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Spontaneous Staggered Polarization of the F-Model

Rodney J. Baxter[1]

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The "order parameter" of the two-dimensional F-model, namely the spontaneous staggered polarization P_0, is derived exactly. At the critical temperature P_0 has an essential singularity, both P_0 and all its derivatives with respect to temperature vanishing.

KEY WORDS: Statistical mechanics; lattice statistics; critical behavior; two-dimensional F-model; antiferroelectric; spontaneous polarization.

1. INTRODUCTION

The F-model of an antiferroelectric on the square lattice was proposed by Rys[(1)] and solved by Lieb.[(2)] It has a phase transition at a critical temperature T_c. Below T_c the system assumes one of two antiferroelectrically ordered thermodynamic states. These states are degenerate, having the same free energy.

Nagle[(3)] has pointed out that it is natural to add a staggered electric field E to the F-model. This breaks the degeneracy of the ordered states and is analogous to applying a magnetic field to the Ising model. Unfortunately, this more general and very interesting problem[(4)] has not yet been solved.

However, we have succeeded in obtaining P_0, the zero-field spontaneous staggered polarization, and give the results (which have already been reported[(5)]) and their derivation here. This P_0 is the "order parameter" of the model (i.e., the analog of the spontaneous magnetization of the Ising model).

[1] Research School of Physical Sciences, The Australian National University, Canberra, Australia.

It varies from unity at zero temperature (complete order) to zero at T_c (disappearance of crystalline order).

We now define the model, which is actually a generalization of the F-model, containing it as a special case.

Consider a rectangular lattice of M rows and N columns, wound on a torus so that cyclic boundary conditions apply. Throughout this paper we take M and N to be even. Thus we can divide the lattice into A and B sublattices such that each A site has only B sites as neighbors and vice versa.

Place arrows on the bonds of the lattice so that at every site, or vertex, there are two arrows pointing in and two out (the "ice condition"[6]). Then there are six possible configurations of arrows at a vertex, as shown in Fig. 1. We associate energies $\epsilon_1, \ldots, \epsilon_6$ with these configurations and suppose that

$$\epsilon_1 = \epsilon_2 , \qquad \epsilon_3 = \epsilon_4 , \qquad \epsilon_5 = \epsilon_6 \tag{1}$$

$$\epsilon_5 < \min(\epsilon_1 , \epsilon_3) \tag{2}$$

[We remark toward the end of this section that the restrictions (1) are not essential. However, they help us fix our ideas.]

We also associate energies E (E') with vertical (horizontal) arrows that point into A sites, and correspondingly energies $-E$ ($-E'$) with arrows that point out. The partition function is then

$$Z = \sum \exp \left\{ -\beta \left[\sum_{j=1}^{6} N_j \epsilon_j + E(N_V - N_V') + E'(N_H - N_H') \right] \right\} \tag{3}$$

where $\beta = 1/kT$, the first summation is over all allowed configurations of arrows on the lattice, N_V and N_H (N_V' and N_H') are the number of vertical and horizontal arrows, respectively, that point into (out of) A sites, and N_j is the number of vertices of type j.

From the ice condition the number of arrows into A sites must equal the number out, so

$$N_V + N_H = N_V' + N_H' \tag{4}$$

From this and (3) it follows that Z depends on E and E' only via their difference $E - E'$. Hence Z is a function of M, N, T, and $E - E'$.

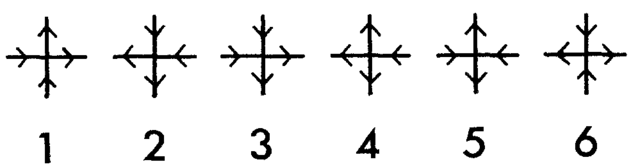

Fig. 1. The six possible configurations of arrows at a vertex.

The free energy per vertex f and the vertical and horizontal staggered polarizations P and P' are defined by

$$-\beta f = \lim_{M,N\to\infty} (MN)^{-1} \ln Z(M, N, T, E - E') \tag{5}$$

$$P = -(\partial f/\partial E)_T, \qquad P' = -(\partial f/\partial E')_T \tag{6}$$

Clearly,

$$P' = -P \tag{7}$$

We define a, b, c, Δ, λ, and t by

$$a = e^{-\beta\epsilon_1}, \qquad b = e^{-\beta\epsilon_3}, \qquad c = e^{-\beta\epsilon_5} \tag{8}$$

$$\Delta = -\cosh\lambda = (a^2 + b^2 - c^2)/(2ab) \tag{9}$$

$$t = e^{-\lambda}$$

When $E = E' = 0$ the system undergoes a phase transition at a temperature T_c given by [2,7]

$$c = a + b \tag{10}$$

Below T_c it follows from (2) that

$$c > a + b, \qquad \Delta < -1 \tag{11}$$

so λ can be chosen real and positive, and $0 < t < 1$. In this regime the system is antiferroelectrically ordered and we expect there to be (see Section 2) a nonzero spontaneous staggered polarization P_0, defined by

$$P_0 = \lim_{E-E'\to 0^+} P \tag{12}$$

We show in this paper that

$$P_0 = \prod_{m=1}^{\infty} (\tanh m\lambda)^2 = \prod_{m=1}^{\infty} (1 - t^{2m})^2/(1 + t^{2m})^2 \tag{13}$$

This result can be expressed in terms of elliptic moduli and integrals. Let k be an elliptic modulus such that

$$\lambda = \pi K'/K \tag{14}$$

where K and K' are the complete elliptic integrals of the first kind, of moduli k and $k' = (1 - k^2)^{1/2}$, respectively. Then from Eq. (8.197.6) of Ref. 8

$$P_0 = 2(k')^{1/2}K/\pi. \tag{15}$$

Further, rearranging Eq. (8.181.1) of Ref. 8 and using (8.192.1), we can show that

$$P_0^{1/2} = 1 + 2 \sum_{m=1}^{\infty} (-1)^m t^{2m^2}$$
$$= 1 - 2t^2 + 2t^8 - 2t^{18} + \cdots \tag{16}$$

This is an extremely rapidly convergent series at low temperatures, when t is small. In an earlier paper [Eq. (7.6) of Ref. 9] we used Nagle's low-temperature series[3] to expand P_0 in powers of t up to and including terms of order t^8. We noted that the result was extremely simple. Equation (16) explains why!

One can apply the Poisson summation formula[10] to (16) and obtain

$$P_0^{1/2} = (2\pi/\lambda)^{1/2} \sum_{m=0}^{\infty} \exp[-(m + \tfrac{1}{2})^2 \pi^2/2\lambda] \tag{17}$$

This series is rapidly convergent when λ is small, i.e., when T is close to T_c. Near T_c we see, using (8) and (9), that

$$P_0 \simeq (2\pi/\lambda) \exp(-\pi^2/4\lambda) \propto (T_c - T)^{-1/2} \exp[-g/(T_c - T)^{1/2}] \tag{18}$$

where g is a positive constant. Thus P_0 has an essential singularity at T_c, both it and all derivatives vanishing.

1.1. Other Thermodynamic Quantities

Such essential singularities seem to be typical of the F-model. Consider the ordered state and let Λ_0, Λ_1, Λ_2 be the three largest (in magnitude) eigenvalues of the transfer matrix, arranged in decreasing order. Then the quantities that have previously been calculated are: the free energy, [2,11] given by Λ_0; the interfacial tension σ [Eqs. (5.11), (5.13) of Ref. 12], given by Λ_0/Λ_1; and the ratio Λ_0/Λ_2 [Eq. (8) of Ref. 13]—this determines the rate of decay of correlations to their asymptotic values.

We define a parameter α by

$$a/b = \sinh[\tfrac{1}{2}(\lambda + \alpha)]/\sinh[\tfrac{1}{2}(\lambda - \alpha)] \tag{19}$$

For the proper F-model, $a = b$, so $\alpha = 0$. For our more general case $a \neq b$, and $|\alpha| < \lambda$.

Both Ref. 12 and 13 concern the eight-vertex model. However, when $k \to 0$ this reduces to the F-model and λ and α in those papers then have the same meaning as here.

We define f_{sing}, the "singular part" of the free energy, to be the difference between the true free energy for $T < T_c$ and the analytic continuation into this regime of f for $T > T_c$. It can be evaluated by methods similar to those used to obtain Eq. (A.13) of Ref. 11.

Using Poisson transforms,[10] or the properties of elliptic functions,[8] we find that

$$-\beta f_{\text{sing}} = i \sum_{m=0}^{\infty} \frac{(-1)^m \{\exp[-(m+\frac{1}{2})\pi^2/\lambda]\} \cos[(m+\frac{1}{2})\pi\alpha/\lambda]}{(m+\frac{1}{2}) \sinh[(m+\frac{1}{2})\pi^2/\lambda]} \tag{20}$$

$$\beta\sigma = \sum_{m=0}^{\infty} \{(m+\tfrac{1}{2}) \sinh[(m+\tfrac{1}{2})\pi^2/\lambda]\}^{-1} \tag{21}$$

$$\ln \frac{\Lambda_0}{\Lambda_2} = -\sum_{m=0}^{\infty} \frac{\cos[(m+\frac{1}{2})\pi\alpha/\lambda]}{(m+\frac{1}{2}) \sinh[(m+\frac{1}{2})\pi^2/\lambda]} \tag{22}$$

These series are rapidly convergent for T near T_c (λ small). Taking their leading terms, we see that near T_c

$$-\beta f_{\text{sing}} \simeq 4i \cos(\tfrac{1}{2}\pi\alpha/\lambda) \exp(-\pi^2/\lambda) \tag{23}$$

$$\beta\sigma \simeq 4 \exp(-\tfrac{1}{2}\pi^2/\lambda) \tag{24}$$

$$ln(\Lambda_0/\Lambda_2) \simeq -4 \cos(\tfrac{1}{2}\pi\alpha/\lambda) \exp(-\tfrac{1}{2}\pi^2/\lambda) \tag{25}$$

Even at T_c, α/λ is an analytic function of T. Thus comparing the above results with (18), we see that all the quantities behave similarly to P_0 at T_c, namely they and their derivatives vanish.

1.2. Scaling Predictions

Such essential singularities are unusual. It is supposed that at T_c the thermodynamic properties of a system normally have branch point singularities, in particular that

$$\begin{aligned} &P_0 \propto (T_c - T)^{\beta'}, \qquad && f_{\text{sing}} \propto (T_c - T)^{2-\alpha'} \\ &\sigma \propto (T_c - T)^{\mu}, \qquad && \ln(\Lambda_0/\Lambda_2) \propto (T_c - T)^{\nu} \end{aligned} \tag{26}$$

Scaling theory[14,15] predicts various relations among such exponents, for instance, that

$$\mu + \nu = d\nu = 2 - \alpha' \tag{27}$$

where d is the dimensionality of the system. Thus if we take the proportionality signs literally in (26), in two dimensions scaling theory predicts that the quantities

$$\sigma^{-1} \ln(\Lambda_0/\Lambda_2) \qquad \text{and} \qquad \sigma^{-2} f_{\text{sing}} \tag{28}$$

tend to finite nonzero limits as $T \to T_c$.

From (23)–(25) we see that this is so for the F-model. Thus in this sense the F-model satisfies the scaling predictions, even though μ, ν, and α' do not exist.

We discussed the possibility of applying such extended scaling predictions to the zero-field staggered susceptibility when we first reported[5] our result for P_0.

1.3. Effect of Direct Fields

Our conditions (1) are equivalent to requiring that no direct (i.e., nonstaggered) electric fields be applied to the lattice. However, if one performs low-temperature series expansions,[3] it soon becomes apparent that for an infinite lattice configurations 1 and 2 (3 and 4; 5 and 6) occur in pairs. Thus adding direct fields does not affect the free energy or the staggered polarization, so long as they are not strong enough to take the system out of the ordered antiferroelectric state.

