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The Transfer Matrix for a Pure Phase in the Two-dimensional Ising Model

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Abstract. The problem of diagonalizing the transfer matrix for the two dimensional Ising model with all boundary spins equal to $+1$ is solved by use of the spinor method. This provides a simple proof that the spontaneous magnetization is actually given by the well known formula for the long range order with toroidal boundary conditions, and this means that the critical temperature is precisely that temperature above which the state is unique and below which it is non unique. An expression for the magnetization at finite distance from the boundary is also given, and a simple derivation of the formula for the surface tension between two coexisting phases is presented. Finally the relation between the degeneracy of the spectrum and the phase transition is discussed.

Introduction

In this paper we consider the problem of calculating the pair correlations and the spontaneous magnetization of a two-dimensional Ising spin system with nearest neighbour interaction and no external field in a rectangular box Λ completely surrounded by $+$ spins. The calculation is achieved by the use of the transfer matrix method appropriately modified to account for the boundary conditions chosen.

The significance of considering the situation where all spins on the boundary of the box are fixed to $+1$ depends on the following facts, which can be proved by simple arguments using the G.K.S. inequalities [9, 10]:

In the presence of an external field $h \geqq 0$ all the correlations $\langle \sigma_A \rangle_{h,\Lambda,+} \equiv \left\langle \prod_{p \in A} \sigma_p \right\rangle_{h,\Lambda,+}$ have limits $\langle \sigma_A \rangle_{h,+}$ as the sides of the box tend to infinity, (when $h > 0$ the limits are completely independent of the boundary condition). The $\langle \sigma_A \rangle_{h,+}$ are translationally invariant and

$$\lim_{d(A,B)\to\infty} \langle \sigma_A \sigma_B \rangle_{h,+} = \langle \sigma_A \rangle_{h,+} \langle \sigma_B \rangle_{h,+} \,.$$

They are continuous from the right in h, and the average magnetization $m(h) \equiv \lim_{\Lambda \to \infty} \frac{1}{|\Lambda|} \sum_{p \in \Lambda} \langle \sigma_p \rangle_{h,\Lambda,+} = \langle \sigma_p \rangle_{h,+}$, $m(h)$ is also equal to the right hand derivative of the limiting free energy: $m(h) = \frac{\partial F(T,h)}{\partial h^+}$. ($F(T,h)$ is completely independent of the boundary condition.) From these facts it follows that the spontaneous magnetization $m^* \equiv \lim_{h \downarrow 0} m(h)$ is equal to $\langle \sigma_p \rangle_{0,+}$ and also equal to the "long range order" $\lim_{d(p,q) \to \infty} \langle \sigma_p \sigma_q \rangle_{0,+}^{1/2}$. In all calculations of this quantity the more symmetric toroidal boundary conditions have been used, but with these it has only been possible to show that one obtains m^* for temperatures outside an interval around the critical one [10]. Our calculations show that $\langle \sigma_p \sigma_q \rangle_{0,+}$ is given by the expression as a Toeplitz determinant valid with toroidal boundary conditions when p and q lie on the same row or column of the lattice and hence that the formula for m^* obtained from it really gives the true value. (Recently this has also been proved by Benedetto, Gallavotti *et al.* (private communication). They show by a general argument that all $\langle \sigma_A \rangle_0$ with $|A|$ even are the same with toroidal and + boundary conditions.)

We also find a formula for the magnetization at finite distance from the boundary of an infinite lattice, whose asymptotic form is left as a challenge to the analysts. Moreover we show how the surface tension between two coexisting phases can be computed very directly.

The idea of considering the + boundary condition is very natural from the point of view of the general theory of infinite Gibbs states of lattice systems in which extremal states describe pure phases of the system. In fact Gallavotti and Miracle-Solé [5] have shown that in the Ising model well below T_c the two states defined by the families of correlations $\langle \sigma_A \rangle_{0,+}$ and $\langle \sigma_A \rangle_{0,-}$ for A finite are in fact precisely the two extremal states, and that they describe a pure up- or down-magnetized phase respectively.

In [9] it was shown for general ferromagnetic spin systems that if one defines the critical temperature T_c as that temperature above which there is a unique Gibbs state (i.e. the $\langle \sigma_A \rangle_0$ are independent of the boundary conditions) and below which there are several different Gibbs states (e.g. those defined by $\langle \sigma_A \rangle_{0,+}$ and $\langle \sigma_A \rangle_{0,-}$), then T_c is precisely that temperature where $m^*(T)$ becomes positive. Our calculation hence conclusively shows that in the Ising model T_c defined in this way is also that temperature where the limiting free energy $F(T,0)$ has a singularity (since $F(T,h)$ is independent of the boundary conditions).

It is interesting to compare the relation between the spectrum of the transfer matrix and the occurrence of the phase transition for the toroidal and + boundary conditions. In the former case the maximum eigenvalue is simple above T_c and asymptotically degenerate below T_c, and this sudden near degeneracy is directly related to the fact that m^* becomes positive [7]. In the latter case the situation turns out to be different; both above and below T_c there is an exact two-fold degeneracy, and above T_c there is an additional near degeneracy of the same order of magnitude as in the toroidal case. However the expression for e.g. m^* in terms of the eigenvectors of the transfer matrix is not changed by the extra degeneracy, so there is no direct relation between it and the positivity of m^* below T_c, which is the characteristic feature of the phase transition [9]. Hence it is not so clear in what sense the degeneracy is related to the phase transition.

1. The Transfer Matrix and Its Diagonalization

We consider a rectangular $(M+1)\times(N+1)$ lattice, with columns and rows numbered by $m=0,\dots,M$, $n=0,\dots,N$ respectively and having interaction energies J_1 and J_2 in the vertical and horizontal directions as indicated in Fig. 1.

In order to impose the boundary condition that all spins on the end rows and columns are equal to $+1$ we use the device of modifying the interaction constant in columns 0 and M to a value J_0, which will become $+\infty$ before N and M tend to infinity. By forcing the spins on rows 0 and N to be all $+1$ we then get the desired boundary condition. The elements $M(\underline{\sigma},\underline{\sigma}')$ of the symmetric transfer matrix are indexed by the possible configurations $\underline{\sigma},\underline{\sigma}'$ on two adjacent rows, and they are equal to the contribution to the Boltzmann factor coming from these rows:

$$
\begin{aligned}
M(\underline{\sigma},\underline{\sigma}') = \exp\Bigg(&\frac{K_2}{2}\sum_1^M \sigma_{m-1}\sigma_m + K_0(\sigma_0\sigma_0'-1) \\
&+K_1\sum_1^{M-1}\sigma_m\sigma_m' + K_0(\sigma_M\sigma_M'-1) + \frac{K_2}{2}\sum_1^M \sigma_{m-1}'\sigma_m'\Bigg)
\end{aligned}
\tag{1}
$$

$$K_i = \frac{J_i}{kT} \qquad i=0,1,2\,.$$

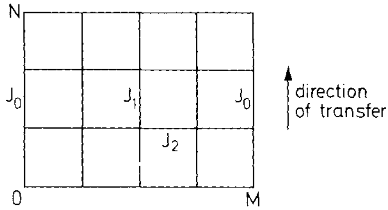

Fig. 1. The rectangular lattice

The partition function is then given by

$$Z_{M,N} = \lim_{J_0 \to \infty} \sum_{\underline{\sigma}_1, \dots, \underline{\sigma}_{N-1}} M(+, \underline{\sigma}_1)\, M(\underline{\sigma}_1, \underline{\sigma}_2), \dots, M(\underline{\sigma}_{N-1}, +) = \lim_{J_0 \to \infty} M^N(+, +) \tag{2}$$

where $+$ denotes the configuration on a row having all $\sigma_m = +1$ and the interaction energy in one end row is included. The pair correlation in a row is given by

$$\langle \sigma_{m_1,n} \sigma_{m_2,n} \rangle = Z_{M,N}^{-1} \sum_{\underline{\sigma}_n} M^n(+, \underline{\sigma}_n)\, \sigma_{m_1,n} \sigma_{m_2,n} M^{N-n}(\underline{\sigma}_n, +) \tag{3}$$

and similar expressions are valid for other averages. (When $J_0 = +\infty$.)

We are going to use the spinor method as explained in [6] and [1] to find the eigenvalues and eigenvectors of the transfer matrix. The initial steps of it is to express the transfer matrix with the help of Pauli spin operators and spinors as follows. Let X be the 2^{M+1} dimensional vector space which is the tensor product of $M+1$ 2-dimensional vector spaces. In each such space choose basis vectors denoted by $|+\rangle_n$, $|-\rangle_n$ $n = 0, \dots, M$, and denote the corresponding basis vectors of X by $|\underline{\sigma}\rangle \equiv \bigotimes_{m=0}^{M} |\sigma_m\rangle_m$, $\sigma_m = \pm 1$.

