Journal of Statistical Physics, Vol. 46, Nos. 1/2, 1987

The Direct Correlation Function of a One-Dimensional Ising Model

C. Borzi,[1] G. Ord,[1] and J. K. Percus[1,2]

Received July 15, 1986; revision received October 6, 1986

The strictly finite range of the direct correlation function for a homogeneous nearest neughbor Ising chain is shown to persist in the presence of arbitrary site-dependent coupling constants and an arbitrary external field. A method is developed to examine the range of the direct correlation function for many-neighbor interactions. It is found from numerical examples that, in general, third-neighbor and higher interactions induce long-range direct correlations, as does the presence of a field in the second-neighbor case.

KEY WORDS: Direct correlation function; one-dimensional Ising model; lattice gas.

1. INTRODUCTION

Among the various ultrasimplified models that have been investigated with a view toward understanding the structure of equilibrium statistical mechanics, the one-dimensional Ising model with nearest neighbor interaction stands out. It possesses a minimal number of degrees of freedom, can accept an arbitrary external field and remain solvable,[(1)] and serves as a fine test of approximation methods. If one had to choose a simple nontrivial property with respect to which it serves as an obvious prototype, this would probably be the strictly finite range of its associated direct correlation function. This is particularly significant because the direct correlation function, in addition to being a primary component of so many approximation methods, is also a primary tool for carrying out direct perturbation expansions.

[1] Courant Institute of Mathematical Sciences, New York University, New York, New York 10012.
[2] Department of Physics, New York University, New York, New York 10012.

The question naturally arises as to whether the nearest neighbor aspect, normally implicit in the term "Ising model," is responsible for the striking simplicity of the direct correlation, or whether it represents but one of a hierarchy of conditions leading to equally simple correlation structure. This question recently took on added significance when Robert[2] showed, using the short-cut best known through the work of Stephenson,[3] that the direct correlation was also of the interaction range for next nearest neighbor (NNN) interactions (with no external field). One possible conjecture at this level would be that with p^{th}-neighbor interaction, the direct correlation would have range p, but a moment's reflection shows that this cannot be: in the one-dimensional continuum limit—as the lattice spacing goes to zero—the direct correlation function does not have the range of the interaction[4] (e.g., with hard core plus square well interaction). A weaker conjecture, with some heuristic justification (the order of the minimal transfer matrix is 2^{p-1}; see Section 5), is that the range goes as 2^{p-1}, and the continuous counterexample would not hold in this case.

In this paper, we will investigate the above question in some detail, via a succession of models of various characteristics, developing effective computational tools as needed. Our conclusion, put briefly, is that the truncated range peculiar to the nearest neighbor model—remaining valid with quite substantial generalization—indeed holds for the field-free second-neighbor model, but does not generally hold for anything beyond this.

2. NEAREST NEIGHBOR INTERACTION

The theater of operations is best entered via the prototypical one-dimensional Ising model with nearest neighbor interaction alone, i.e., with Boltzmann factor

$$e^{-\beta\phi(\sigma_0,\sigma_1,\dots,\sigma_N)} = \prod_{i=1}^{N} e^{J\sigma_{i-1}\sigma_i} \tag{2.1}$$

corresponding to free-spin boundary conditions. J is the (negative) interaction strength in units of kT, and each $\sigma_i = \pm 1$. The corresponding partition function is

$$\Xi = \sum_{\{\sigma_i\}} e^{-\beta\phi} = \langle\omega|\, M^N \,|\omega\rangle \tag{2.2}$$

where

$$M = \begin{pmatrix} e^J & e^{-J} \\ e^{-J} & e^J \end{pmatrix}, \qquad \omega = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

In terms of standard Pauli spin matrices

$$M = e^J + e^{-J}\sigma_x, \qquad \sigma = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_z \tag{2.3}$$

We will also need the spin expectations

$$\langle \sigma_i \rangle = \langle \omega | \, M^i \sigma_z M^{N-i} \, | \omega \rangle / \Xi \tag{2.4}$$

and the pair spin expectation

$$\begin{aligned} \langle \sigma_i \sigma_j \rangle &= \langle \omega | \, M^i \sigma_z M^{j-i} \sigma_z M^{N-j} \, | \omega \rangle / \Xi, \qquad j \geqslant i \\ &= \langle \omega | \, M^i (\sigma_z M \sigma_z)^{j-i} \, M^{N-j} \, | \omega \rangle / \Xi \end{aligned} \tag{2.5}$$

where

$$\sigma_z M \sigma_z = e^J - e^{-J}\sigma_x$$

Since the eigenvalues of σ_x are ± 1 and, except in (2.4), which vanishes by parity, only functions of σ_x appear, computations are trivial: we simply use

$$f(\sigma_x) = \frac{1}{2}(1 + \sigma_x) f(1) + \frac{1}{2}(1 - \sigma_x) f(-1) \tag{2.6}$$

and find at once

$$\begin{aligned} \Xi &= 2(2 \cosh J)^N \\ \langle \sigma_i \rangle &= 0 \\ \langle \sigma_i \sigma_j \rangle &= (\tanh J)^{j-i}, \qquad j \geqslant i \end{aligned} \tag{2.7}$$

