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Correlation near the free surface of an Ising ferromagnet

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Abstract. The two-spin and four-spin correlation functions involving one and two pairs of nearest neighbours respectively are evaluated near the free surface of an Ising ferromagnet and the departure from the bulk value is found. These correlation functions could be termed the energy density and the energy density–energy density correlation functions. Near the critical temperature T_c the energy density in the surface layer is found to behave as $t^2 \ln t$ with $t = |T - T_c|$. This contrasts with the bulk energy density which has a $t \ln t$ singularity. Correlations between a surface and a bulk spin are evaluated above and below T_c. Correlations between surface spins when the coupling between the surface spins is different from those in the bulk are examined.

1. Introduction

A cylindrical Ising model is investigated using the transfer matrix V' parallel to the axis of the cylinder. In particular, certain correlations between spins a finite distance from the edge of the lattice will be calculated.

The problem of a non-toroidal lattice has been investigated by McCoy and Wu (1967) who gave an exhaustive analysis of properties such as magnetisation and correlation in the boundary layer itself. This problem has also been examined by Abraham (1971) and Abraham and Martin-Lof (1973). Here correlations between spins near, but not necessarily both in, the surface layer will be investigated. This problem was investigated by Camp and Fisher (1972) who obtained a high temperature expression for the spin–spin correlation when the spins are an arbitrary distance from a free surface. In a few cases the approach of a correlation function to its bulk value can be easily calculated at a variety of temperatures. It is these correlation functions that will be of interest here.

In § 2 a brief review of the model is given. In § 3 the expectation of a pair of nearest neighbour spins is calculated at an arbitrary distance from the free surface and the approach to the bulk value found for $T \lessgtr T_c$ and $T = T_c$. Also in § 3 the energy density–energy density correlation function is calculated at $T = T_c$, and to leading order this behaves as

$$\frac{1}{l^2} - \frac{1}{(l+2r)^2}$$

where l is the separation and r is the distance of the nearer pair of spins from the free surface. The above has the form of a direct correlation minus an image correlation. This means that the second term has the form of a direct correlation between a pair of spins at $l + r$ and $-r$ (i.e. a distance r from the free surface, but on the other side). This form of a direct term minus an image term occurs for other correlations near a free surface (Bray and Moore 1977). The exponent for the decay of the energy density–energy density correlation function is 2 for $r<l$ and 3 for $r>l$. This change in the critical exponent can be related to the change in critical behaviour of the energy density as the surface is approached. The bulk energy density has a $t \ln t$ ($t=|T-T_c|$) singularity; however, it is shown in § 4 that the surface energy density has a $t^2 \ln t$ singularity. Scaling would then predict a change in exponent from 2 to 3 as found explicitly.

In § 4 the correlation between a surface and bulk spin is found for $T \lessgtr T_c$. In both cases the Ornstein–Zernike form is found. This contrasts with the bulk case when only for $T>T_c$ is the Ornstein–Zernike form found there being an anomalous r^2 term in the denominator of the correlation function for low temperatures. Also in § 4, consideration is given to surface correlations when the coupling between surface spins is different from those in the bulk.

2. Model

A cylindrical Ising ferromagnet with M columns (M is even) and N rows is considered. At each lattice site i, j there is a spin $\sigma_{ij}=\pm 1$ interacting with its nearest neighbours only. The energy of any configuration is taken as

$$E=-\sum_{ij} J(\sigma_{ij}\sigma_{i+1\,j}+\sigma_{ij}\sigma_{i\,j+1}). \tag{2.1}$$

The partition function Z is given by

$$Z=\sum W_1(\sigma_1)\,e^{-\beta E}\,W_N(\sigma_N). \tag{2.2}$$

$W_1(\sigma_1)$ and $W_N(\sigma_N)$ are statistical weights assigned to configurations of the first and last rows respectively. It is well known (Camp and Fisher 1972, Schultz *et al* 1964) that (2.2) can be expressed as the expectation of an abstract operator as follows:

$$Z=\langle W_1|(V_2V_1)^{N-1}V_2|W_N\rangle,$$

with

$$V_2=(\sinh 2K)^{M/2}\exp\Big(-K\sum \sigma_j^x\sigma_{j+1}^x\Big),$$
$$V_1=\exp\Big(-K^*\sum \sigma_j^z\Big), \tag{2.3}$$

and

$$K=J\beta, \qquad \beta=(kT)^{-1}, \qquad \exp(-2K^*)=\tanh K.$$

$\sigma_1^{x,z}$ are Pauli spin matrices, and $\langle W_1|$ and $|W_N\rangle$ are kets representing the boundary conditions that are imposed. Similarly, if A and B are functions of spins in the i and $i+r$ rows respectively, then the expectation of AB can be written as

$$Z^{-1}\langle W_1|(V_2V_1)^i\boldsymbol{A}(V_2V_1)^r\boldsymbol{B}(V_2V_1)^{N-(r+i+1)}V_2|W_N\rangle \tag{2.3}$$

where $\boldsymbol{A}$ and $\boldsymbol{B}$ are suitable operator representations of A and B. Typically A and B are single spins. The generalisation of (2.3) to the expectation of the product of any number of operators is obvious. The diagonalisation of the symmetrised product

$V' = V_1^{1/2} V_2 V_1^{1/2}$ essentially calculated the partition function. This was first done by Onsager (1944) and the details are contained in many places (Schultz *et al* 1964, Abraham 1972); the result is:

$$V' = \tfrac{1}{2}[1+(-1)^\sigma] V'(\beta) + \tfrac{1}{2}[1-(-1)^\sigma] V'(\alpha) \tag{2.4}$$

$$V'(\omega) = (2 \sinh 2K)^{M/2} \exp\left(-\sum_\omega \gamma(\omega)(G_\omega^+ G_\omega - \tfrac{1}{2})\right). \tag{2.5}$$