In each 2-dimensional space let the Pauli spin operators be defined by the matrices

$$\sigma^x = \begin{matrix} & + & - \\ + & 1 & 0 \\ - & 0 & -1 \end{matrix}, \quad \sigma^y = \begin{matrix} & + & - \\ + & 0 & -i \\ - & i & 0 \end{matrix}, \quad \sigma^z = \begin{matrix} & + & - \\ + & 0 & -1 \\ - & -1 & 0 \end{matrix} \tag{4}$$

and let the corresponding operators in X be defined by

$$\sigma_m^u = \underset{0}{I} \otimes \cdots \otimes \underset{m}{\sigma^u} \otimes \cdots \otimes \underset{M}{I}, \qquad m = 0, \dots, M, \; u = x, y, z\,.$$

Then the σ_m^u commute for different m-values and anticommute for the same m-values, and $\sigma_m^x \sigma_m^y = i \sigma_m^z$ (cycl.). The transfer matrix defines an operator in X which can be written as

$$M = (2\,\mathrm{Sh}\,2K_0)(2\,\mathrm{Sh}\,2K_1)^{\frac{M-1}{2}}\, e^{-2K_0}\, V_2^{1/2}\, V_1\, V_2^{1/2} \tag{5}$$

with

$$V_1 = \exp\left(-K_0^* \sigma_0^z - K_1^* \sum_{1}^{M-1} \sigma_m^z - K_0^* \sigma_M^z\right) \tag{6}$$

$$V_2 = \exp\left(K_2 \sum_{1}^{M} \sigma_{m-1}^x \sigma_m^x\right) \tag{7}$$

where K_0^*, K_1^* are defined by the equations $(\mathrm{Sh}\,2K)\,\mathrm{Sh}(2K^*) = 1$ as explained in [6].

When we let K_0 tend to infinity K_0^* tends to zero, so from now on V_1 is given by

$$V_1 = \exp\left(-K_1^* \sum_1^{M-1} \sigma_m^z\right) \tag{6'}$$

and $(2\,\mathrm{Sh}\,2K_0)e^{-2K_0} = 1$.

In (6) and in (7) the terms in each sum commute. The next step is the introduction of spinor operators $\Gamma_0, \ldots, \Gamma_{2M+1}$ by the Jordan-Wigner transformation:

$$\begin{aligned} \Gamma_0 &= \sigma_0^x \qquad & \Gamma_{2j} &= \prod_0^{j-1} (-\sigma_m^z)\sigma_j^x \\ \Gamma_1 &= \sigma_0^y \qquad & \Gamma_{2j+1} &= \prod_0^{j-1} (-\sigma_m^z)\sigma_j^y \end{aligned} \qquad j = 1, \ldots, M \tag{8}$$

which satisfy the anticommutation relations

$$[\Gamma_i, \Gamma_j]_+ = 2\delta_{ij} I \qquad i, j = 0, \ldots, 2M+1\,. \tag{9}$$

In terms of them

$$\begin{aligned} \sigma_m^z &= -i\Gamma_{2m}\Gamma_{2m+1} \qquad & m &= 0, \ldots, M \\ \sigma_{m-1}^x \sigma_m^x &= i\Gamma_{2m-1}\Gamma_{2m} \qquad & m &= 1, \ldots, M \end{aligned} \tag{10}$$

so that

$$V_1 = \exp\left(iK_1^* \sum_1^{M-1} \Gamma_{2m}\Gamma_{2m+1}\right) \tag{11}$$

$$V_2 = \exp\left(iK_2 \sum_1^{M} \Gamma_{2m-1}\Gamma_{2m}\right). \tag{12}$$

The spinor method makes use of the fact that an operator $\exp(iK\Gamma_m\Gamma_n)$ acts on the spinors as a simple rotation:

$$\exp(iK\Gamma_m\Gamma_n)\Gamma_j \exp(-iK\Gamma_m\Gamma_n) = \begin{cases} \Gamma_j & j \neq m, n \\ \Gamma_m(\mathrm{Ch}\,2K) - \Gamma_n(i\,\mathrm{Sh}\,2K) & j = m \\ \Gamma_m(i\,\mathrm{Sh}\,2K) + \Gamma_n(\mathrm{Ch}\,2K) & j = n \end{cases}$$

so that the action of V_1 and V_2 on $\Gamma^T \equiv (\Gamma_0, \ldots, \Gamma_{2M+1})$ is given by:

$$V_1 \Gamma^T V_1^{-1} = \Gamma^T R_1 \tag{13}$$

$$V_2 \Gamma^T V_2^{-1} = \Gamma^T R_2 \tag{14}$$

where R_1 and R_2 are the $2(M+1)\times 2(M+1)$ rotation matrices defined by:

$$R_1=\begin{bmatrix} 1 & & & & & & \\ & 1 & & & & & \\ & & A(v_1) & & & & \\ & & & \ddots & & & \\ & & & & A(v_1) & & \\ & & & & & 1 & \\ & & & & & & 1 \end{bmatrix} \tag{15}$$

$$R_2=\begin{bmatrix} 1 & & & & \\ & A(v_2) & & & \\ & & \ddots & & \\ & & & A(v_2) & \\ & & & & 1 \end{bmatrix} \tag{16}$$

with

$$A(v)=\begin{bmatrix} \mathrm{Ch}\,v & i\,\mathrm{Sh}\,v \\ -i\,\mathrm{Sh}\,v & \mathrm{Ch}\,v \end{bmatrix} \tag{17}$$

and $v_1=2K_1^*$, $v_2=2K_2$.

R_1 and R_2 are hermitian and orthogonal, i.e. $R_i=R_i^\dagger$ and $R_i^{-1}=R_i^T$, $i=1,2$.

The transfer operator $V=V_2^{1/2}\,V_1\,V_2^{1/2}$ hence acts on Γ^T as $R\equiv R_2^{1/2}\,R_1\,R_2^{1/2}$.

The diagonalization of V is then achieved in two steps. First we try to find new spinors g_k, $k=0,\ldots,2M+1$ by an orthogonal transformation $g^T=\Gamma^T S$ such that the action of V on g^T consists of simple rotations:

$$V g^T V^{-1}=g^T\begin{bmatrix} 1 & & & & \\ & A(\gamma_1) & & & \\ & & \ddots & & \\ & & & A(\gamma_M) & \\ & & & & 1 \end{bmatrix} \tag{18}$$

This will be achieved if

$$RS=S\begin{bmatrix} 1 & & & & \\ & A(\gamma_1) & & & \\ & & \ddots & & \\ & & & A(\gamma_M) & \\ & & & & 1 \end{bmatrix} \tag{19}$$

This will imply that V can be expressed as

$$V = \exp\left(\frac{i}{2} \sum_{1}^{M} \gamma_k g_{2k-1} g_{2k}\right). \tag{20}$$

Then in terms of the fermi operators f_k, $f_k^\dagger$ $k=0, \ldots, M$ given by

$$\begin{aligned} f_0 &= \tfrac{1}{2}(g_0 + i g_{2M+1}) \quad & f_k &= \tfrac{1}{2}(g_{2k} + i g_{2k-1}) \\ f_0^\dagger &= \tfrac{1}{2}(g_0 - i g_{2M+1}) \quad & f_k^\dagger &= \tfrac{1}{2}(g_{2k} - i g_{2k-1}) \end{aligned} \qquad k = 1, \ldots, 2M \tag{21}$$

having the anticommutation relations

$$[f_k, f_l]_+ = [f_k^\dagger, f_l^\dagger]_+ = 0, \; [f_k^\dagger, f_l]_+ = \delta_{kl} I$$

V can be written as

$$V = \exp\left(-\tfrac{1}{2} \sum_{0}^{M} \gamma_k (2 f_k^\dagger f_k - I)\right) \tag{22}$$

if we put $\gamma_0 = 0$.

It then follows directly that the orthonormal basis defined by f_k consisting of the "vacum" $|\Phi\rangle$ determined by $f_l|\Phi\rangle = 0$ for all l and the "excited states" $|L\rangle = f_{l_1}^\dagger \ldots f_{l_j}^\dagger |\Phi\rangle$ for all sequences $L = (l_1 < \cdots < l_j)$ $j \leqq M$ are the eigenvectors of V; the vacum having the maximum eigenvalue

$$\Lambda_\Phi = \exp\left(+\tfrac{1}{2} \sum_k \gamma_k\right) \tag{23}$$

and $|L\rangle$ having the eigenvalue

$$\Lambda_L = \Lambda_\Phi \exp\left(-\sum_{l \in L} \gamma_l\right). \tag{24}$$

(We will see that $\gamma_k > 0$ for all $k > 0$.)

Since $\gamma_0 = 0$ we see that all eigenvalues have twofold degeneracy; $|L\rangle$ and $|0, L\rangle$ both having the eigenvalue Λ_L for $L \not\ni 0$. The eigenvalue problem for V is now reduced to that of solving the Eqs. (19).

2. The Solution of the Associated Eigenvalue Problem

Consider now the Eqs. (19) and write the orthogonal matrix S as follows:

$$S = \left[\begin{array}{c|c|c|c|c|c} 1 & & & & & 0 \\ 0 & \eta(\omega_1) & \xi(\omega_1) & \ldots & \eta(\omega_M) & 0 \\ & & & & & 1 \end{array}\right] \tag{25}$$

with $\eta_0(\omega_k) = \eta_{2M+1}(\omega_k) = \xi_0(\omega_k) = \xi_{2M+1}(\omega_k) = 0$.

(Anticipating the form of the solution we label the columns by a variable ω in the interval $(0, \pi)$.) The equations are then:

$$\begin{aligned} R\eta(\omega_k) &= \eta(\omega_k)\,\mathrm{Ch}\,\gamma_k - i\xi(\omega_k)\,\mathrm{Sh}\,\gamma_k \\ R\xi(\omega_k) &= i\eta(\omega_k)\,\mathrm{Sh}\,\gamma_k + \xi(\omega_k)\,\mathrm{Ch}\,\gamma_k \end{aligned} \tag{26}$$

or

$$\begin{aligned} R(\xi(\omega_k) + i\eta(\omega_k)) &= (\xi(\omega_k) + i\eta(\omega_k))\,e^{\gamma_k} \\ R(\xi(\omega_k) - i\eta(\omega_k)) &= (\xi(\omega_k) - i\eta(\omega_k))\,e^{-\gamma_k}. \end{aligned} \tag{27}$$

Hence $y(\omega_k) = \xi(\omega_k) + i\eta(\omega_k)$ are determined as those eigenvectors of R which correspond to eigenvalues $e^{\gamma_k} > 1$ and $\bar{y}(\omega_k)$ as those with eigenvalues $e^{-\gamma_k} < 1$.