1.4. Long-Range Order

One can relate the spontaneous staggered polarization to the long-range behavior of the arrow-arrow correlation function by arguments similar to those used for the Ising model [Eqs. (5.15)–(5.16) of Ref. 16]. If $\sigma_J{}^z$ is the Pauli operator acting on the arrow in column J in some particular row of the lattice, then

$$P_0{}^2 = \lim_{J\to\infty} (-1)^{J-1} \langle \sigma_1{}^z \sigma_J{}^z \rangle \tag{29}$$

Here $\langle\cdots\rangle$ means a thermal average over all configurations of the lattice, in the limit when the lattice is infinitely large.

The transfer matrix $\mathbf{T}$ commutes[2] with the Heisenberg chain operator

$$\mathscr{H} = -\tfrac{1}{2} \sum_{J=1}^{N} (\sigma_J{}^x \sigma_{J+1}^x + \sigma_J{}^y \sigma_{J+1}^y + \Delta \sigma_J{}^z \, \sigma_{J+1}^z) \tag{30}$$

and the eigenvector corresponding to the maximum eigenvalue of $\mathbf{T}$ also corresponds to the minimum eigenvalue of $\mathscr{H}$. It follows that we can also use (29) to determine the long-range order of the Heisenberg chain, taking $\langle\cdots\rangle$ now to mean a ground-state expectation value for an infinite chain.

1.5. Outline of Working

We have now stated and discussed our result (13). The rest of this paper is concerned with deriving it.

In Section 2 we generalize the model so that it becomes inhomogeneous, a set of parameters $w_1, \ldots, w_N$ $(w_1', \ldots, w_M')$ being associated with the columns (rows) of the lattice, and a staggered field $E_{I,J}$ with each site (I, J). This enables us to define a local spontaneous staggered polarization $P_0(I, J)$.

In Section 3 we consider the row-to-row transfer matrices (one for each row) of this inhomogeneous model. In zero fields these all commute and have the same eigenvectors. In particular there are two eigenvectors $|0\rangle$ and $|1\rangle$ corresponding to the asymptotically degenerate (in magnitude) maximum eigenvalues of each transfer matrix. We express $P_0(I, J)$ as the matrix element of σ_J^z between these eigenvectors. This shows that $P_0(I, J)$ is in fact independent of I, J, $w_1, \ldots, w_N$, and $w_1', \ldots, w_M'$, and is simply the spontaneous polarization of the normal homogeneous model.

We make a number of mathematical assumptions (which we believe to be exactly correct) in Sections 2 and 3. To clarify the situation we summarize in Section 4 the results of these sections that we need.

The rest of the paper is completely rigorous. In Sections 5 and 6 we derive exact general formulas for the eigenvectors and the matrix elements. In Section 7 we consider the inhomogeneous lattice with $w_J = \frac{1}{2}\pi(2J - N - 1)/N$ for $J = 1, \ldots, N$. In this case the required matrix elements can be evaluated exactly, for finite N. This enables us to calculate P_0. Since P_0 is independent of $w_1, \ldots, w_N$, this gives us P_0 in general, and in particular for the homogeneous system.

Note that the generalization to an inhomogeneous lattice is essential to this derivation.

Where possible, detailed working is confined to the appendices.

2. INHOMOGENEOUS MODEL

Here we generalize the homogeneous model discussed in Section 1 to an inhomogeneous model which is exactly soluble in zero staggered fields.[9]

Consider first the case of zero staggered fields and let the Boltzmann weights a, b, c defined by (1) and (8) vary from site to site, in such a way that at the site on row I and column J their values are

$$\begin{aligned} a_{I,J} &= \rho_{I,J} \sin(\eta + w_I' - w_J) \\ b_{I,J} &= \rho_{I,J} \sin(\eta - w_I' + w_J) \\ c_{I,J} &= \rho_{I,J} \sin(2\eta) \end{aligned} \tag{31}$$

where $I = 1,\ldots, M$ and $J = 1,\ldots, N$. Thus η is some fixed parameter, and $w_1',\ldots, w_M'$ ($w_1,\ldots, w_N$) are parameters associated with the rows (columns) of the lattice. The $\rho_{I,J}$ are simply normalization factors.

We can verify that

$$\Delta = [a_{I,J}^2 + b_{I,J}^2 - c_{I,J}^2]/(2a_{I,J}b_{I,J}) = -\cos(2\eta) \tag{32}$$

Thus Δ is the same for each site of the lattice. We consider here only the ordered state, when

$$\Delta < -1 \tag{33}$$

Comparing this with (9), we see that η can be chosen pure imaginary, such that

$$\eta = \tfrac{1}{2}i\lambda \tag{34}$$

where λ is real and positive.

In the *physical regime* (PR) the Boltzmann weights must be positive. The parameters $\rho_{I,J}$, w_I', and w_J can then all be chosen to be pure imaginary, such that

$$|\operatorname{Im}(w_I' - w_J)| < \tfrac{1}{2}\lambda, \qquad \text{all} \quad I, J \tag{35}$$

Note that the normal homogeneous case is contained in this regime, occuring when $w_1' = \cdots = w_M'$ and $w_1 = \cdots = w_N$.

We shall find it convenient to extend the PR to the *fundamental regime* (FR), where λ is still real and positive, (33)–(35) are satisfied, but the complex numbers w_I', and w_J need not be pure imaginary. On the contrary, we shall find it helpful at times to focus attention on the case when they are real.

2.1. Staggered Fields

Now add the staggered fields E, E'. If we share the resulting energy of each arrow between its end points, then these energies can be incorporated into $\epsilon_1,\ldots, \epsilon_6$. From Fig. 1 we see that the effect of this for the homogeneous lattice is to add (subtract) an energy $E - E'$ to ϵ_6 (ϵ_5) on A sites, and to ϵ_5 (ϵ_6) on B sites. Energies ϵ_1, ϵ_2, ϵ_3, ϵ_4 are unchanged.

Again we generalize to an inhomogeneous lattice and suppose that instead of adding two fields E, E', we add a set of "vertex staggered fields" $E_{I,J}$ such that at site (I, J) the vertex energies ϵ_j are incremented by $\Delta\epsilon_j$, where

$$\Delta\epsilon_j = 0, \quad j = 1, 2, 3, 4; \qquad \Delta\epsilon_5 = \mp E_{I,J}; \qquad \Delta\epsilon_6 = \pm E_{I,J} \tag{36}$$

The upper choice of sign in (36) applies on A sites, the lower on B sites.

2.2. Local Staggered Polarizations

We now want to define a site-dependent spontaneous staggered polarization corresponding to the field $E_{I,J}$ (for some particular values of I and J). We encounter a problem in that unless we specify the w_I', w_J, and $E_{I,J}$ (which we do not want to do), the limiting free energy per vertex f of a large lattice, normally given by (5), is not defined.

The easiest, though nonrigorous, way out of this dilemma seems to be to regard f as defined by its "low-temperature" series expansion. At low temperatures we see from (2), (8), and (9) that for the homogeneous system $c \gg (a, b)$, $\Delta \ll -1$, λ is large and $t \ll 1$.

Similarly, for the inhomogeneous system defined above we can consider the purely ordered state when $\lambda \to \infty$, while $\lambda^{-1} w_I'$, $\lambda^{-1} w_J$, and $\beta E_{I,J}$ remain fixed, satisfying (35). From (31) it follows that at each site

$$| c_{I,J} | \gg \max(| a_{I,J} |, | b_{I,J} |) \tag{37}$$

The dominant contribution to the partition function therefore comes from arrangements of arrows on the lattice such that at each vertex the arrows are in configuration 5 or 6 of Fig. 1. There are two such arrangements, as shown in Fig. 2. Neglecting all other arrangements, it follows that in the completely ordered state the partition function is

$$Z = 2Z_0 \cosh \left(\beta \sum_{I=1}^{M} \sum_{J=1}^{N} E_{I,J}\right) \tag{38}$$

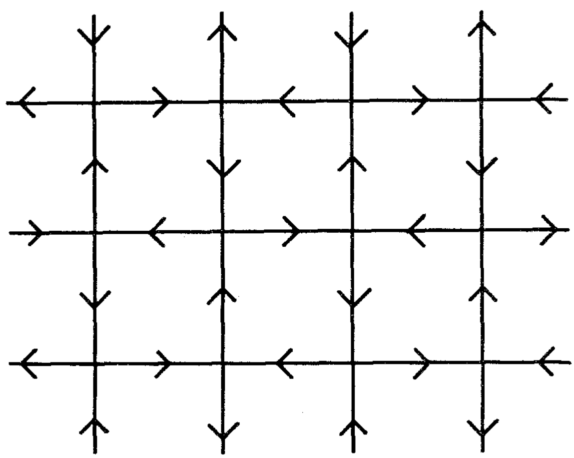

Fig. 2. One of the two zero-temperature purely ordered states of the lattice. The other state is obtained by reversing all arrows.

where

$$Z_0 = \prod_{I=1}^{M} \prod_{J=1}^{N} c_{I,J} \tag{39}$$

is the partition function in zero staggered fields.

In principle one can generalize the methods used by Nagle[3] for the homogeneous system and develop a perturbation expansion of Z in increasing powers of t. To any given order in this expansion the only contributions come from arrow arrangements on the lattice that differ from the two completely ordered arrangements by reversing a finite (i.e., independent of M, N) number of arrows. Thus to any given order we can take M, N sufficiently large that these arrangements can be classified uniquely as being either perturbations on the state shown in Fig. 2, or on the state obtained by reversing all arrows in Fig. 2. Calling the contribution from the former states Z_+ and the latter Z_-, we have

$$Z = Z_+ + Z_- \tag{40}$$

Further, on performing the expansion, we soon find ourselves expecting that

$$\ln Z_\pm = -\beta \sum_{I=1}^{M} \sum_{J=1}^{N} f_\pm(I, J) \tag{41}$$

where to any given order in the perturbation expansion $f_\pm(I, J)$ is independent of M and N, being a function only of the Boltzmann weights of the sites in some neighborhood of (I, J). For instance, to order t^2 we can choose

$$\begin{aligned} f_\pm(I, J) = {} & \epsilon_5(I, J) \mp E_{I,J} \\ & + t^2 \exp[\mp \beta(E_{I,J} + E_{I,J+1} + E_{I+1,J} + E_{I+1,J+1})] \\ & + O(t^3) \end{aligned} \tag{42}$$

Thus we can think of $f_\pm(I, J)$ as local free energies corresponding to the two possible ordered thermodynamic states of the lattice.

We define a local staggered polarization $P(I, J)$ by

$$P(I, J) = \beta^{-1}\, \partial(\ln Z)/\partial E_{I,J} \tag{43}$$

Suppose we hold the mean of the $E_{I,J}$ fixed at some positive value and let M, N become large. Then from (38) and the above equations, for sufficiently small t, Z_- will be exponentially small compared with Z_+. Thus in this rather ill-defined but plausible limit

$$P(I, J) = \beta^{-1}\, \partial(\ln Z_+)/\partial E_{I,J} \tag{44}$$

To any given order in perturbation expansion, only a finite (i.e., independent of M, N) number of local free energies in (41) depend on $E_{I,J}$, so we expect the r.h.s. of (44) to be independent of M, N for a sufficiently large lattice.

Having taken (in some sense) the limit of a large lattice, we now define a spontaneous local staggered polarization $P_0(I, J)$ by

$$P_0(I, J) = [P(I, J)]_{E_{1,1},\dots,E_{M,N}\to 0^+} \tag{45}$$

Comparing the above procedure with (5), (6), and (12), we see that P_0 for homogeneous staggered fields is obtained by setting all $E_{I,J}$ equal to E and differentiating $(MN\beta)^{-1}\, ln\, z_+$ with respect to E. Thus

$$P_0 = (MN)^{-1} \sum_{I=1}^{M} \sum_{J=1}^{N} P_0(I, J) \tag{46}$$

i.e., P_0 is the average of the local polarizations.

In an earlier paper[9] we evaluated $P_0(I, J)$ to order t^4 and found that

$$P_0(I, J) = 1 - 4t^2 + 4t^4 + \cdots \tag{47}$$

which is a remarkably simple result. It suggests that $P_0(I, J)$ may in fact be independent of I and J, and of $w_1',\dots, w_M'$ and $w_1,\dots, w_N$. In the next section we shall present a plausible (but unfortunately again nonrigorous) argument that this is so.