Our major interest will be in the spin–spin correlation function,

$$S_{ij} = \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle \tag{2.8}$$

and its reciprocal, the spin direct correlation,

$$C_{ij} = (S^{-1})_{ij} \tag{2.9}$$

(Since $\sigma = 2v - 1$, where v is the site occupation number, these differ by a factor of 4 from the lattice gas structure factor and direct correlation function.) In the present case, we have, and readily compute,

$$\begin{aligned} S_{ij} &= (\tanh J)^{|i-j|} \\ C_{ij} &= -\tfrac{1}{2} \sinh 2J \qquad && \text{for} \quad |i-j| = 1 \\ &= \cosh 2J && \text{for} \quad i = j \neq 0, N \\ &= \cosh^2 J && \text{for} \quad i = j = 0 \text{ or } N \\ &= 0 && \text{otherwise} \end{aligned} \tag{2.10}$$

Thus, the range of C_{ij} is 1, coinciding with the range of the force. If, on the other hand, one adopts periodic boundary conditions, $\sigma_N = \sigma_0$, the force is effectively of range N and the direct correlation is no longer of short range. It becomes so, however, as $N \to \infty$, in which case the expectations of (2.7) are impervious to boundary conditions, while

$$(\Xi_{pbc})^{1/N} = (\operatorname{Tr} M^N)^{1/N} = [(2\cosh J)^N + (2\sinh J)^N]^{1/N} \to \Xi^{1/N}$$

We will later take advantage of this fact, suitably extended.

3. GENERALIZATION

The short-range character of C is maintained even for site-dependent coupling, as is shown by a fairly straightforward argument. We locate each bond between two sites, $J_{i+1/2}$, and define the normalized transfer matrix

$$T_{i+1/2} = \frac{1}{2}\begin{pmatrix} e^{J_{i+1/2}} & e^{-J_{i+1/2}} \\ e^{-J_{i+1/2}} & e^{J_{i+1/2}} \end{pmatrix} = \frac{1}{2}\left(e^{J_{i+1/2}} + e^{-J_{i+1/2}}\sigma_x\right) \tag{3.1}$$

Since T reduces to a projection when $J = 0$, we can allow the system to become doubly infinite if $J_{i+1/2} \to 0$ as $|i| \to \infty$. The boundary conditions are then irrelevant, and we choose them as periodic. We now have [Ξ normalized to accord with (3.1)]

$$\begin{aligned} \Xi = \operatorname{Tr} \prod_j T_{j+1/2} &= \operatorname{Tr}\left[\frac{1}{2}(1+\sigma_x)\prod_j \cosh J_{j+1/2} \right. \\ &\qquad \left. + \frac{1}{2}(1-\sigma_x)\prod_j \sinh J_{j+1/2}\right] \\ &= \prod_j \cosh J_{j+1/2} \end{aligned} \tag{3.2}$$

Of course, $\langle \sigma_j \rangle = 0$, and since

$$\sigma_z T_{j+1/2} \sigma_z = \frac{1}{2}\left(e^{J_{j+1/2}} - e^{-J_{j+1/2}}\sigma_x\right)$$

then similarly, for $i < j$,

$$\begin{aligned} \Xi S(i,j) &= \operatorname{Tr}\left[\prod_{k<i} T_{k+1/2} \prod_{k=i}^{j-1} (\sigma_z T_{k+1/2} \sigma_z) \prod_{k>j} T_{k+1/2}\right] \\ &= \prod_{k<i} \cosh J_{k+1/2} \prod_{k=i}^{j-1} \sinh J_{k+1/2} \prod_{k>i} \cosh J_{k+1/2} \end{aligned} \tag{3.3}$$

or [clearly $S(i, i) = 1 - \langle \sigma_i \rangle^2 = 1$]

$$S(i, j) = \prod_{k=1}^{j-1} \tanh J_{k+1/2} \qquad \text{for} \quad i \leqslant j \tag{3.4}$$

It is convenient to define

$$K_j = \prod_{k<j} \tanh J_{k+1/2} \tag{3.5}$$

so that (3.4) translates to

$$S(i, j) = K_j / K_i \qquad \text{for} \quad i \leqslant j \tag{3.6}$$

Thus, the spin–spin direct correlation, defined via

$$\sum_k S(i, k)\, C(k, j) = \delta_{ij} \tag{3.7}$$

satisfies

$$\sum_{k>i} \frac{K_k}{K_i} C(k, j) + \sum_{k \leqslant i} \frac{K_i}{K_k} C(k, j) = \delta_{ij} \tag{3.8}$$

The solution of (3.8) is found, after a certain amount of algebra, to be

$$\begin{aligned} C(i, i) &= \left(\frac{K_{i+1}}{K_{i-1}} - \frac{K_{i-1}}{K_{i+1}} \right) \Bigg/ \left(\frac{K_i}{K_{i-1}} - \frac{K_{i-1}}{K_i} \right) \left(\frac{K_i}{K_{i+1}} - \frac{K_{i+1}}{K_i} \right) \\ C(i-1, i) &= \left(\frac{K_i}{K_{i-1}} - \frac{K_{i-1}}{K_i} \right)^{-1}, \quad C(i+1, i) = \left(\frac{K_{i+1}}{K_i} - \frac{K_i}{K_{i+1}} \right)^{-1} \\ C(i, j) &= 0 \qquad \text{for} \quad |i-j| > 1 \end{aligned} \tag{3.9}$$