The eigenvalue equation $R_2^{1/2} R_1 R_2^{1/2} y = e^{\gamma} y$ can also be written as

$$R_1(R_2^{1/2} y) = e^{\gamma} R_2^T (R_2^{1/2} y) \tag{28}$$

or more explicitly with $x = R_2^{1/2} y$ using (15) and (16):

row no. $2n-1$:

$$-(i\,\mathrm{Sh}\,v_1)x_{2n-2} + (\mathrm{Ch}\,v_1 - e^{\gamma}\,\mathrm{Ch}\,v_2)x_{2n-1} + e^{\gamma}(i\,\mathrm{Sh}\,v_2)x_{2n} = 0 \tag{29}$$

row no $2n$:

$$-e^{\gamma}(i\,\mathrm{Sh}\,v_2)x_{2n-1} + (\mathrm{Ch}\,v_1 - e^{\gamma}\,\mathrm{Ch}\,v_2)x_{2n} + (i\,\mathrm{Sh}\,v_1)x_{2n+1} = 0$$

for $n = 1, \ldots, M$

if we add the boundary conditions

$$\begin{aligned} -(i\,\mathrm{Sh}\,v_1)x_0 + (\mathrm{Ch}\,v_1 - 1)x_1 &= 0 \\ (\mathrm{Ch}\,v_1 - 1)x_{2M} + (i\,\mathrm{Sh}\,v_1)x_{2M+1} &= 0 \end{aligned} \tag{30}$$

and afterwards put $x_0 = x_{2M+1} = 0$.

The ansatz

$$\begin{aligned} x_{2n} &= b z^{2n} \\ x_{2n+1} &= a z^{2n+1} \end{aligned} \qquad n = 0, \ldots, M \tag{31}$$

solves (29) if

$$\begin{aligned} (-iz^{-1}\,\mathrm{Sh}\,v_1)b + (\mathrm{Ch}\,v_1 - e^{\gamma}\,\mathrm{Ch}\,v_2)a + e^{\gamma}(iz\,\mathrm{Sh}\,v_2)b &= 0 \\ e^{\gamma}(-iz^{-1}\,\mathrm{Sh}\,v_2)a + (\mathrm{Ch}\,v_1 - e^{\gamma}\,\mathrm{Ch}\,v_2)b + (iz\,\mathrm{Sh}\,v_1)a &= 0. \end{aligned} \tag{32}$$

If we put

$$T_1 = \begin{bmatrix} \mathrm{Ch}\,v_1 & -iz^{-1}\,\mathrm{Sh}\,v_1 \\ iz\,\mathrm{Sh}\,v_1 & \mathrm{Ch}\,v_1 \end{bmatrix} \qquad T_2 = \begin{bmatrix} \mathrm{Ch}\,v_2 & iz\,\mathrm{Sh}\,v_2 \\ -iz^{-1}\,\mathrm{Sh}\,v_2 & \mathrm{Ch}\,v_2 \end{bmatrix} \tag{33}$$

(32) can be written as

$$T_1 \begin{bmatrix} a \\ b \end{bmatrix} = e^{\gamma} T_2^{-1} \begin{bmatrix} a \\ b \end{bmatrix} = 0 \tag{34}$$

or equivalently as

$$(T_2^{1/2} T_1 T_2^{1/2}) T_2^{-1/2} \begin{bmatrix} a \\ b \end{bmatrix} = e^{\gamma} T_2^{-1/2} \begin{bmatrix} a \\ b \end{bmatrix}. \tag{35}$$

When $|z| = 1$ the eigenvalues and eigenvectors of $T = T_2^{1/2} T_1 T_2^{1/2}$ can easily be found by inspection if we recall the following elementary facts about the Klein model of hyperbolic geometry: The hyperbolic plane is represented by the interior of the unit disc $|t| < 1$ in the complex t-plane with the metric defined by $dl = \frac{2|dt|}{1-|t|^2}$. The geodesics are the circles orthogonal to the unit circle, and the hyperbolic distance from a point t to the origin is determined by $|t| = \operatorname{th} l/2$. The transformations $t \to \frac{t \operatorname{Ch} v + u \operatorname{Sh} v}{t\bar{u} \operatorname{Sh} v + \operatorname{Ch} v}$ with $|u| = 1$ and v real preserve distances and hence transform geodesics into geodesics. Such a transformation has fixpoints $\pm u$, and any point $t = u \operatorname{th} l/2$ is moved a distance $2v$ towards u into $T(t) = u \operatorname{th}\left(\frac{l+2v}{2}\right)$. Any other point is moved along the circle determined by it and the two fixpoints $\pm u$. The matrix $\begin{bmatrix} \operatorname{Ch} v & u \operatorname{Sh} v \\ \bar{u} \operatorname{Sh} v & \operatorname{Ch} v \end{bmatrix}$ has eigenvectors $\begin{bmatrix} \pm u \\ 1 \end{bmatrix}$ with eigenvalues $e^{\pm v}$.

We see that T_1 and T_2 have fixpoints $\pm u_1 = \pm (iz)^{-1}$ $\pm u_2 = \pm (iz)$ respectively. Call that of Tu, so that

$$T = \begin{bmatrix} \operatorname{Ch} \gamma & u \operatorname{Sh} \gamma \\ \bar{u} \operatorname{Sh} \gamma & \operatorname{Ch} \gamma \end{bmatrix} \tag{36}$$

u and γ can be found if we follow the point $t = -u \operatorname{th} \gamma/2$ under the action of $T_2^{1/2} T_1 T_2^{1/2}$ to the point $T(t) = u \operatorname{th} \gamma/2$ as shown in Fig. 2.

We write $z^2 = e^{i\omega}$ with $0 \leqq \omega \leqq \pi$.

Consider the triangle $00'0''$ where $0', 0''$ is the line carried into $T(t), 0$ by $T_2^{1/2}$. Since $l(0'', 0) = v_2$ and $l(0', 0'') = \gamma$ and the angle $0, 0'', 0'$ is equal to the angle $u_2, 0, u$ we see that $u = u_2 e^{i\delta^*} = iz e^{i\delta^*}$, and that $\gamma, \delta^*, \delta'$ are the parameters indicated of the triangle $00'0''$, which is congruent to that considered by Onsager. Here it is seen in a natural way why it comes into the argument. The well known formulae of hyperbolic trigonometry determining

$$\gamma(\omega) = \gamma(-\omega), \quad \delta^*(\omega) = -\delta^*(-\omega), \quad \delta'(\omega) = -\delta'(-\omega)$$

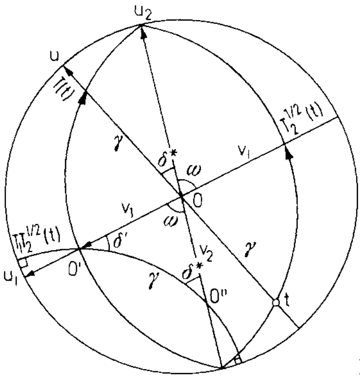

Fig. 2. The action of $T_2^{1/2} T_1 T_2^{1/2}$

are

$$\begin{aligned} \operatorname{Ch}\gamma &= \operatorname{Ch} v_1 \operatorname{Ch} v_2 - \operatorname{Sh} v_1 \operatorname{Sh} v_2 \operatorname{Cos}\omega \\ (\operatorname{Sh}\gamma)\operatorname{Cos}\delta' &= \operatorname{Sh} v_1 \operatorname{Ch} v_2 - \operatorname{Ch} v_1 \operatorname{Sh} v_2 \operatorname{Cos}\omega \\ (\operatorname{Sh}\gamma)\operatorname{Cos}\delta^* &= \operatorname{Ch} v_1 \operatorname{Sh} v_2 - \operatorname{Sh} v_1 \operatorname{Ch} v_2 \operatorname{Cos}\omega \\ \frac{\operatorname{Sin}\delta'}{\operatorname{Sh} v_2} &= \frac{\operatorname{Sin}\delta^*}{\operatorname{Sh} v_1} = \frac{\operatorname{Sin}\omega}{\operatorname{Sh}\gamma}. \end{aligned} \tag{37}$$