3. TRANSFER MATRICES

We now set up the row-to-row transfer matrices of the model and express $P_0(I, J)$ as a matrix element.

We consider the inhomogeneous model, with Boltzmann weights given by (31). Thus there are M transfer matrices $\mathbf{T}_1,\dots, \mathbf{T}_M$, one for each row of the lattice.

Again we first consider the case of zero staggered fields. Let Φ and Φ' be the configurations of the arrows on the rows of vertical bonds below and above row I of sites. (In each row there are N bonds, each arrow can be up or down, so Φ and Φ' each have 2^N values.)

The 2^N by 2^N transfer matrix $\mathbf{T}_I$ for row I then has elements

$$T_I(\Phi, \Phi') = \sum_{C} \omega(C, I, 1)\omega(C, I, 2) \cdots \omega(C, I, N) \tag{48}$$

where the sum is over all arrangements C of intervening horizontal arrows and $\omega(C, I, J)$ is the corresponding Boltzmann weight (a, b, or c) of the arrow configuration at the site (I, J).

The zero-field partition function of the lattice is then

$$Z_0 = \mathrm{Tr}(\mathbf{T}_1\mathbf{T}_2 \cdots \mathbf{T}_M) \tag{49}$$

Now add the local staggered fields $E_{1,1}, \ldots, E_{M,N}$ as in (36). We can do this by sharing the field energies between the vertical arrows, giving an energy $\frac{1}{2}E_{I,J}$ to vertical arrows that point into A sites (I, J) or out of B sites (I, J), and $-\frac{1}{2}E_{I,J}$ for other arrows. (Thus each arrow gets two contributions, one from each end point.)

Define operators $\mathbf{S}_1, \ldots, \mathbf{S}_M$ by

$$\mathbf{S}_I = \sum_{J=1}^{N} (-1)^J E_{I,J}\sigma_J^z \tag{50}$$

where σ_J^z is the Pauli operator acting on the arrow (or "spin") in column J. Further, let

$$\mathbf{V}_I = \exp(-\tfrac{1}{2}\beta\mathbf{S}_I) \tag{51}$$

then the transfer matrix for row I in the presence of fields is

$$\begin{aligned} \mathscr{T}_I &= \mathbf{V}_I\mathbf{T}_I\mathbf{T}_I^{-1} \qquad \text{if} \quad I \text{ is even} \\ &= \mathbf{V}_I^{-1}\mathbf{T}_I\mathbf{V}_I \qquad \text{if} \quad I \text{ is odd} \end{aligned} \tag{52}$$

and the partition function is

$$Z = \mathrm{Tr}(\mathscr{T}_1\mathscr{T}_2 \cdots \mathscr{T}_M) \tag{53}$$

3.1. Eigenvalue Degeneracy

Again we find it helpful to consider a perturbation expansion about the completely ordered state of Fig. 2.

Let

$$\Phi_+ = \downarrow\uparrow\downarrow\uparrow \cdots \downarrow\uparrow, \qquad \Phi_- = \uparrow\downarrow\uparrow\downarrow \cdots \uparrow\downarrow \tag{54}$$

We see from Fig. 2 that only these row configurations occur in the completely ordered state. Thus the dominant elements of the transfer matrix $\mathbf{T}_I$ are

$$T_I(\Phi_+, \Phi_-) = T_I(\Phi_-, \Phi_+) = \prod_{J=1}^{N} c_{I,J} \tag{55}$$

Let $\Lambda_{0,I}$ and $\Lambda_{1,I}$ be the two largest (in magnitude) eigenvalues of $\mathbf{T}_I$, and $|0\rangle$ and $|1\rangle$ their corresponding eigenvectors. Suppose we develop perturbation expansions for these about the completely ordered state, e.g., in increasing powers of t. Then to order t^r we find the only elements of $\mathbf{T}_I$ that enter the calculation are $T_I(\Phi, \Phi')$ and $T_I(\Phi', \Phi)$, where Φ differs from Φ_+, and Φ' from Φ_-, by at most r reversals of arrows.

If $r < \frac{1}{2}N$ the transfer matrix therefore effectively breaks up into two blocks, one at top right, the other at the lower left, and the eigenvalue problem naturally decomposes into finding vectors $|+\rangle$ and $|-\rangle$ and an eigenvalue μ_I such that

$$\mathbf{T}_I \mid +\rangle \simeq \mu_I \mid -\rangle, \qquad \mathbf{T}_I \mid -\rangle \simeq \mu_I \mid +\rangle \tag{56}$$

Here $\mid +\rangle$ has nonzero elements only for configurations differing from Φ_+ by reversing at most r arrows. Similarly for $|-\rangle$ and Φ_-. Thus if $r < \frac{1}{2}N$, there are no configurations for which $\mid +\rangle$ and $|-\rangle$ both have nonzero elements. Since $\sigma_J{}^z$, $\mathbf{S}_I$ are diagonal operators (independent of t), it follows that

$$\begin{aligned} \langle + \mid -\rangle \simeq \langle - \mid +\rangle \simeq \langle + \mid \sigma_J{}^z \mid -\rangle \simeq \langle - \mid \sigma_J{}^z \mid +\rangle \\ \simeq \langle + \mid \mathbf{S}_I \mid -\rangle \simeq \langle - \mid \mathbf{S}_I \mid +\rangle \simeq 0 \end{aligned} \tag{57}$$

We use the approximation signs to denote the fact that the equations are true only to order t^r, $r < \frac{1}{2}N$. For nonzero t and finite (but large) N we expect (56) and (57) to be in error by terms that decay exponentially with N.

The matrix $\mathbf{T}_I$ is symmetric with respect to reversing all arrows, i.e., it commutes with the operator

$$\mathbf{R} = \sigma_1{}^x \sigma_2{}^x \cdots \sigma_N{}^x \tag{58}$$

From (56) it follows that

$$|-\rangle = \mathbf{R} \mid +\rangle, \qquad \mid +\rangle = \mathbf{R} \mid -\rangle \tag{59}$$

Also, from (50), $\mathbf{S}_I$ anticommutes with $\mathbf{R}$, so we can define

$$s_I = \langle + \mid \mathbf{S}_I \mid +\rangle = -\langle - \mid \mathbf{S}_I \mid -\rangle \tag{60}$$

Here $\langle + \mid$ and $\langle - \mid$ are row vectors having nonzero elements only for the same configurations as $\mid +\rangle$ and $|-\rangle$, respectively, and satisfying an analog of (56), namely

$$\langle + \mid \mathbf{T}_I \simeq \mu_I \langle - \mid, \qquad \langle - \mid \mathbf{T}_I \simeq \mu_I \langle + \mid \tag{61}$$

This ensures that if $\langle +' \mid$ is a solution of (61) for some other eigenvalue μ_I', then $\langle +' \mid +\rangle = 0$. In this sense the vectors are orthogonal.

The reader who finds this confusing is advised to focus his attention on the case when the w_I' and w_J are real. The transfer matrix $\mathbf{T}_I$ is then Hermitian and in the usual way $\langle \pm \mid$ is the complex conjugate of the transpose of $\mid \pm\rangle$.

In any event we require for the moment that the vectors be normalized, so that

$$\langle + \mid + \rangle = \langle - \mid - \rangle = 1 \tag{62}$$

From (56) it is apparent that the largest eigenvalues of $\mathbf{T}_I$ are

$$\Lambda_{0,I} \simeq \mu_I, \qquad \Lambda_{1,I} \simeq -\mu_I \tag{63}$$

and the corresponding eigenvectors are

$$\mid 0\rangle = \mid +\rangle + \mid -\rangle, \qquad \mid 1\rangle = \mid +\rangle - \mid -\rangle \tag{64}$$

Thus to order $r < \frac{1}{2}N$ in perturbation theory the largest eigenvalues are degenerate in the sense that they have the same magnitude. We have observed this phenomenon explicitly in earlier papers.[9,12]

The inhomogeneous model defined by (31) has one very important property, namely that the transfer matrices $\mathbf{T}_1, \ldots, \mathbf{T}_M$ all commute and have the same eigenvectors, i.e., the eigenvectors of $\mathbf{T}_I$ do not depend on the row parameter w_I' (nor of course on any other of $w_1', \ldots, w_M'$).

Thus the vectors $\mid 0\rangle$, $\mid 1\rangle$, $\mid +\rangle$, and $\mid -\rangle$ are all independent of I. From (49) it follows that in zero field and for M large (and even)

$$Z_0 \simeq 2\mu_1\mu_2 \cdots \mu_M \tag{65}$$

The argument is now similar to that used by Yang[17] and Schultz *et al.*[16] for the spontaneous magnetization of the Ising model. Introduce the fields $E_{I,J}$ and suppose they are sufficiently small that $\mathbf{S}_I$ can be treated by first-order perturbation theory in (51) and (52), but that M is large enough for the cumulative effect of $\mathbf{S}_1, \ldots, \mathbf{S}_M$ in (53) to be appreciable.

In the representation which diagonalizes $\mathbf{T}_1, \ldots, \mathbf{T}_M$, each $\mathscr{T}_I$ is still "almost diagonal," and its largest elements lie in the subspace spanned by $\mid 0\rangle$ and $\mid 1\rangle$. For large M we expect the effect of all other elements to become negligible. Thus we replace each $\mathscr{T}_I$ by its 2 by 2 projection onto the subspace spanned by $\mid 0\rangle$ and $\mid 1\rangle$, or equivalently and more conveniently by $\mid +\rangle$ and $\mid -\rangle$. Thus from (56), (57), and (60) we can set

$$\mathbf{T}_I = \mu_I \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \mathbf{S}_I = s_I \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{66}$$

Substituting these into (51)–(53), we obtain

$$Z = 2Z_0 \cosh[\beta(s_1 + s_2 + \cdots + s_M)] \tag{67}$$

Let

$$P_J = (-1)^J \langle + \mid \sigma_J^z \mid + \rangle \tag{68}$$

Then from (50) and (60)

$$s_I = \sum_{J=1}^{N} E_{I,J} p_J \tag{69}$$

so

$$Z = 2Z_0 \cosh \left(\beta \sum_{I=1}^{M} \sum_{J=1}^{N} E_{I,J} p_J \right) \tag{70}$$

From (54) and (68) we can see that the p_J are all positive, at least for sufficiently small t, so from (40) and the discussion after (43)

$$Z_+ = Z_0 \exp \left(\beta \sum_{I=1}^{M} \sum_{J=1}^{N} E_{I,J} p_J \right) \tag{71}$$

From (44) and (45) the local spontaneous staggered polarization is

$$P_0(I, J) = p_J \tag{72}$$

Thus $P_0(I, J)$ is independent of I. Also, since $| + \rangle$ is independent of $w_1', \ldots, w_M'$, so is $P_0(I, J)$.

However, instead of dividing the vertex field energies $E_{I,J}$ among the vertical arrows as we did to obtain (50), we can divide them among the horizontal arrows and perform the above reasoning with column, rather than row, transfer matrix matrices. In this way we find that $P_0(I, J)$ is also independent of J and $w_1, \ldots, w_N$.

Thus, using (46), the overall and local spontaneous staggered polarizations P_0 and $P_0(I, J)$, together with the matrix elements p_J, must all be the same function of λ (or t) only, as we surmised from our series expansion (47).

This is a truly remarkable result—it means that to obtain P_0 for the normal homogeneous lattice, it is sufficient to evaluate the matrix element (68) for any J and any values of $w_1, \ldots, w_N$, so long as the system is sufficiently close to the completely ordered state.

"Sufficiently close" presumably means that the perturbation expansions in powers of $t = e^{-\lambda}$ should converge, and that the parameters should lie in some region including the completely ordered state where no other eigenvalue crosses (in magnitude) $\Lambda_{0,I}$ or $\Lambda_{1,I}$. From the result (13) (as well as the other previous results given in Section 1) the first condition is apparently satisfied if $\lambda > 0$. The second condition is more difficult, but from the behavior when $\lambda \to \infty$, and in the physical regime of the homogeneous model, we conjecture that it is sufficient for the system to be in the FR, i.e., for (35) to be satisfied.