The Onsager function $\gamma(\omega)$ is defined by

$$\cosh \gamma(\omega) = \cosh 2K^* \cosh 2K - \cos \omega. \tag{2.6}$$

G_ω^+ and G_ω are derived from the following transformations:

$$G_\omega^+ = \cos Q_\omega F_\omega^+ - \mathrm{i} \sin Q_\omega F_{-\omega}$$

$$F_\omega^+ = M^{1/2} \sum_{j=1}^{M} \mathrm{e}^{\mathrm{i}j\omega} f_j^+ \tag{2.7}$$

$$f_j^+ = \prod_{p=1}^{j-1} \exp[\tfrac{1}{2}\mathrm{i}\pi(1+\sigma_p^z)] \tfrac{1}{2}(\sigma_j^x + \mathrm{i}\sigma_j^y).$$

α and β in (2.4) are generated by the following conditions:

$$\mathrm{e}^{\mathrm{i}M\alpha} = 1 \qquad \mathrm{e}^{\mathrm{i}M\beta} = -1, \tag{2.8}$$

$(-1)^\sigma$ is the parity operator and Q_ω, the transformation angle in the Bogoliubov–Valatin transformation, is defined by:

$$\exp(-2\mathrm{i}Q_\omega) = \frac{1}{(AB)^{1/2}} \left(\frac{Z-A}{Z-A^{-1}} \frac{Z-B}{Z-B^{-1}} \right)^{1/2} \tag{2.9}$$

with

$$Z = \mathrm{e}^{\mathrm{i}\omega} \qquad A = \exp 2(K+K^*) \qquad B = \exp 2(K-K^*). \tag{2.10}$$

The appropriate branch of the square root in (2.9) is determined by the conditions:

$$Q_0 = \begin{cases} 0 & K^* > K \quad (T > T_c) \\ \tfrac{1}{2}\pi & K^* < K \quad (T < T_c). \end{cases} \tag{2.11}$$

The vacuum state of V' is defined to be $|\phi_+\rangle$ for $T > T_c$ and $|\phi_+\rangle$, $|\phi_-\rangle$ for $T < T_c$.

3. Calculation of $\langle \sigma_{r+1,1} \sigma_{r,1} \rangle$

The energy density may be expressed as the expectation of the product of a pair of neighbouring spins. The bulk value of the energy density was one of the first correlation functions to be calculated for the two-dimensional Ising ferromagnet (Kaufman and Onsager 1949, Montrol *et al* 1962). Here the energy density is investigated as a function of distance from the free boundary spins. The asymptotic approach of the energy density to its bulk value is found in the three temperature regions $T > T_c$, $T < T_c$ and $T = T_c$. All results have the scaling form and in the regions $T < T_c$ and $T > T_c$ the approach to the bulk value is governed by a single exponential term and not by a decreasing sequence of exponentials.

Firstly, a boundary state is found on which all other states have equal projections. This state then represents a free boundary. The appropriate state to choose is the σ_j^z vacuum state $2^{-M}|0\rangle$. From (2.2) the partition function is

$$Z=\frac{1}{2^{2M}}\mathrm{e}^{MK^*}\langle 0|V'^N|0\rangle. \tag{3.1}$$

After making a spectral decomposition using the even spectrum of V' this becomes:

$$\begin{aligned} Z&=2^{-2M}\lambda_+^N\prod_{\beta>0}\cos Q_\beta+\mathrm{O}(\mathrm{e}^{-N\gamma(0)}),\\ \lambda_+&=(\sinh 2K)^{M/2}\exp\tfrac{1}{2}\sum_\beta\gamma(\beta). \end{aligned} \tag{3.2}$$

Using (2.3) and the periodicity of the system, the following is found:

$$\langle\sigma_{r,1}\sigma_{r+1,1}\rangle=\cosh 2K^*+\frac{\mathrm{e}^{MK^*}}{ZM}\sinh 2K^*\sum_{j=1}^{M}\langle 0|V'^{N-r}\sigma_j^z V'^r|0\rangle. \tag{3.3}$$

The matrix element in (3.3) is calculated by the method of Schultz *et al* (1964) and the result is found to be in the limit $N\to\infty$, $M\to\infty$,

$$\langle\sigma_{r+1,1}\sigma_{r,1}\rangle=\cosh 2K^*-\sinh 2K^*\frac{1}{\pi}\int_0^\pi\cos\delta'_\omega-\sinh 2K^*\frac{2}{\pi}\int_0^\pi\mathrm{e}^{-2r\gamma(\omega)}\left(\sin\frac{\delta'_\omega}{2}\right)^2 \tag{3.4}$$

δ'_ω is defined in Onsager (1944) and is related to Q_ω by $\delta'_\omega=2Q_\omega$. The first two terms of (3.4) give the bulk value of the energy density. This is evaluated in Kaufman and Onsager (1949). The third term of (3.4) gives the deviation from the bulk value and will be evaluated by steepest descent. Using some results from Onsager (1944) the last term of (3.4) can be written

$$D(T)=\sinh 2K^*\times\int_{\gamma(0)}^{\gamma(\pi)}\mathrm{e}^{-2rx}\frac{\sinh x-\cosh 2K\sinh 2K^*-\cosh 2K^*\sinh 2K(d-\cosh x)}{[1-(d-\cosh x)^2]^{1/2}} \tag{3.5}$$

with $d=\cosh 2K\cosh 2K^*$. (3.5) will be evaluated for $T\lessgtr T_\mathrm{c}$ and $T=T_\mathrm{c}$. For $T\lessgtr T_\mathrm{c}$ the integral is dominated by its value near $\gamma(0)$ and the leading behaviour of the integral is found by expanding the integrand about this point and using steepest descent. Thus for $r\gamma(0)>1$:

$$\begin{aligned} D(T<T_\mathrm{c})&\simeq-\frac{\mathrm{e}^{-2r\gamma(0)}}{r^{1/2}}\left(\frac{\sinh\gamma(0)}{\pi}\right)^{1/2}\sinh 2K^*\left(1+\mathrm{O}\left(\frac{1}{r}\right)\right)\\ D(T>T_\mathrm{c})&\simeq-\frac{\mathrm{e}^{-2r\gamma(0)}}{4r^{3/2}}\left(\frac{\cosh\gamma(0)-\cosh 2K^*\sinh 2K\sinh\gamma(0)}{(2\pi\sinh\gamma(0))^{1/2}}+\mathrm{O}\left(\frac{1}{r}\right)\right). \end{aligned} \tag{3.6}$$