Therefore, the short-range character of $C(i, j)$ is indeed maintained in the face of nonuniform coupling as well. Expressed in terms of the coupling, we have explicitly

$$\begin{aligned} C(i-1, i) &= -\frac{1}{2} \sinh(2J_{i-1/2}) \\ C(i, i) &= \frac{1}{2} \cosh(2J_{i-1/2}) + \frac{1}{2} \cosh(2J_{i+1/2}) \\ C(i+1, i) &= -\frac{1}{2} \sinh(2J_{i+1/2}) \end{aligned} \tag{3.10}$$

A further step can now be taken, and that is to introduce a nonuniform external potential u_j (in units of kT), in addition to the nonuniform coupling. We need as well the site transfer matrix

$$U_j = \begin{pmatrix} e^{-u_j} & 0 \\ 0 & e^{u_j} \end{pmatrix} \tag{3.11}$$

and will assume that $U_j \to I$ as $|j| \to \infty$. Since the left- and right-hand T's project onto the state ω of (2.2), we can write

$$\Xi = \frac{1}{2} \langle \omega | \prod_j U_j T_{j+1/2} | \omega \rangle \tag{3.12}$$

(a u_j limit other than I requires a sech u to accompany each factor). Although Ξ, $\bar{\sigma}(j) = \langle \sigma_j \rangle$, and $S(i, j)$ cannot be solved explicitly in terms of the u_j (with the $J_{j+1/2}$ fixed once and for all), the corresponding inverse problem, in which the $\bar{\sigma}(j)$ are given rather than the u_j, yields fairly easily. Given j, we define the 2×2 matrix

$$Q_j(\sigma, \sigma') = \frac{1}{2\Xi} \langle \omega | \prod_{k<j} (T_{k-1/2} U_k) | \sigma \rangle \langle \sigma' | \prod_{k>j} (U_k T_{k+1/2}) | \omega \rangle \tag{3.13}$$

where $\sigma, \sigma' = \pm 1$ and denote the associated unit vectors as well. Then, it is clear that

$$\begin{aligned}
&\sum_{\sigma,\sigma'} \langle \sigma | T_{j-1/2} U_j T_{j+1/2} | \sigma' \rangle \, Q_j(\sigma, \sigma') = 1 \\
&\sum_{\sigma,\sigma'} \langle \sigma | \sigma_z T_{j-1/2} U_j T_{j+1/2} | \sigma' \rangle \, Q_j(\sigma, \sigma') = \bar{\sigma}(j-1) \\
&\sum_{\sigma,\sigma'} \langle \sigma | T_{j-1/2} \sigma_z U_j T_{j+1/2} | \sigma' \rangle \, Q_j(\sigma, \sigma') = \bar{\sigma}(j) \\
&\sum_{\sigma,\sigma'} \langle \sigma | T_{j-1/2} U_j T_{j+1/2} \sigma_z | \sigma' \rangle \, Q_j(\sigma, \sigma') = \bar{\sigma}(j+1)
\end{aligned} \tag{3.14}$$

These four equations can now be solved in terms of $J_{j-1/2}$, u_j, $J_{j+1/2}$ to yield the four $Q(\sigma, \sigma')$ in the form

$$Q_j(\sigma, \sigma') = f_j^{\sigma\sigma'}(e_{j-1/2}, w_j, e_{j+1/2}, \bar{\sigma}(j-1), \bar{\sigma}(j), \bar{\sigma}(j+1)) \tag{3.15}$$

where

$$e_{j+1/2} = e^{J_{j+1/2}}, \qquad w_j = e^{-u_j}$$

But from the definition (3.13), $Q_j(\sigma, \sigma')$ is of rank 1, implying the relation

$$Q_j(1, 1) \, Q_j(-1, -1) = Q_j(1, -1) \, Q_j(-1, 1) \tag{3.16}$$

Substituting (3.15) into (3.16), we can solve in principle— and in practice—for u_j, in the form

$$u_j = g_j(e_{j-1/2}, e_{j+1/2}, \bar{\sigma}(j-1), \bar{\sigma}(j), \bar{\sigma}(j+1)) \tag{3.17}$$

Equation (3.17) suffices to establish the short range of the direct correlation $C(i, j)$. We recall that

$$\begin{aligned} \bar{\sigma}(i) &= -\partial \ln \Xi/\partial u_i \\ S(i, j) &= \partial^2 \ln \Xi/\partial u_i\, \partial u_j = -\partial\bar{\sigma}(i)/\partial u_j \end{aligned} \tag{3.18}$$

so that

$$C(i, j) = -\partial u_j/\partial\bar{\sigma}(i) \tag{3.19}$$

According to (3.17), then,

$$C(i, j) = 0 \qquad \text{when} \quad |i-j| > 1 \tag{3.20}$$

as desired.