From (57), (59), (62), and (64) we can verify that

$$\langle 0 \mid 0 \rangle = \langle 1 \mid 1 \rangle = 2 \tag{73}$$

$$\langle 0 \mid \sigma_J{}^z \mid 1 \rangle = \langle 1 \mid \sigma_J{}^z \mid 0 \rangle = 2\langle + \mid \sigma_J{}^z \mid + \rangle \tag{74}$$

So from (68)

$$p_J{}^2 = \langle 0 \mid \sigma_J{}^z \mid 1 \rangle \langle 1 \mid \sigma_J{}^z \mid 0 \rangle / \langle 0 \mid 0 \rangle \langle 1 \mid 1 \rangle \tag{75}$$

This expression for p_J has the advantage that it involves only the eigenvectors of $\mathbf{T}_I$, for which exact expressions are available,[2,9] and is independent of their normalizations.

4. ASSUMPTIONS

Almost the only rigorous remark made so far is that $\mathbf{T}_1, \ldots, \mathbf{T}_M$ commute and have the same eigenvectors. It therefore seems worthwhile consolidating our assumptions, which we can list as follows.

(i) If λ, $w_1', \ldots, w_M'$ and $w_1, \ldots, w_N$ lie in some closed subregion of the FR, then the limit (taken through even values of N)

$$P_0 = \lim_{N \to \infty} [(\langle 0 \mid \sigma_N{}^z \mid 1 \rangle \langle 1 \mid \sigma_N{}^z \mid 0 \rangle / \langle 0 \mid 0 \rangle \langle 1 \mid 1 \rangle)^{1/2}] \tag{76}$$

exists and is independent of $w_1', \ldots, w_M'$, and $w_1, \ldots, w_N$.

(ii) P_0 thus defined is the spontaneous staggered polarization.

(iii) $\Lambda_{0,I}$ and $\Lambda_{1,I}$ are the largest (in magnitude) eigenvalues of $\mathbf{T}_I$ throughout the FR, all other eigenvalues being strictly less in magnitude.

Since $\mid 0 \rangle$ and $\mid 1 \rangle$ are independent of $w_1', \ldots, w_M'$, obviously P_0 must be, too. The justifications for the other assumptions in (i) and (ii) have been given above. When these are taken into account, assumptions (i) and (ii) appear to be little worse than those commonly made for the spontaneous magnetization of the Ising model.[16]

Assumption (iii) ensures that no third eigenvalue crosses (in magnitude) $\Lambda_{0,I}$ or $\Lambda_{1,I}$ inside the FR. This enables us to identify the vectors $\mid 0 \rangle$ and $\mid 1 \rangle$ by continuity arguments from the solution in the completely ordered state. The assumption fits the behavior in the completely ordered state and makes sense in the physical regime (a, b, c positive), where the FR becomes the region $c > a + b$. If necessary, we could weaken this assumption by contracting the FR—our results would then simply be valid only in this contracted region.

The rest of the working is completely rigorous. We evaluate the square root in (76) exactly for finite, even N (taking $\frac{1}{2}N$ to be a prime number) when

$$w_J = \tfrac{1}{2}\pi(2J - N - 1)/N, \qquad J = 1,..., N \tag{77}$$

[Thus $w_1 ,..., w_N$ are all real and we can certainly satisfy (35).] We then take the limit $N \to \infty$ and obtain P_0.

5. EIGENVECTORS AND EIGENVALUE OF T_I

The elements $T_I(\Phi, \Phi')$ of the transfer matrix are zero unless Φ and Φ' have the same number n of down arrows. Thus $\mathbf{T}_I$ breaks up into $N + 1$ diagonal blocks ($n = 0,..., N$) and we can look at one such diagonal block with a given value of n.

A configuration Φ can then be specified by $x_1 ,..., x_n$, the locations of the down arrows, arranged so that

$$1 \leqslant x_1 < x_2 < \cdots < x_n \leqslant N \tag{78}$$

We write $|f\rangle$ for a typical eigenvector, and $f(x_1 ,..., x_n)$ for its element corresponding to the configuration Φ. These elements can be obtained by a generalized Bethe ansatz[9].

We find it convenient to introduce a direct electric field H acting on the single column of horizontal bonds between columns N and 1. (Later we shall let $H \to 0$; this avoids some mathematical problems in calculating normalization factors.)

Then from Ref. 9, after making several notational changes, we find that

$$f(x_1 ,..., x_n) = \sum_U \left\{ \prod_{1 \leqslant i < j \leqslant n} \frac{\sin(u_i - u_j + 2\eta)}{\sin(u_i - u_j)} \right\} \times \varphi(u_1 , x_1)\varphi(u_2 , x_2) \cdots \varphi(u_n , x_n) \tag{79}$$

where the functions $\varphi(u, x)$ are defined by

$$\varphi(u, x) = \frac{1}{\sin(u - w_x - \eta)} \prod_{y=1}^{x-1} - \frac{\sin(u - w_y + \eta)}{\sin(u - w_y - \eta)} \tag{80}$$

The summation in (79) is over all $n!$ permutations U of $u_1 ,..., u_n$. These are to be chosen so as to satisfy the equations

$$\prod_{J=1}^{N} - \frac{\sin(u_i - w_J + \eta)}{\sin(u_i - w_J - \eta)} = -h^2 \prod_{j=1}^{n} \frac{\sin(u_i - u_j + 2\eta}{\sin(u_i - u_j - 2\eta)} \tag{81}$$

for $i = 1,..., n$, where

$$h = e^{-\beta H} \tag{82}$$

The corresponding eigenvalue Λ_I of $\mathbf{T}_I$ is

$$\Lambda_I = \left[h^{-1} a_{I,1} \cdots a_{I,N} \prod_{j=1}^{n} \sin(w_I' - u_j - 2\eta) + h b_{I,1} \cdots b_{I,N} \prod_{j=1}^{n} \sin(w_I' - u_j + 2\eta) \right] \times \left[\prod_{j=1}^{n} -\sin(w_I' - u_j) \right]^{-1} \tag{83}$$

Note that Eqs. (79)–(81) do not involve w_I'. Thus $\mathbf{T}_1, \ldots, \mathbf{T}_M$ all have the same eigenvectors, as we have stated.

We define $\langle f |$ to be the row vector whose transpose is the eigenvector of the transpose of $\mathbf{T}_I$, with eigenvalue Λ_I. This ensures that two eigenvectors $| f \rangle$ and $| f' \rangle$ with different eigenvalues are orthogonal in the sense that

$$\langle f | f' \rangle = \langle f' | f \rangle = 0 \tag{84}$$

Transposing $\mathbf{T}_I$ is equivalent to interchanging the Boltzmann weights $a_{I,J}$ and $b_{I,J}$ (for all J) and negating H. From (32) this is accomplished by negating η, $\rho_{I,J}$, and H. From (81) we can leave $u_1, \ldots, u_n$ unchanged, while from (83) Λ_I is then unchanged.

Thus the elements of $\langle f |$ are given by (79) and (80) with only η negated.

Perhaps this will appear clearer if we consider the case when the w_I' and w_J are real but η and the $\rho_{I,J}$ are pure imaginary. (This lies in the FR and is a case we shall return to later.) The $a_{I,J}$ and $b_{I,J}$ are then complex conjugates, while $c_{I,J}$ is real. Thus $\mathbf{T}_I$ is a Hermitian matrix. Provided $u_1, \ldots, u_n$ are real (they are for the two maximum eigenvalues), negating η in (79) and (80) is equivalent to complex conjugation. Thus $\langle f |$ is then the complex conjugate of the transpose of $| f \rangle$, as we expect.

We shall also consider another eigenvector $| g \rangle$, defined in the same way as $| f \rangle$, but with $u_1, \ldots, u_n$ replaced by $v_1, \ldots, v_n$ and the direct field H set equal to zero, i.e., $h = 1$. Some quantities that we shall need frequently are

$$\mu = (\sin 2\eta)^n \tag{85a}$$

$$\gamma = \prod_{1 \leqslant i < j \leqslant n} \sin(u_i - u_j) \tag{85b}$$

$$\gamma' = \prod_{1 \leqslant i < j \leqslant n} \sin(v_j - v_i) \tag{85c}$$

$$\delta = \prod_{i=1}^{n} \prod_{j=1}^{n} \sin(u_i - v_j) \tag{85d}$$

$$A_N(u) = \prod_{J=1}^{N} \sin(u - w_J - \eta) \tag{85e}$$

$$B_N(u) = \prod_{J=1}^{N} \sin(u - w_J + \eta) \tag{85f}$$

$$\xi_N = \prod_{i=1}^{n} A_N(u_i), \qquad \xi_N{}' = \prod_{i=1}^{n} B_N(v_i) \tag{85g}$$

5.1. Analytic Properties of Eigenvectors

We can think of the elements of $|f\rangle$, as defined by (79) and (80) [ignoring (81) for the moment], as functions of $u_1 ,..., u_n$. Possible poles occur when $u_i = u_j$ or $u_i = w_x + \eta$ for any i, j, x $(i \neq j)$. These poles can be removed by defining

$$F(X) = \gamma \xi_N f(X) \tag{86}$$

Regard $F(X)$ as a function of u_1 (say). Then it is a sum of n terms, each of the form

$$\text{const} \times \prod_{j=1}^{N+n-2} \sin(u_1 - d_j) \tag{87}$$

where $d_1 ,..., d_{N+n-2}$ are independent of u_1. Expanding each sine as $-\frac{1}{2}i$ times the difference of two imaginary exponentials, it follows that $F(X)$ is of the form

$$p_m(u_1) \equiv \sum_{j=0}^{m} C_j \exp[i(2j - m)u_1] \tag{88}$$

where $m = N + n - 2$ and the C_j are independent of u_1.

Equation (88) defines a class of entire functions of u_1. We encounter such functions often enough in the working to warrant giving them a name. Let us call them *p-functions of degree m.*

We now establish an elementary theorem that we shall use frequently.

Theorem 1. If two p-functions of degree m are equal at $m + 1$ values of their argument, these values being distinct to modulus π, then the functions are identically equal.

Proof. Consider $e^{imu}p_m(u)$. From the definition (88) this is a polynomial of degree m in the variable e^{2iu}. If two polynomials of degree m are equal for $m + 1$ distinct values of their argument, then they are identically equal. This proves the theorem.

From now on we use "distinct" to mean "distinct to modulus π".

Returning to considering $f(X)$ as defined by (79), note that it is by construction a symmetric function of $u_1, \ldots, u_n$. Thus the apparent simple pole occurring when a u_i equals a u_j ($i \neq j$) must be spurious, having residue zero. [If it were nonzero, then sufficiently close to $u_i = u_j$ we would have $f(X) \propto 1/\sin(u_i - u_j)$, which is antisymmetric in u_i, u_j.]

It follows that $\xi_N f(X)$ is an entire function of $u_1, \ldots, u_n$ and more strongly that

$$\xi_N f(X) = \text{symmetric function of } u_1, \ldots, u_n \text{, being a } p\text{-function of degree } N-1 \text{ in each of } u_1, \ldots, u_n \tag{89}$$

6. MATRIX ELEMENTS

Defining $|f\rangle$, $|g\rangle$, and $\langle g|$ as in Section 5, we see that

$$\begin{aligned}
\xi_N \xi_N' \langle g \mid f\rangle &= \xi_N \xi_N' \sum_X g^*(x_1, \ldots, x_n) f(x_1, \ldots, x_n) \\
&= \sum_U \sum_V \prod_{1 \leqslant i < j \leqslant n} \{[\sin(u_i - u_j + 2\eta) \sin(v_j - v_i + 2\eta)] \\
&\quad \times [\sin(u_i - u_j) \sin(v_j - v_i)]^{-1}\} \\
&\quad \times \sum_X \prod_{j=1}^{n} \prod_{y=1}^{x_j - 1} [\sin(v_j - w_y - \eta) \sin(u_j - w_y + \eta)] \\
&\quad \times \prod_{y=x_j+1}^{N} [\sin(v_j - w_y + \eta) \sin(u_j - w_y - \eta)]
\end{aligned} \tag{90}$$

where the summation over U (V) is over all $n!$ permutations of $u_1, \ldots, u_n$ ($v_1, \ldots, v_n$), and the X summation is over all integers $x_1, \ldots, x_n$ satisfying (78).

