeta) \neq 0$ . However,  $\text{ind} a_1(\zeta) = 0$ , where  $a_1(\zeta) = \zeta a(\zeta)$ ,<sup>9</sup> so that the canonical factorization  $a_1^{-1}(\zeta) = G_+(\zeta) G_-(\zeta)$  exists. We can repeat the procedure of Sec. 3 and we see immediately that all correlation functions containing an odd number of sites

vanish identically, as we should expect. Those with an even number of sites are given by (4.2).

(ii) Let us assume that there are impurity bonds between the sites  $(1, 1+\lambda_i)$  and  $(1, 2+\lambda_i)$ ,  $i=1, \dots, f$ , of weight  $x_i'$ , respectively, so that  $B = \{1+\lambda_1, \dots, 1+\lambda_f\}$ . By an expansion into correlation functions similar to that of Sec. 2 followed by a substitution from (4.1), we see that

$$\langle \sigma_{1,1} \rangle_B = M \det(N_f) / \det(D_f), \quad (4.4)$$

$$N_f = \begin{pmatrix} 1+K_1\gamma_{\lambda_1\lambda_1} & K_1\gamma_{\lambda_2\lambda_1} & \dots & K_1\gamma_{\lambda_f\lambda_1} \\ K_2\gamma_{\lambda_1\lambda_2} & 1+K_2\gamma_{\lambda_2\lambda_2} & \dots & K_2\gamma_{\lambda_f\lambda_2} \\ \vdots & \vdots & \ddots & \vdots \\ K_f\gamma_{\lambda_1\lambda_f} & \dots & \dots & 1+K_f\gamma_{\lambda_f\lambda_f} \end{pmatrix}, \quad (4.5)$$

$$D_f = \begin{pmatrix} 1+K_1c_0 & K_1c_{\lambda_1-\lambda_2} & \dots & K_1c_{\lambda_1-\lambda_f} \\ K_2c_{\lambda_2-\lambda_1} & 1+K_2c_0 & \dots & K_2c_{\lambda_2-\lambda_f} \\ \vdots & \vdots & \ddots & \vdots \\ K_fc_{\lambda_f-\lambda_1} & \dots & \dots & 1+K_fc_0 \end{pmatrix}, \quad (4.6)$$

$$K_i = (x_i' - x_i) / (1 - x_i x_i'), \quad i = 1, \dots, f. \quad (4.7)$$

$D_f$  is obtained from  $N_f$  by letting all the  $\lambda_n \rightarrow \infty$  keeping every  $\lambda_i - \lambda_m$  fixed. Equation (4.4) can be applied to the case of a dislocation<sup>17</sup> by putting all  $x_i' = 0$ .

(iii) Finally, we can use (4.1) to see how reliable certain decoupling methods are. Matsudaira<sup>2</sup> has used such a method in calculating the frequency-dependent magnetic susceptibility, from a general formula which he has derived, for the square lattice. He is particularly interested in the behavior near the critical point and has pointed out that his decoupling method does not give the correct analytic behavior. Let us see where the difference arises for a simple case. Consider  $\langle \sigma_{1,1} \sigma_{1,1+r} \sigma_{1,2+r} \rangle$ , where  $r$  is very large, which is decoupled as

$$M [ \langle \sigma_{1,1} \sigma_{1,1+r} \rangle + \langle \sigma_{1,1} \sigma_{1,2+r} \rangle + \langle \sigma_{1,1+r} \sigma_{1,2+r} \rangle - 2M^2 ]. \quad (4.8)$$

By using the results of Wu<sup>9</sup> for the asymptotic form of the pair correlation function, we see that for  $J_1=J_2=J$ ,  $\epsilon \ll 1$ , and  $\epsilon(r+1) \gg 1$ , the decoupling approximation gives

$$\langle \sigma_{1,1} \sigma_{1,1+r} \sigma_{1,2+r} \rangle - M c_0 \sim M^3 [32\pi\epsilon^2(r+1)^2]^{-1}, \quad (4.9)$$

because the pair correlation functions are asymptotically proportional to  $M^3$ . This expression vanishes like  $(T_c - T)^{3/8}$ . The asymptotic form of the exact result can be derived from (4.1) and (3.24), was given in P, and is proportional to  $M\epsilon$  near the critical point.

It is

$$\langle \sigma_{1,1} \sigma_{1,1+r} \sigma_{1,2+r} \rangle - M c_0 \sim M \epsilon [8\pi\epsilon^2(r+1)^2]^{-1}, \quad (4.10)$$

which vanishes like  $(T_c - T)^{9/8}$ .

<sup>16</sup> J. Stephenson, J. Math. Phys. 7, 1123 (1966).

<sup>17</sup> S. Melinckx, *The Direct Observation of Dislocations* (Academic Press Inc., New York, 1964), p. 294.