To each possible $\gamma > 0$ there are two values of ω, $\omega' = \omega > 0$ and $\omega'' = -\omega$. Hence $z' = z$, $z'' = z^{-1}$, $u' = u$ and $u'' = -u^{-1}$. If we call $\frac{a}{b} \equiv q = T_2^{1/2}(u)$ we find that also $q' = q$, $q'' = -q^{-1}$, so that also

$$\begin{bmatrix} x_{2n} \\ x_{2n+1} \end{bmatrix} = b' z^{2n} \begin{bmatrix} 1 \\ qz \end{bmatrix} + a'' z^{-2n-1} \begin{bmatrix} -qz \\ 1 \end{bmatrix} \qquad n = 0, \ldots, M \tag{38}$$

satisfy (29). The boundary conditions (30) can be written as

$$\begin{aligned} \left(\operatorname{Ch}\frac{v_1}{2}\right) x_0 + \left(i \operatorname{Sh}\frac{v_1}{2}\right) x_1 &= 0 \\ \left(-i \operatorname{Sh}\frac{v_1}{2}\right) x_{2M} + \left(\operatorname{Ch}\frac{v_1}{2}\right) x_{2M+1} &= 0 \end{aligned} \tag{39}$$

or in terms of b', a'' as

$$\begin{aligned} & b'\left(\operatorname{Ch}\frac{v_1}{2} + q\left(iz \operatorname{Sh}\frac{v_1}{2}\right)\right) + a''\left(-q \operatorname{Ch}\frac{v_1}{2} + \left(iz^{-1} \operatorname{Sh}\frac{v_1}{2}\right)\right) = 0 \\ & b' z^{2M+1}\left(\left(-iz^{-1} \operatorname{Sh}\frac{v_1}{2}\right) + q \operatorname{Ch}\frac{v_1}{2}\right) \\ & \qquad + a'' z^{-2M-1}\left(q\left(iz \operatorname{Sh}\frac{v_1}{2}\right) + \operatorname{Ch}\frac{v_1}{2}\right) = 0\,. \end{aligned} \tag{40}$$

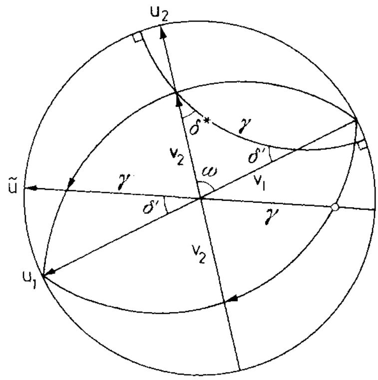

Fig. 3. Determination of $\tilde{u}$

Hence we must have

$$\frac{b'}{a''} = T_1^{1/2}(q) = -\frac{z^{-4M-2}}{T_1^{1/2}(q)}. \tag{41}$$

It is easy to verify that $\tilde{u} \equiv T_1^{1/2}(q) = T_1^{1/2}\, T_2^{1/2}(u)$ is the fixpoint of the other symmetrized product $\tilde{T} = T_1^{1/2}\, T_2\, T_1^{1/2}$, so that it can be found by a construction like that used to find u as shown in Fig. 3.

We see that $\tilde{u} = u_1 e^{-i\delta'} = (iz)^{-1} e^{-i\delta'}$ and hence that (38) is a solution if

$$\frac{b'}{a''} = (iz)^{-1} e^{-i\delta'} \tag{42}$$

and ω satisfies the eigenvalue equation $z^{4M+2} = z^2 e^{2i\delta'}$, which can be written as

$$e^{i\omega M} = \alpha e^{i\delta'(\omega)} \qquad \alpha = \pm 1\,. \tag{43}$$

Since $\dfrac{a''}{b'} = ize^{i\delta'} = (i\alpha) z^{2M+1}$ (38) gives

$$\begin{bmatrix} x_{2n-1} \\ x_{2n} \end{bmatrix} = b' z^{2n} \begin{bmatrix} qz^{-1} \\ 1 \end{bmatrix} + b'(\mathrm{i}\alpha) z^{2(M+1-n)} \begin{bmatrix} 1 \\ -qz^{-1} \end{bmatrix} \qquad n = 1, \ldots, M \tag{44}$$

and finally $y = R_2^{-1/2} x$, $u = T_2^{-1/2}(q)$ give us the eigenvectors y:

$$\begin{aligned} y_{2n-1}(\omega) &= b(\omega)\left(uz^{2n-1} + (i\alpha) z^{2(M+1-n)}\right) \\ y_{2n}(\omega) &= b(\omega)\left(z^{2n} - (i\alpha) u z^{2(M+1-n)-1}\right) \end{aligned} \qquad n = 1, \ldots, M \tag{45}$$

with $u = ize^{i\delta^*(\omega)}$, $z^2 = e^{i\omega}$, $z^{2M} = e^{i\omega M} = \alpha e^{i\delta'(\omega)}$ and some constant $b(\omega)$ whose modulus is determined by the normalization $\sum_1^{2M} |y_n|^2 = 1$ to be given by

$$|b(\omega)|^{-2} = 4\left(M + \frac{\operatorname{Cos}\delta^*(\omega)\operatorname{Sin}\delta'(\omega)}{\operatorname{Sin}\omega}\right) \equiv 4N^2(\omega)\,. \tag{46}$$

From the relations (37) it is found that

$$N^2(\omega) = M - \frac{d\delta'(\omega)}{d\omega} \tag{47}$$

which will be of use later.

If we choose $2b(\omega) = N^{-1}(\omega)e^{-i\frac{\delta^*(\omega)}{2} - i\frac{(M+1)\omega}{2}}$ the eigenvectors are given by:

$$\begin{aligned} y_{2n-1}(\omega) &= N^{-1}(\omega)\, i \operatorname{Cos}\left(\frac{\delta^*(\omega)}{2} + \left(n - \frac{M+1}{2}\right)\omega\right) \\ y_{2n}(\omega) &= N^{-1}(\omega) \operatorname{Cos}\left(\frac{-\delta^*(\omega)}{2} + \left(n - \frac{M+1}{2}\right)\omega\right) \end{aligned} \tag{48}$$

when $\alpha(\omega) = +1$, and by

$$\begin{aligned} y_{2n-1}(\omega) &= -N^{-1}(\omega) \operatorname{Sin}\left(\frac{\delta^*(\omega)}{2} + \left(n - \frac{M+1}{2}\right)\omega\right) \\ y_{2n}(\omega) &= N^{-1}(\omega)\, i \operatorname{Sin}\left(\frac{-\delta^*(\omega)}{2} + \left(n - \frac{M+1}{2}\right)\omega\right) \end{aligned} \tag{49}$$

when $\alpha(\omega) = -1$. $n = 1, \ldots, M$ and $y_0(\omega) = y_{2M+1}(\omega) = 0$. The matrix S is hence determined by (25) with $\xi(\omega) = \sqrt{2}\operatorname{Re} y(\omega)$, $\eta(\omega) = \sqrt{2}\operatorname{Im} y(\omega)$, and

$$\begin{aligned} \xi_{2n-1}(\omega) &= 0 \\ \xi_{2n}(\omega) &= \sqrt{2}N^{-1}(\omega) \operatorname{Cos}\left(\frac{-\delta^*(\omega)}{2} + \left(n - \frac{M+1}{2}\right)\omega\right) \end{aligned} \tag{50}$$

$$n = 1, \ldots, M$$

$$\begin{aligned} \eta_{2n-1}(\omega) &= \sqrt{2}N^{-1}(\omega) \operatorname{Cos}\left(\frac{\delta^*(\omega)}{2} + \left(n - \frac{M+1}{2}\right)\omega\right) \\ \eta_{2n}(\omega) &= 0 \end{aligned} \tag{51}$$

for $\alpha(\omega) = +1$

$$\begin{aligned} \xi_{2n-1}(\omega) &= -\sqrt{2}N^{-1}(\omega) \operatorname{Sin}\left(\frac{\delta^*(\omega)}{2} + \left(n - \frac{M+1}{2}\right)\omega\right) \\ \xi_{2n}(\omega) &= 0 \end{aligned} \tag{52}$$

$$n = 1, \ldots, M$$

$$\begin{aligned} \eta_{2n-1}(\omega) &= 0 \\ \eta_{2n}(\omega) &= \sqrt{2}N^{-1}(\omega) \operatorname{Sin}\left(\frac{-\delta^*(\omega)}{2} + \left(n - \frac{M+1}{2}\right)\omega\right) \end{aligned} \tag{53}$$

for $\alpha(\omega) = -1$.

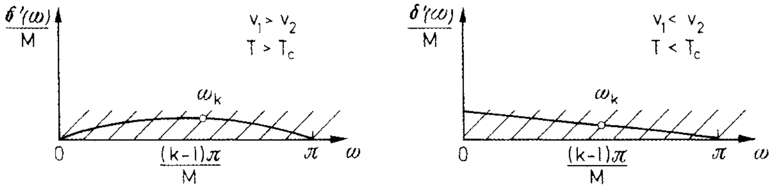

Fig. 4. The location of the roots of the eigenvalue equation

It remains to locate the roots of the eigenvalue Eq. (43) and to check that they give rise the appropriate number of eigenvectors. (43) can be written

$$\frac{\delta'(\omega)}{M} = \omega - \left(\frac{k-1}{M}\right)\pi \tag{54}$$

with integer k and $\alpha = (-1)^{k-1}$.

The roots of (54) in the interval $0 \leqq \omega \leqq \pi$ can be located graphically as indicated in Fig. 4.

