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Crystal Statistics. III. Short-Range Order in a Binary Ising Lattice

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The degree of order in a binary lattice is described in terms of a family of "correlation" functions. The correlation function for two given lattice sites states what is the probability that the spins of the two sites are the same; this probability is, of course, a function of temperature, as well as of the distance and orientation of the atoms in the pair. It is shown that each correlation function is given by the trace of a corresponding 2^n-dimensional matrix. To evaluate this trace, we make use of the apparatus of spinor analysis, which was employed in a previous paper to evaluate the partition function for the lattice. The trace is found in terms of certain functions of temperature, Σ_a, and these are then calculated with the aid of an elliptic substitution.

Correlations for the five shortest distances (without restriction as to the orientation of the pair within the plane) are plotted as functions of temperature. In addition, the correlation for sites lying within the same row is given to any distance. For the critical temperature this correlation is plotted as a function of distance. It is shown that the correlation tends to zero as the distance increases, that is to say: there is no long-range order at the critical temperature.

1. DEFINITION OF THE DEGREE OF ORDER

THE "degree of order" in a crystal composed of several kinds of atoms is an observable, as is shown by x-ray diffraction studies.[1] Several attempts[2] have been made to interpret the degree of order quantitatively, so that a functional dependence of order upon temperature could be stated. In this paper we use a statistical approach to find the average, taken over all configurations of the crystal, of the correlation between a pair of atoms within the crystal. This correlation will be a function of the temperature, and will depend on the relative position of the atoms in the pair. Since only relative positions enter here, we may keep one of the atoms fixed and consider the family of correlation curves for all pairs in which our fixed atom is a member. This family of curves will describe the degree of order within the crystal.

In order to define, and evaluate, the correlation functions in a formal way, we must rely upon the results of previous papers, I and II;[3] we will make use of the spinor-analysis method introduced in II.

The model we use is, as in the previous papers, a two-dimensional rectangular lattice, with a spin variable $\mu=\pm 1$ at each lattice site. It is assumed that only nearest neighbors interact, and that at zero temperature the perfectly ordered crystal has all its spins aligned in one direction (either $\mu=+1$ for all lattice sites, or $\mu=-1$ for all sites). It has been shown[4] that all the information about probabilities of configurations could be presented in a compact way with the help of a matrix **V** having 2^n rows and columns, such that for example the partition function for the lattice becomes

$$Z=\sum_{\substack{\text{all}\\ \text{configurations}}}(\text{probability of configuration})$$

$$=\sum_{1,2,\cdots}\mathbf{V}_{\nu_1\nu_2}\mathbf{V}_{\nu_2\nu_3}\cdots\mathbf{V}_{\nu_m\nu_1}=\operatorname{trace}\mathbf{V}^m. \quad \text{(II. 3)}$$

Here ν_i is the configuration of the ith row, that is to say, the specification of the values of μ for all the n atoms in this row ($1\leqslant\nu_i\leqslant 2^n$ for all $1\leqslant i\leqslant m$).

Using the matrix **V**, we can also write the average values of various functions of the configurations of the lattice. Such functions must be weighted in each configuration by the probability of the configuration, and so we find that the average of the function $f_{\nu_1\nu_2\ldots}$ is

$$\bar{f}=\frac{1}{Z}\sum_{\nu_1,\nu_2,\cdots}f_{\nu_1\nu_2\ldots}\mathbf{V}_{\nu_1\nu_2}\mathbf{V}_{\nu_2\nu_3}\cdots\mathbf{V}_{\nu_m\nu_1}. \quad (1)$$

The Correlation Functions

The spin of the jth site in any given row (say row k) is clearly a function of the configuration of the lattice. It depends only on the configuration of its own row, i.e., on ν_k. And it is easy to see that as ν_k goes through its range of values ($1\leqslant\nu_k\leqslant 2^n$), the spin under consideration takes on the values $+1$ or -1 in a particular order, which is the order of the diagonal elements in the (diagonal) matrix $\mathbf{s}_j\equiv 1\times 1\times\cdots\times\mathbf{s}\times 1\times 1\cdots$ (n factors). (The notation is as in I:

$$1\equiv\begin{pmatrix}1&0\\0&1\end{pmatrix},\quad \mathbf{s}\equiv\begin{pmatrix}1&0\\0&-1\end{pmatrix},\quad \mathbf{C}\equiv\begin{pmatrix}0&1\\1&0\end{pmatrix}$$

are the Pauli matrices; $\times$ stands for direct product of

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[1] G. C. Nix and W. Shockley, Rev. of Mod. Phys. **10**, 1 (1938).

[2] W. L. Bragg and E. J. Williams, Proc. Roy. Soc. London **145A'** 699 (1934); **151A**, 540 (1935); **152A**, 231 (1935). H. A. Bethe, Proc. Roy. Soc. **150A**, 552 (1935).

[3] L. Onsager, Phys. Rev. **65**, 117 (1943) will be referred to as I. B. Kaufman, Phys. Rev. **76**, 1232 (1949) (preceding paper) will be referred to as II.

[4] H. A. Kramers and G. H. Wannier, Phys. Rev. **60**, 252, 263 (1941); E. N. Lassettre and J. P. Howe, J. Chem. Phys. **9**, 747 (1941).

matrices). As an example, consider the simple case $n=2$. ν_k has $2^2=4$ possibilities: $++$, $+-$, $-+$, $--$. Correspondingly, the spin of the left-hand site is: $+1$, $+1$, -1, -1. But these are the diagonal elements (in that order) of $\mathbf{s}\times\mathbf{1}$. The spin of the right-hand site is: $+1$, -1, $+1$, -1, which can be read off the diagonal of the matrix $\mathbf{1}\times\mathbf{s}$. In general the spin of the jth site in the kth row, when the crystal is in configuration $\{\nu_1, \nu_2, \cdots, \nu_m\}$, is $(\mathbf{s}_j)_{\nu_k\nu_k}$.

We can now find the average value of this spin:

$$\begin{aligned}\bar{s}_j&=1/Z \sum_{\nu_1,\nu_2,\cdots} (\mathbf{s}_j)_{\nu_k\nu_k}\mathbf{V}_{\nu_1\nu_2}\mathbf{V}_{\nu_2\nu_3}\cdots\\ &\qquad\times\mathbf{V}_{\nu_{k-1}\nu_k}\mathbf{V}_{\nu_k\nu_{k+1}}\cdots\mathbf{V}_{\nu_m\nu_1}\\ &=1/Z \sum_{\nu_1,\nu_2,\cdots} \mathbf{V}_{\nu_1,\nu_2}\mathbf{V}_{\nu_2\nu_3}\cdots\\ &\qquad\times\mathbf{V}_{\nu_{i-1}\nu_1}(\mathbf{s}_j)_{\nu_k\nu_k}\mathbf{V}_{\nu_k\nu_{k+1}}\cdots\mathbf{V}_{\nu_m\nu_1}\\ &=1/Z\cdot\operatorname{trace}\{\mathbf{V}^{k-1}\mathbf{s}_j\mathbf{V}^{m-k+1}\}.\end{aligned}\tag{2}$$

Since the trace is invariant with respect to cyclic changes in the order of factors we have

$$\bar{s}_j=(1/Z)\operatorname{trace}(\mathbf{s}_j\mathbf{V}^m).\tag{3}$$

This result is independent of k, as it should be. It will be seen later that $\bar{s}_j$ vanishes identically for every j, and this is not surprising because *a priori* every site has the same probability of being occupied by a positive spin as by a negative one, at all temperatures.

The situation is different for the correlation between two sites. Consider the product of the spins of site k in row j and site b in row a. The average of this product will be:

$$\begin{aligned}\langle s_{jk}s_{ab}\rangle_{\mathsf{Av}}&=(1/Z)\sum_{\nu_1,\nu_2,\cdots}\mathbf{V}_{\nu_1\nu_2}\cdots\mathbf{V}_{\nu_{j-1}\nu_j}(\mathbf{s}_k)_{\nu_j\nu_j}\mathbf{V}_{\nu_j\nu_{j+1}}\cdots\\ &\qquad\times\mathbf{V}_{\nu_{a-1}\nu_a}(\mathbf{s}_b)_{\nu_a\nu_a}\mathbf{V}_{\nu_a\nu_{a+1}}\cdots\\ &=(1/Z)\operatorname{trace}\{\mathbf{V}^{j-1}\mathbf{s}_k\mathbf{V}^{a-j}\mathbf{s}_b\mathbf{V}^{m-a+1}\}\\ &=(1/Z)\operatorname{trace}\{\mathbf{s}_k\mathbf{V}^{a-j}\mathbf{s}_a\mathbf{V}^{m-a+j}\}.\end{aligned}\tag{4}$$

This average value will not vanish. At zero temperature, all spins are aligned, so that $(\mathbf{s}_k)_{\nu_j\nu_j}=(\mathbf{s}_b)_{\nu_a\nu_a}=+1$ and therefore $(\mathbf{s}_k)_{\nu_j\nu_j}(\mathbf{s}_b)_{\nu_a\nu_a}=+1$. As a result

$$\langle s_{jk}s_{ab}\rangle_{\mathsf{Av}}=1/Z\cdot Z=+1$$

for all pairs of sites. This is the state of perfect order. At higher temperatures $\langle s_{jk}s_{ab}\rangle_{\mathsf{Av}}$ decreases, and tends to zero for very high T.