4. NEXT NEAREST NEIGHBOR INTERACTIONS

We proceed next to interactions of range 2. It is convenient to specify the lattice sites as $-N,..., -1, 0, 1,..., N$, so that the field-free energy becomes

$$\beta\phi(\sigma_{-N},..., \sigma_N) = -J \sum_{1-N}^{N} \sigma_{j-1}\sigma_j - K \sum_{2-N}^{N} \sigma_{j-2}\sigma_j \tag{4.1}$$

Stephenson's transformation to new independent spin variables

$$\tau_j = \sigma_{j-1}\sigma_j, \qquad j = 1-N,..., N \tag{4.2}$$

lets σ_{-N} vary freely, yielding the partition function

$$\begin{aligned} \Xi &= 2 \sum_{\{\tau_j\}} \exp\left(J \sum_{1-N}^{N} \tau_j + K \sum_{2-N}^{N} \tau_{j-1}\tau_j\right) \\ &= 2 \sum_{\{\tau_j\}} \left[\exp\left(\frac{1}{2} J\tau_{1-N}\right)\right] T(\tau_{1-N}, \tau_{2-N}) \cdots T(\tau_{N-1}, \tau_N) \exp\left(\frac{1}{2} J\tau_N\right) \\ &= 2\langle\omega'|\, T^{2N-1}\, |\omega'\rangle \end{aligned} \tag{4.3}$$

where

$$T(\tau, \tau') = \exp\left[K\tau\tau' + \frac{1}{2} J(\tau + \tau')\right], \qquad \omega' = \begin{pmatrix} \exp(-j/2) \\ \exp(j/2) \end{pmatrix}$$

Similarly,

$$S(i, j)\,\Xi = \sum_{\{\tau_k\}} \sigma_i \sigma_j \exp\left(J \sum_{1-N}^{N} \tau_k + K \sum_{2-N}^{N} \tau_{k-1}\tau_k\right), \quad \text{for } i \leqslant j$$

$$= 2 \sum_{\{\tau_k\}} \tau_{i+1}\tau_{i+2} \cdots \tau_j \exp\left(J \sum_{1-N}^{N} \tau_k + K \sum_{2-N}^{N} \tau_{k-1}\tau_k\right)$$

$$= 2 \sum_{\{\tau_k\}} \left[\exp\left(\frac{1}{2} J\tau_{1-N}\right)\right] \tau_{i+1}$$

$$\times \cdots \tau_j T(\tau_{1-N}, \tau_{2-N}) \cdots T(\tau_{N-1}, \tau_N) \exp\left(\frac{1}{2} J\tau_N\right)$$

or

$$S(i, j)\,\Xi = 2\langle \omega' |\, T^{N-1+i} (T\tau)^{j-i}\, T^{N-j}\, |\omega'\rangle \tag{4.4}$$

where τ is the diagonal matrix τ_z.

Equation (4.4) can now be analyzed without using the detailed structure of T. Suppose that λ_0 and v_0 are the maximal eigenvalue and corresponding eigenvector of T. Then, since

$$(T/\lambda_0)^N \rightarrow |v_0\rangle\langle v_0| \tag{4.5}$$

for large N (in standard Dirac notation), we have from (4.3) and (4.4) in the thermodynamic limit $N \rightarrow \infty$,

$$S(i, j) = \langle v_0|\, (T\tau/\lambda_0)^{|j-i|}\, |v_0\rangle \tag{4.6}$$

To invert (4.6), we take the lattice Fourier transform

$$\tilde{S}(\theta) = \sum_j e^{ij\theta} S(0, j) \tag{4.7}$$

which works out to

$$\tilde{S}(\theta) = \langle v_0|\, \frac{\lambda_0/T\tau - T\tau/\lambda_0}{\lambda_0/T\tau + T\tau/\lambda_0 - 2\cos\theta}\, |v_0\rangle \tag{4.8}$$

Then, if λ_1 and λ_2 are the eigenvalues of $T\tau$, and P_1 and P_2 are the corresponding orthogonal projections, so that

$$T\tau = \lambda_1 P_1 + \lambda_2 P_2, \qquad I = P_1 + P_2 \tag{4.9}$$

then (4.8) becomes

$$\langle v_0|\, \frac{\lambda_0/\lambda_1 - \lambda_1/\lambda_0}{\lambda_0/\lambda_1 + \lambda_1/\lambda_0 - 2\cos\theta} P_1 + \frac{\lambda_0/\lambda_2 - \lambda_2/\lambda_0}{\lambda_0/\lambda_2 + \lambda_2/\lambda_0 - 2\cos\theta} P_2\, |v_0\rangle$$

or

$$\left(\frac{\lambda_0}{\lambda_1}+\frac{\lambda_1}{\lambda_0}-2\cos\theta\right)\left(\frac{\lambda_0}{\lambda_2}+\frac{\lambda_2}{\lambda_0}-2\cos\theta\right)\tilde{S}(\theta)$$

$$= \langle v_0|\left(\frac{\lambda_0}{\lambda_1}-\frac{\lambda_1}{\lambda_0}\right)\left(\frac{\lambda_0}{\lambda_2}+\frac{\lambda_2}{\lambda_0}-2\cos\theta\right)P_1 \tag{4.10}$$

$$+\left(\frac{\lambda_0}{\lambda_2}-\frac{\lambda_2}{\lambda_0}\right)\left(\frac{\lambda_0}{\lambda_1}+\frac{\lambda_1}{\lambda_0}-2\cos\theta\right)|v_0\rangle$$