At T_c, $\gamma(0)=0$ and there is a removable singularity at $x=0$. *However, the integral is* *still dominated by the behaviour of the integrand for small x.* The following is found for $r > 1$:

$$D(T_c) = -\frac{1}{r}\left(\frac{\sinh 2K^*}{2\pi} + O\left(\frac{1}{r}\right)\right). \tag{3.7}$$

The summation of (3.7) over r is divergent. This is to be expected in view of the logarithmic infinity in the surface entropy at $T = T_c$. It is perhaps worth noting that (3.7) would not be reproduced if the energy density was to be calculated at a distance r from some point defect in the bulk. In this case the departure from the bulk value would behave like the energy density–energy density correlation function for the bulk system.

3.1. Calculation of $\langle \sigma_{r,1}\sigma_{r+1,1}\sigma_{r+l+1,1}\sigma_{r+l+2,1}\rangle$

From considering the energy density as a function of distance from the free boundary, consideration is now given to the energy density–energy density correlation function. This may be expressed as the expectation of the product of four spins consisting of two pairs of nearest neighbours. This correlation function will be investigated at the critical temperature only.

Associated with any correlation function is an exponent x such that at the critical temperature this correlation function decays as r^{-x}, with r being the separation between the spins. For correlations between spins near a free boundary x will depend on the distance from the free boundary. Some effort has recently been given to the problem of extracting the dependence of x on the distance from the boundary (Bray and Moore 1977). For the energy density–energy density correlation function the dependence of x on distance from the free boundary can be readily found, and this will now be done.

Consider two pairs of nearest-neighbour spins lying in the same column; one pair a distance r from the surface, the other a distance $r + l$. Define:

$$C(l, r) = \langle \sigma_{r,1}\sigma_{r+1,1}\sigma_{r+l+1,1}\sigma_{r+l+2,1}\rangle - \langle \sigma_{r,1}\sigma_{r+1,1}\rangle\langle \sigma_{r+l+1,1}\sigma_{r+l+2,1}\rangle. \tag{3.8}$$

Using (2.4) and making a spectral decomposition, with the aid of the even spectrum of V', the following is found:

$$C(l, r) = \frac{\langle \phi_+|\hat{\sigma}_1^z V'^l \hat{\sigma}_1^z V'^r|0\rangle + O(e^{-(N-l-r)\gamma(0)})}{\lambda_+^{l+r}\Pi_{\beta>0}\cos Q_\beta + O(e^{-N\gamma(0)})} - \langle \sigma_{r,1}\sigma_{r+1,1}\rangle\langle \sigma_{r+l+1,1}\sigma_{r+l+2,1}\rangle \tag{3.9}$$

with

$$\hat{\sigma}_1^z = \cosh 2K^* + \sigma_1^z \sinh 2K^*.$$

In the limit $N \to \infty$, $e^{-(N-l-r)\gamma(0)}$ and $e^{-N\gamma(0)}$ both tend to zero and will be ignored. Only the first term of (3.9) needs to be calculated, the other terms having already been found. The transfer matrices are eliminated from (3.1) using the following substitution for σ_1^z:

$$\sigma_1^z = \frac{2}{M}\sum_{\beta_1\beta_2} e^{i(\beta_1-\beta_2)}(-i \sin Q_{\beta_2} \cos Q_{\beta_1} G_{\beta_1}^+ G_{-\beta_2}^+ + \cos Q_{\beta_1} \cos Q_{\beta_2} G_{\beta_1}^+ G_{\beta_2}$$
$$+ i \sin Q_{\beta_1} \cos Q_{\beta_2} G_{-\beta_1} G_{\beta_2} + \sin Q_{\beta_1} \sin Q_{\beta_2} G_{-\beta_1} G_{-\beta_2}^+) - 1.$$

Using this in (3.9) only leaves fourth- and second-order matrix elements of the form

$\langle\phi_+|G_{\beta_1}G_{\beta_2}G_{\beta_3}G_{\beta_4}|0\rangle$ and $\langle\phi_+|G_{\beta_1}G_{\beta_2}|0\rangle$ respectively and these are readily calculated using (2.7). Finally, for $T=T_c$ the following is found:

$$\lim_{\substack{N\to\infty\\M\to\infty}} C(l,r)=\frac{2}{\pi^2}\int_0^{\gamma(\pi)}\int_0^{\gamma(\pi)} e^{-l(x_1+x_2)} \times\frac{\cosh\frac{1}{2}x\cosh x_2(1-\cosh 2K\tanh\frac{1}{2}x_1)(1+\cosh 2K\tanh x_2)}{(3-\cosh x_1)^{1/2}(3-\cosh x_2)^{1/2}}$$
$$-\frac{2}{\pi^2}\left(\int_0^{\gamma(\pi)} e^{-(l+2r)x}\frac{\cosh\frac{1}{2}x(1-\cosh 2K\tanh\frac{1}{2}x)}{(3-\cosh x)^{1/2}}\right)^2$$
$$+\frac{4}{\pi^2}\int_0^{\gamma(\pi)}\int_0^{\gamma(\pi)} e^{-lx_1}e^{-(l+2r)x_2}\frac{\cosh 2K\tanh\frac{1}{2}x_1(1-\cosh 2K\tanh\frac{1}{2}x_2)}{(3-\cosh x_1)^{1/2}(3-\cosh x_2)^{1/2}}. \tag{3.10}$$