We will refer to $\langle s_{jk}s_{ab}\rangle_{\mathsf{Av}}$ as the *correlation* between the two sites (j, k) and (a, b), and will take the set of all these functions to be a measure of the degree of order within the crystal. Short-range order is described by the correlations for finite (small) distances between the sites. Long-range order is the limit for great distances, and will be discussed in Part IV.

In what follows, we will show how to evaluate the correlations as functions of temperature for successive distances between pairs of sites. Part of the work in the evaluation of these averages is algebraic: it is necessary to find the trace of the appropriate matrices, as given in (4). This will be simple for $a-j=0, 1$. For larger distances between rows the procedure, while still straightforward, is quite tedious. The algebraic work will give the correlation in terms of sums of the form

$$\frac{1}{n}\sum_{s=1}^{n}\cos(a(s\pi/n)+\delta_s')\equiv\Sigma_a\quad(a=0, 1, 2, \cdots).$$

These sums are then evaluated (with the help of an elliptic substitution) for the case of a quadratic crystal: $H=H'$. A particularly simple result obtains at the critical temperature, where $\Sigma_a\sim[-2/\pi(2a-1)]$. The value of $\langle s_{1,1}s_{1,k}\rangle_{\mathsf{Av}}\equiv\langle s_1s_k\rangle_{\mathsf{Av}}$ can then be computed to any desired distance. It is found that

$$\lim_{k\to\infty}\langle s_1s_k\rangle_{\mathsf{Av}}=0,$$

but this limit is approached very slowly.

2. PROCEDURE FOR EVALUATING AVERAGES

In our basic Eq. (4) we will employ an approximation: we will neglect all eigenvalues of $\mathbf{V}$ as compared with the largest one, when the power of the eigenvalues is high enough. (This approximation was justified in II, in the discussion of the partition function.) In order to make use of the approximation we transform (4) by $\mathbf{\Psi}$, which brings $\mathbf{V}$ to its diagonal form:

$$\langle s_{1,1}s_{1+a,b}\rangle_{\mathsf{Av}}=\left\{\sum_{i=1}^{2^n}\lambda_i^m\right\}^{-1}\cdot\left\{\sum_{i=1}^{2^n}\lambda_i^{m-a}\cdot(\mathbf{\Psi}\mathbf{s}_1\mathbf{V}^a\mathbf{s}_b\mathbf{\Psi}^{-1})_{ii}\right\}.\tag{5}$$

It was shown (see I.101) that for $T>T_c$ the largest eigenvalue, $\lambda_{\max}=\exp\{\frac{1}{2}(\gamma_1+\cdots+\gamma_{2n-1})\}$ is non-degenerate. On the other hand, for $T<T_c$ there is a twofold degeneracy:

$$\lambda^+{}_{\max}\simeq\lambda^-{}_{\max}=\exp\{\tfrac{1}{2}(\gamma_0+\cdots+\gamma_{2n-2})\}.$$

If we write, for both cases, $\lambda^+{}_{\max}\equiv\lambda$, we have above the critical temperature

$$\langle s_{1,1}s_{1+a,b}\rangle_{\mathsf{Av}}\simeq\lambda^{-a}\{\mathbf{\Psi}_+\mathbf{s}_1\mathbf{V}^a\mathbf{s}_b\mathbf{\Psi}_+{}^{-1}\}_{11},\tag{6}$$

and below the critical temperature

$$\begin{aligned}\langle s_{1,1}s_{1+a,b}\rangle_{\mathsf{Av}}\simeq\tfrac{1}{2}\lambda^{-a}[&\{\mathbf{\Psi}_+\mathbf{s}_1\mathbf{V}^a\mathbf{s}_b\mathbf{\Psi}_+{}^{-1}\}_{11}\\ &+\{\mathbf{\Psi}_-\mathbf{s}_1\mathbf{V}^a\mathbf{s}_b\mathbf{\Psi}_-{}^{-1}\}_{11}].\end{aligned}\tag{7}$$

$\mathbf{\Psi}_+$ and $\mathbf{\Psi}_-$ differ only in that $\mathbf{\Psi}_+$ involves the even-indexed angles $\omega_{2r}=(2r\pi/n)$ and δ_{2r}', while $\mathbf{\Psi}_-$ contains the odd-indexed ones. For simplicity of notation, we will no longer differentiate between odd- and even-indexed angles, but will use the neutral index t, which is to take on the values $2r$ or $2r-1$ as needed for the evaluation

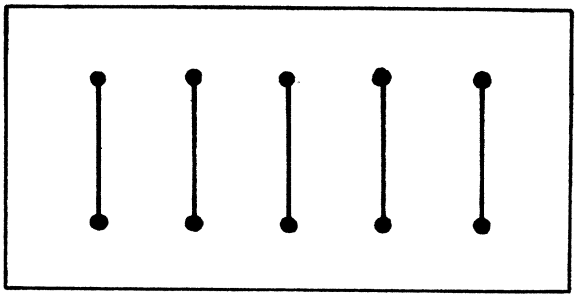

FIG. 1. Correlation of nearest neighbors in adjacent rows.

of the averages (6) and (7). Later on it will be seen that for large n, m both terms in (7) are equal, so that (6) may be used at *all* temperatures.

The quantity $\mathbf{\Psi}$ is completely known in terms of the rotation which it induces in the spinor base $\mathbf{P}_1$, $\mathbf{Q}_1$, $\mathbf{P}_2$, $\cdots$, $\mathbf{P}_n$, $\mathbf{Q}_n$. We had

$$\mathbf{\Psi}=\mathbf{g}\cdot\mathbf{S}(\mathbf{TH}), \qquad \text{(II. 62, 69)}$$

where

$$\begin{aligned}\mathbf{H}:\quad &\mathbf{P}_r\to\cosh H^*\cdot\mathbf{P}_r-i\sinh H^*\cdot\mathbf{Q}_r\\ &\qquad\qquad\qquad\qquad\qquad (1\leqslant r\leqslant n),\\ &\mathbf{Q}_r\to i\sinh H^*\cdot\mathbf{P}_r+\cosh H^*\cdot\mathbf{Q}_r \qquad \text{(II. 63)}\end{aligned}$$

$$\begin{aligned}\mathbf{T}:\quad &\mathbf{P}_a\to\sum_{r=1}^{n}\sigma_{ra}\mathbf{P}_r+\sum_{r=1}^{n}\tau_{ra}\mathbf{Q}_r\\ &\qquad\qquad\qquad\qquad (1\leqslant a\leqslant n), \qquad \text{(II. 57)}\\ &\mathbf{Q}_a\to\sum_{r=1}^{n}\sigma_{ra}'\mathbf{P}_r+\sum_{r=1}^{n}\tau_{ra}'\mathbf{Q}_r\end{aligned}$$

with

$$\begin{aligned}\sigma_{ra}&=\frac{1}{n^{\frac{1}{2}}}\cos\left(\frac{ta\pi}{n}+\tfrac{1}{2}\delta_t'\right),\\ \tau_{ra}&=\frac{-1}{n^{\frac{1}{2}}}\sin\left(\frac{ta\pi}{n}+\tfrac{1}{2}\delta_t'\right),\\ \sigma_{ra}'&=\frac{1}{n^{\frac{1}{2}}}\sin\left(\frac{ta\pi}{n}-\tfrac{1}{2}\delta_t'\right),\\ \tau_{ra}'&=\frac{-1}{n^{\frac{1}{2}}}\cos\left(\frac{ta\pi}{n}-\tfrac{1}{2}\delta_t'\right).\end{aligned} \qquad \text{(II. 58)}$$

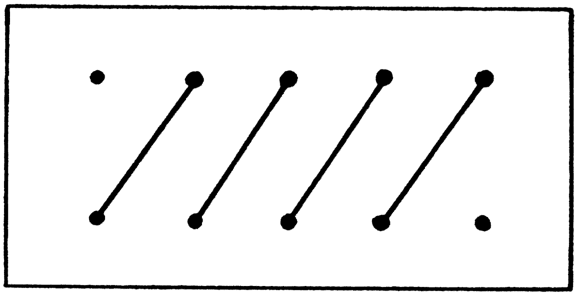

FIG. 2. Correlation of next-nearest neighbors.