## APPENDIX

If we write

$$a^{-1}(\zeta) = \sum_{j=-\infty}^{\infty} v_j \zeta^j, \quad (\text{A1})$$

it follows from (3.7) and (3.8) that

$$\sum_{n=0}^{\infty} \gamma_{n+j}^{(+)} \gamma_n^{(-)} = v_j, \quad j \geq 0 \quad (\text{A2})$$

$$\sum_{n=0}^{\infty} \gamma_n^{(+)} \gamma_{n+j}^{(-)} = v_{-j}, \quad j \geq 0.$$

If we then make use of the fact that here  $a^{-1}(\zeta^{-1}) = a(\zeta)$ , we see that  $v_j = c_{-j}$ . Finally, in (3.13), for  $k < n$  we put

$k - m = l$  to obtain

$$\gamma_{kn} = \sum_{l=0}^{\infty} \gamma_l^{(+)} \gamma_{l+n-k}^{(-)} - \Omega_{k-n}^{n+1}, \quad (\text{A3})$$

and for  $k > n$  we put  $n - m = l$ , which gives

$$\gamma_{kn} = \sum_{l=0}^{\infty} \gamma_{l+k-n}^{(+)} \gamma_l^{(-)} - \Omega_{k-n}^{n+1}. \quad (\text{A4})$$

By using (A2), we see that (3.20) is verified.

It should be noted that (A2) follows almost immediately, in a way identical to that of Appendix 3 of P, from the theorem concerning inverses of Fourier series proven by Edrei and Szego.<sup>18</sup> In passing, we might also note that we can easily prove these results by means of the contour integration procedure used in P.

<sup>18</sup> A. Edrei and G. Szego, Proc. Am. Math. Soc. 4, 323 (1953).

Two-Dimensional Antiferromagnetism in  $\text{Mn}(\text{HCOO})_2 \cdot 2\text{H}_2\text{O}^\dagger$ 

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Long-range two-dimensional magnetic correlations have been observed in  $\text{Mn}(\text{HCOO})_2 \cdot 2\text{H}_2\text{O}$  by the quasi-elastic scattering of neutrons. A direct indication of the two-dimensional magnetic character of the system is the occurrence of the scattering near "lines" in the reciprocal lattice. The "lines" are parallel to  $a^*$ , indicating that long-range correlations are occurring in planes of atoms parallel to (100). The two-dimensional character is observed below  $T_N = 3.6^\circ\text{K}$  and persists to at least  $2T_N$ . Observation of the  $q$  dependence of the scattering above  $T_N$  is consistent with a decreasing two-dimensional correlation length as the temperature increases. Another interesting property of this crystal is the different degree of ordering exhibited by two types of Mn moments which occur in the primitive cell at two pairs of inequivalent positions ( $A$  sites and  $B$  sites). The  $A$  sites and  $B$  sites form alternating layers of atoms parallel to (100) and strong intraplanar antiferromagnetic coupling exists only for the  $A$  sites. Measurements of magnetic Bragg peaks below  $T_N$  indicate that  $\langle \mu_A \rangle$  is an order of magnitude larger than  $\langle \mu_B \rangle$ , which is in agreement with a molecular field model with very small interplanar coupling. The sublattice magnetization  $\langle \mu_A \rangle$  was found to vary as  $(3.62 - T)^{0.23 \pm 0.01}$  from 2.00 to  $3.48^\circ\text{K}$ , the initial slope of the magnetization just below  $T_N$  being larger than that obtained in isotropic three-dimensional systems.

## INTRODUCTION

NEUTRON diffraction techniques have recently been utilized by Birgeneau *et al.*<sup>1</sup> to give direct evidence for long-range two-dimensional magnetic correlations in  $\text{K}_2\text{NiF}_4$  over a wide range of temperatures. Structural, thermal, and magnetic measurements of several other compounds suggest the existence of a similar two-dimensional character. One of the most

attractive is  $\text{Mn}(\text{HCOO})_2 \cdot 2\text{H}_2\text{O}$ , a well-studied antiferromagnet with a Néel temperature at  $3.7^\circ\text{K}$ .

The structure of  $\text{Mn}(\text{HCOO})_2 \cdot 2\text{H}_2\text{O}$  has been determined by Osaki *et al.*<sup>2</sup> and an (010) projection is indicated in Fig. 1. The space group is  $P2_1/c$  with four molecules in the primitive cell, and the Mn atoms occupy two pairs of inequivalent positions. The two sets of sites ( $A$  and  $B$ ) are contained alternately in planes parallel to (100). An  $A$  site is coordinated through formate groups to four other  $A$  sites within a plane and

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<sup>1</sup> R. J. Birgeneau, H. J. Guggenheim, and G. Shirane, Phys. Rev. Letters 22, 720 (1969).

<sup>2</sup> K. Osaki, Y. Nakai, and T. Watanabe, J. Phys. Soc. Japan 19, 717 (1964).