This is a very complicated expression to handle. Hitherto the only progress has been made by Gaudin[18] for the similar problem of the one-dimensional Bose gas, but then only for scattered states on an infinite line.

It turns out, however, that the r.h.s. of (90) can be simplified to a form which makes its dependence on N and $w_1, \ldots, w_N$ clearer. We state the result here and give an inductive proof in Appendix A. We find that

$$\begin{aligned}
\xi_N \xi_N' \langle g \mid f\rangle &= (\mu\gamma\gamma')^{-1} \sum_V \epsilon_V \sum_1 \sum_2 \cdots \sum_n \\
&\quad \times \prod_{i=1}^{n} \left[\frac{A_N(u_i) B_N(v_i)}{\sin(u_i - v_i)} \prod_{j=1 \neq i}^{n} \sin(u_i - v_j + 2\eta) \right]
\end{aligned} \tag{91}$$

where ϵ_V is the signature ($+1$ or -1) of the permutation V, and $\sum_i$ means we are to add the summand and the summand with (u_i, v_i) interchanged, i.e., to sum over the two permutations of (u_i, v_i). Thus there are $n! \times 2^n$ additive terms on the r.h.s. of (91).

To make these points clearer, we write (91) explicitly for $n = 2$. Define

$$\begin{aligned} S(u, u \mid v, v') = {} & A_N(u)\, A_N(u')\, B_N(v)\, B_N(v') \\ & \times \sin(u - v' + 2\eta) \sin(u' - v + 2\eta) \\ & [\sin(u - v) \sin(u' - v')]^{-1} \end{aligned} \tag{92}$$

Then the r.h.s. of (92) becomes (performing the summations progressively from right to left)

$$\begin{aligned} & (\mu\gamma\gamma')^{-1}[S(u_1, u_2 \mid v_1, v_2) + S(u_1, v_2 \mid v_1, u_2) \\ & \quad + S(v_1, u_2 \mid u_1, v_2) + S(v_1, v_2 \mid u_1, u_2) - S(u_1, u_2 \mid v_2, v_1) \\ & \quad - S(u_1, v_1 \mid v_2, u_2) - S(v_2, u_2 \mid u_1, v_1) - S(v_2, v_1 \mid u_1, u_2)] \end{aligned} \tag{93}$$

To evaluate (76), we also need $\langle g \mid \sigma_N^z \mid f \rangle$. Let

$$\tau_N = \tfrac{1}{2}(1 + \sigma_N^z) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{94}$$

be an operator acting on the arrow in column N. Then

$$\langle g \mid \sigma_N^z \mid f \rangle = 2\langle g \mid \tau_N \mid f \rangle - \langle g \mid f \rangle \tag{95}$$

Now $\langle g \mid \tau_N \mid f \rangle$ is formed in the same way as $\langle g \mid f \rangle$, except that no down arrow is allowed in column N. Thus $\langle g \mid \tau_N \mid f \rangle$ is given by Eq. (90) for $\langle g \mid f \rangle$, but with the X summation restricted to the domain $1 \leqslant x_1 < \cdots < x_n \leqslant N - 1$. Noting that N does not explicitly enter Eqs. (79) and (80), it follows that

$$\begin{aligned} \langle g \mid \tau_N \mid f \rangle = {} & \langle g \mid f \rangle \text{ as given by (91), but with } N \\ & \text{replaced by } N - 1 \text{ in} \\ & \xi_N, \xi_N', A_N(u), B_N(v) \end{aligned} \tag{96}$$

6.1. Elimination of *N*

From (85g) and (91) we see that N enters the expression (91) for $\langle g \mid f \rangle$ only via the ratios $B_N(u_i)/A_N(u_i)$ and $A_N(v_i)/B_N(v_i)$ ($i = 1, \ldots, n$). These are precisely the ratios that occur on the l.h.s. of (81) (and its analog for $v_1, \ldots, v_n$ with $h = 1$).

We first explicitly consider the effect of interchanging (u_i, v_i) for $i = k_1, ..., k_r$ in (91) and then use Eq. (81) and its v analog. This gives

$$\langle g \mid f \rangle = (\mu\delta)^{-1} R_n(u_1, ..., u_n \mid v_1, ..., v_n) \tag{97}$$

where

$$\begin{aligned}
&R_n(u_1, ..., u_n \mid v_1, ..., v_n) \\
&\quad = (\gamma\gamma')^{-1} \delta \sum_V \epsilon_V \Big\{ \prod_{i=1}^{n} [\sin(u_i - v_i)]^{-1} \\
&\qquad \times \sum_{r=0}^{n} (-h^2)^r \sum_{1 \leqslant k_1 < \cdots < k_r \leqslant n} \Big[\prod_{i \neq K} \prod_{j \neq K, i} \sin(u_i - v_j + 2\eta) \Big] \\
&\qquad \times \Big[\prod_{i = K} \prod_{j = K \neq i} \sin(v_i - u_j + 2\eta) \Big] \\
&\qquad \times \Big\{ \prod_{i \neq K} \prod_{j = K} [\sin(u_j - u_i + 2\eta) \sin(v_i - v_j + 2\eta)] \Big\} \Big\}
\end{aligned} \tag{98}$$

Here K denotes the set of integers $k_1, ..., k_r$. The products denoted $i = K$ are over the r values $i = k_1, k_2, ..., k_r$; those denoted $i \neq K$ are over the $n - r$ values $i = 1, ..., n$ excluding $k_1, ..., k_r$. Similarly for j. Each summation applies to *all* the terms following it.

Similarly, from (96) we find that $\langle g \mid \tau_N \mid f \rangle = \langle g \mid f \rangle$ as given by (97) and (98) but with an extra term in the summand of (98), namely

$$\prod_{i=K} [\sin(u_i - w_N - \eta) \sin(v_i - w_N + \eta) / \sin(u_i - w_N + \eta) \sin(v_i - w_N - \eta)] \tag{99}$$

6.2. Recursive Definition of R_n

The expression (98) is still extremely complicated. (It is interesting to note that it reduces to an expression similar to Gaudin's $\tilde{\Delta}$ when $h = 0$.) However, it turns out that R_n can be defined by a comparatively simple recurrence relation.

Regard $u_1, ..., u_n$ and $v_1, ..., v_n$ as independent variables and R_n as defined by (85b)–(85d) and (98). The sum in (98) is by construction an antisymmetric function of $v_1, ..., v_n$, so it contains γ' as a factor. Also, the summand of the V summation is unaffected by applying the same permutation to both $u_1, ..., u_n$ and $v_1, ..., v_n$, so the V summation (with signature ϵ_V) could be replaced by a U summation (with signature ϵ_U). Hence the sum is also an antisymmetric function of $u_1, ..., u_n$ and must contain γ as a factor.

Also, the possible poles arising when a u_i equals a v_j are cancelled by the factor δ. Thus R_n is an entire function of $u_1, ..., v_n$.

Noting the symmetries and growth rates as any u_j or v_j tend to $\pm i\infty$, it follows that

$$R_n(u_1, ..., u_n \mid v_1, ..., v_n)$$
$$= \text{symmetric function of } u_1, ..., u_n \text{ and of } v_1, ..., v_n, \text{ being a } p\text{-function of degree } n-1 \text{ in each of } u_1, ..., u_n \text{ and } v_1, ..., v_n \tag{100}$$

Suppose that $u_n \to v_n = x$. Then the sum in (98) is dominated by those terms containing a factor $1/\sin(u_n - v_n)$, i.e., by those permutations V that leave v_n unchanged.

Considering the terms in the $r, k_1, ..., k_r$ summation, we find that if $k_r < n$, they are the same as if we replaced n by $n - 1$ and multiplied by a factor

$$\prod_{i=1}^{n-1} \sin(u_i - x + 2\eta) \sin(x - v_i + 2\eta) \tag{101a}$$

Alternatively, if $k_r = n$, they are the same as if we replaced n and r by $n - 1$ and $r - 1$ and multiplied by

$$-h^2 \prod_{i=1}^{n-1} [\sin(x - u_i + 2\eta) \sin(v_i - x + 2\eta)] \tag{101b}$$

Allowing also for the effects of letting $u_n \to v_n$ in γ, γ', δ, it follows that

$$R_n(u_1, ..., u_{n-1}, x \mid v_1, ..., v_{n-1}, x)$$
$$= \left\{ \prod_{i=1}^{n-1} [\sin(u_i - x + 2\eta) \sin(x - v_i + 2\eta)] - h^2 \prod_{i=1}^{n-1} [\sin(x - u_i + 2\eta)\, sin(v_i - x + 2\eta)] \right\}$$
$$\times R_{n-1}(u_1, ..., u_{n-1} \mid v_1, ..., v_{n-1}) \tag{102}$$

When $n = 1$ it is easy to see from (98) and (85a)–(85g) that

$$R_1(u \mid v) = 1 - h^2 \tag{103}$$

These equations (100), (102), and (103) are sufficient to determine R_n uniquely. To see this, suppose R_{n-1} is known and regard R_n as a function of u_n. It is a p-function of degree $n - 1$. Equation (102) gives its value when $u_n = v_n$. By symmetry it also determines R_n when $u_n = v_1, ..., v_n$. Thus R_n is known at n values, and if $v_1, ..., v_n$ are distinct, it follows from Theorem 1 that R_n is uniquely determined. The cases when two or more v_j's are equal can then be determined by continuity.

Note that when $h = 1$ the solution of (100), (102), and (103) is clearly $R_n \equiv 0$. Thus if $|f\rangle$ and $|g\rangle$ are both eigenvectors of the zero-field transfer matrix and $\delta \neq 0$ (i.e., no u_i equals any v_j), then from (97)

$$\langle g | f \rangle = 0 \tag{104}$$

Thus in this sense two distinct eigenvectors are orthogonal. This is a gratifying result, verifying elementary algebra, but does not help us calculate normalization factors. It is for this reason that we have asymmetrically introduced the parameter h, since it enables us to usefully define $\langle g | f \rangle$ for distinct $u_1, ..., u_n$ and $v_1, ..., v_n$, and later to take limits such as $h \to 1$, $u_i \to v_i$, $i = 1, ..., n$.

6.3. Relation Between $\langle g | f \rangle$ and $\langle g | \sigma_N^z | f \rangle$

One can obtain similar recursive relations for the expression (99) for $\langle g | \tau_N | f \rangle$, and hence $\langle g | \sigma_N^z | f \rangle$. We do this in Appendix B and find a rather remarkable result, namely that

$$\frac{\langle g | \sigma_N^z | f \rangle}{\langle g | f \rangle} = \frac{1 + h^2}{1 - h^2} - \frac{2h^2}{1 - h^2} \prod_{i=1}^{n} \frac{\sin(u_i - w_N - \eta)\sin(v_i - w_N + \eta)}{\sin(u_i - w_N + \eta)\sin(v_i - w_N - \eta)} \tag{105}$$

Thus if we can calculate R_n for arbitrary $h, u_1, ..., v_n$, then we can calculate $\langle g | f \rangle$ and $\langle g | \sigma_N^z | f \rangle$. Substituting the appropriate values of $u_1, ..., v_n$, we can then obtain the various matrix elements in (97) and hence the spontaneous staggered polarization.

An interesting check on our calculation is to evaluate the ratio (105) for the homogeneous lattice ($w_1 = \cdots = w_N = w$) when $h \to 1$ and $|g\rangle \to |f\rangle$. Taking products over $i = 1, ..., n$ of both sides of (81), we obtain

$$\prod_{i=1}^{n} \left[-\frac{\sin(u_i - w + \eta)}{\sin(u_i - w - \eta)} \right]^N = h^{2n} \tag{106}$$

From the v analog of (81) we get a similar equation, with u_i replaced by v_i and h by 1.