(t is $2r$ or $2r-1$, as explained above). Finally

$$\mathbf{g}=\mathbf{g}^{-1}=2^{-n}\cdot\begin{pmatrix}1&1\\1&-1\end{pmatrix}\times\begin{pmatrix}1&1\\1&-1\end{pmatrix}\times\cdots \quad (n\text{ factors}), \qquad \text{(II. 16)}$$

and $\mathbf{g}$ has the property that $\mathbf{g}\mathbf{s}_r\mathbf{g}=\mathbf{C}_r$, $\mathbf{g}\mathbf{C}_r\mathbf{g}=\mathbf{s}_r$.

Since $\mathbf{S}(\mathbf{T})$ is a complicated matrix we do not give its components, and so we cannot write $\mathbf{\Psi}$ explicitly. Nevertheless, it will be seen that the $\{\ \}_{11}$ member of matrices transformed by $\mathbf{\Psi}$ can be found without much difficulty if we study the effect of the successive operations: $\mathbf{S}(\mathbf{H})$, $\mathbf{S}(\mathbf{T})$ and $\mathbf{g}$ on $(\mathbf{s}_1\mathbf{V}^a\mathbf{s}_b)$.

3. AVERAGES FOR 2-SPINOR MATRICES

Consider first $a=0$, $b=2$. We have then $\mathbf{s}_1\mathbf{V}^a\mathbf{s}_b=\mathbf{s}_2\mathbf{s}_1=-i\mathbf{P}_2\mathbf{Q}_1$. The average of this quantity will give us the correlation between two neighbors in a row. However, it is useful for the following problems to treat the more general 2-spinor quantities $\mathbf{X}=\mathbf{P}_k\mathbf{P}_l$, $\mathbf{P}_k\mathbf{Q}_l$, or $\mathbf{Q}_k\mathbf{Q}_l$. We will therefore investigate $\{\mathbf{g}\cdot\mathbf{S}(\mathbf{TH})\cdot\mathbf{X}\cdot\mathbf{S}(\mathbf{TH})^{-1}\mathbf{g}\}_{11}$, where $\mathbf{X}$ is a 2nd rank spinor. Clearly, transformation by $\mathbf{S}(\mathbf{TH})$ will send $\mathbf{X}$ into a linear combination of 2-spinor quantities. These are still to be transformed by $\mathbf{g}$, and the $\{\ \}_{11}$ member has to be taken. However, we know that the only matrices which have diagonal elements are the matrices $\mathbf{s}_r$ (or their products, which, as we shall see, do not enter here). Therefore, $\{\ \}_{11}=0$ unless the bracketed quantity is a product of $\mathbf{s}_r$ matrices. But this means that before transformation by $\mathbf{g}$ the bracketed quantity was a product of $\mathbf{C}_r$ matrices. Now $\mathbf{C}_r=i\mathbf{P}_r\mathbf{Q}_r$ is already a 2-spinor quantity so that no products of $\mathbf{C}_r$ matrices appear. We thus have the following result: In the transform of $\mathbf{X}$ by $\mathbf{S}(\mathbf{TH})$ only the terms of the form $\mathbf{P}_r\mathbf{Q}_r$ will contribute to the average.

Up to now we have not yet made use of the special properties of the rotation $\mathbf{T}$. These will lead to further simplifications. Choose for example $\mathbf{X}=\mathbf{P}_k\mathbf{Q}_l$. By (II. 63), cited above,

$$\begin{aligned}\mathbf{H}:\quad \mathbf{P}_k\mathbf{Q}_l\to\cosh^2H^*\mathbf{P}_k\mathbf{Q}_l&+i\cosh H^*\\ \times\sinh H^*(\mathbf{P}_k\mathbf{P}_l-\mathbf{Q}_k\mathbf{Q}_l)&-\sinh^2H^*\mathbf{P}_l\mathbf{Q}_k\\ &=\mathbf{S}(\mathbf{H})\cdot\mathbf{P}_k\mathbf{Q}_l\cdot\mathbf{S}(\mathbf{H})^{-1}. \qquad (8)\end{aligned}$$

This linear combination must now be transformed by $\mathbf{S}(\mathbf{T})$. Consider the term $\mathbf{P}_k\mathbf{P}_l$.

$$\mathbf{T}:\quad \mathbf{P}_k\mathbf{P}_l\to\sum_{r=1}^{n}\begin{vmatrix}\sigma_{rk}&\tau_{rk}\\ \sigma_{rl}&\tau_{rl}\end{vmatrix}\cdot\mathbf{P}_r\mathbf{Q}_r+\text{other terms.} \qquad (9)$$

The "other terms" are of the form $\mathbf{P}_r\mathbf{P}_s$ or $\mathbf{Q}_r\mathbf{Q}_s$ or $\mathbf{P}_r\mathbf{Q}_s$, and we have seen above that they will not contribute to the average. Now we put in the values of σ_{rk} etc., from (II. 58), and we get:

$$\mathbf{T}:\quad \mathbf{P}_k\mathbf{P}_l\to\frac{1}{n}\sum_{r=1}^{n}\sin(k-l)\frac{t\pi}{n}\cdot\mathbf{P}_r\mathbf{Q}_r+\text{other terms.}$$

Therefore

$$\mathbf{g}\cdot\mathbf{S}(\mathbf{T})\cdot\mathbf{P}_k\mathbf{P}_l\cdot\mathbf{S}(\mathbf{T})^{-1}\cdot\mathbf{g}$$

$$=\frac{i}{n}\sum_{r=1}^{n}\sin(k-l)\frac{t\pi}{n}\cdot(\mathbf{s}_r)+\text{other terms.}$$

Finally, we have to take the $\{\ \}_{11}$ member of this matrix. But $\{\mathbf{s}_r\}_{11}=1$ for all r, so that

$$\{\mathbf{g}\cdot\mathbf{S}(\mathbf{T})\cdot\mathbf{P}_k\mathbf{P}_l\cdot\mathbf{S}(\mathbf{T})^{-1}\mathbf{g}\}_{11}=\frac{i}{n}\sum_{t}\sin(k-l)\frac{t\pi}{n}=0. \qquad (10)$$

In exactly the same way we find that

$$\{\mathbf{g}\cdot\mathbf{S}(\mathbf{T})\cdot\mathbf{Q}_k\mathbf{Q}_l\cdot\mathbf{S}(\mathbf{T})^{-1}\mathbf{g}\}_{11}=0. \qquad (11)$$

On the other hand, for $\mathbf{P}_k\mathbf{Q}_l$ we have

$$\mathbf{T}:\quad \mathbf{P}_k\mathbf{Q}_l\rightarrow\frac{1}{n}\sum_{r=1}^{n}\cos\left[(k-l)\frac{t\pi}{n}+\delta_t'\right]\cdot\mathbf{P}_r\mathbf{Q}_r+\text{other terms.}$$

As a result

$$\{\mathbf{g}\cdot\mathbf{S}(\mathbf{T})\cdot i\mathbf{P}_k\mathbf{Q}_l\cdot\mathbf{S}(\mathbf{T})^{-1}\cdot\mathbf{g}\}_{11}$$

$$=\frac{1}{n}\sum_{t}\cos\left[(k-l)\frac{t\pi}{n}+\delta_t'\right]\equiv\Sigma_{k-l}. \qquad (12)$$

Thus we see that we could disregard, in (8), all the terms in the transform of $\mathbf{X}$ which did not have the form $\mathbf{P}_k\mathbf{Q}_l$, and then we read off the average of $\mathbf{X}$ directly from (8):

$$i\bar{\mathbf{X}}=\langle i\mathbf{P}_k\mathbf{Q}_l\rangle_{\text{Av}}=\{\mathbf{g}\cdot\mathbf{S}(\mathbf{TH})\cdot i\mathbf{P}_k\mathbf{Q}_l\cdot\mathbf{S}(\mathbf{TH})^{-1}\cdot\mathbf{g}\}_{11}$$

$$=\cosh^2H^*\cdot\Sigma_{k-l}-\sinh^2H^*\cdot\Sigma_{l-k}. \qquad (13)$$

In particular

$$\bar{\mathbf{C}}_k=\langle i\mathbf{P}_k\mathbf{Q}_k\rangle_{\text{Av}}=\Sigma_0. \qquad (14)$$

Similarly, one finds

$$\langle\mathbf{P}_k\mathbf{P}_l\rangle_{\text{Av}}=\tfrac{1}{2}\sinh 2H^*\cdot(\Sigma_{k-l}-\Sigma_{l-k}), \qquad (15)$$

$$\langle\mathbf{Q}_k\mathbf{Q}_l\rangle_{\text{Av}}=-\tfrac{1}{2}\sinh 2H^*\cdot(\Sigma_{k-l}-\Sigma_{l-k}). \qquad (16)$$

The Σ_a can be evaluated exactly for large n, when the sum may be replaced by an integral. See below for the calculation of the Σ_a, and the derived results.