We have to distinguish the two cases $v_1 > v_2$ i.e. $T > T_c$ and $v_1 < v_2$ i.e. $T < T_c$. In the former case it is seen from the triangle $0, 0', 0''$ in Fig. 2 that $\delta'(0) = 0$ and in the latter case that $\delta'(0) = \pi$. Hence we find $M-1$ roots ω_k corresponding to $k = 2, \ldots, M$ when $v_1 > v_2$ and M roots ω_k for $k = 1, \ldots, M$ when $v_1 < v_2$ which give rise to non zero eigenvectors, since the roots $\omega = 0$ and $\omega = \pi$ give $y_n \equiv 0$. For $T < T_c$ we have hence found all eigenvectors, but for $T > T_c$ one is missing. This is similar to what was found in [1] for the transfer matrix with free boundary conditions, but in that case one root was missing when $T < T_c$. As in [1] the missing root is found for ω imaginary near the value determined by $e^{i\omega} = \dfrac{\operatorname{th} K_2}{\operatorname{th} K_1{}^*}$ if we use the well known formulae

$$e^{i\delta'(\omega)} = (AB)^{-1/2}\left[\frac{(e^{i\omega}-A)(e^{i\omega}-B)}{(e^{i\omega}-A^{-1})(e^{i\omega}-B^{-1})}\right]^{1/2}$$

$$e^{i\delta^*(\omega)} = \left(\frac{B}{A}\right)^{1/2}\left[\frac{(e^{i\omega}-A)(e^{i\omega}-B^{-1})}{(e^{i\omega}-A^{-1})(e^{i\omega}-B)}\right]^{1/2} \tag{55}$$

$$\operatorname{th}\frac{\gamma(\omega)}{2} = \left[\frac{(e^{i\omega}-B)(e^{i\omega}-B^{-1})}{(e^{i\omega}-A)(e^{i\omega}-A^{-1})}\right]^{1/2}$$

with $A = \dfrac{1}{\operatorname{th} K_2 \operatorname{th} K_1{}^*}$ $B = \dfrac{\operatorname{th} K_2}{\operatorname{th} K_1{}^*}$ and the square roots being positive for $e^{i\omega} = -1$.

When $v_1 > v_2$ $A^{-1} < B < 1 < B^{-1} < A$ and the missing root having $\alpha = +1$ is approximatively given by

$$e^{i\omega} - B \approx B^{2M}(AB)\frac{(B-A^{-1})(B^{-1}-B)}{(A-B)} \tag{56}$$

and the corresponding value of γ by

$$\frac{\gamma_1}{2} \approx \left(\frac{B^{-1}-B}{A-B}\right) B^M (AB)^{1/2}. \tag{57}$$

so it is exponentially small when M is large.

We have hence the following description of the spectrum of the transfer matrix as mentioned in the introduction:

The eigenvalues $\Lambda_L = \Lambda_\Phi \exp\left(-\sum_{l\in L}\gamma_l\right)$ with $L \subsetneqq \{1, \ldots, M\}$ occur in "bands" according to the size of L. The addition of a new element to L decreases Λ_L by at least $\min_l \gamma_l$ which is at least $\gamma(0) = |v_1 - v_2|$ for $T < T_c$ and equal to γ_1 for $T > T_c$. Each eigenvalue is doubly degenerate, $\Lambda_L = \Lambda_{\{0,L\}}$, and for $T > T_c$ there is an additional asymptotic degeneracy, $\Lambda_{\{1,L\}} = \Lambda_L e^{-\gamma_1} \approx \Lambda_L(1 - 0(B^M))$.

3. The Pair Correlation and the Spontaneous Magnetization

The pair correlation in a row can be written as in (3) in terms of the transfer operator:

$$\langle \sigma_{m,n}\sigma_{m+r,n}\rangle = \frac{\langle + | V^n \sigma_m^x \sigma_{m+r}^x V^{N-n} | + \rangle}{\langle + | V^N | + \rangle}. \tag{58}$$

When N and $N-n$ tend to infinity only the contribution corresponding to the largest eigenvalue Λ_Φ contributes, so that V^N can be approximated by $\Lambda_\Phi^N(|\Phi\rangle\langle\Phi| + |0\rangle\langle 0|) \equiv \Lambda_\Phi^N Q$, and in the limit:

$$\langle \sigma_{m,n}\sigma_{m+r,n}\rangle = \frac{\langle + | Q \sigma_m^x \sigma_{m+r}^x Q | + \rangle}{\langle + | Q | + \rangle} \equiv C_{m,m+r}. \tag{59}$$

(In Appendix A we show that $\langle + | Q | + \rangle > 0$ so that the approximation is allowed. By the argument used in [9] to show that the correlations have limits as the box increases it follows that the limit is independent of how N and M tend to infinity, so we first let $N \to \infty$ and then $M \to \infty$.)

In evaluating the matrix elements occurring in (59) it is important to consider the symmetries related to the parity operator

$$P = \prod_{m=0}^{M} (-\sigma_m^z) = (i)^{M+1}(\Gamma_0 \Gamma_1 \ldots \Gamma_{2M+1}). \tag{60}$$

Since $P = P^\dagger$ and $P^2 = I$ it splits X into the orthogonal sum of an even and an odd subspace according to if $P|x\rangle = \pm|x\rangle$. Since $P\Gamma_m = -\Gamma_m P$ P anticommutes with a product of an odd no. of Γ_m:s and commutes with a product of an even no. of Γ_m:s. Hence P commutes with V_1, V_2 and V. In order to see the parity of $|\Phi\rangle$ and the other eigenvectors we use the fact that $P = (i)^{M+1}(g_0 g_1 \dots g_{2M+1})|S|$ as noted in [8]. In Appendix B we show that $|S| = +1$, so

$$P = (i)^{M+1}(g_0 g_1 \dots g_{2M+1}) = -(i)^{M+1}(g_{2M+1} g_0)(g_1 g_2)\dots(g_{2M-1} g_{2M}) \quad (61)$$

as well. From (21) follows that $g_{2k-1} g_{2k}|\Phi\rangle = (-i)(f_k - f_k^\dagger)(f_k + f_k^\dagger|\Phi\rangle = (-i)|\Phi\rangle$, so $P|\Phi\rangle = -|\Phi\rangle$ and the parity of $|L\rangle = f_{l_1}^\dagger \dots f_{l_j}^\dagger|\Phi\rangle$ is $(-1)^{j+1}$. We also need to know the action of P and f_0 on the boundary vectors $|+\rangle$ and $|-\rangle$. From (4) follows that $\sigma^x|\pm\rangle_m = \pm|\pm\rangle_m$ and $-\sigma^z|\pm\rangle_m = |\mp\rangle_m$, so $\sigma_m^x|\pm\rangle = \pm|\pm\rangle$ and $P|\pm\rangle = |\mp\rangle$. Since

$$\begin{aligned} f_0 &= \tfrac{1}{2}(g_0 + i g_{2M+1}) = \tfrac{1}{2}(\Gamma_0 + i\Gamma_{2M+1}) \\ &= \tfrac{1}{2}\left(\sigma_0^x + i\prod_0^{M-1}(-\sigma_m^z)\sigma_M^y\right) = \tfrac{1}{2}(\sigma_0^x - iP\sigma_M^z\sigma_M^y) \\ &= \tfrac{1}{2}(\sigma_0^x - P\sigma_M^x) \end{aligned} \quad (62)$$

we have

$$f_0|\pm\rangle = \frac{\pm 1}{2}(|\pm\rangle - |\mp\rangle) = \frac{|+\rangle - |-\rangle}{2} \equiv |\text{od}\rangle \quad (63)$$

with $|\text{od}\rangle = \dfrac{|+\rangle - |-\rangle}{2}$, $|\text{ev}\rangle = \dfrac{|+\rangle + |-\rangle}{2}$, $|+\rangle = |\text{ev}\rangle + |\text{od}\rangle$. We can now turn to the matrix elements in (59): In the denominator

$$\langle +|0\rangle = \langle +|f_0^\dagger|\Phi\rangle = \overline{\langle\Phi|f_0|+\rangle} = \overline{\langle\Phi|\text{od}\rangle} = \langle\text{od}|\Phi\rangle = \langle +|\Phi\rangle,$$

so

$$\langle +|Q|+\rangle = 2|\langle\text{od}|\Phi\rangle|^2.$$

Since

$$\sigma_m^x\sigma_{m+r}^x = \sigma_m^x\sigma_{m+1}^x\sigma_{m+1}^x\sigma_{m+2}^x \dots \sigma_{m+r-1}^x\sigma_{m+r}^x = (i)^r(\Gamma_{2m+1}\Gamma_{2m+2}\dots\Gamma_{2m+2r})$$

it preserves parity, and mixed matrix elements in the numerator vanish. Hence we find that

$$C_{m,m+r} = \tfrac{1}{2}(\langle\Phi|\sigma_m^x\sigma_{m+r}^x|\Phi\rangle + \langle 0|\sigma_m^x\sigma_{m+r}^x|0\rangle).$$

The two terms are equal however, because from (62) follows that f_0 commutes with $\sigma_m^x\sigma_{m+r}^x$ so that $\langle 0|\sigma_m^x\sigma_{m+r}^x|0\rangle = \langle\Phi|f_0\sigma_m^x\sigma_{m+r}^x f_0^\dagger|\Phi\rangle = \langle\Phi|\sigma_m^x\sigma_{m+r}^x|\Phi\rangle$, and

$$C_{m,m+r} = (i)^r\langle\Phi|\Gamma_{2m+1}\Gamma_{2m+2}\dots\Gamma_{2m+2r}|\Phi\rangle. \quad (64)$$

In order to evaluate (64) by Wick's theorem we need to know the averages $\langle\Phi|\Gamma_m\Gamma_n|\Phi\rangle$, $m, n=0, \ldots, M+1$, $m \neq n$. They are directly obtained from $\Gamma^T = g^T S^T$ and (21) which implies that

$$\langle\Phi|g_{2k}g_{2l}|\Phi\rangle = \langle\Phi|g_{2k-1}g_{2l-1}|\Phi\rangle = i\langle\Phi|g_{2k-l}g_{2l}|\Phi\rangle = \delta_{kl} \quad (65)$$

and hence

$$\begin{aligned}\langle\Phi|\Gamma_m\Gamma_n|\Phi\rangle &= \sum_{k=1}^{M} S_{m,2k}S_{n,2k-1} - S_{m,2k-1}S_{n,2k} \\ &= i\sum_{k=1}^{M} \xi_m(\omega_k)\,\eta_n(\omega_k) - \eta_m(\omega_k)\,\xi_n(\omega_k) \qquad 1 \leqq m < n \leqq 2M \\ \langle\Phi|\Gamma_0\Gamma_{2M+1}|\Phi\rangle &= \langle\Phi|g_0 g_{2M+1}|\Phi\rangle = i\end{aligned} \quad (66)$$