The coefficient of $-2\cos\theta$ on the right is

$$\langle v_0|\left(\frac{\lambda_0}{\lambda_1}-\frac{\lambda_1}{\lambda_0}\right)P_1+\left(\frac{\lambda_0}{\lambda_2}-\frac{\lambda_2}{\lambda_0}\right)P_2\,|v_0\rangle$$

$$= \langle v_0|\frac{\lambda_0}{T\tau}-\frac{T\tau}{\lambda_0}|v_0\rangle$$

$$= \langle v_0|\,(T\tau)^{-1}\,T-T^{-1}T\tau\,|v_0\rangle=0$$

Setting

$$\Delta=\langle v_0|\,P_1-P_2\,|v_0\rangle \tag{4.11}$$

and using $P_1+P_2=I$, we conclude that

$$\tilde{C}(\theta)=\frac{1}{\tilde{S}(\theta)}=\frac{(\lambda_0/\lambda_1+\lambda_1/\lambda_0-2\cos\theta)(\lambda_0/\lambda_2+\lambda_2/\lambda_0-2\cos\theta)}{(\lambda_0^2/\lambda_1\lambda_2-\lambda_1\lambda_2/\lambda_0^2)+(\lambda_2/\lambda_1-\lambda_1/\lambda_2)\,\Delta} \tag{4.12}$$

containing at most second harmonics. In other words, $C(i, j)$ is of range 2.

On the other hand, the NNN model with an arbitrary external field is not expected to have a short-range direct correlation. To see this, we extend the analysis of (3.11)–(3.20) by first building up the full Boltzmann factor using internal interaction third-rank tensors $T(\sigma, \sigma', \sigma'')$ as well as external scalars $U(\sigma)$:

$$e^{-\beta\phi}=\prod_{i=-\infty}^{\infty} T_i(\sigma_{i-1}, \sigma_i, \sigma_{i+1})\,U_i(\sigma_i) \tag{4.13}$$

NNN interactions can certainly be encompassed—although not uniquely—in this fashion. At fixed j, we then isolate that part of the probability kernel that contains no functions of σ_{j-1}, σ_j, or σ_{j+1}, but for which $\sigma_{j-3}, \sigma_{j-2},..., \sigma_{j+3}$ are fixed:

$$Q_j(\sigma\sigma', \sigma''\sigma''')$$
$$= \frac{1}{\Xi} \sum_{\{\cdots \sigma_{j-4}, \sigma_{j+4}, \ldots\}} \left[\prod_{-\infty}^{j-6} (T_{i+1}(\sigma_i, \sigma_{i+1}, \sigma_{i+2})\, U_{i+1}(\sigma_{i+1})) \right.$$
$$\times T_{j-4}(\sigma_{j-5}, \sigma_{j-4}, \sigma)\, U_{j-4}(\sigma_{j-4})$$
$$\times T_{j-3}(\sigma_{j-4}, \sigma, \sigma')\, U_{j-3}(\sigma)\, U_{j-2}(\sigma')$$
$$\times U_{j+2}(\sigma'')\, U_{j+3}(\sigma''')\, T_{j+3}(\sigma''\sigma'''\sigma_{j+4})\, T_{j+4}(\sigma'''\sigma_{j+4}\sigma_{j+5})$$
$$\left. \times \prod_{j+4}^{\infty} (T_{i+1}(\sigma_i, \sigma_{i+1}, \sigma_{i+2})\, U_{i+1}(\sigma_{i+1})) \right] \tag{4.14}$$

Just as in (3.14), the eight quantities 1, $\bar{\sigma}(j-3)$, $\bar{\sigma}(j-2)$,..., $\bar{\sigma}(j+3)$ can then be expressed in terms of the 16 elements $Q_j(\sigma\sigma', \sigma''\sigma''')$ and the unknowns u_{j-1}, u_j, u_{j+1}. Since $Q_j(\sigma\sigma', \sigma''\sigma''')$ is again of rank 1, as a 4×4 matrix, only $2 \times 4 - 1 = 7$ of its 16 elements are independent. This, however, leaves $7 + 3 = 10$ unknowns and only eight equations. Thus, we cannot in general solve for u_j in terms of the $\bar{\sigma}(i)$ for $|i-j| \leqslant 3$, and the corresponding proof of the short range of $C(i, j)$, as in (3.17)–(3.20) does not go through.

To be sure, the lack of a proof does not constitute a disproof. But we can be much more explicit. Suppose the lattice has nearest neighbor coupling $-J$, next nearest neighbor $-K$, and a *constant* external potential u, with corresponding Boltzmann factors

$$e = e^{-u}, \qquad w = e^{J}, \qquad w' = e^{K} \tag{4.15}$$

Then the full Boltzmann factor can be written as the product of the third-rank factors

$$T(\sigma, \sigma', \sigma'') = e^{\sigma} w^{\sigma\sigma'} w'^{\sigma\sigma''} \tag{4.16}$$