Taking the ratio of this with (106) and then taking the Nth root, remembering that we wish to choose the branch so that each $u_i \to v_i$ when $h \to 1$, and then substituting into (105), we get

$$\langle f | \sigma_N^z | f \rangle / \langle f | f \rangle = \lim_{h \to 1} (1 + h^2 - 2h^{2-2n/N})/(1 - h^2) = (N - 2n)/N \tag{107}$$

This is correct, being simply the mean difference of the number of up and down arrows in each row of the lattice, i.e., the direct vertical polarization (Lieb's[2] parameter y).

7. EVALUATION OF R_n AND P_0 FOR A SPECIAL INHOMOGENEOUS LATTICE

Unfortunately, we have not been able to obtain tractable expressions for the function $R_n(u_1,..., u_n \mid v_1,..., v_n)$ in general. However, in Appendix C we show that we can evaluate it exactly if

$$u_j = -ix + \tfrac{1}{2}\pi(2j - n - 1)/n \tag{108a}$$

$$v_j = -iy + \tfrac{1}{2}\pi(2j - n - 1)/n, \qquad j = 1,..., n \tag{108b}$$

where x and y are arbitrary constants, in general complex. Thus $u_1,..., u_n$ are uniformly distributed along a line segment of length π parallel to the real axis, with average value $-ix$. (Similarly for $v_1,..., v_n$, y.)

We find that

$$\begin{aligned} R_n = {} & (2i)^{n-n^2}(1 - t^2)^{-n}(1 - h^2)(1 - t^{2n}) \\ & \times \prod_{m=1}^{n-1} [(t^{m-n} - t^{n-m})(t^{-m} - h^2 t^m)e^{n(y-x)} \\ & - (t^{-m} - t^m)(h^2 t^{m-n} - t^{n-m})e^{n(x-y)}] \end{aligned} \tag{109}$$

The proof of this result that is given in Appendix C is valid only when n is a prime number. From assumption (i) in Section 4 this is sufficient for our purposes. However, it seems likely that (109) should be true for any integer n (it is for $n = 4$).

Given (108b), one can readily establish (e.g., by comparing zeros and growth rates at infinity the identity

$$\prod_{j=1}^{n} \sin(u - v_j) \equiv 2^{1-n} \cos[n(u + iy - \tfrac{1}{2}\pi)] \tag{110}$$

for all complex numbers u. Using (108a) and (85d), it then follows that

$$\delta = 2^{n-n^2} i^{-n^2} [\sinh n(x - y)]^n \tag{111}$$

while from (34) and (85a)

$$\mu = i^n (\sinh \lambda)^n \tag{112}$$

Substituting these results into (97), using $t = e^{-\lambda}$, and rearranging the terms in (109), we get

$$\begin{aligned} \langle g \mid f \rangle = {} & \alpha(\sinh \lambda)^{-2n} \sinh(n\lambda) \prod_{m=1}^{n-1} [\alpha(\sinh n\lambda) \cosh n(x - y) \\ & - 2(1 + h^2)(\sinh m\lambda) \sinh(n - m)\lambda \\ & - (1 - h^2) \sinh(n - 2m)\lambda] \end{aligned} \tag{113}$$

where

$$\alpha = (1 - h^2)/\sinh n(x - y) \tag{114}$$

7.1. A Special Inhomogeneous Lattice

Fortunately, there are values of $w_1, \ldots, w_N$, lying in the FR, for which the u_j (or v_j) corresponding to the eigenvectors $|0\rangle$ and $|1\rangle$ do satisfy (108a) and (108b), for all values of h. Thus we can use the above results to calculate matrix elements and the spontaneous staggered polarization P_0.

Let

$$N = 2n \tag{115}$$

(we expect[2] this subspace to contain the maximum eigenvalues), and

$$w_J = \tfrac{1}{2}\pi(2J - N - 1)/N \tag{116}$$

Thus $w_1, \ldots, w_N$ are spaced evenly along the line segment $(-\frac{1}{2}\pi, \frac{1}{2}\pi)$ of the real axis. The conditions (35) can be satisfied (e.g., by choosing each $w_I' = 0$) and the lattice parameters then lie in the FR.

Consider the equations (81) for $u_1, \ldots, u_n$ and suppose a solution of the form (108a) exists. Substituting (108a) and (116) into (81) and using identities analogous to (110), the equations become

$$\frac{\cos N(u_j + \eta - \frac{1}{2}\pi)}{\cos N(u_j - \eta - \frac{1}{2}\pi)} = -h^2 \frac{\cos n(u_j + ix + 2\eta - \frac{1}{2}\pi)}{\cos n(u_j + ix - 2\eta - \frac{1}{2}\pi)} \tag{117}$$

for $j = 1, \ldots, n$. Using (108a) once more, and also using (115) and (34), we obtain

$$\cosh N(x - \tfrac{1}{2}\lambda)/\cosh N(x + \tfrac{1}{2}\lambda) = h^2 \tag{118}$$

Thus the equations (181) are satisfied, provided x is chosen to satisfy (118), i.e.,

$$x = x_L \equiv (\tfrac{1}{2}i\pi L/n) + d(h) \tag{119}$$

where L is any integer and

$$d(h) = (4n)^{-1} \ln[(1 - h^2 t^N)/(h^2 - t^N)] \tag{120}$$

We choose the branch of the logarithm in (120) so as to be zero when $h = 1$.

From (108a) we see that incrementing L by two simply relabels the u_j and moves the end ones by π. This merely multiplies the eigenvector (79) by ± 1, so is not a new solution. It follows that there are just two solutions of (118) corresponding to distinct eigenvectors, namely $x = x_0$ and $x = x_1$.

For both solutions the u_j are then equally spaced along a line segment parallel to the real axis, those of one solution sitting in the middle of the spaces of the other.

From (83), the eigenvalue Λ_I is the ratio of two entire functions of w_I'. The conditions (81) ensure that the denominator is a factor of the numerator, so Λ_I is an entire function of w_I'. (As it must be, since the eigenvectors are independent of w_I' and the elements of the transfer matrix are entire functions —we have made these points before in connection with the eight-vertex model.[7]

Substituting (108a) and (116) into (83) and dividing the denominator into the numerator, using (119), we obtain

$$\begin{aligned}\Lambda_{L,I} = {} & (1 - t^2)^{-N} \left(\prod_{J=1}^{N} c_{I,J}\right) \\ & \times \{(-1)^L(1 - t^N)\,[(1 - h^2t^N)(1 - h^{-2}t^N)]^{1/2} \\ & + 2(-1)^n t^N(h + h^{-1}) \cos(2nw_I')\}\end{aligned} \tag{121}$$

for $L = 0, 1$ and $I = 1, \ldots, M$. The branch of the square root in (121) is to be chosen to be positive when $t^N < h^2 < t^{-N}$.

In the completely ordered state $t \to 0$. From (55) we see that the eigenvalues $\Lambda_{0,I}$ and $\Lambda_{1,I}$ given by (119) and (121) are then indeed the maximum eigenvalues of the transfer matrix, and that $\Lambda_{0,I}$ ($\Lambda_{1,I}$) corresponds to an eigenvector which is symmetric (antisymmetric) with respect to reversing all arrows.

From assumption (iii) (Section 4) we therefore expect that for all positive λ (i.e., $0 < t < 1$) the two maximum eigenvalues and their associated eigenvectors are given by (108a), (108b), and (119)–(121).

Remember that $v_1, \ldots, v_n$ are also required to satisfy (81), with h set equal to one. From (108b) and the above it follows that $y = y_0$ or y_1, where

$$y_L = \tfrac{1}{2} i\pi L/n, \qquad L = 0, 1 \tag{122}$$

7.2. Matrix Elements $\langle 0 \mid 0 \rangle$ and $\langle 1 \mid 1 \rangle$

Now let $\mid 0\rangle$ and $\mid 1\rangle$ be the eigenvectors of the zero-field transfer matrix (with ($h = 1$), corresponding to the maximum eigenvalues. Substituting the appropriate values of x and y into (113) and (114), it follows that

$$\langle L' \mid L\rangle = \lim_{h \to 1} [\text{r.h.s. of } (113)]_{x=x_L, y=y_{L'}} \tag{123}$$

for $L, L' = 0$ or 1.

With these substitutions we see from (114), (115), (119), and (122) that

$$\lim_{h\to 1} \alpha = 0 \qquad \text{if} \quad L \neq L' \tag{124a}$$

$$= \lim_{h\to 1} (1 - h^2)/[nd(h)] = 4 \tanh(n\lambda) \qquad \text{if} \quad L = L' \tag{124b}$$

From (113) and (124a) it is apparent that

$$\langle 0 \mid 1\rangle = \langle 1 \mid 0\rangle = 0 \tag{125}$$

as we expect. Also, substituting (124b) into (113), letting $h \to 1$ and $x \to y$, and rearranging the remaining terms inside the product, we obtain

$$\langle 0 \mid 0\rangle = \langle 1 \mid 1\rangle = 4^n(\sinh \lambda)^{-2n} \tanh(n\lambda) \sinh(n\lambda) \times \prod_{m=1}^{n-1} [(\cosh m\lambda) \cosh(n-m)\lambda - \operatorname{sech} n\lambda] \tag{126}$$

7.3. Matrix Elements $\langle 0 \mid \sigma_N{}^z \mid 1\rangle$ and $\langle 1 \mid \sigma_N{}^z \mid 0\rangle$

We now go back to Eq. (105) and use the identity (110), together with its analog when the u_j replace the v_j, and (116). Multiplying by $1 - h^2$, setting $x = x_1$ and $y = y_0$, and taking the limit $h \to 1$, we obtain

$$\begin{aligned} &\lim_{h\to 1} [(1 - h^2)\langle 0 \mid \sigma_N{}^z \mid 1\rangle/\langle 0 \mid 1\rangle] \\ &\quad = \lim_{h\to 1} [1 + h^2 - 2h^2 \cos^2(n\eta + \tfrac{1}{4}\pi) \sec^2(n\eta - \tfrac{1}{4}\pi)] \\ &\quad = 4ie^{i\theta} \tanh(n\lambda) \end{aligned} \tag{127}$$

where θ is real and is given by

$$\theta = 2 \operatorname{artan}(e^{-n\lambda}) - \tfrac{1}{2}\pi \tag{128}$$

The limiting value of $\langle 0 \mid 1\rangle/(1 - h^2)$ is readily obtained from (113), (114), and (124a), giving

$$\langle 0 \mid \sigma_N{}^z \mid 1\rangle = 4^n(-1)^{n-1} e^{i\theta}(\sinh \lambda)^{-2n} \tanh(n\lambda) \sinh(n\lambda) \times \prod_{m=1}^{n-1} (\sinh m\lambda) \sinh(n-m)\lambda \tag{129}$$

Interchanging $\mid 0\rangle$ and $\mid 1\rangle$ is equivalent to negating η, λ, and θ in (127) and to complex conjugation in (113). Thus

$$\langle 1 \mid \sigma_N{}^z \mid 0\rangle = \langle 0 \mid \sigma_N{}^z \mid 1\rangle^* \tag{130}$$

Substituting these results (127), (130), and (131) into (76) and taking the positive square root, we obtain

$$P_0 = \prod_{m=1}^{n-1} [(\coth m\lambda) \coth(n-m)\lambda \\ - (\operatorname{sech} n\lambda)(\operatorname{cosech} m\lambda) \operatorname{cosech}(n-m)\lambda]^{-1} \tag{131}$$

We emphasize that this result is exact for finite N, n (at least for n a prime number) satisfying (115), provided $w_1 ,..., w_N$ are given by (116).