We are now in position to find the three simplest correlation functions.

Neighboring atoms in a row:

$$\langle s_1s_2\rangle_{\text{Av}}=\langle\mathbf{s}_1\mathbf{s}_2\rangle_{\text{Av}}=\langle -i\mathbf{P}_2\mathbf{Q}_1\rangle_{\text{Av}}$$

$$=-\cosh^2H^*\cdot\Sigma_1+\sinh^2H^*\cdot\Sigma_{-1}. \qquad (17)$$

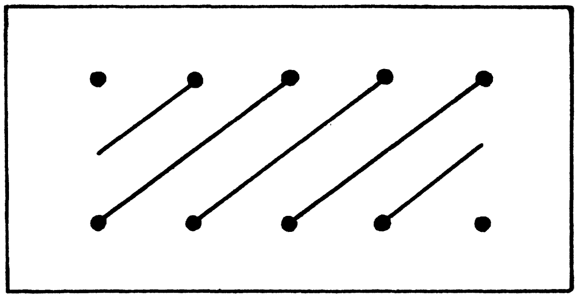

FIG. 3. Correlation between the sites (1, 1) and (2, 3).

(17) may also be written in the following useful form:

$$\langle s_1s_2\rangle_{\text{Av}}=-\cosh^2H^*\cdot\frac{1}{n}\sum_t\cos\left(\frac{t\pi}{n}+\delta_t'\right)$$

$$+\sinh^2H^*\cdot\frac{1}{n}\sum_t\cos\left(-\frac{t\pi}{n}+\delta_t'\right)$$

$$=-\frac{1}{n}\sum_t\left(\cos\frac{t\pi}{n}\cos\delta_t'-\sin\frac{t\pi}{n}\sin\delta_t'\cosh 2H^*\right)\equiv\frac{1}{n}\sum_t\cos\delta_t^*. \qquad (18)$$

(We recognize, from its definition, that δ^* is the third angle in the hyperbolic triangle of Fig. 4 in I.) Neighboring atoms in adjacent rows are shown in Fig. 1. We need

$$\langle s_{1,1}s_{2,1}\rangle_{\text{Av}}=\lambda^{-1}\{\mathbf{\Psi}\mathbf{s}_1\mathbf{V}\mathbf{s}_1\mathbf{\Psi}^{-1}\}_{11}.$$

Now

$$\mathbf{s}_1\mathbf{V}\mathbf{s}_1=\mathbf{s}_1\cdot\exp(H^*\mathbf{B})\cdot\exp(H'\mathbf{A})\cdot\mathbf{s}_1$$

$$=\mathbf{s}_1\cdot\exp(H^*\Sigma\mathbf{C}_r)\cdot\exp(H'\Sigma\mathbf{s}_r\mathbf{s}_{r+1})\cdot\mathbf{s}_1$$

$$=\exp(-2H^*\mathbf{C}_1)\cdot\mathbf{V}.$$

This is a result of the fact that all factors in $\mathbf{V}$ commute with $\mathbf{s}_1$, except for $\exp(H^*\mathbf{C}_1)$. Therefore

$$\langle s_{1,1}s_{2,1}\rangle_{\text{Av}}=\cosh 2H^*-\sinh 2H^*\cdot\Sigma_0. \qquad (19)$$

Next-nearest neighbors are shown in Fig. 2.

$$\langle s_{1,1}s_{2,2}\rangle_{\text{Av}}=\lambda^{-1}\{\mathbf{\Psi}\mathbf{s}_1\mathbf{V}\mathbf{s}_2\mathbf{\Psi}^{-1}\}_{11}.$$

Here

$$\mathbf{s}_1\mathbf{V}\mathbf{s}_2=\mathbf{s}_1\mathbf{s}_2\exp(-2H^*\mathbf{C}_2)\cdot\mathbf{V}$$

$$=(\cosh 2H^*\cdot\mathbf{s}_1\mathbf{s}_2-\sinh 2H^*\cdot\mathbf{s}_1\mathbf{s}_2\mathbf{C}_2)\mathbf{V},$$

and

$$\mathbf{s}_1\mathbf{s}_2\mathbf{C}_2=\mathbf{Q}_2\mathbf{Q}_1,$$

so that

$$\langle s_{1,1}s_{2,2}\rangle_{\text{Av}}=\cosh 2H^*\cdot\langle s_1s_2\rangle_{\text{Av}}-\tfrac{1}{2}\sinh^2 2H^*(\Sigma_1-\Sigma_{-1}). \qquad (20)$$

Several remarks may be made here:

(a) $\langle s_{1,1}s_{2,1}\rangle_{\text{Av}}$ must, of course, equal $\langle s_1s_2\rangle_{\text{Av}}$ in the case of a crystal with $H=H'$. Comparing (17) and (19), we

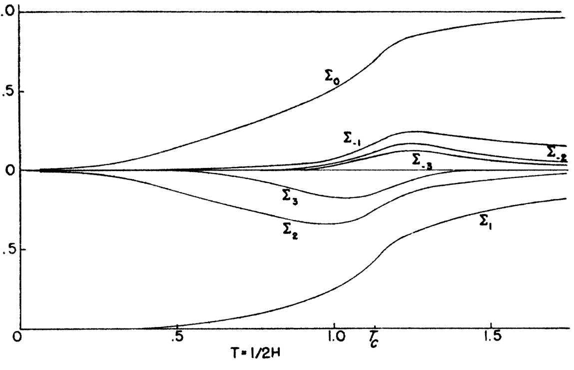

FIG. 4. Dependence of the functions Σ_a upon temperature. At low temperatures all Σ_a are negligible, except for Σ_1 which is $\sim+1$. At high temperatures only Σ_0 is significant.

see that this cannot be a term-by-term equality. But it it is to be expected that the complete expressions will equal one another. And indeed, this will be shown to be the case when the Σ_a are evaluated. See Section 5.

(b) $mn\langle s_1s_2\rangle_{\text{Av}}$ is, by its meaning, the average energy of a quadratic crystal (if J be normalized to unity). It should therefore equal the logarithmic derivative of the partition function, Z, with respect to H. Now

$$dZ/dH=d/dH\sum_i \lambda_i^m=m\sum_i (d\lambda_i/dH)\lambda_i^{m-1}; \quad (21)$$

but

$$\frac{d\lambda_i}{dH}=\frac{d}{dH}\exp[\tfrac{1}{2}(\cdots\pm\gamma_t\pm\gamma_{t+2}\pm\cdots)]$$

$$=\tfrac{1}{2}\lambda_i\frac{d}{dH}(\cdots\pm\gamma_t\pm\gamma_{t+2}\pm\cdots)=\tfrac{1}{2}\lambda_i\sum_t(\pm)\frac{d\gamma_t}{dH}. \quad (22)$$

(The sign-combination is determined by i; for $i=1$ we know that all signs are $+$.)

Furthermore, we have, from the definition of γ (see I. 89 and I. 112)

$$(d\gamma_t/dH)=2\cos\delta_t^*. \quad (23)$$

Combining the last three expressions, we get:

$$dZ/dH=m\sum_i \lambda_i^m\cdot\{\sum_t\pm\cos\delta_t^*\}_i. \quad (24)$$

Using only the largest eigenvalue, we have

$$1/Z\cdot dZ/dH\sim m\sum_t \cos\delta_t^*\sim mn\langle s_1s_2\rangle_{\text{Av}}. \quad (25)$$

These two entirely different methods of obtaining the average energy in the crystal have thus been shown to check with each other.