(50)–(53) then imply that

$$\langle\Phi|\Gamma_{2m}\Gamma_{2n}|\Phi\rangle = \langle\Phi|\Gamma_{2m-1}\Gamma_{2n-1}|\Phi\rangle = 0$$

$$\begin{aligned}\langle\Phi|\Gamma_{2m-1}\Gamma_{2n}|\Phi\rangle &= i\sum_{k\,\mathrm{odd}} -\eta_{2m-1}(\omega_k)\,\xi_{2n}(\omega_k) + i\sum_{k\,\mathrm{even}} \xi_{2m-1}(\omega_k)\quad \eta_{2n}(\omega_k) \\ &= -2i\sum_{k\,\mathrm{odd}} N^{-2}(\omega_k)\,\mathrm{Cos}\left(\frac{\delta^*(\omega_k)}{2} + \left(m-\frac{M+1}{2}\right)\omega_k\right) \\ &\qquad \cdot \mathrm{Cos}\left(\frac{-\delta^*(\omega_k)}{2} + \left(n-\frac{M+1}{2}\right)\omega_k\right) \\ &\quad -2i\sum_{k\,\mathrm{even}} N^{-2}(\omega_k)\,\mathrm{Sin}\left(\frac{\delta^*(\omega_k)}{2} + \left(m-\frac{M+1}{2}\right)\omega_k\right) \\ &\qquad \cdot \mathrm{Sin}\left(\frac{-\delta^*(\omega_k)}{2} + \left(n-\frac{M+1}{2}\right)\omega_k\right)\end{aligned} \quad (67)$$

which when $M \to \infty$ and $m - \dfrac{M+1}{2}$ $n - \dfrac{M+1}{2} = \mathrm{const}$ converges to

$$-i a_{m-n} \equiv \frac{-i}{\pi}\int_0^{\pi} \mathrm{Cos}(\delta^*(\omega) + (m-n)\omega)\, d\omega = \frac{-i}{2\pi}\int_{-\pi}^{\pi} e^{i\delta^*(\omega) + i(m-n)\omega}\, d\omega\,. \quad (68)$$

From (64), which can be written

$$\begin{aligned}C_{m,m+r} = (-1)^{\frac{r(r-1)}{2}} &\langle\Phi|(i\Gamma_{2m+1})(i\Gamma_{2m+3})\ldots \\ &\ldots(i\Gamma_{2(m+r)-1})(\Gamma_{2m+2})\ldots(\Gamma_{2(m+r)})|\Phi\rangle\,.\end{aligned}$$

Wick's theorem then gives us the following Pfaffian expression for $C_r \equiv \lim_{M\to\infty} C_{\frac{M+1}{2}, \frac{M+1}{2}+r}$:

$$C_r = \begin{array}{|cc|ccc|cc|} 0 & 0 & a_0 & a_{-1} & a_{-r+1} & & \\ & 0 & a_1 & a_0 & a_{-r+2} & & \\ & & a_{r-1} & a_1 & a_0 & & \\ & & & & & 0 & 0 \\ & & & & & & 0 \end{array} (-1)^{\frac{r(r-1)}{2}} = \begin{vmatrix} a_0 & a_{-1} & a_{-r+1} \\ a_1 & a_0 & a_{-r+2} \\ a_{r-1} & a_1 & a_0 \end{vmatrix} \tag{69}$$

This is the well known Toeplitz determinant of Montroll, Potts, and Ward valid with toroidal boundary conditions, from which the spontaneous magnetization is obtained directly by the Szegö-Kac theorem [11]:

$$\begin{aligned} (m^*)^2 = \lim_{r\to\infty} C_r &= (1-(\mathrm{Sh}\,2K_1\,\mathrm{Sh}\,2K_2)^{-2})^{1/4} \qquad T<T_c \\ &= 0 \qquad\qquad\qquad\qquad\qquad\qquad T>T_c. \end{aligned} \tag{70}$$

4. A Formula for the Magnetization at Finite Distance from the Boundary

In the limit $N\to\infty$ $N-n\to\infty$ the average $\langle\sigma_{m,n}\rangle$ is given as in (59) by:

$$\langle\sigma_{m,n}\rangle = \frac{\langle +|Q\sigma_m^x Q|+\rangle}{\langle +|Q|+\rangle}. \tag{71}$$

From (8) and (10) we see that $\sigma_m^x = i^m(\Gamma_0\Gamma_1 \dots \Gamma_{2m})$, a product of an odd no. of P : s. Hence only mixed matrix elements in the numerator of (71) contribute, and

$$\begin{aligned} \langle\sigma_{m,n}\rangle &= \tfrac{1}{2}(\langle 0|\sigma_m^x|\Phi\rangle + \langle\Phi|\sigma_m^x|0\rangle) \\ &= \tfrac{1}{2}(\langle\Phi|f_0\sigma_m^x|\Phi\rangle + \langle\Phi|\sigma_m^x f_0^\dagger|\Phi\rangle \\ &= i^m\langle\Phi|\Gamma_1\Gamma_2\dots\Gamma_{2m}|\Phi\rangle \end{aligned} \tag{72}$$

since $f_0+f_0^\dagger = g_0 = \Gamma_0$.

In evaluating this using Wick's theorem we need to find the limit of (67) when $M\to\infty$ and m,n finite. This is easily done if we express the sums as contour integrals as follows. The ω_k are the roots of the equation

$$F(\omega_k) \equiv e^{iM\omega_k - i\delta'(\omega_k)} = (-1)^{k-1} \equiv \alpha(\omega_k)$$

with $\mathrm{Re}\, e^{i\omega_k} \geqq 0$, and

$$F'(\omega_k) = i\left(M - \frac{d\delta'(\omega_k)}{d\omega}\right)\alpha(\omega_k) = iN^2(\omega_k)\,\alpha(\omega_k)$$

by (47).

Hence for any analytic function $g(\omega)$

$$\sum_{\alpha(\omega_k)=\alpha} N^{-2}(\omega_k)\, g(\omega_k) = \frac{1}{2\pi} \int_\gamma g(\omega)\, \alpha(F(\omega)-\alpha)^{-1}\, d\omega \qquad \alpha = \pm 1 \tag{73}$$

where γ is a contour surrounding all the roots in the upper halfplane and no others.

Hence (67) can be written as

$$\begin{aligned}
i\langle\Phi|\Gamma_{2m-1}\Gamma_{2n}|\Phi\rangle
&= \frac{1}{2\pi}\int_\gamma 2\,\mathrm{Cos}\left(\frac{\delta^*(\omega)}{2} + \left(m - \frac{M+1}{2}\right)\omega\right)\\
&\qquad \cdot\ \mathrm{Cos}\left(\frac{-\delta^*(\omega)}{2} + \left(n - \frac{M+1}{2}\right)\omega\right)(F(\omega)-1)^{-1}\, d\omega\\
&\quad - \frac{1}{2\pi}\int_\gamma 2\,\mathrm{Sin}\left(\frac{\delta^*(\omega)}{2} + \left(m - \frac{M+1}{2}\right)\omega\right) \qquad\qquad (74)\\
&\qquad \cdot\ \mathrm{Sin}\left(\frac{-\delta^*(\omega)}{2} + \left(n - \frac{M+1}{2}\right)\omega\right)(F(\omega)+1)^{-1}\, d\omega\\
&= \frac{1}{2\pi}\int_\gamma 2(\mathrm{Cos}(m+n-M-1)\omega)\, F(\omega)\,(F^2(\omega)-1)^{-1}\, d\omega\\
&\quad + \frac{1}{2\pi}\int_\gamma 2(\mathrm{Cos}(\delta^*(\omega)+(m-n)\omega))\,(F^2(\omega)-1)^{-1}\, d\omega\,.
\end{aligned}$$

Using (56) and (55) it is easy to check that the contribution from ω_1 when $T > T_c$ vanishes as $M \to \infty$, and considering separately the contributions with $|e^{i\omega}| < 1$ and $|e^{i\omega}| > 1$ in (74) we obtain in the limit $M \to \infty$:

$$\begin{aligned}
i\langle\Phi|\Gamma_{2m-1}\Gamma_{2n}|\Phi\rangle &= \frac{1}{\pi}\int_0^\pi \mathrm{Cos}(\delta^*(\omega)+(m-n)\omega)\\
&\quad + \mathrm{Cos}(\delta'(\omega)+(m+n-1)\omega)\, d\omega \qquad\qquad (75)\\
&= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{i\delta^*(\omega)+i(m-n)\omega} + e^{i\delta'(\omega)+i(m+n-1)\omega}\, d\omega \equiv a_{m,n}\,.
\end{aligned}$$

Finally, as in (69) we obtain

$$\lim_{M\to\infty} \lim_{\substack{N\to\infty \\ N-n\to\infty}} \langle\sigma_{m,n}\rangle = \begin{vmatrix} a_{1,1} & \cdots & a_{1,m} \\ a_{m,1} & \cdots & a_{m,m} \end{vmatrix}. \tag{76}$$

The study of how rapidly this expression converges to m^* as $m \to \infty$ requires a generalized refined Szegö-Kac theorem which has yet to be found.