The last term of (3.10) is an order of magnitude smaller than the first two terms. For $l\gg 1$ it is seen that each integral is dominated by the value of the integrand near the origin. Hence the large-l behaviour of the integral can be found by expanding the integrand to smallest value in x and integrating. The following is found:

$$C(l,r)=\frac{1}{\pi^2}\left(\frac{1}{l^2}-\frac{1}{(l+2r)^2}+\frac{\cosh 2K}{l^2(l+2r)}+O(l^{-4})\right). \tag{3.11}$$

To leading order in l this correlation function has the form of a direct correlation plus an image correlation. The first term is just the bulk value of the energy density–energy density correlation function (Niemeijer 1967). In the two limits $r<l$ and $r>l$ $C(l,r)$ becomes:

$$C(l,r)=\begin{cases} l^{-2}, & r>l,\\ 2rl^{-3}, & r<l.\end{cases} \tag{3.12}$$

(3.12) gives the criteria for the cross-over from bulk to surface behaviour. The two forms given in (3.12) are consistent with scaling. Firstly, the bulk energy density has a $t\ln t$ singularity as the critical temperature is approached. This would lead to a predicted l^{-2} decay in the bulk energy density–energy density correlation function. Later it will be shown that the energy density in the surface has a $t^2\ln t$ singularity leading to an expected decay rate of l^{-3} in the energy density–energy density correlation function.

4. Calculation of $\langle\sigma_{r,1}\sigma_{1,1}\rangle$

Correlations between spins in a free boundary of an Ising ferromagnet have been investigated by McCoy and Wu (1967) and Abraham (1971) using different techniques. Here correlations between a spin in the boundary layer and one in the bulk will be investigated at temperatures both greater and less than T_c. Correlations between surface spins will also be investigated when the coupling between the surface spins is allowed to be different from the bulk coupling.

Consider the correlation between a spin in the surface and a spin a distance r lattice spacings from it and lying in the same column. This from (2.3) is expressible as

$$\langle\sigma_{r,1}\sigma_{1,1}\rangle = e^{K^*}\langle 0|V'^{N-r}\hat{\sigma}_1^x V'^r\sigma_1^x|0\rangle(\langle 0|V'^N|0\rangle)^{-1} \tag{4.1}$$

with $\hat{\sigma}_1^x = \cosh(K^*)\sigma_1^x - \mathrm{i}\sinh(K^*)\sigma_1^y$. To evaluate (4.1) a spectral decomposition is made in both numerator and denominator using the even spectrum of V' to give:

$$\frac{e^{K^*}\langle\phi_+|\hat{\sigma}_1^x V'^r\sigma_1^x|0\rangle + O(e^{-(N-r)\gamma(0)})}{\lambda_+^r \cos Q_\beta + O(e^{-N\gamma(0)})}. \tag{4.2}$$

Terms of order $e^{-(N-r)\gamma(0)}$ and $e^{-N\gamma(0)}$ both vanish in the limit $N\to\infty$ and will be ignored. (4.2) is investigated for $T<T_c$ and $T>T_c$. Firstly the more involved case for $T<T_c$ is investigated. A spectral decomposition of (4.1) is made using the odd spectrum of V'. (4.2) becomes

$$\begin{aligned} e^{K^*}\langle\phi_+|\hat{\sigma}_1^x|\phi_-\rangle\Big[\langle\phi_-|\sigma_1^x|0\rangle\Big(\prod_{\beta>0}\cos Q_\beta\Big)^{-1}\Big] \\ + e^{K^*}\sum_{\alpha_1\alpha_2} e^{-r(\gamma(\alpha_1)+\gamma(\alpha_2))}\langle\phi_+|\hat{\sigma}_1^x G_{\alpha_2}^+ G_{\alpha_1}^+|\phi_-\rangle\langle\phi_-|G_{\alpha_1}G_{\alpha_2}\sigma_1^x|0\rangle \\ + O(e^{-4\gamma(0)}). \end{aligned} \tag{4.3}$$

The final term of (4.3) is a bound on the sum of higher terms in the spectral decomposition. $\langle\phi_+|\hat{\sigma}_1^x|\phi_-\rangle$ is the spontaneous magnetisation for the Ising ferromagnet (Yang 1952) its value being

$$m^* = \langle\phi_+|\hat{\sigma}_1^x|\phi_-\rangle = [1-(\sinh 2K)^{-2}]^{1/8}. \tag{4.4}$$

Now

$$\langle\phi_-|\sigma_1^x|0\rangle = M^{-1/2}\prod_{\alpha>0}\cos Q_\alpha,$$

and let

$$m_1 = M^{-1/2} e^{K^*}\prod_{\alpha>0}\cos Q_\alpha\Big(\prod_{\beta>0}\cos Q_\beta\Big)^{-1}.$$

m_1 is not such a well known quantity. It is in fact the spontaneous magnetisation for spins in the boundary. It is evaluated in appendix 1 where it is shown to be:

$$m_1 = \left(\frac{\cosh 2K - \coth 2K}{\cosh 2K - 1}\right)^{1/2} \tag{4.5}$$

$\langle\phi_-|G_{\alpha_1}G_{\alpha_2}|0\rangle$ is evaluated using (2.7) and the result is found to be:

$$\begin{aligned} M^{-1/2}\prod_{\alpha>0}\cos Q_\alpha[\mathrm{i}\,e^{-\mathrm{i}\alpha_2}(\cos Q_{\alpha_2})^{-1}\delta_{\alpha_1 0} - \mathrm{i}\,e^{-\mathrm{i}\alpha_1}(\cos Q_{\alpha_1})^{-1}\delta_{\alpha_2 0} \\ - e^{-\mathrm{i}Q_{\alpha_1}}(\cos Q_{\alpha_1})^{-1}\delta_{\alpha_1 - \alpha_2} + \delta_{\alpha_1\alpha_2}]. \end{aligned} \tag{4.6}$$