(c) An even closer analysis can be made, which will at the same time check the result for

$$\bar{\mathbf{C}}_a=\Sigma_0=(1/n)\sum_t \cos\delta_t'.$$

Taking the general case, $H\neq H'$, we will express $\partial Z/\partial H'$ and $\partial Z/\partial H^*$ in terms of the angles δ^* and δ', respectively.

$$\frac{\partial Z}{\partial H'}=\frac{\partial}{\partial H'}\operatorname{trace}(\mathbf{V}^m)$$

$$=\frac{\partial}{\partial H'}\operatorname{trace}\{(\exp(H^*\mathbf{B})\cdot\exp(H'\mathbf{A}))^m\}$$

$$=\operatorname{trace}\{\mathbf{AV}^m+\mathbf{VAV}^{m-1}+\mathbf{V}^2\mathbf{AV}^{m-2}+\cdots\}$$

$$=m\operatorname{trace}\{\mathbf{AV}^m\}=m\operatorname{trace}\{\mathbf{\Psi A\Psi}^{-1}\cdot\mathbf{\Lambda}^m\}$$

$$=m\sum_i \lambda_i^m\{\mathbf{\Psi A\Psi}^{-1}\}_{ii}=mn\sum_i\lambda_i^m\{\mathbf{\Psi s}_1\mathbf{s}_2\mathbf{\Psi}^{-1}\}_{ii}.$$

This can now be compared by term with (24), giving

$$\{\mathbf{\Psi s}_1\mathbf{s}_2\mathbf{\Psi}^{-1}\}_{ii}=(1/n)\{\sum_t\pm\cos\delta_t^*\}_i. \quad (26)$$

For the special case $i=1$ we rederive (18).

Consider how the derivative of Z with respect to H^*.

$$\partial Z/\partial H^*=m\operatorname{trace}\{\mathbf{BV}^m\}=mn\textstyle\sum_i\lambda_i^m\{\mathbf{\Psi C}_a\mathbf{\Psi}^{-1}\}_{ii}; \quad (27)$$

but we also have, as in the case of $\langle s_1s_2\rangle_{\text{Av}}$,

$$\partial Z/\partial H^*=\partial/\partial H^*\textstyle\sum_i\lambda_i^m, \quad (28)$$

and (see I. 112)

$$\partial\gamma_t/\partial H^*=2\cos\delta_t'. \quad (29)$$

Therefore

$$\partial Z/\partial H^*=m\sum_i\lambda_i^m\{\sum_t\pm\cos\delta_t'\}_i. \quad (30)$$

Comparing the two expressions for $\partial Z/\partial H^*$ we find

$$\{\mathbf{\Psi C}_a\mathbf{\Psi}^{-1}\}_{ii}=1/n\{\sum_t\pm\cos\delta_t'\}_{ii}. \quad (31)$$

For $i=1$, then, all signs are $+$, and $\bar{\mathbf{C}}_a=\Sigma_0$, as should be.

4. EXTENSION TO GREATER DISTANCES

The next farthest correlation introduces a new type of problem. In $\langle s_1s_3\rangle_{\text{Av}}$ we find that we need the transform of $\mathbf{P}_3\mathbf{Q}_2\mathbf{P}_2\mathbf{Q}_1$. There is no difficulty in applying $\mathbf{H}$, especially since $\mathbf{P}_2\mathbf{Q}_2$ remains invariant under $\mathbf{H}$. However, we must investigate the effect of the other operations on a 4-spinor matrix, say $\mathbf{P}_a\mathbf{Q}_b\mathbf{P}_c\mathbf{Q}_d$.

It will be helpful here to introduce a notation for an intermediate step in the averaging procedure. Let $\mathbf{X}$ be the quantity to be averaged, i.e., we want to evaluate $\bar{\mathbf{X}}=\{\mathbf{gS}(\mathbf{T})\cdot\mathbf{S}(\mathbf{H})\mathbf{XS}(\mathbf{H})^{-1}\cdot\mathbf{S}(\mathbf{T})^{-1}\mathbf{g}\}_{11}$. Denote by $\mathbf{Y}$ the the result of transforming $\mathbf{X}$ by $\mathbf{S}(\mathbf{H})$: $\mathbf{Y}=\mathbf{S}(\mathbf{H})\mathbf{XS}(\mathbf{H})^{-1}$. Then $\bar{\mathbf{X}}=\{\mathbf{gS}(\mathbf{T})\cdot\mathbf{YS}(\mathbf{T})^{-1}\cdot\mathbf{g}\}_{11}\equiv\langle\{\mathbf{Y}\}\rangle_{\text{Av}}$. This notation is useful because the transformation by $\mathbf{S}(\mathbf{T})$ is the main step, whereas $\mathbf{S}(\mathbf{H})$ can be performed by inspection for the quantities $\mathbf{X}$ with which we will be dealing.

In this new notation we can rewrite (10), (11) and (12):

$$\langle\{\mathbf{P}_k\mathbf{P}_l\}\rangle_{\text{Av}}=\langle\{\mathbf{Q}_k\mathbf{Q}_l\}\rangle_{\text{Av}}=0, \quad (32)$$

$$\langle\{i\mathbf{P}_k\mathbf{Q}_l\}\rangle_{\text{Av}}=\Sigma_{k-l}. \quad (33)$$

We will now show that

$$\langle\{\mathbf{P}_a\mathbf{Q}_b\mathbf{P}_c\mathbf{Q}_d\}\rangle_{\mathrm{Av}}=\langle\{\mathbf{P}_a\mathbf{Q}_b\}\rangle_{\mathrm{Av}}\cdot\langle\{\mathbf{P}_c\mathbf{Q}_d\}\rangle_{\mathrm{Av}} +\langle\{\mathbf{P}_a\mathbf{P}_c\}\rangle_{\mathrm{Av}}\cdot\langle\{\mathbf{Q}_b\mathbf{Q}_d\}\rangle_{\mathrm{Av}}+\langle\{\mathbf{P}_a\mathbf{Q}_d\}\rangle_{\mathrm{Av}}\cdot\langle\{\mathbf{Q}_b\mathbf{P}_c\}\rangle. +\text{a negligible correction term.} \quad (34)$$

Reasoning as in Section 3, we know that $\mathbf{T}$ sends $\mathbf{P}_a\mathbf{Q}_b\mathbf{P}_c\mathbf{Q}_d$ into a linear combination of 4-spinor matrices, but that only those which are of the form

$$\mathbf{P}_r\mathbf{Q}_r\mathbf{P}_u\mathbf{Q}_u=-\mathbf{s}_r\mathbf{s}_u$$

can contribute to $\langle\{\mathbf{P}_a\mathbf{Q}_b\mathbf{P}_c\mathbf{Q}_d\}\rangle_{\mathrm{Av}}$.

Now

$$\mathbf{T}:\quad \mathbf{P}_a\mathbf{Q}_b\rightarrow 1/n\sum_t \cos[(a-b)t\pi/n+\delta_t']\mathbf{P}_r\mathbf{Q}_r +\text{other terms,} \quad (35)$$

$$\mathbf{P}_c\mathbf{Q}_d\rightarrow 1/n\sum_v \cos[(c-d)v\pi/n+\delta_v']\mathbf{P}_u\mathbf{Q}_u +\text{other terms.} \quad (36)$$

If we multiply the $\mathbf{P}_r\mathbf{Q}_r$ terms in (35) by the $\mathbf{P}_u\mathbf{Q}_u$ terms in (36) we get a set of matrices all having the desired form $\mathbf{P}_r\mathbf{Q}_r\mathbf{P}_u\mathbf{Q}_u$. The products in which $r=u$ (and, therefore, $\mathbf{P}_r\mathbf{Q}_r\mathbf{P}_u\mathbf{Q}_u=-1$) must be excluded, since the transform of $\mathbf{P}_a\mathbf{Q}_b\mathbf{P}_c\mathbf{Q}_d$ must contain only 4-spinor matrices.

We will therefore have, as a set of contributing matrices:

$$\{1/n\sum_t \cos[(a-b)t\pi/n+\delta_t']\cdot\mathbf{P}_r\mathbf{Q}_r\} \cdot\{1/n\sum_v \cos[(c-d)v\pi/n+\delta_v']\mathbf{P}_u\mathbf{Q}_u\} -1/n^2\sum_t \cos[(a-b)t\pi/n+\delta_t'] \cdot\cos[(c-d)t\pi/n+\delta_t']\cdot\mathbf{P}_r\mathbf{Q}_r\mathbf{P}_r\mathbf{Q}_r, \quad (37)$$

and its contribution will be

$$\langle\{\mathbf{P}_a\mathbf{Q}_b\}\rangle_{\mathrm{Av}}\langle\{\mathbf{P}_c\mathbf{Q}_d\}\rangle_{\mathrm{Av}}+1/n^2\sum_t \cos[(a-b)t\pi/n+\delta_t'] \cdot\cos[(c-d)t\pi/n+\delta_t']. \quad (38)$$

However, this set does not exhaust all contributing matrices in the transform of $\mathbf{P}_a\mathbf{Q}_b\mathbf{P}_c\mathbf{Q}_d$. (For example, a $\mathbf{P}_k\mathbf{Q}_l$ matrix in (35) when multiplied by $\mathbf{P}_l\mathbf{Q}_k$ in (36), is also of the desired form.) The reason for this is that we had restricted the pair $\mathbf{P}_r\mathbf{Q}_r$ to be taken from the transform of $\mathbf{P}_a\mathbf{Q}_b$, and $\mathbf{P}_u\mathbf{Q}_u$ to be taken from the transform of $\mathbf{P}_c\mathbf{Q}_d$. Two other possibilities are:

$\mathbf{P}_r\mathbf{Q}_r$ from the transform of $\mathbf{P}_a\mathbf{P}_c$ and $\mathbf{P}_u\mathbf{Q}_u$ from the transform of $\mathbf{P}_b\mathbf{Q}_d$,

$\mathbf{P}_r\mathbf{Q}_r$ from the transform of $\mathbf{P}_a\mathbf{Q}_d$ and $\mathbf{P}_u\mathbf{Q}_u$ from the transform of $\mathbf{Q}_b\mathbf{P}_c$.