5. Calculation of the Surface Tension between the Two Phases

The machinery developed in the previous sections also allows us in a very simple way to calculate the surface tension associated with the boundary between two oppositely magnetized phases which can be forced to coexist for $T < T_c$ by a suitable choice of boundary condition as follows:

Consider a box with $2N+1$ rows and let the boundary spins on the top half of it be $+1$ and on the bottom half -1. If we represent a configuration by drawing the contours separating opposite spins we realize that an arbitrary configuration will then include one contour going between the two breaks in the boundary configuration. It separates two regions where all contours are closed, the top region having boundary condition $+1$ and the bottom one -1. These will hence consist of pure $+$ and $-$ phases. The difference in free energy with this boundary condition and the one used before for which all contours are closed will be due to the presence of the phase boundary, so the surface tension should be defined by

$$\tau = \lim_{N,M \to \infty} M^{-1} \log Z^{+-}/Z^{++} \tag{77}$$

Z^{+-} and Z^{++} being the partition functions with the two different boundary conditions respectively. (The definition is discussed in more detail in [3] and [4].)

Since the operator $-\sigma^z$ changes $|\pm\rangle_m$ into $|\mp\rangle_m$ we have $Z^{+-} = \langle - | V^N \sigma_0^z \sigma_M^z V^N | + \rangle$, and hence

$$\tau = \lim_{M \to \infty} M^{-1} \log \langle - | Q \sigma_0^z \sigma_M^z Q | + \rangle / \langle + | Q | + \rangle . \tag{78}$$

From (10) we have $\sigma_0^z \sigma_M^z = -\Gamma_0 \Gamma_1 \Gamma_{2M} \Gamma_{2M+1} = -g_0 \Gamma_1 \Gamma_{2M} g_{2M+1}$, and mixed matrix elements in Z^{+-} vanish. From (63) follows that $\langle - | 0 \rangle = -\langle - | \Phi \rangle = \langle + | \Phi \rangle = \langle + | 0 \rangle$, which allows us to simplify the ratio in (78) to $\frac{1}{2}(\langle 0 | \sigma_0^z \sigma_M^z | 0 \rangle - \langle \Phi | \sigma_0^z \sigma_M^z | \Phi \rangle)$. The first quantity is

$$\langle \Phi | f_0 \sigma_0^z \sigma_M^z f_0^\dagger | \Phi \rangle = \langle \Phi | \Gamma_0 \Gamma_0 \Gamma_1 \Gamma_{2M} \Gamma_{2M+1} \Gamma_0 | \Phi \rangle$$

$$= \langle \Phi | \Gamma_0 \Gamma_1 \Gamma_{2M} \Gamma_{2M+1} | \Phi \rangle = \text{the second quantity} = i \langle \Phi | \Gamma_1 \Gamma_{2M} | \Phi \rangle$$

since $\Gamma_0 \Gamma_{2M+1}|\Phi\rangle = i|\Phi\rangle$, and hence

$$\tau = \lim_{M\to\infty} M^{-1} \log i\langle\Phi|\Gamma_1 \Gamma_{2M}|\Phi\rangle . \tag{79}$$

In (74) the integral can be changed into $\frac{1}{2}\left(\int_{\gamma+} - \int_{\gamma-}\right)$ with $\gamma_\pm$ defined by $|e^{i\omega}| = r_\pm$ if $B^{-1} < r_- < 1 < r_+ < B$, and since $F(-\omega) = F(\omega)^{-1}$ the change of variables $\omega \to -\omega$ in $\int_{\gamma+}$ gives:

$$i\langle\Phi|\Gamma_1 \Gamma_{2M}|\Phi\rangle = \frac{1}{2\pi} \int_{\gamma-} (2F(\omega) + 2\,\mathrm{Cos}(\delta^*(\omega) - (M-1)\omega)) \cdot (1 - F^2(\omega))^{-1} d\omega - \frac{1}{2\pi} \int_{\gamma-} \mathrm{Cos}(\delta^*(\omega) - (M-1)\omega)\, d\omega. \tag{80}$$

Remembering that $F(\omega) = e^{iM\omega - i\delta'(\omega)}$ and using the method of deforming γ_- to a path along the cut $[A^{-1}, B^{-1}]$ in the $e^{i\omega}$-plane one sees that $i\langle\Phi|\Gamma_1 \Gamma_{2M}|\Phi\rangle = 0(B^{-M})$ as $M \to \infty$ when $T < T_c$. (From (55) we see that $A^{-1} < B^{-1} < 1 < B < A$ for $T < T_c$.) We hence obtain

$$\tau = -\log B = -2K_1 - \log \mathrm{th} K_2 . \tag{81}$$

This is the same value as that computed by Onsager [12] using his different definition, and it was shown in [3] that it is obtained from several other definitions as well.

6. On the Relation between the Degeneracy of the Spectrum and the Phase Transition

When toroidal boundary conditions are used it is found [2, 7] that if we consider e, g, the pair correlation in a column and express it in terms of the transfer matrix as

$$C_r = \langle \sigma_{m,n} \sigma_{m,n+r} \rangle = \lim_{M\to\infty} \lim_{N\to\infty} \frac{\mathrm{Tr}(V^{N-r} \sigma_m^x V^r \sigma_m^x)}{\mathrm{Tr}(V^N)} \tag{82}$$

and then study its limit as $r \to \infty$ we obtain a formula for $(m^*)^2$ which is drastically dependent on the degeneracy arising below T_c. Above T_c the limit of C_r is identically zero, but below T_c it is equal to a contribution from the asymptotically degenerate eigenvector, so the occurrence of spontaneous magnetization is directly related to the onset of degeneracy.

Let us consider an expression analogous to (82) with our boundary conditions. In order to get rid of the boundary effects coming from the end columns in a simple way let us first consider the average $C=\langle(\sigma_{m,n}\sigma_{m,n+r})(\sigma_{m+s,n}\sigma_{m+s,n+r})\rangle$. By the general argument given in [9] mentioned in the introduction we know that if we let N, M, m, s tend to infinity in that order C will have the limit C_r^2. In terms of the transfer matrix we have when $N\to\infty$:

$$\begin{aligned} C &= \frac{\langle +|Q\,\sigma_m^x\sigma_{m+s}^x V^r \sigma_m^x\sigma_{m+s}^x Q|+\rangle}{\langle +|Q|+\rangle \Lambda_\Phi^r} \\ &= \langle +|Q|+\rangle^{-1}\sum_L |\langle +|Q\,\sigma_m^x\sigma_{m+s}^x|L\rangle|^2\left(\frac{\Lambda_L}{\Lambda_\Phi}\right)^r. \end{aligned} \tag{83}$$

As mentioned before mixed matrix elements of $\sigma_m^x\sigma_{m+s}^x$ vanish, so $\langle\Phi|\sigma_m^x\sigma_{m+s}^x|L\rangle=0$ if $|L|$ odd, and then also

$$\begin{aligned} \langle 0|\sigma_m^x\sigma_{m+s}^x|L\rangle &= \langle\Phi|f_0\,\sigma_m^x\sigma_{m+s}^x|L\rangle = \langle\Phi|\sigma_m^x\sigma_{m+1}^x f_0|L\rangle \\ &= \begin{cases} 0 & \text{if} \quad 0\notin L \\ \langle\Phi|\sigma_m^x\sigma_{m+s}^x|L'\rangle & \text{if} \quad L=(0,L') \end{cases} \end{aligned} \tag{84}$$

$$\langle\Phi|\sigma_m^x\sigma_{m+s}^x|0,L\rangle = \langle\Phi|\sigma_m^x\sigma_{m+s}^x f_0^\dagger|L\rangle = \langle\Phi|f_0^\dagger\,\sigma_m^x\sigma_{m+s}^x|L\rangle = 0\,.$$

Hence

$$C=\sum_{\substack{|L|\,\text{even}\\ 0\notin L}} |\langle\Phi|\sigma_m^x\sigma_{m+s}^x|L\rangle|^2\left(\frac{\Lambda_L}{\Lambda_\Phi}\right)^r \tag{85}$$

and we see that the leading term having $\lim\limits_{M\to\infty}\left(\frac{\Lambda_L}{\Lambda_\Phi}\right)=1$ will always be that coming from $L=\Phi$ which contributes precisely the quantity $(m^*)^2$ defined by (69), (70). When $T>T_c$ any term with $1\in L$ will also have $l\in L$ for some $l>1$, so that $\left(\frac{\Lambda_L}{\Lambda_\Phi}\right)\leqq e^{-r\gamma(0)}$, and it will hence not contribute to the leading term.

The change in the multiplicity of the spectrum taking place at T_c is thus not as directly related to the occurrence of spontaneous magnetization as in the toroidal case.