However, it can also be written as a product of transfer matrices if, as suggested by (4.14), the indices correspond to successive pairs of spins, e.g., (4.16) is interpreted as the interaction of the pair (σ, σ') with the pair (σ', σ''), with a vanishing weight unless the second spin of the left pair equals the first spin of the right pair. Equation (4.16) hence translates to the 4×4 transfer matrix

$$T = \begin{array}{c} \\ ++ \\ +- \\ -- \\ -+ \end{array} \begin{pmatrix} ++ & +- & -- & -+ \\ eww' & ew/w' & 0 & 0 \\ 0 & 0 & e/ww' & ew'/w \\ 0 & 0 & ww'/e & w/ew' \\ 1/eww' & w'/ew & 0 & 0 \end{pmatrix} \tag{4.17}$$

and in this representation the spin σ, entered on the left, becomes simply

$$\sigma = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{4.18}$$

In the notation of (4.17) and (4.18), spin and pair spin averages proceed exactly as in the NN case. We assume periodic boundary conditions, subsequent to which the thermodynamic limit will be taken. Thus

$$\begin{aligned} \Xi &= \mathrm{Tr}\ T^N \\ \Xi\langle\sigma\rangle &= \mathrm{Tr}\ T^i\sigma T^{N-i} = \mathrm{Tr}\ T^N\sigma \\ i \leqslant j: \quad \Xi\langle\sigma(i)\,\sigma(j)\rangle &= \mathrm{Tr}\ T^i\sigma T^{j-i}\sigma T^{N-j} \\ &= \mathrm{Tr}\ T^{N-(j-i)}\sigma T^{j-i}\sigma \end{aligned} \tag{4.19}$$

If λ_0 is the maximum eigenvalue of T, with eigenvector v_0 and dual eigenvector $\hat{v}_0$, it follows as usual that

$$\begin{aligned} \langle\sigma\rangle &= \langle\hat{v}_0|\,\sigma\,|v_0\rangle \\ \langle\sigma(i)\,\sigma(j)\rangle &= \langle\hat{v}_0|\,\sigma(T/\lambda_0)^{|j-i|}\,\sigma\,|v_0\rangle \end{aligned} \tag{4.20}$$

In terms of the remaining eigenvalues λ_α, $\alpha = 1, 2, 3$, of T and corresponding eigenvectors v_α and dual eigenvectors $\hat{v}_\alpha$, we then have

$$\begin{aligned} S(i, j) &= \sum_{\alpha=0}^{3} \langle\hat{v}_0|\,\sigma\,|v_\alpha\rangle \left(\frac{\lambda_\alpha}{\lambda_0}\right)^{|j-i|} \langle\hat{v}_\alpha|\,\sigma\,|v_0\rangle \\ &\quad - \langle\hat{v}_0|\,\sigma\,|v_0\rangle\langle\hat{v}_0|\,\sigma\,|v_0\rangle \\ &= \sum_{\alpha=1}^{3} \langle\hat{v}_0|\,\sigma\,|v_\alpha\rangle \left(\frac{\lambda_\alpha}{\lambda_0}\right)^{|j-i|} \langle\hat{v}_\alpha|\,\sigma\,|v_0\rangle \end{aligned} \tag{4.21}$$

with Fourier transform

$$\tilde{S}(\theta) = \sum_{\alpha=1}^{3} \langle\hat{v}_0|\,\sigma\,|v_\alpha\rangle \frac{1-(\lambda_\alpha/\lambda_0)^2}{1+(\lambda_\alpha/\lambda_0)^2 - 2(\lambda_\alpha/\lambda_0)\cos\theta} \langle\hat{v}_\alpha|\,\sigma\,|v_0\rangle \tag{4.22}$$

Since the $\alpha = 0$ term in (4.22) would vanish, except at $\theta = 0$, we have as well

$$\tilde{S}(\theta) = \langle\hat{v}_0|\,\sigma \frac{1-(T/\lambda_0)^2}{1+(T/\lambda_0)^2 - 2(T/\lambda_0)\cos\theta}\,\sigma\,|v_0\rangle \tag{4.23}$$

or, alternatively,

$$\tilde{S}(\theta) = \langle \hat{v}_0 | \frac{1 - (\sigma T \sigma / \lambda_0)^2}{1 + (\sigma T \sigma / \lambda_0)^2 - 2(\sigma T \sigma / \lambda_0) \cos \theta} | v_0 \rangle \tag{4.24}$$

Inversion to find $\tilde{C}(\theta)$ is now tedious but straightforward, in version (4.22), (4.23), or (4.24). Using (4.24), for example, we expand out in a power series in $\cos \theta$:

$$\tilde{S}(\theta) = \sum_{j=0}^{\infty} \langle \hat{v}_0 | \frac{1 - (\sigma T \sigma / \lambda_0)^2}{1 + (\sigma T \sigma / \lambda_0)^2} \left[\frac{2 \sigma T \sigma / \lambda_0}{1 + (\sigma T \sigma / \lambda_0)^2} \right]^j | v_0 \rangle (\cos \theta)^j \tag{4.25}$$

and compute $\tilde{C}(\theta) = 1/\tilde{S}(\theta)$ numerically as a power series in $\cos \theta$. If $C(i, j)$ is of range r, $\tilde{C}(\theta)$ will be a polynomial of degree r in $\cos \theta$, and to check this, one only needs to retain powers in (4.25) substantially larger than r in number. Doing so with various examples of (4.17), one finds indeed that the next-nearest neighbor interaction, with constant external field, does not in general have a truncated direct correlation. See Fig. 1 for a typical result: c has a distinct oscillating tail.