In the limit of n large the term containing sech $n\lambda$ in (131) becomes negligible, giving

$$P_0 = \lim_{n\to\infty} \prod_{m=1}^{n-1} [(\tanh m\lambda)\tanh (n-m)\lambda]$$

$$= \lim_{n\to\infty} \left(\prod_{m=1}^{n-1} \tanh m\lambda\right)^2 = \prod_{m=1}^{\infty} \tanh^2 m\lambda \tag{132}$$

This is our result, which we quoted and discussed in Section 1.

APPENDIX A

Let

$$I \equiv \text{r.h.s. of (90)}, \qquad I' \equiv \text{r.h.s. of (91)} \tag{A.1}$$

We prove here that

$$I \equiv I' \tag{A.2}$$

for all complex numbers η, $u_1 ,..., u_n$, $v_1 ,..., v_n$, and $w_1 ,..., w_N$. We do *not* use the relations (81), nor their analog for $v_1 ,..., v_n$.

We first establish four properties.

(i) I and I' are p-functions of degree $N - 1$ of each of the variables $u_1 ,..., u_n$. For I this follows directly from (89). For I' we first note that the summand in (91) is unaffected by applying the same permutation to both $u_1 ,..., u_n$ and $v_1 ,..., v_n$. The V summation, with weight ϵ_V , can therefore be replaced by a U summation, with weight ϵ_U . Thus the sum in (91) is an antisymmetric periodic function of $u_1 ,..., u_n$. It must therefore contain γ as a factor.

Further, the summations $\sum_i$ ensure that the apparent poles in (91) at $u_j = v_j$ are spurious, having residue zero. Thus I' is an entire function of $u_1 ,..., u_n$. Considering the periodicity properties and the growth rates at $u_j = \pm i\infty$, it follows that I' is a p-function of degree $N - 1$ of the variable u_j , for $j = 1,..., n$.

(ii) I and I' are symmetric functions of $u_1, \dots, u_n$. This follows from (89) and the above remarks.

(iii) I and I' are symmetric functions of $w_1, \dots, w_N$. For I' this is obvious from (91) and (85a)–(85g). To prove it for I, consider the effect of interchanging w_J and w_{J+1} in (90). We distinguish three types of terms occurring in the X summation:

(a) No down arrow in columns J or $J+1$: No x_j equals either J or $J+1$. Such terms in (90) are by construction symmetric functions of w_J, w_{J+1}.

(b) One down arrow in columns J and $J+1$: One x_j equals J, or $J+1$. Considering both possibilities, removing all factors in (90) that are by construction symmetric functions of w_J and w_{J+1}, we are left with a term

$$\begin{aligned}\sin(v_j - w_{J+1} + \eta)\sin(u_j - w_{J+1} - \eta) + \sin(v_j - w_J - \eta)\sin(u_j - w_J + \eta)\\ = \cos(u_j - v_j)\cos 2\eta - \cos(u_j + v_j - w_J - w_{J+1})\cos(w_J - w_{J+1}) \quad \text{(A.3)}\end{aligned}$$

which is symmetric.

(c) Two down arrows in columns J and $J+1$. There exists j such that $x_j = J$ and $x_{j+1} = J+1$. Look simply at the corresponding elements of $|f\rangle$, as given by (79). Including the effect of interchanging u_j and u_{j+1}, we find that the only possibly asymmetric factor of the summand in (79) is

$$\begin{aligned}&\sin(u_j - u_{j+1} + 2\eta)\sin(u_j - w_{J+1} - \eta)\sin(u_{j+1} - w_J + \eta)\\ &\quad - \sin(u_{j+1} - u_j + 2\eta)\sin(u_{j+1} - w_{J+1} - \eta)\sin(u_j - w_J + \eta)\\ &\quad = \sin(u_{j+1} - u_j)[\cos(u_j + u_{j+1} - w_J - w_{J+1})\cos(2\eta)\\ &\qquad - \cos(u_{j+1} - u_j)\cos(w_j - w_{J+1})] \qquad \text{(A.4)}\end{aligned}$$

which is symmetric. Similarly, so are the corresponding elements of $\langle g|$, and hence this contribution to $\langle g|f\rangle$.

Thus I, defined as the r.h.s. of (90), is a symmetric function of w_J and w_{J+1} for $J = 1, \dots, N$. It is therefore a symmetric function of $w_1, \dots, w_N$.

(iv) $I = I' = 0$ if $u_i + \eta = u_j - \eta = w_J$, $i \neq j$.

Set $u_1 = w_1 - \eta$ in (79) and (80). Then $\varphi(u_1, x)$ vanishes unless $x = 1$. Thus $f(x_1, \dots, x_n)$ vanishes unless $x_1 = 1$ and only permutations U that leave u_1 unchanged give a nonzero contribution to (79). Multiplying by ξ_N removes the poles in (80), so $\xi_N f$, and hence I, contains a factor

$$\prod_{j=2}^{n} \sin(u_1 - u_j + 2\eta) = \prod_{j=2}^{n} \sin(w_1 - u_j + \eta) \qquad \text{(A.5)}$$

Also, set $u_1 = w_1 - \eta$ in (91). Then $B_N(u_1) = 0$, so the term in $\sum_1$ corresponding to interchanging u_1 and v_1 is not allowed. All remaining terms contain either a factor $A_N(u_j)$, or, if u_j and v_j are interchanged, a factor $\sin(u_1 - u_j + 2\eta)$. In either case they contain the factors $\sin(w_1 - u_j + \eta)$ for $j = 2,..., n$. Thus I and I' both contain (A.5) as a factor.

Hence I and I' vanish if $u_1 + \eta = u_j - \eta = w_1$ ($j = 2,..., n$). From the symmetry properties (ii) and (iii) the general property (iv) follows.

Proof of Identity: Stage 1

Define, for $m = 0, 1,..., n$,

$$K_m = I - I' \qquad \text{with} \quad u_i = w_i - \eta \quad \text{for} \quad i = 1,..., m \tag{A.6}$$

Thus K_0 is simply $I - I'$ for arbitrary $u_1,..., u_n$. We assert that

$$K_0 \equiv 0 \qquad \text{if} \quad K_n \equiv 0 \tag{A.7}$$

The proof is obtained recursively by taking $m = n - 1, n - 2,..., 1, 0$ in the following argument.

Suppose that for some value of m

$$K_{m+1} \equiv 0 \tag{A.8}$$

From property (i) and (A.6), K_m is a p-function of degree $N - 1$ of the variable u_{m+1}. From property (iv) and (A.6) it vanishes if

$$u_{m+1} = w_i + \eta, \qquad i = 1,..., m \tag{A.9}$$

From (A.6) and (A.8), K_m also vanishes if

$$u_{m+1} = w_{m+1} - \eta \tag{A.10}$$

However, from the symmetry property (iii) and (A.6), K_m is a symmetric function of $w_{m+1},..., w_N$. Thus (A.10) can be generalized to state that K_m vanishes if

$$u_{m+1} = w_J - \eta, \qquad J = m + 1,..., N \tag{A.11}$$

We assume that $w_1 \pm \eta,..., w_N \pm \eta$ are distinct complex numbers. Then from (A.9) and (A.11) K_m as a function of u_{m+1} has N distinct zeros. From Theorem 1 it therefore vanishes identically.

Thus if $K_n \equiv 0$, so are K_{n-1}, $K_{n-2},..., K_1$, K_0. This proves (A.7).

By continuity the result is also true even if $w_1 \pm \eta,..., w_N \pm \eta$ are not all distinct.

Stage 2

We now show that $K_n \equiv 0$. From (A.7) our desired identity $I \equiv I'$ then follows.

To obtain K_n, set

$$u_i = w_i - \eta, \qquad i = 1,\dots, n \tag{A.12}$$

in (90) and (91). Then the summand in (90) vanishes unless

$$x_j = j, \qquad j = 1,\dots, n \tag{A.13}$$

and U is the identity permutation. Also, since $B_N(u_i) = 0$ for $i = 1,\dots, n$, all terms in (91) arising from interchanging any u_i, v_i vanish. Hence the summations $\sum_1,\dots, \sum_n$ can be ignored in (91).

Using these facts, we find from (85a)–(85g), (90), (91), and (A.6) that

$$K_n = (-1)^n(\mu\gamma\gamma')^{-1}\left[\prod_{j=1}^{n}\prod_{y=1}^{N} \sin(w_j - w_y - 2\eta) \times \prod_{j=1}^{n}\prod_{y=n+1}^{N} \sin(v_j - w_y + \eta)\right] L_n \tag{A.14}$$

where

$$L_n = \sum_V \epsilon_V \left[\prod_{1\leqslant i<j\leqslant n} \sin(w_i - w_j)\sin(v_j - v_i + 2\eta) \times \sin(v_j - w_i - \eta)\sin(v_i - w_j + \eta) - \prod_{i=1}^{n}\prod_{j=1\neq i}^{n} \sin(w_i - v_j + \eta)\sin(v_i - w_j + \eta)\right] \tag{A.15}$$

Thus L_n is a function of $v_1,\dots, v_n$ and $w_1,\dots, w_n$. We now prove inductively that L_1, $L_2,\dots, L_n$ are identically zero. We need four properties.

(a) L_n is a p-function of degree $2(n-1)$ of $w_1,\dots, w_n$. This follows from the analyticity and periodicity of (A.15), together with the growth rates as $w_j \to \pm i\infty$.

(b) L_n is an antisymmetric function of $v_1,\dots, v_n$ and of $w_1,\dots, w_n$. The first statement is obvious from (A.15). The second can be verified indirectly from properties (ii) and (iii) of $I - I'$, together with (A.12) and (85b).

(c) If $w_n = v_n + \eta$, then

$$L_n = L_{n-1}\prod_{i=1}^{n-1} [\sin(w_i - v_n - \eta)\sin(v_n - v_i + 2\eta) \times \sin(v_n - w_i - \eta)\sin(v_i - v_n)] \tag{A.16}$$

This follows from (A.15) by noting that only permutations V that leave v_n unchanged give a nonzero contribution, and then removing all factors containing v_n or w_n.

The proof is now simple. Suppose that for some m ($m = 1,..., n$) L_{m-1} is identically zero. Regard L_m as a function of w_m. From (*b*) it vanishes if

$$w_m = w_1, ..., w_{m-1} \tag{A.17}$$

From (c) and our assumption that $L_{m-1} \equiv 0$, L_m also vanishes if

$$w_m = v_m + \eta \tag{A.18}$$

However, from the first of the properties (b), it must then vanish if

$$w_m = v_j + \eta, \qquad j = 1,..., m \tag{A.19}$$

Thus L_m has $2m - 1$ zeros, in general distinct. From property (a) and Theorem 1 it must therefore vanish identically.

Finally, from (A.15)

$$L_1 = 1 - 1 = 0 \tag{A.20}$$

Thus $L_1, L_2, ..., L_n$ are identically zero. Hence from (A.14) K_n is zero, and from (A.7) K_0 is zero, i.e.,

$$I \equiv I' \tag{A.21}$$

This completes the proof.

APPENDIX B

Here we derive (105) from (98) and (99).