Appendix A. A Lower Bound for $\langle +|Q|+\rangle$

Such a bound can easily be found for any matrix element $\langle\underline{\sigma}|Q|\underline{\sigma}\rangle$ by comparing the partition function with a fixed configuration $\underline{\sigma}$ on the top and bottom row to that with cyclic boundary conditions in the vertical direction:

$$\langle \underline{\sigma} | Q | \underline{\sigma} \rangle = \lim_{N \to \infty} \frac{\langle \underline{\sigma} | V^N | \underline{\sigma} \rangle}{\Lambda_\Phi{}^N} = \lim_{N \to \infty} \frac{\langle \underline{\sigma} | V^N | \underline{\sigma} \rangle}{\frac{1}{2} \operatorname{Tr} V^N} . \tag{A 1}$$

For any two configurations differing only in the top and bottom row the energies differ at most by $(2J_2 + 4J_1)M$, so that the ratio of the Boltzmann factors lies between $e^{\pm(2K_2+4K_1)M}$, and hence $e^{-(2K_2+4K_1)M} \leqq \frac{\langle \underline{\sigma} | V^N | \underline{\sigma} \rangle}{\langle \underline{\sigma}' | V^N | \underline{\sigma}' \rangle} \leqq e^{(2K_2+4K_1)M}$ for any $\underline{\sigma}$, $\underline{\sigma}'$ also. It follows from this that $\operatorname{Tr} V^N = \sum_{\underline{\sigma}'} \langle \underline{\sigma}' | V^N | \underline{\sigma}' \rangle \leqq 2^M e^{(2K_2+4K_1)M} \langle \underline{\sigma} | V^N | \underline{\sigma} \rangle$, and the bound $\langle \underline{\sigma} | Q | \underline{\sigma} \rangle \geqq 2^{-M+1} e^{-(2K_2+4K_1)M} > 0$ is valid.

Appendix B. Proof that $|S| = +1$

S is given by (25), and it is seen that by elementary column operations the columns can be replaced by $y(\omega_k)$, $\bar{y}(\omega_k)$:

$$|S| = (2i)^{-M} \begin{vmatrix} 1 & & & & & & \\ & y(\omega_1) & \bar{y}(\omega_1) & \dots & y(\omega_M) & \bar{y}(\omega_M) & \\ & & & & & & 1 \end{vmatrix} . \tag{B 1}$$

Since $x(\omega_k) = R_2^{1/2}\, y(\omega_k)$, $\bar{x}(\omega_k) = (R_2^T)^{1/2}\, \bar{y}(\omega_k)$ and $|R_2| = 1$ we also have

$$|S| = C_+ i^{-M} \begin{vmatrix} x_1(\omega_1) & \dots & \bar{x}_1(\omega_M) \\ \vdots & & \\ x_{2M}(\omega_1) & \dots & \bar{x}_{2M}(\omega_M) \end{vmatrix} . \tag{B 2}$$

C_+ will denote an arbitrary positive constant, and we can assume that the $x(\omega_k)$ are normalized by $x_1(\omega_k) = 1$. The Eqs. (29), (30) for $x(\omega_k)$, $\bar{x}(\omega_k)$ can be written

$$\begin{aligned} x_{2n} &= (i \operatorname{Sh} v_2)^{-1} [-(\lambda^{-1} \operatorname{Ch} v_1 - \operatorname{Ch} v_2) x_{2n-1} + \lambda^{-1} (i \operatorname{Sh} v_1) x_{2n-2}] \\ x_{2n+1} &= (i \operatorname{Sh} v_1)^{-1} [-(\operatorname{Ch} v_1 - \lambda \operatorname{Ch} v_2) x_{2n} + \lambda (i \operatorname{Sh} v_2) x_{2n-1}] \\ x_1 &= \frac{i \operatorname{Sh} v_1}{\operatorname{Ch} v_1 - 1} x_0 \end{aligned} \tag{B 3}$$

with $\lambda = e^{\gamma_k} \equiv \lambda_k$ and $\lambda = e^{-\gamma_k} \equiv \lambda_{-k}$ respectively, $k = 1, \dots, M$. ($\lambda_1 < \lambda_2 < \dots < \lambda_M$, since $\gamma(\omega)$ is increasing.)

From (B 3) it is seen that the x_n are polynomials in λ, λ^{-1} as follows:

$$\begin{aligned} x_{2n} &= a_{2n}\lambda^{n-1} + \cdots + b_{2n}\lambda^{-n} \qquad n=0,\ldots,M \\ x_{2n+1} &= a_{2n+1}\lambda^{n} + \cdots + b_{2n+1}\lambda^{-n} \qquad n=1,\ldots,M \end{aligned} \tag{B4}$$

if $a_0=0$, $b_0=x_0$. We also put $a_1=b_1=1$, so that $x_1=1=\frac{a_1+b_1}{2}$.

By substituting (B 4) into (B 3) it is found that the leading coefficients are given by the relations:

$$\left.\begin{aligned} a_{2n} &= (i\,\mathrm{Sh}\,v_2)^{-1}(\mathrm{Ch}\,v_2)a_{2n-1} \\ b_{2n} &= (i\,\mathrm{Sh}\,v_2)^{-1}[-(\mathrm{Ch}\,v_1)b_{2n-1}+(i\,\mathrm{Sh}\,v_1)b_{2n-2}] \\ a_{2n+1} &= (i\,\mathrm{Sh}\,v_1)^{-1}[(\mathrm{Ch}\,v_2)a_{2n}+(i\,\mathrm{Sh}\,v_2)a_{2n-1}] \\ b_{2n+1} &= -(i\,\mathrm{Sh}\,v_1)^{-1}(\mathrm{Ch}\,v_1)b_{2n} \end{aligned}\right\} \quad n=1,\ldots,M \tag{B5}$$

which imply that

$$\left.\begin{aligned} a_{2n+1} &= -(\mathrm{Sh}\,v_1\,\mathrm{Sh}\,v_2)^{-1}a_{2n-1} \\ b_{2n+2} &= -(\mathrm{Sh}\,v_1\,\mathrm{Sh}\,v_2)^{-1}b_{2n} \end{aligned}\right\} \quad n=1,\ldots,M\,. \tag{B6}$$

In (B 2) we can hence factorize the matrix into a lower triangular matrix and a Van der Monde type matrix:

$$\begin{bmatrix} x_1(\omega_1) & \bar{x}_1(\omega_1) & \ldots & \bar{x}_1(\omega_M) \\ \vdots & \vdots & & \vdots \\ & & & \\ x_{2M}(\omega_1) & \bar{x}_{2M}(\omega_M) & & \bar{x}_{2M}(\omega_M) \end{bmatrix} = \begin{bmatrix} a_1 & & & \\ \vdots & b_2 & 0 & \\ & & \ddots\; a_3 & \\ & & \ldots\ldots\ldots & b_{2M} \end{bmatrix} \begin{bmatrix} 1 & 1 & \ldots & 1 \\ \lambda_1^{-1} & \lambda_{-1}^{-1} & & \lambda_{-M}^{-1} \\ \lambda_1^{1} & \lambda_{-1}^{1} & & \lambda_{-M}^{1} \\ \vdots & \vdots & & \vdots \\ \lambda_1^{-M} & \lambda_{-1}^{-M} & \ldots & \lambda_{-M}^{-M} \end{bmatrix}. \tag{B7}$$

The determinant of the latter matrix can be found if we permute the columns into the order $\lambda_{-M} < \lambda_{-M+1} < \cdots \lambda_M$ and the rows by the same permutation into the order $\lambda^{-M} < \lambda^{-M+1} < \cdots \lambda^M$, and then multiply the columns by λ_k^M, $k=-M,\ldots,M$. These operations transform it into the standard Van der Monde determinant

$$\begin{vmatrix} 1 & \ldots & 1 \\ \lambda_{-M} & & \lambda_M \\ \vdots & & \vdots \\ \lambda_{-M}^{2M-1} & & \lambda_M^{2M-1} \end{vmatrix} = \prod_{k>l}(\lambda_k-\lambda_l) = C_+\,,$$

so $|S| = C_+ i^{-M}\prod_1^M a_{2k-1}b_{2k}$. From (B6) follows that $a_{2k-1}b_{2k}=C_+(a_1b_2)$, so $|S|=C_+ i^{-M} b_2^M$. From (B 5) and the boundary condition we see that $b_2=(i\,\mathrm{Sh}\,v_2)^{-1}(-\mathrm{Ch}\,v_2+\mathrm{Ch}\,v_2-1)=iC_+$ and finally that $|S|=C_+=+1$, since S is orthogonal.

References

1. Abraham, D. B.: Studies in Appl. Math. **L**, 71 (1971).
2. Abraham, D. B.: Studies in appl. Math. **LI**, 199 (1972).
3. Abraham, D. B., Gallavotti, G., Martin-Löf, A.: Surface Tension on the two dimensional Ising Model, Preprint 1972.
4. Gallavotti, G., Martin-Löf, A.: Commun. math. Phys. **25**, 87 (1972).
5. Gallavotti, G., Miracle-Solé, S.: Phys. Rev. **5B**, 2555 (1972).
6. Huang, K.: Statistical Mechanics, New York: John Wiley 1963.
7. Kac, M.: Proc. Brandeis Univ. Summer Inst. in Theor. Phys. 1966, vol. 1, ed. by M. Chrétien, New York: Gordon and Breach 1968.
8. Kaufmann, B., Onsager, L.: Phys. Rev. **76**, 1232 (1949).
9. Lebowitz, J., Martin-Löf, A.: Commun. math. Phys. **25**, 176 (1972).
10. Martin-Löf, A.: Commun. math. Phys. **24**, 253 (1972).
11. Montroll, E., Potts, R., Ward, J.: Journ. Math. Phys. **4**, 308 (1963).
12. Onsager, L.: Phys. Rev. **65**, 117 (1944).

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Note added in proof: The calculation of the surface tension in Section 5 is not quite correct. The formulas should be based on the other symmetrised product $V_1^{1/2} V_2 V_1^{1/2}$ instead of on V. The final result is however correct. The argument in Appendix A is also not quite right, but it can easily be completed for $\sigma = +$. The correct proofs will appear in forthcoming papers by the authors.