Using results contained in Abraham (1972) the matrix element $\langle\phi_+|\hat{\sigma}_1^x G_{\alpha_2}G_{\alpha_1}|\phi_-\rangle$ is given by:

$$\langle\phi_+|\hat{\sigma}_1^x G_{\alpha_2} G_{\alpha_1}|\phi_-\rangle = M^{-1}\,\mathrm{e}^{\mathrm{i}(\alpha_1+\alpha_2)}\,\mathrm{e}^{\mathrm{i}(Q_{\alpha_1}+Q_{\alpha_2})} m^* f(\alpha_1, \alpha_2)$$

$$f(\alpha_1, \alpha_2) = \frac{\cosh K^*}{1-z_1 z_2}\left[z_1\left(\frac{A-z_2}{1-z_1 A}\,\frac{B-z_2}{1-z_1 B}\right)^{1/2} - z_2\left(\frac{A-z_1}{1-z_2 A}\,\frac{B-z_{1-}}{1-z_2 B}\right)^{1/2}\right]$$
$$-AB\sinh K^*(z_2-z_1)[(1-z_1A)(1-z_1B)(1-z_2A)(1-z_2B)]^{-1/2} \tag{4.7}$$

with $\mathrm{e}^{\mathrm{i}\alpha_1} = z_1$, $\mathrm{e}^{\mathrm{i}\alpha_2} = z_2$.

Using (4.7) and (4.6) in (4.3):

$$\lim_{\substack{N\to\infty\\ M\to\infty}} \langle\sigma_{r,1}\sigma_{1,1}\rangle = m_1 m^*\left[1 - \frac{\mathrm{e}^{K^*}}{\pi}\int_{-\pi}^{\pi}\frac{\mathrm{e}^{\mathrm{i}Q_\omega}}{\cos Q_\omega}\left(f(\omega, 0)\,\mathrm{e}^{-r(\gamma(\omega)+\gamma(0))} + f(\omega, -\omega)\frac{\mathrm{e}^{-2r\gamma(\omega)}}{2}\right)\right]. \tag{4.8}$$

The saddle point of $\gamma(\omega)$ is at $\omega = 0$ and in the limit $r\,\gamma(0) \gg 1$ the integral is dominated by the contribution from small values of ω. Thus the leading behaviour of the integral is obtained by expanding the integrand in powers of ω and using steepest descent. Thus for $r\gamma(0) \gg 1$,

$$\lim_{\substack{M\to\infty\\ N\to\infty}} \langle\sigma_{r,1}\sigma_{1,1}\rangle = m_1 m^*\left(1 + \frac{\mathrm{e}^{-2r\gamma(0)}}{(r\sinh\gamma(0))^{1/2}}[C + \mathrm{O}(1/r)]\right) \tag{4.9}$$

with

$$C = (\cosh 2K - 1)\frac{\mathrm{e}^{K^*}}{\pi^{1/2}}\left(2\frac{\sinh K^*(\tanh 2K - \mathrm{e}^{-2K}) + \cosh K^*(\cosh 2K - \coth 2K)}{\cosh 2K - \coth 2K}\right.$$
$$\left. + 2^{1/2}[\mathrm{e}^{2K} + 2(\cosh 2K - \coth 2K)]\right).$$

(4.9) has the Ornstein–Zernike form, the correlation length being $(2\gamma(0))^{-1}$ which is the same as the bulk correlation length. The correlation for $T > T_c$ between a spin in the surface and a spin in the bulk will now be calculated. It will be found that this correlation function also has the Ornstein–Zernike form. Thus these perpendicular surface correlation functions are quite different from the corresponding bulk correlation functions where only for $T > T_c$ is the Ornstein–Zernike form found.

For $T > T_c$ a spectral decomposition is again made of (4.1) and the limit $N \to \infty$ taken. The result is

$$\lim_{N\to\infty} \langle\sigma_{r,1}\sigma_{1,1}\rangle = \sum_\alpha \mathrm{e}^{K^*}\,\mathrm{e}^{-r\gamma(\omega)}\left(\prod_{\beta>0}\cos Q_\beta\right)^{-1} \langle\phi_+|\hat{\sigma}_1^x G_\alpha^+|\phi_-\rangle\langle\phi_-|G_\alpha\sigma_1^x|0\rangle + \mathrm{O}(\mathrm{e}^{-2r\gamma(0)}). \tag{4.10}$$

The final term of (4.10) is a bound on higher terms in the spectral decomposition. From (2.7) the following is found:

$$\langle\phi_-|G_\alpha\hat{\sigma}_1^x|0\rangle = M^{-1/2}\,\mathrm{e}^{\mathrm{i}\alpha}(\cos Q_\alpha)^{-1}\prod_{\alpha>0}(\cos Q_\alpha). \tag{4.11}$$

$\langle\phi_+|\hat{\sigma}_1^x G_\alpha|\phi_-\rangle$ is evaluated by the method of Abraham (1972) the result being

$$M^{-1/2}\,\mathrm{e}^{\mathrm{i}\alpha}\,\mathrm{e}^{\mathrm{i}Q_\alpha}\langle\phi_+|\phi_-\rangle\left[\cosh K^*\left(\frac{1-A^{-1}\,\mathrm{e}^{\mathrm{i}\alpha}}{1-B\,\mathrm{e}^{\mathrm{i}\alpha}}\right)^{1/2} + \sinh K^*\left(\frac{B-\mathrm{e}^{\mathrm{i}\alpha}}{A^{-1}-\mathrm{e}^{\mathrm{i}\alpha}}\right)^{1/2}\right]$$
$$= \mathrm{e}^{\mathrm{i}\alpha}\,\mathrm{e}^{\mathrm{i}Q_\alpha} M^{-1/2} f(\alpha). \tag{4.12}$$