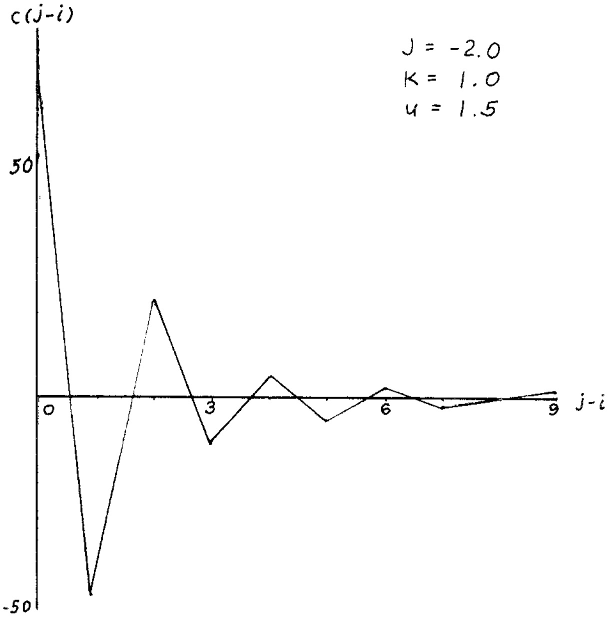

Fig. 1. Direct correlation function for parameters $J = -2.0$, $K = 1.0$, $u = 1.5$.

5. LONGER RANGE INTERACTION

The situation simplifies, in a sense, when one has third-neighbor interactions or higher. Now it is no longer necessary to apply an external field to break the short range of the direct correlation. This is demonstrated by extending the formalism of (4.17)–(4.25) in the obvious way, necessitating $2^p \times 2^p$ matrices for interactions of range p. In fact, it is helpful to process the formalism a bit to recover the reduced pattern of (4.8), either by extending the Stephenson approach or more directly, as follows.

To start, we choose the transfer matrix between successive p-tuplets of sites, so that just two elements in each row or column are nonvanishing. Then the 2^p-dimensional index space of $(\sigma_1,..., \sigma_p)$ configurations is ordered by having the first 2^{p-1} indices allocated to $\sigma_1 = +1$, with any allocation of the remaining species; the second block of 2^{p-1} indices is obtained by reversing all spins of the corresponding first-block entries. For the Boltzmann factor in $T(\sigma_1,..., \sigma_p; \sigma'_1,..., \sigma'_p)$ we may choose the interaction energy of σ_1 alone with all σ'_j. It is readily seen that in the absence of an external field, T and σ (the left spin insertion) take the compartmental form

$$T = \begin{pmatrix} A & B \\ B & A \end{pmatrix}, \qquad \sigma = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \tag{5.1}$$

where A and B have no nonvanishing rows in common. Now only T and $\sigma T \sigma$ appear in the ensuing computation, and both have the spaces $\{(\substack{u \\ u})\}$ and $\{(\substack{u \\ -u})\}$ as invariant subspaces,

$$\begin{aligned} T\binom{u}{u} &= \begin{pmatrix} (A+B)\,u \\ (A+B)\,u \end{pmatrix}, & T\binom{u}{-u} &= \begin{pmatrix} (A-B)\,u \\ -(A-B)\,u \end{pmatrix} \\ \sigma T \sigma\binom{u}{u} &= \begin{pmatrix} (A-B)\,u \\ (A-B)\,u \end{pmatrix}, & \sigma T \sigma\binom{u}{-u} &= \begin{pmatrix} (A+B)\,u \\ -(A+B)\,u \end{pmatrix} \end{aligned} \tag{5.2}$$

Hence

$$\operatorname{Tr} f(T, \sigma T \sigma) = \operatorname{Tr} f(A+B, A-B) + \operatorname{Tr} f(A-B, A+B) \tag{5.3}$$

But only expressions of the form $\operatorname{Tr} T^a(\sigma T \sigma)^b$ occur, and of course $\operatorname{Tr} T^a(\sigma T \sigma)^b = \operatorname{Tr}(\sigma T \sigma)^a T^b$, so that

$$\operatorname{Tr} T^a(\sigma T \sigma)^b = 2 \operatorname{Tr}(A+B)^a (A-B)^b \tag{5.4}$$

Finally, since A and B have no nonvanishing row in common, we can write

$$A - B = \tau(A+B) \tag{5.5}$$

for a suitable spin matrix (diagonal, with ± 1's) τ. We conclude that

$$\operatorname{Tr} T^a(\sigma T\sigma)^b = 2 \operatorname{Tr} T'^a(\tau T')^b \tag{5.6}$$

where $T' = A + B$ and τ are $2^{p-1} \times 2^{p-1}$ matrices.