There are no other possibilities, and the three given ones contain no common terms, except for the matrices $\mathbf{P}_r\mathbf{Q}_r\mathbf{P}_r\mathbf{Q}_r$, which are everywhere to be excluded, as in (37). When n is very large, the sum of the excluded terms is negligible compared to all the rest, and will henceforth be neglected. We have thus proved (34). Making use of (32) and (33), we get finally:

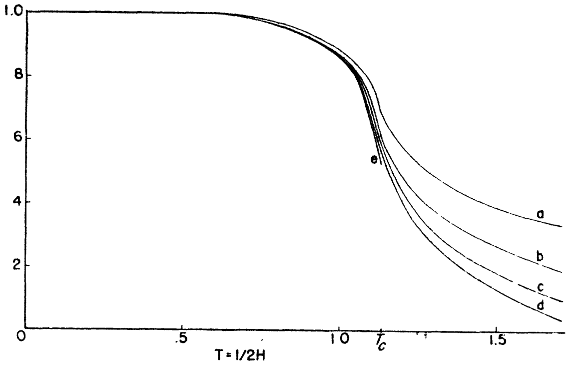

Fig. 5. Correlations for small distances, as functions of temperature. (a) $\langle s_1s_2\rangle_{\mathrm{Av}}$; (b) $\langle s_{1,1}s_{2,2}\rangle$; (c) $\langle s_1s_3\rangle_{\mathrm{Av}}$; (d) $\langle s_{1,1}s_{2,3}\rangle_{\mathrm{Av}}$; (e) $\langle s_1s_4\rangle_{\mathrm{Av}}$.

$$\langle\{\mathbf{P}_a\mathbf{Q}_b\mathbf{P}_c\mathbf{Q}_d\}\rangle_{\mathrm{Av}}=\Sigma_{a-b}\Sigma_{c-d}-\Sigma_{a-d}\Sigma_{c-b} =\begin{vmatrix}\Sigma_{a-b} & \Sigma_{a-d}\\ \Sigma_{c-b} & \Sigma_{c-d}\end{vmatrix}. \quad (39)$$

From (32) there results the further useful simplification that $\langle\{\mathbf{X}\}\rangle_{\mathrm{Av}}=0$ for $\mathbf{X}=\mathbf{P}_a\mathbf{P}_b\mathbf{P}_c\mathbf{P}_d$, $\mathbf{P}_a\mathbf{P}_b\mathbf{P}_c\mathbf{Q}_d$, etc., i.e., whenever it is impossible to group all factors in $\mathbf{X}$ into $\mathbf{P}-\mathbf{Q}$ pairs. Therefore $\mathbf{X}$ must contain equal numbers of $\mathbf{P}$'s and $\mathbf{Q}$'s.

Equation (39) can be generalized to any number of factors:

If $\mathbf{X}=\mathbf{P}_{a1}\mathbf{Q}_{b1}\mathbf{P}_{a2}\mathbf{Q}_{b2}\cdots\mathbf{P}_{af}\mathbf{Q}_{bf}$ $(a_i, b_i=1, 2, \cdots n)$, *then* $\langle\{\mathbf{X}\}\rangle_{\mathrm{Av}}$ *is equal to an f-rowed determinant whose (k, l)-member is* $\Sigma_{a_k-b_l}$. (40)

Further Correlations

Returning to the correlation functions, we have:

$$\langle s_1s_3\rangle_{\mathrm{Av}}=-\langle\{\mathbf{S}(\mathbf{H})\mathbf{P}_3\mathbf{Q}_2\mathbf{P}_2\mathbf{Q}_1\mathbf{S}(\mathbf{H})^{-1}\}\rangle_{\mathrm{Av}}.$$

$$\mathbf{H}:\quad -\mathbf{P}_3\mathbf{Q}_2\mathbf{P}_2\mathbf{Q}_1\rightarrow\cosh^2 H^*\cdot\mathbf{P}_3\mathbf{Q}_2\mathbf{P}_2\mathbf{Q}_1 -\sinh^2 H^*\mathbf{P}_1\mathbf{Q}_2\mathbf{P}_2\mathbf{Q}_3+\text{other terms.}$$

The "other terms" here do not contain equal numbers of $\mathbf{P}$'s and $\mathbf{Q}$'s, and will therefore not contribute to

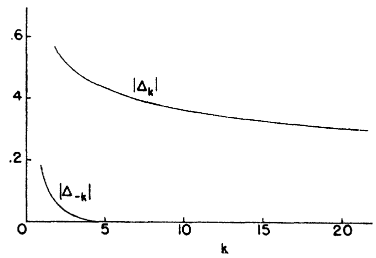

Fig. 6. The quantity $|\Delta_k|$ is proportional to the correlation $\langle s_1s_{1+k}\rangle_{\mathrm{Av}}$ at the critical temperature. Δ_k tends to zero as $k\rightarrow\infty$. There is no long-range order at T_c.

$\langle s_1 s_3\rangle_{\text{Av}}$. Hence:

$$\langle s_1 s_3\rangle_{\text{Av}}=\cosh^2 H^*\begin{vmatrix}\Sigma_1 & \Sigma_2\\ \Sigma_0 & \Sigma_1\end{vmatrix}+\sinh^2 H^*\begin{vmatrix}\Sigma_{-1} & \Sigma_{-2}\\ \Sigma_0 & \Sigma_{-1}\end{vmatrix}$$

$$\equiv\cosh^2 H^*\cdot\Delta_2+\sinh^2 H^*\cdot\Delta_{-2}. \qquad (41)$$

For the correlation indicated in Fig. 3, we have:

$$\langle s_{1,1}s_{2,3}\rangle_{\text{Av}}=\lambda^{-1}\{\mathbf{\Psi}\mathbf{s}_1\mathbf{V}\mathbf{s}_3\mathbf{\Psi}^{-1}\}_{11}$$
$$=\cosh 2H^*\langle s_1 s_3\rangle_{\text{Av}}+i\sinh 2H^*\{\mathbf{\Psi}\mathbf{Q}_1\mathbf{P}_2\mathbf{Q}_2\mathbf{Q}_3\mathbf{\Psi}^{-1}\}_{11};$$

but

$$\mathbf{H}:\quad \mathbf{Q}_1\mathbf{P}_2\mathbf{Q}_2\mathbf{Q}_3\rightarrow i/2\sinh 2H^*(-\mathbf{P}_1\mathbf{Q}_2\mathbf{P}_2\mathbf{Q}_3+\mathbf{P}_3\mathbf{Q}_2\mathbf{P}_2\mathbf{Q}_1)$$
$$+\text{other terms.}$$

Hence:

$$\langle s_{1,1}s_{2,3}\rangle_{\text{Av}}=\cosh 2H^*\langle s_1 s_3\rangle_{\text{Av}}+\tfrac{1}{2}\sinh^2 2H^*(\Delta_2-\Delta_{-2}). \qquad (42)$$

It is not necessary to evaluate $\langle s_{1,1}s_{3,2}\rangle_{\text{Av}}$, for this is equal to $\langle s_{1,1}s_{2,3}\rangle_{\text{Av}}$; also $\langle s_{1,1}s_{3,1}\rangle_{\text{Av}}$ equals $\langle s_{1,3}\rangle_{\text{Av}}$.