Using (4.12) and (4.11) in (4.10) and taking the limit $M \to \infty$ yields:

$$\lim_{\substack{N\to\infty \\ M\to\infty}} \langle \sigma_{r,1}\sigma_{1,1}\rangle = \frac{e^{K^*}}{2\pi}\int_{-\pi}^{\pi} \frac{e^{iQ_\alpha}}{\cos Q_\alpha} e^{-r\gamma(\alpha)} f(\alpha). \tag{4.13}$$

Again the minimum value of $\gamma(\alpha)$ is for $\alpha = 0$ and thus for $r\gamma(0) \gg 1$ the integral is dominated by the small-α behaviour of the integrand. Hence the leading behaviour of the integral can be found by expanding the integrand to smallest powers in α. Hence for $r\gamma(0) \gg 1$ the following is found:

$$\lim_{\substack{N\to\infty \\ M\to\infty}} \langle \sigma_{r,1}\sigma_{1,1}\rangle = \frac{e^{-r\gamma(0)}}{(r \sinh \gamma(0))^{1/2}}[C_1 + O(1/r)] \tag{4.14}$$

$$C_1 = \langle \phi_+|\phi_-\rangle\, e^{K^*} \frac{\cosh K^*(e^{-2K} - \tanh K)^2 + \sinh K^*(e^{-2K} - \coth K)^2}{(e^{-2K} - \tanh K)(e^{-2K} - \coth K)}.$$

Thus the Ornstein–Zernike form has again ensued. If both spins had been allowed to be an arbitrary distance from the surface then for $T > T_c$ (4.14) would not have ensued. The correlation function would have been the difference between a 'direct correlation' and 'image correlation' (Camp and Fisher 1972). This would change the exponent in the denominator from $\frac{1}{2}$ to $\frac{3}{2}$. The problem of correlations between spins in the surface has been examined by McCoy and Wu (1967) and Abraham (1971). Using the formalism developed so far it is an easy matter to extend the discussion to surface correlation. It is also possible to extend the discussion to the case where the couplings between the surface spins is altered from J to J^-. This case was not discussed above.

Equation (2.3) is quite general and holds even if the couplings between spins are not all the same. Thus the spin–spin correlation between spins in the boundary row when the coupling between the surface spins is altered from J to J^- can be expressed as

$$\begin{aligned} \langle \sigma_{1,1}\sigma_{1,P}\rangle &= \langle 0|\, V'^N V_1^{1/2} \bar{V}_2 \sigma_1^x \sigma_P^x |0\rangle (\langle 0|\, V'^N V_1^{1/2} \bar{V}_2 |0\rangle)^{-1} \\ \bar{V} &= \exp\Big(-\bar{K} \sum \sigma_i^x \sigma_{i+1}^x\Big), \qquad \bar{K} = J^-\beta. \end{aligned} \tag{4.15}$$

Using the ordinary properties of transfer matrices (4.15) becomes in the limit $N \to \infty$, $M \to \infty$

$$\frac{1}{2\pi i}\int_{-\pi}^{\pi} e^{i\omega(P-1)} \tan Q_\omega \frac{\cosh 2\bar{K} + \sinh 2\bar{K} \cos\omega - \cot Q_\omega\, e^{2K^*} \sin\omega \sinh 2\bar{K}}{e^{2K^*}(\cosh 2\bar{K} - \sinh 2\bar{K}\cos\omega) - \tan Q_\omega \sin\omega \sinh 2\bar{K}}. \tag{4.16}$$

For the case of $J = J^-$ this becomes equal to

$$\frac{e^{2K^*}}{2\pi i}\int_{-\pi}^{\pi} e^{i\omega(P-1)} \tan Q_\omega \tag{4.17}$$

which, though derived by different methods, has been investigated by McCoy and Wu (1967) and an equivalent integral has been investigated by Abraham (1971). Here (4.16) will be investigated at all temperatures. Define $C(T)$ to be (4.16) and denote the integrand of (4.16) by $e^{i\omega(P-1)}P(\omega, T)$. The singularities of $P(\omega, T)$ which will be of importance in evaluation of (4.16) are outlined below.

(i) For $0<T<T_c$ there is a pole at $\omega=0$ and branch singularities at $\omega=\pm\mathrm{i}\ln B$, $\omega=\pm\mathrm{i}\ln A$, $A>B>1$.

(ii) For $T=T_c$ there is no pole on the axis and there are branch singularities at $\omega=\pm\mathrm{i}\ln A$.

(iii) For $T>T_c$ there is again no pole term and there are branch points at $\omega=\pm\ln B$, $\omega=\pm\mathrm{i}\ln A$, $A>1>B$.

(iv) For $T=0$ the branch singularities disappear but extra poles may appear on the axis of integration.

In all cases the integrals will be evaluated in the limit of large P. Consider $0<T<T_c$, then (4.16) becomes

$$C(T<T_c)=\frac{m_1^2\,\mathrm{e}^{2(\bar{K}-K^*)}}{\mathrm{e}^{2(K-K^*)}+2\,\mathrm{e}^{-2K^*}m_1^2\sinh 2\bar{K}}+\frac{1}{2\pi\mathrm{i}}\oint \mathrm{e}^{\mathrm{i}\omega(P-1)}P(\omega, 0<T<T_c). \tag{4.18}$$