Equation (4.24) can now be taken over directly:

$$\tilde{S}(\theta) = \langle \hat{v}_0 | \frac{1 - (\tau T'/\lambda_0)^2}{1 + (\tau T'/\lambda_0)^2 - 2(\tau T'/\lambda_0)\cos\theta} | v_0 \rangle \tag{5.7}$$

and analyzed similarly as a function of $\cos\theta$. If p is not too large, little subtlety is required. We rewrite (5.7) as

$$\tilde{S}(\theta) = \frac{\langle \hat{v}_0 | \left[1 - (\tau T'/\lambda_0)^2\right] \operatorname{Adj}\left[(1 + \tau T'/\lambda_0)^2 - 2(\tau T'/\lambda_0)\cos\theta\right] | v_0 \rangle}{\operatorname{Det}\left[1 + (\tau T'/\lambda_0)^2 - 2(\tau T'/\lambda_0)\cos\theta\right]}$$

$$= \frac{P_{2^{p-1}-1}(\cos\theta)}{Q_{2^{p-1}}(\cos\theta)} \tag{5.8}$$

a ratio of polynomials of indicated degree in $\cos\theta$. Here Adj A stands for the matrix of cofactors of A. We then ask whether

$$\tilde{C}(\theta) = Q_{2^{p-1}}(\cos\theta)/P_{2^{p-1}-1}(\cos\theta)$$

is also a polynomial, which in principle could be of degree 2^{p-1}. In any event, $\tilde{C}(\theta)$ and hence $C(j-i)$ to any required degree of accuracy are readily computed, resulting in the aforementioned conclusion that field-free Ising lattices with longer than NNN interaction do not in general have short-range direct correlation. See Fig. 2 for a typical example: here c has an exponential tail, which, however, decays very rapidly.

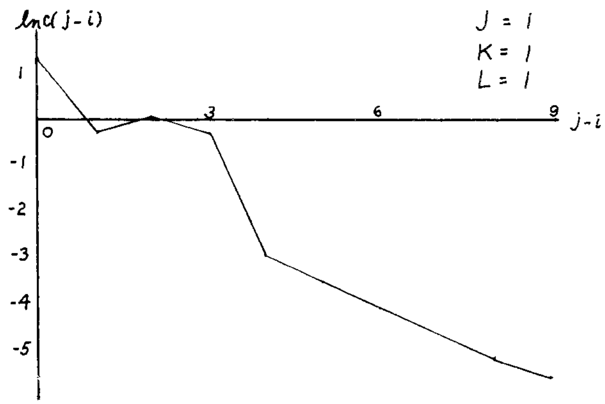

Fig. 2. Direct correlation function for parameters $J = 1.0$, $K = 1.0$, $L = 1.0$.

An obvious question in the context of this survey is whether there are special longer range interactions for which the $C(i, j)$ are short range. At least three possibilities exist. The first is that in which the range is extended, but only a few of the interactions are nonvanishing. If matters are so arranged that the lattice Λ breaks up into noninteracting sublattices $\{\Lambda_\alpha\}$, each with short-range interaction, then matters simplify dramatically: sites from distinct sublattices are then independent—a trivial observation—

$$S(\alpha i, \beta j) = \delta_{\alpha\beta} S_\alpha(i, j) \tag{5.9}$$

and correspondingly

$$C(\alpha i, \beta j) = \delta_{\alpha\beta} S_\alpha^{-1}(i, j) \tag{5.10}$$

Thus pure second-neighbor interaction with an arbitrary external field has short range C, as does second- plus fourth-neighbor interaction in the absence of an external field.

Are there nondecomposing interaction patterns for which C is short range? There are certainly hints from (5.8) that special cases of this type exist, but they have not yet been categorized. But several periodically nonhomogeneous special cases with finite range C have been found and will be reported in due course; they typically involve interacting clusters of sites.

A third category is that of interactions that are strictly hard core exclusion, of any range. Here, it is easy to show by other methods[5] that the direct correlation has precisely the range of the core, and in the presence of an arbitrary external field. Indeed, the hard core makes sense only in the context of a lattice gas, rather than a spin model, and so even the field-free lattice gas maps into an Ising model with constant external field.

6. CONCLUSION

We have seen that the strictly finite-range direct correlation function, a striking aspect of the nearest neighbor Ising model, extends to a few more or less obvious longer range interaction cases, but not beyond. Thus, it does not mimic in a consistent way the short range of the interaction, as Ornstein and Zernike hoped it would. There are of course other ways of satisfying the primitive result, the set–set direct correlation function of Green[6] being one that has not been extensively investigated. It is also true that other modes of extension, e.g., to Bethe lattices, are called for, and in fact it has been shown[7] that the finite range of C for hard cores in an arbitrary external field—for Ising lattices—extends to this wider domain. It certainly is not known whether analogous results obtain for any true higher dimensional lattice. Thus, there is still work to be done at the categorization level before proceeding to deeper and more incisive descriptions of the microscopic correlation structure of lattices.

ACKNOWLEDGMENTS

This work was supported in part by NSF grant CHE-823-05238 and DOE contract DE-ACO2-76ERO3077.

REFERENCES

1. J. K. Percus, *J. Stat. Phys.* **15**:505 (1976).
2. M. Robert, *Phys. Rev. A* **29**:2856 (1984); **33**:2825 (1985).
3. J. Stephenson, *Can. J. Phys.* **48**:1724 (1970).
4. J. L. Lebowitz, J. K. Percus, and I. J. Zucker, *Bull. Am. Phys. Soc.* **7**:415 (1962).
5. A. Robledo, *J. Chem. Phys.* **72**:1701 (1980).
6. M. S. Green, *J. Math. Phys.* **9**:875 (1968).
7. J. K. Percus and A. Robledo, to be published.