Define $S_n(u_1, ..., u_n \mid v_1, ..., v_n)$ = r.h.s. of (98) with an extra term in the summand, namely

$$\prod_{i=K} [\sin(u_i - w_N - \eta) \sin(v_i - w_N + \eta)] \times \prod_{i \neq K} [\sin(u_i - w_N + \eta) \sin(v_i - w_N - \eta)] \tag{B.1}$$

Then from (97)–(99)

$$\langle g \mid \tau_N \mid f \rangle / \langle g \mid f \rangle = R_n^{-1} S_n \Big/ \prod_{i=1}^{n} [\sin(u_i - w_N + \eta) \sin(v_i - w_N - \eta)] \tag{B.2}$$

Using reasoning similar to that used to derive (100), but taking account of the extra factor (B.1), we find that

$$S_n(u_1, ..., u_n \mid v_1, ..., v_n)$$
= symmetric function of $u_1, ..., u_n$ and of $v_1, ..., v_n$, being a p-function of degree n in each of $u_1, ..., u_n$ and $v_1, ..., v_n$ (B.3)

Further, we can derive the analog of (102) and (103), namely

$$
\begin{aligned}
S_n(u_1, \ldots, u_{n-1}, x \mid v_1, \ldots, v_{n-1}, x) \\
&= \sin(x - w_N - \eta)\sin(x - w_N + \eta) \\
&\quad\times \left\{ \prod_{i=1}^{n-1} [\sin(u_i - x + 2\eta)\sin(x - v_i + 2\eta)] \right. \\
&\quad \left. - h^2 \prod_{i=1}^{n-1} [\sin(x - u_i + 2\eta)\sin(v_i - x + 2\eta)] \right\} \\
&\quad\times S_{n-1}(u_1, \ldots, u_{n-1} \mid v_1, \ldots, v_{n-1})
\end{aligned} \tag{B.4}
$$

$$
\begin{aligned}
S_1(u \mid v) &= \sin(u - w_N + \eta)\sin(v - w_N - \eta) \\
&\quad - h^2 \sin(u - w_N - \eta)\sin(v - w_N + \eta)
\end{aligned} \tag{B.5}
$$

Unfortunately, Eqs. (B.3)–(B.5) do not define S_n uniquely, it being a p-function of degree n, rather than $n - 1$ (as R_n is). We need one more piece of information. This can be obtained by noting from (B.1) that if

$$u_n = w_N + \eta \tag{B.6}$$

then the summand vanishes unless $k_r < n$. From (98) and (B.1) the summand therefore contains a factor

$$\prod_{j=K} \sin(u_j - u_n + 2\eta) \prod_{j \neq K} \sin(u_j - w_N + \eta) = \sin(2\eta) \prod_{j=1}^{n-1} \sin(u_j - w_N + \eta) \tag{B.7}$$

Using symmetry, it follows that

$$S_n = 0 \qquad \text{if} \quad u_i - \eta = u_j + \eta = w_N \qquad (i \neq j) \tag{B.8}$$

Equations (B.3)–(B.5) and (B.8) determine S_n uniquely. To see this, suppose S_{n-1} is known and let $u_{n-1} = w_N - \eta$. Then from (B.4) and (B.8) we can evaluate S_n at the $n + 1$ points (in general distinct) $u_n = v_1, \ldots, v_n$, $w_N + \eta$. Since S_n is a p-function of degree n of u_n, this determines S_n for all u_n, provided that $u_{n-1} = w_N - \eta$.

By symmetry, this also determines S_n for $u_n = w_N - \eta$ and all u_{n-1}. We can also evaluate S_n from (B.3) and (B.4) for $u_n = v_1, \ldots, v_n$, and hence for $n + 1$ values of u_n (for all u_{n-1}). This determines S_n for *all* values of $u_1, \ldots, u_n$.

A rather startling result follows, namely that

$$
\begin{aligned}
S_n = &\left\{ \prod_{i=1}^{n} [\sin(u_i - w_N + \eta)\sin(v_i - w_N - \eta)] \right. \\
&\left. - h^2 \prod_{i=1}^{n} [\sin(u_i - w_N - \eta)\sin(v_i - w_N + \eta)] \right\} R_n/(1 - h^2)
\end{aligned} \tag{B.9}
$$

From (100), (102), and (103) this expression (B.9) for S_n satisfies (B.3)–(B.5) and (B.8). It is therefore correct.

Substituting (B.9) into (B.2) and the result into (95), we obtain Eq. (105).

APPENDIX C

Here we show that if $u_1,..., u_n$ and $v_1,..., v_n$ are given by (108a) and (108b), then R_n is given by (109).

Let

$$\bar{R}_n = (2i)^{n(n-1)} \exp\left[i(n-1) \sum_{j=1}^{n} (u_j + v_j + 2\eta)\right] R_n \tag{C.1}$$

Then from (100) and the definition (88) of a p-function, $\bar{R}_n$ is a polynomial of degree $n - 1$ in each of the variables

$$\bar{u}_j = e^{2iu_j}, \qquad \bar{v}_j = e^{2iv_j}, \qquad j = 1,..., n \tag{C.2}$$

It is a symmetric function of $u_1,..., u_n$, and hence a symmetric multinomial in $\bar{u}_1,..., \bar{u}_n$ (and similarly in $\bar{v}_1,..., \bar{v}_n$). Thus it can be written as a (simpler) multinomial in the symmetric variables

$$U_j = (-1)^j \sum \bar{u}_{k_1} \cdots \bar{u}_{k_j}, \qquad V_j = (-1)^j \sum \bar{v}_{k_1} \cdots \bar{v}_{k_j} \tag{C.3}$$

where $j = 1,..., n$ and the summations are over all integers $k_1,..., k_j$ such that

$$1 \leqslant k_1 < k_2 < \cdots < k_j \leqslant n \tag{C.4}$$

Defining

$$U_0 = V_0 = 1 \tag{C.5}$$

it is an elementary algebraic identity that

$$\prod_{j=1}^{n} (1 - \bar{u}_j z) \equiv \sum_{m=0}^{n} U_m z^m \tag{C.6}$$

for all complex numbers z. (Similarly for $\bar{v}_j$ and V_m.)

Each U_j(or V_j) is a linear function of any $\bar{u}_k$ (or $\bar{v}_k$). It follows that there exist a unique set of coefficients c_n such that

$$\bar{R}_n = \sum c_n(j_1,..., j_{n-1} \mid k_1,..., k_{n-1}) U_{j_1} \cdots U_{j_{n-1}} V_{k_1} \cdots V_{k_{n-1}} \tag{C.7}$$

Further, from (85a)–(85g) and (98) R_n is unchanged by adding the same constant to each of $u_1,..., u_n$ and $v_1,..., v_n$. This implies that the summation in (C.7) is restricted to nonnegative integers $j_1, \dots, k_{n-1}$ (each not greater than n) such that

$$j_1 + \cdots + j_{n-1} + k_1 + \cdots + k_{n-1} = n(n-1) \tag{C.8}$$

We now regard $\bar{R}_n$ as a function of the U_j and V_j of the form (C.7), and write it as

$$\bar{R}_n(U_j \mid V_j) \equiv \bar{R}_n(U_0, \dots, U_n \mid V_0, \dots, V_n) \tag{C.9}$$

We set

$$z = e^{2ix}, \qquad t = e^{2i\eta} \tag{C.10}$$

[From (34) this t is the same as that in (9).] Defining U_j and V_j as above, but with n replaced by $n-1$, expanding the sines in (102) in terms of the difference of imaginary exponentials, then using (C.1) and (C.6), the recurrence relation (102) becomes the identity

$$\bar{R}_n(U_j - zU_{j-1} \mid V_j - zV_{j-1})$$
$$\equiv (-1)^{n-1} \sum_{l=0}^{n-1} \sum_{m=0}^{n-1} t^{2(n-1+l-m)} z^{2n-2-l-m} (U_l V_m - h^2 V_l U_m) \bar{R}_{n-1}(U_j \mid V_j) \tag{C.11}$$

for all complex numbers z, $U_0, \dots, U_{n-1}$ and $V_0, \dots, V_{n-1}$. Here U_{-1}, U_n, V_{-1}, and V_n on the l.h.s. are to be interpreted as zero.

Also, (103) becomes

$$\bar{R}_1 = 1 - h^2 \tag{C.12}$$

Substituting (C.7) into (C.11) and equating coefficients, we obtain equations for the coefficients c_n that determine them uniquely if the c_{n-1} are known. For instance, it is quite easy to verify that

$$\begin{aligned} \bar{R}_2 = (1 - h^2)[&(1 + t^2)(1 - t^2h^2)U_0V_2 \\ &- t^2(1 - h^2)U_1V_1 + (1 + t^2)(t^2 - h^2)U_2V_0] \end{aligned} \tag{C.13}$$

Despite these simplications, we have not been able to obtain useful general expressions for $\bar{R}_n$. However, it turns out that we can handle the case when

$$U_1 = \cdots = U_{n-1} = V_1 = \cdots = V_{n-1} = 0 \tag{C.14}$$

as we shall now show. This corresponds to $u_1, \dots, v_n$ being of the form (108a) and (108b), with

$$U_n = (-1)^n e^{2nx}, \qquad V_n = (-1)^n e^{2ny} \tag{C.15}$$

In the recurrence identity (C.11) set

$$\begin{aligned} U_j &= z^j, \qquad j = 0, 1, \ldots, n-1 \\ V_j &= z^j, \qquad j = 0, 1, \ldots, m-1 \\ &= -z^{j-n}\beta, \qquad j = m, m+1, \ldots, n-1 \end{aligned} \tag{C.16}$$

where m is some integer between 1 and $n - 1$, and β is an arbitrary complex number. Then the l.h.s. of (88) becomes

$$\bar{R}_n(1, 0, \ldots, 0, -z^n \mid 1, 0, \ldots, 0, -z^{m-n}\beta - z^m, 0, \ldots, 0, \beta) \tag{C.17}$$

i.e., all arguments of the function $\bar{R}_n$ are zero except U_0, U_n, V_0, V_m, and V_n.

Now imagine evaluating (C.17) from (C.7), and consider possible terms involving only U_0, U_n, V_0, V_m, V_n. If V_m occurs r times, then from (C.8) we must have

$$rm = n \times \text{integer} \tag{C.18}$$

where $r = 0, 1, \ldots, n - 1$. If n is a prime number, the only solution of this Diophantine equation is $r = 0$. Thus V_m does not occur, i.e., $\bar{R}_n$ is independent of V_m.

It follows that we can replace the argument $-z^{m-n}\beta - z^m$ in (C.17) by zero. Equation (C.11) then becomes, using (C.16) on the r.h.s.,

$$\begin{aligned} &\bar{R}_n(1, 0, \ldots, 0, \alpha \mid 1, 0, \ldots, 0, \beta) \\ &\quad = (-1)^n z^{n-2} A_n [A_m(t^{2n-2m} - h^2)\alpha \\ &\qquad + A_{n-m}(1 - h^2 t^{2m})\beta] \, \bar{R}_{n-1}(U_j \mid V_j) \end{aligned} \tag{C.19}$$

where we have set

$$\alpha = -z^n \tag{C.20}$$

$$A_m = 1 + t^2 + t^4 + \cdots + t^{2m-2} = (1 - t^{2m})/(1 - t^2) \tag{C.21}$$

Since $\bar{R}_{n-1}$ is an entire function, the bracketted expression preceding it on the r.h.s. of (C.19) must be a factor of the l.h.s. Taking $m = 1, \ldots, n - 1$, we obtain $n - 1$ such factors, each linear in α (and β). However, from (C.7) the l.h.s. of (C.19) is a polynomial of degree $n - 1$ in α (and β). Thus

$$\begin{aligned} &\bar{R}_n(1, 0, \ldots, 0, \alpha \mid 1, 0, \ldots, 0, \beta) \\ &\quad = C_n \prod_{m=1}^{n-1} [A_m(t^{2n-2m} - h^2)\alpha + A_{n-m}(1 - h^2 t^{2m})\beta] \end{aligned} \tag{C.22}$$

where C_n is a constant, independent of α and β.

To obtain this constant, note from (C.7) and (C.8) that if the arguments $V_1, \ldots, V_n$ of $\bar{R}_n$ are all zero, then $\bar{R}_n$ must be of the form

$$\bar{R}_n = d_n(U_n V_0)^{n-1} \tag{C.23}$$

where d_n is some constant.

Now set $m = 1$ and $\beta = 0$ in (C.16). Then $V_1 = \cdots = V_{n-1} = 0$ and we can use (C.23) for both $\bar{R}_n$ and $\bar{R}_{n-1}$ in (C.19). Using (C.20), we obtain

$$d_n = A_n(t^{2n-2} - h^2)d_{n-1} \tag{C.24}$$

Solving this recursively, using $d_1 = 1 - h^2$, and comparing the result with (C.22) for $\beta = 0$ we see that

$$C_n = (1 - h^2)A_n \tag{C.25}$$

Noting that $\alpha = U_n$ and $\beta = V_n$ and using (C.1), (C.15), and (C.22), we obtain the result quoted in Eq. (109).

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