It is easy to generalize (41) and (42) to any distance. One finds:

$$(-1)^k\langle s_1 s_{1+k}\rangle_{\text{Av}}=\cosh^2 H^*\Delta_k+\sinh^2 H^*\Delta_{-k}, \qquad (43)$$

and

$$\langle s_{1,1}s_{2,1+k}\rangle_{\text{Av}}=\cosh 2H^*\cdot\langle s_1 s_{1+k}\rangle_{\text{Av}}$$
$$-(-1)^k/2\sinh^2 2H^*\cdot(\Delta_k-\Delta_{-k}), \qquad (44)$$

where

$$\Delta_k=\begin{vmatrix}\Sigma_1 & \Sigma_2 & \Sigma_3 & \Sigma_4 & \cdots & \Sigma_k\\ \Sigma_0 & \Sigma_1 & \Sigma_2 & \Sigma_3 & \cdots & \Sigma_{k-1}\\ \Sigma_{-1} & \Sigma_0 & \Sigma_1 & \Sigma_2 & \cdots & \Sigma_{k-2}\\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot\\ \Sigma_{-k+2} & \cdot & \cdot & \cdot & \cdot & \Sigma_1\end{vmatrix},$$

$$\Delta_{-k}=\begin{vmatrix}\Sigma_{-1} & \Sigma_{-2} & \Sigma_{-3} & \Sigma_{-4} & \cdots & \Sigma_{-k}\\ \Sigma_0 & \Sigma_{-1} & \Sigma_{-2} & \Sigma_{-3} & \cdots & \Sigma_{-k+1}\\ \Sigma_1 & \Sigma_0 & \Sigma_{-1} & \Sigma_{-2} & \cdots & \Sigma_{-k+2}\\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot\\ \Sigma_{k-2} & \cdot & \cdot & \cdot & \cdot & \Sigma_{-1}\end{vmatrix}. \qquad (45)$$

5. EVALUATION OF THE Σ_a

For large n, the sum in Σ_a may be replaced by an integral;

$$\Sigma_a=\frac{1}{n}\sum_{r=1}^{n}\cos\left[a\frac{2r\pi}{n}+\delta_{2r}'\right]$$

$$\simeq\frac{1}{\pi}\int_0^{\pi}\cos[a\omega+\delta'(\omega)]d\omega. \qquad (46)$$

(It obviously makes no difference now if one replaces the even-indexed angles in Σ_a by odd-indexed ones. This justifies the statements made on p. 1245–6.)

δ' is a function of H and ω through the relations (for the case $H=H'$; see (I. 89)):

$$\sin\delta'=\sinh 2H(\sin\omega/\sinh\gamma), \qquad (47)$$

$$\sinh\gamma\cos\delta'=(\cosh 2H/\sinh 2H)-\cosh 2H\cdot\cos\omega, \qquad (48)$$

and

$$\cosh\gamma=(\cosh^2 2H/\sinh 2H)-\cos\omega. \qquad (49)$$

An elliptic substitution[5] is now made separately for values of H below and above the critical point. (The critical point itself occurs at $\sinh 2H_c=1$.) The variable u_1 is introduced, and both ω and δ' are expressed in terms of this variable.

Below the critical temperature ($T<T_c$, $H>H_c$). First choose for the elliptic modulus

$$k\equiv\sinh^{-2}2H<1 \qquad (50)$$

and

$$\cos\delta'\equiv cn(u,k),\quad \sin\delta'\equiv sn(u,k). \qquad (51)$$

As a result (see I. 2.4),

$$\cos\omega=k^{\frac{1}{2}}\frac{(1+k)sn^2u-dnu\,cnu}{1+k\,sn^2u}. \qquad (52)$$

The limits of integration in (46) become: 0 to $2K(k)$, where K is the complete elliptic integral of the first kind. Now make one further substitution,[6] which serves to eliminate the denominator in (52):

$$u_1\equiv u(1+k),\quad k_1\equiv 2k^{\frac{1}{2}}/1+k. \qquad (53)$$

Then we have

$$cn(u_1,k_1)=\frac{cn(u,k)\,dn(u,k)}{1+k\,sn^2(u,k)},$$

$$dn(u_1,k_1)=\frac{1-k\,sn^2(u,k)}{1+k\,sn^2(u,k)} \qquad (54)$$

and

$$K_1\equiv K(k_1)=K(k)\cdot(1+k). \qquad (55)$$

As a result, we get

$$\cos\omega=\frac{1}{k_1}[1-dn(u_1,k_1)]-cn(u_1,k_1), \qquad (56)$$

and the limits of integration become: 0 to $2K_1$. Since the integrals of powers of dnu and cnu are all known, it is now possible to evaluate any integral of the form

$$\int_0^{2K_1}\cos^a\omega\cdot du_1. \qquad (57)$$

In order to express δ' in terms of u_1, we make use of the relationship (see I. 2.4 and I. 2.5)

$$\partial\omega/\partial u=-\sinh\gamma/k^{\frac{1}{2}}. \qquad (58)$$

This we insert into $\cos\delta'\cdot d\omega$:

$$\cos\delta'\cdot d\omega=\cos\delta'\cdot\partial\omega/\partial u\cdot du$$
$$=-(\cos\delta'\sinh\gamma/k^{\frac{1}{2}})du. \qquad (59)$$

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[5] See I, especially Section 2 of the Appendix.

[6] See, for example, E. Jahnke and F. Emde, *Tables of Functions* (B. G. Teubner, Leipzig and Berlin, 1933).

We now use (48) and (50), and get

$$\cos\delta'\cdot d\omega=(1+k)^{\frac{1}{2}}(k^{\frac{1}{2}}-\cos\omega)\cdot du. \tag{60}$$

Finally we replace u by u_1:

$$\cos\delta'\cdot d\omega=\frac{1}{(1+k)^{\frac{1}{2}}}(k^{\frac{1}{2}}-\cos\omega)\cdot du_1. \tag{61}$$

Similarly we get for $\sin\delta'$:

$$\sin\delta' d\omega=\sin\omega\, du=\frac{\sin\omega\, du_1}{(1+k)}. \tag{62}$$

And now, we can apply these results to the integrand of Σ_a:

$$\begin{aligned}\cos(a\omega+\delta')d\omega&=\cos a\omega\cdot\cos\delta' d\omega-\sin a\omega\,\sin\delta' d\omega\\ &=\frac{1}{(1+k)^{\frac{1}{2}}}\sum_{s=1}^{a}\alpha_s\cdot\cos^s\omega(k^{\frac{1}{2}}-\cos\omega)du_1\\ &=\frac{1}{1+k}\sum_{s=1}^{a-1}\beta_s\cos^s\omega\,\sin^2\omega\cdot du_1,\end{aligned}$$

where we have expanded $\cos a\omega$ and $\sin a\omega$ into polynomials in $\cos\omega$. The integral of $\cos(a\omega+\delta')$ now involves only integrals of the form (57). Thus the procedure for evaluating any Σ_a is completed.

As an example we will now give the details of the computation for Σ_0.

$$\begin{aligned}\Sigma_0&=\frac{1}{\pi}\int_0^\pi\cos\delta' d\omega=\frac{1}{\pi(1+k)^{\frac{1}{2}}}\int_0^{2K_1}(k^{\frac{1}{2}}-\cos\omega)du_1\\ &=\frac{1}{\pi}\left(\frac{k}{1+k}\right)^{\frac{1}{2}}2K_1-\frac{(1+k)^{\frac{1}{2}}}{\pi}\int_0^{2K_1}\cos\omega du_1.\end{aligned}$$

And from (56):

$$\int_0^{2K_1}\cos\omega\, du_1=\int_0^{2K_1}\left[\frac{1}{k_1}(1-dnu_1)-cnu_1\right]du_1=\frac{2K_1-\pi}{2k^{\frac{1}{2}}}.$$

Altogether

$$\Sigma_0=1/\pi(1+k/k)^{\frac{1}{2}}\{\pi/2-(1-k)K\}\quad (T<T_c). \tag{63}$$

(This result is the same as that already obtained in (I. 5.1).)

Above the critical temperature ($T>T_c$, $H<H_c$). Choose

$$k=\sinh^2 2H<1, \tag{64}$$

$$\cos\delta'=dnu,\quad \sin\delta'=k\, snu. \tag{65}$$

And find, as above:

$$\cos\delta' d\omega=\frac{1}{(1+k)^{\frac{1}{2}}}(1-k^{\frac{1}{2}}\cos\omega)du_1, \tag{66}$$

$$\sin\delta' d\omega=\frac{k}{1+k}\sin\omega\cdot du_1. \tag{67}$$

(52) and (56) hold at all temperatures. Applying to Σ_0 we find:

$$\Sigma_0=(1+k)^{\frac{1}{2}}/\pi\{\pi/2+(1-k)K\}\quad (T>T_c). \tag{68}$$

Σ_0 is continuous and bounded at the critical point. The reason for this is that, although $K\rightarrow\infty$ as $k\rightarrow 1$, $(1-k)K\rightarrow 0$. At the critical point then,

$$\Sigma_0=1/\sqrt{2}. \tag{69}$$

In the same way we find:

$$\pi\Sigma_{\pm 1}=\begin{cases}(1+k)^{\frac{1}{2}}/k\{(\pi/2)-k(1-k)\cdot K-(1+k)E_1\}\\ \qquad\mp(1+k/k)\{(\pi/2)-E_1\}\quad\text{for } T<T_c\\ (1+k/k)^{\frac{1}{2}}\{k(\pi/2)+(1-k)\cdot K-(1+k)E_1\}\\ \qquad\mp(1+k)\{(\pi/2)-E_1\}\quad\text{for } T>T_c.\end{cases} \tag{70}$$

Here E_1 is an abbreviation for $E(2k^{\frac{1}{2}}/(1+k))$. Graphs of Σ_0, $\Sigma_{\pm 1}$, $\Sigma_{\pm 2}$, $\Sigma_{\pm 3}$ are shown in Fig. 4. It is seen that, for $|a|>2$, all Σ_a are very small except in the immediate neighborhood of the critical point.