The first term is just the square of the spontaneous magnetisation in a boundary row with perturbed bonds. For a discussion of the spontaneous magnetisation in a boundary row with perturbed bonds see Au-Yang (1973). The second term is the integral round the branch cut from $\omega=\mathrm{i}\ln B$ to $\omega=\mathrm{i}\ln A$. In the limit $P\ln B>1$ this integral is dominated by the contribution from $\omega=\mathrm{i}\ln B$ and hence in the limit $P\ln B>1$ the following is found:

$$\begin{aligned}C(T<T_c)&=\frac{m_1^2\,\mathrm{e}^{2(\bar{K}-K^*)}}{\mathrm{e}^{2(K^*-\bar{K})}+2m_1^2\,\mathrm{e}^{-2K^*}\sinh 2\bar{K}}+\left(\frac{\mathrm{e}^{2(K-K^*)}(\mathrm{e}^{4K^*}-1)}{2\pi(\mathrm{e}^{4K}-1)\sinh 2(K-K^*)}\right)^{1/2}\\&\quad\times\frac{\sinh^2 2(K-K^*)\,\mathrm{e}^{2K^*}+\coth^2 2\bar{K}-\cosh^2 2(K-K^*)}{\{\mathrm{e}^{2K^*}[\coth 2\bar{K}-\cosh 2(K-K^*)]+\sinh 2(K-K^*)\}^2}\,\frac{\mathrm{e}^{-2(K-K^*)(P-1)}}{(P-1)^{3/2}}\\&\quad\times(1+\mathrm{O}(1/P)).\end{aligned} \tag{4.19}$$

$[2(K-K^*)]^{-1}$ is the bulk correlation length, at $T=T_c$, $K-K^*=0$. At the critical temperature the analytic properties of $P(\omega, T_c)$ change; however it is still possible to Taylor expand $P(\omega, T_c)$ about $\omega=0$ and the following is obtained in the limit $P>1$:

$$C(T_c)=\frac{1}{P-1}[\mathrm{e}^{4\bar{K}-2K^*}+\mathrm{O}(1/P^2)]. \tag{4.20}$$

For $T_c<T$ the following is obtained:

$$\begin{aligned}C(T_c<T)&=\left(\frac{\mathrm{e}^{2(K^*-K)}(\mathrm{e}^{4K^*}-1)}{2\pi(\mathrm{e}^{4K}-1)\sinh 2(K^*-K)}\right)^{1/2}\\&\quad+\frac{\mathrm{e}^{2K^*}\sinh^2 2(K^*-K)+\coth^2 2\bar{K}-\cosh^2 2(K^*-K)}{\mathrm{e}^{2K^*}[\coth 2\bar{K}-\cosh 2(K^*-K)]+\sinh 2(K^*-K)}\,\frac{\mathrm{e}^{-2(K^*-K)(P-1)}}{(P-1)^{3/2}}\\&\quad\times(1+\mathrm{O}(1/P)).\end{aligned} \tag{4.21}$$

(4.21), (4.20) and (4.19) reduce to the results of McCoy and Wu (1967) for the case $J=J^-$. For $T=0$ (4.16) can be evaluated exactly to give:

$$C(0)=\lim_{T\to 0}\frac{-1}{2\pi\mathrm{i}}\int_{-\pi}^{\pi}\frac{\sin\omega[\mathrm{e}^{4\bar{K}+2K}-2(1-\cos\omega)]\,\mathrm{e}^{\mathrm{i}(P-1)\omega}}{(\cos\omega-1)\,\mathrm{e}^{4\bar{K}+2K}-2\sin^2\omega}.$$

For K positive and $4\bar{K}+2K>0$:

$$C(0)=1.$$

For $4\bar{K}+2K<0$:

$$C(0)=(-1)^{p-1}$$

For $4\bar{K}+2K=0$:

$$C(0)=\frac{1}{5}+\frac{(5^{1/2}-1)(13-45^{1/2})}{(5^{1/2}-3)(55^{1/2}-5)}\left(\frac{5^{1/2}-3}{2}\right)^{p-1}.$$

For $K>0$ and $4\bar{K}+2K=0$ correlations in the surface behave like those in a one-dimensional Ising antiferromagnet in a magnetic field of magnitude equal to twice the coupling constant. For this special case only there will also be entropy associated with the surface. Equation (4.17) can be used to examine the energy density in the surface layer. This will now be done and the critical behaviour of the surface energy density will be found. The bulk energy density has a $t\ln t$ singularity; however, the surface energy density has a $t^2\ln t$ singularity. This change in critical behaviour can be associated with the change in the decay rate of the energy density–energy density correlation function as explained in § 3. For neighbouring spins (4.17) becomes

$$\frac{e^{2K^*}}{2\pi i}\int_{-\pi}^{\pi} e^{i\beta}\tan Q_\beta$$

and consider $T>T_c$. The branch points of $\tan Q_\beta$ can be seen from (2.9) to be at $\beta=\pm 2i(K^*-K)$ and $\beta=\pm 2i(K+K^*)$. Define $\tau=(K^*-K)$ and choose T such that $|K^*-K|\ll 1$, and define

$$C(\tau)=\frac{e^{2K^*}}{2\pi}\int_{-\pi}^{\pi} e^{i\beta}\tan Q_\beta. \tag{4.22}$$

The critical behaviour of the above can be found by analytic continuation of $C(\tau)$ into the complex τ plane. Consider $C(e^{2\pi i}\tau)$, where the contour of integration of this is shown in figure 1(*b*). Now consider

$$\hat{C}(\tau)=C(e^{2\pi i}\tau)-C(\tau)$$

then the contour of integration of $\hat{C}(\tau)$ is the Pochhammer contour shown in figure 1(*c*). Using (2.9) and (4.22) the following is found:

$$\hat{C}(\tau)=i\tau^2(e^{2K^*}+O(\tau^2))$$

which implies:

$$C(\tau)=\tau^2\ln\tau(e^{2K^*}+O(\tau^2))+\text{Taylor series in }\tau.$$

So far only the non-analytic part of $C(\tau)$ has been found and there may be a linear term in the Taylor series so that the critical behaviour of $C(\tau)$ is not yet identified. Now consider

$$C'(\tau)=C(e^{i\pi}\tau)-C(\tau).$$

This expression will contain contributions from the non-analytic part of $C(\tau)$ and from terms linear in τ. The contour of integration for $C'(\tau)$ is shown in figure 1(*d*).