At the critical temperature. A fairly good approximation[7] gives $\delta'\sim\pi/2-\omega/2$ at the critical point, so that

$$\Sigma_a\sim 1/\pi\int_0^\pi\cos(a\omega+\pi/2-\omega/2)=-2/[\pi(2a-1)]. \tag{71}$$

Exact values at the critical point are

$$\Sigma_0=1/\sqrt{2}=0.7070,$$

$$\Sigma_{\pm 1}=\sqrt{2}\left(\frac{1}{2}-\frac{2}{\pi}\right)\mp\left(1-\frac{2}{\pi}\right)=\begin{cases}-0.5566\\ \ \ 0.1702\end{cases},$$

$$\Sigma_{\pm 2}=\sqrt{2}\left(\frac{5}{2}-\frac{8}{\pi}\right)\mp\left(4-\frac{12}{\pi}\right)=\begin{cases}-0.2461,\\ \ \ 0.1145\end{cases},$$

$$\Sigma_{\pm 3}=\sqrt{2}\left(\frac{25}{2}-\frac{118}{3\pi}\right)\mp\left(19-\frac{178}{3\pi}\right)=\begin{cases}-0.1421\\ \ \ 0.0853\end{cases}.$$

The Correlation Curves

A few qualitative statements can be made immediately about the behavior of the correlation curves at the ends of their range, i.e., for very low and very high temperatures. As $T\rightarrow 0$, $\delta'\sim\pi-\omega$, therefore

$$\cos(a\omega+\delta')=-\cos(a-1)\omega;$$

as a result $\Sigma_a=0$ for all a, except that $\Sigma_{+1}=-1$. On the other hand, as $T\rightarrow\infty$, $\delta'\sim 0$, therefore $\cos(a\omega+\delta')=\cos a\omega$. This gives $\Sigma_a=0$ for all a, except that $\Sigma_0=+1$. Thus $\langle s_1 s_k\rangle_{\text{Av}}=1$ at low temperatures, and $=0$ at high ones, for all k. This results from the fact that we chose a model in which the energy of like neighbors, $-J$, is lower than that of unlike neighbors, $+J$. In other words, the completely ordered state, at absolute zero temperature, is a configuration with all spins alike; it is left unstated whether these spins are all + or all

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[7] It can be shown that $\delta'=\pi/2-\omega/2$ at the critical temperature for correlations along a 45° diagonal of the lattice.

—. The model with the opposite assignment of interaction energies would give $\langle s_1 s_k\rangle_{\text{Av}}=0$ in the completely ordered state (0°K).

Figure 5 shows exact curves for $\langle s_1 s_2\rangle_{\text{Av}}$, $\langle s_{1,1}s_{2,2}\rangle_{\text{Av}}$, $\langle s_1 s_3\rangle_{\text{Av}}$, $\langle s_{1,1}s_{2,3}\rangle_{\text{Av}}$, $\langle s_1 s_4\rangle_{\text{Av}}$ which correspond to the geometric distances 1, $2^{\frac{1}{2}}$, 2, $5^{\frac{1}{2}}$, 3, respectively. It is seen that the curve for $\langle s_{1,1}s_{2,2}\rangle_{\text{Av}}$ lies between $\langle s_1 s_2\rangle_{\text{Av}}$ and $\langle s_1 s_3\rangle_{\text{Av}}$: similarly $\langle s_{1,1}s_{2,3}\rangle_{\text{Av}}$ lies between $\langle s_1 s_3\rangle_{\text{Av}}$ and $\langle s_1 s_4\rangle_{\text{Av}}$. At the critical point the values have been computed exactly for the first few correlations of the type $\langle s_1 s_k\rangle_{\text{Av}}$, and, for the ones farther out, the approximation $\Sigma_a \sim -2/[\pi(2a-1)]$ was used. With these values for Σ_a one has[8]

$$|\Delta_k| = \frac{2}{\pi}\prod_{s=1}^{k}\frac{\Gamma(s+1)\Gamma(s+1)}{\Gamma(s+\frac{1}{2})\Gamma(s+\frac{3}{2})}$$

and

$$|\Delta_{-k}| = \frac{2}{\pi}\prod_{s=1}^{k}\frac{\Gamma(s+1)\Gamma(s+1)}{\Gamma(s+\frac{3}{2})\Gamma(s+(5/2))} \tag{72}$$

Both Δ_k and Δ_{-k} tend to zero as $k\to\infty$, although Δ_k approaches this limit very slowly.[8] The quantities $|\Delta_k|$ and $|\Delta_{-k}|$ are plotted as functions of k in Fig. 6. Since Δ_{-k} is negligible compared to Δ_k, certainly for $k\geqslant 4$, we have from (43) and (44) at the critical point:

$$\begin{gathered}(-1)^k\langle s_1 s_{1+k}\rangle_{\text{Av}} = (1+\sqrt{2}/2)\Delta_k,\\ (-1)^k\langle s_{1,1}s_{2,1+k}\rangle_{\text{Av}} \cong (1+\sqrt{2}/2)\Delta_k = (-1)^k\langle s_1 s_{1+k}\rangle_{\text{Av}},\end{gathered}$$

which is to be expected, since the geometrical distances are almost equal. Finally, it is of interest to verify the statement made on p. 1247 that $\langle s_1 s_2\rangle_{\text{Av}} = \langle s_{1,1}s_{2,1}\rangle_{\text{Av}}$. From (17) we have:

$$\begin{aligned}\langle s_1 s_2\rangle_{\text{Av}} &= -\tfrac{1}{2}(\cosh 2H^*+1)\Sigma_1+\tfrac{1}{2}(\cosh 2H^*-1)\Sigma_{-1}\\ &= \tfrac{1}{2}\cosh 2H^*(\Sigma_1-\Sigma_{-1})-\tfrac{1}{2}(\Sigma_1+\Sigma_{-1}).\end{aligned}$$

Also

$$\cosh 2H^* = \coth 2H = \begin{cases}(1+k)^{\frac{1}{2}} & \text{for } T<T_c,\\ (1+k/k)^{\frac{1}{2}} & \text{for } T<T_c.\end{cases}$$

Therefore, by (70),

$$\langle s_1 s_2\rangle_{\text{Av}} = \begin{cases}\dfrac{(1+k)^{\frac{3}{2}}}{\pi k}\left\{\dfrac{\pi}{2}-E_1\right\}-\dfrac{(1+k)^{\frac{1}{2}}}{\pi k}\\ \quad\times\left\{\dfrac{\pi}{2}-k(1-k)K-(1+k)E_1\right\} & \text{for } T<T_c\\ \dfrac{(1+k)^{\frac{3}{2}}}{\pi k^{\frac{1}{2}}}\left\{\dfrac{\pi}{2}-E_1\right\}-\dfrac{(1+k)^{\frac{1}{2}}}{\pi k^{\frac{1}{2}}}\\ \quad\times\left\{k\dfrac{\pi}{2}+(1-k)K-(1+k)E_1\right\} & \text{for } T>T_c.\end{cases}$$

On the other hand, from Eqs. (19), (63), and (68) we have:

$$\langle s_{1,1}s_{2,1}\rangle_{\text{Av}} = \cosh 2H^* - \sinh 2H^*\Sigma_0$$

$$= \begin{cases}(1+k)^{\frac{1}{2}}-\dfrac{(1+k)^{\frac{1}{2}}}{\pi}\left\{\dfrac{\pi}{2}-(1-k)K\right\} & \text{for } T<T_c\\ \left(\dfrac{1+k}{k}\right)^{\frac{1}{2}}-\dfrac{1}{\pi}\left(\dfrac{1+k}{k}\right)^{\frac{1}{2}}\left\{\dfrac{\pi}{2}+(1-k)K\right\} & \\ & \text{for } T>T_c.\end{cases} \tag{74}$$

Equations (73) and (74) are identical except for their algebraic form.

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[8] T. Muir, *A Treatise on the Theory of Determinants*, revised and enlarged by W. H. Meltzer (private publication, Albany, New York, 1930), p. 437.