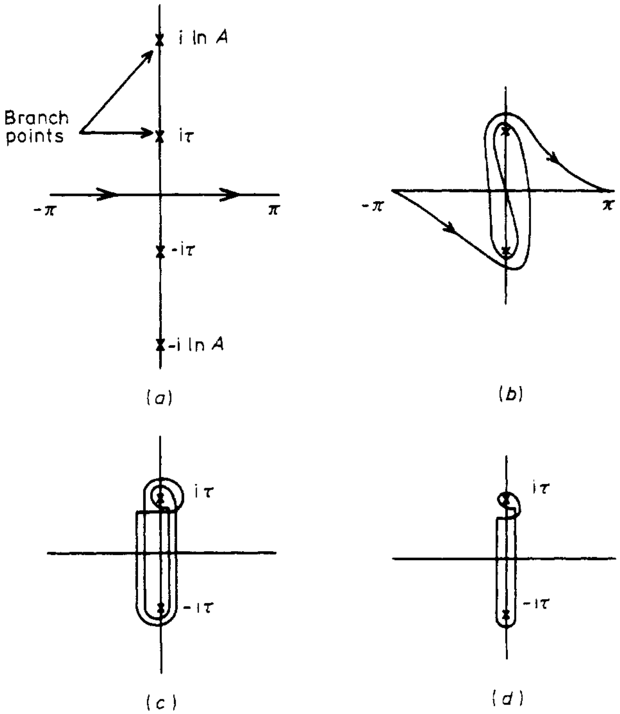

Figure 1. Contours of integration for: (*a*) $C(\tau)$; (*b*) $C(e^{2\pi i}\tau)$; (*c*) $C(\tau)$; (*d*) $C'(\tau)$.

However it is easy to show that

$$\hat{C}(\tau)-2C'(\tau)=0$$

so there are no linear terms in $C(\tau)$. A similar calculation can be made for $T<T_c$ and it is found that the critical part of the energy density behaves as $\tau^2 \ln|\tau|$.

5. Conclusion

Using simple techniques the energy density and the energy density–energy density correlation functions have been calculated near the free surface of an Ising ferromagnet and the results are given in § 2. The correlation between a bulk and a surface spin have been calculated in the limit when the separation is greater than the correlation length. Both above and below T_c this correlation function has the Ornstein–Zernike form. Asymptotic forms for the surface correlations with perturbed surface bonds have been found and the results given in § 4. The non-analytic part of the surface energy density has been found to be $t^2 \ln t$. This contrasts with a bulk singularity of $t \ln t$.

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Appendix 1.

Consider

$$m_1 = \lim_{M\to\infty} M^{-1/2} e^{K^*} \prod_{\alpha>0} \cos Q_\alpha \Big(\prod_{\beta>0} \cos Q_\beta\Big)^{-1}. \tag{A.1}$$

From (2.8) it is seen that

$$\alpha = \beta + (\pi/M) \tag{A.2}$$

therefore

$$Q_\alpha = Q_\beta + \frac{\pi}{M}\frac{\partial Q_\beta}{\partial \beta} + O\Big(\frac{1}{M^2}\Big). \tag{A.3}$$

Only terms of order less than $1/M^2$ need be retained. Define

$$m_0 = \lim_{M\to\infty} M^{-1/2} \prod_{\alpha>0} \sin\tfrac{1}{2}\alpha \Big(\prod_{\beta>0} \sin\tfrac{1}{2}\beta\Big)^{-1}. \tag{A.4}$$

Then using (A.2) and (A.3) in (A.4) and (A.1)

$$\ln\Big(\frac{m_1}{m_0}\Big) = \lim_{M\to\infty} \sum_\beta \ln\Big(1 - \frac{\pi}{M} Q'_\beta \tan Q_\beta\Big) - \ln\Big(1 + \frac{\pi}{M}\cot\tfrac{1}{2}\beta\Big) + K^*. \tag{A.5}$$

The summation in (A.5) can be written as an improper integral

$$\lim_{M\to\infty} \frac{M}{2\pi}\int_{\pi/M}^{\pi-(\pi/M)} \ln\Big(1 - \frac{\pi}{M} Q'_\beta \tan Q_\beta\Big) - \ln\Big(1 + \frac{\pi}{M}\cot\tfrac{1}{2}\beta\Big). \tag{A.6}$$

Expanding each logarithm in (A.6) and retaining the first term from each logarithm yields

$$-\frac{1}{2}\ln\frac{AB-1}{(1-A)(1-B)}. \tag{A.7}$$

Now all other terms coming from the expansion of the logarithms cancel in pairs. Hence from (A.5)

$$\frac{m_1}{m_0} = e^{K^*}\Big(\frac{(1-A)(1-B)}{AB-1}\Big)^{1/2}.$$

Now $m_0 = 1$, so that

$$m_1 = e^{K^*}\Big(\frac{(1-A)(1-B)}{AB-1}\Big)^{1/2} = \Big(\frac{\cosh 2K - \coth 2K}{\cosh 2K - 1}\Big)^{1/2}.$$

The above is identical to the spontaneous magnetisation found by McCoy and Wu (1967).

References

Abraham D B 1971 *Studies Appl. Math.* **50** 71
—— 1972 *Studies Appl. Math.* **51** 179
Abraham D B and Martin-Lof A 1973 *Commun. Math. Phys.* **32** 245

Au-Yang H 1973 *J. Math. Phys.* **14** 937
Bray A and Moore M A 1977 *Phys. Rev. Lett.* **38** 735
Camp W J and Fisher M E 1972 *Phys. Rev.* B **6** 946
Kaufman B and Onsager L 1949 *Phys. Rev.* **76** 1244
McCoy B and Wu T T 1967 *Phys. Rev.* **162** 436
Montroll E W, Potts R B and Ward J C 1962 *J. Math. Phys.* **4** 308
Niemeijer T 1967 *Physica* **36** 377
Onsager L 1944 *Phys. Rev.* **65** 117
Schultz T D, Mattis D C and Lieb E H 1964 *Rev. Mod. Phys.* **36** 856
Yang C N 1952 *Phys. Rev.* **84** 808