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Transfer-matrix-like properties of the XY model

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Abstract. Although the XY model cannot have a transfer matrix in the sense of an Ising model, it is shown that the partition function is as if there were one. The partition function for the closed anisotropic XY chain with N sites and arbitrary external field is shown to take the form $\lambda_0^N + \Sigma_{k=1}^{\infty} g_k \lambda_k^N$ where the g_k are integers. This means that there could be a transfer matrix of infinite size, the λ_k being its eigenvalues and the g_k being the corresponding degeneracies.

1. Introduction

1.1. *Purpose of this paper*

For those one-dimensional models which can be solved by the method of transfer matrices the partition function, Z_N, for a chain of N sites takes the form

$$Z_N = \sum_k g_k \lambda_k^N$$

where $|\lambda_k| \geqslant |\lambda_{k+1}|$. The number of k may not exceed the number of states per site and may be infinite as in the case of the classical Ising model. A grand partition function, $\mathscr{z}(w)$ may be constructed as follows:

$$\mathscr{z}(w) \equiv \sum_{N=N_0}^{\infty} Z_N w^{N-1} \qquad \text{for some } N_0.$$

Provided that $\Sigma_k |g_k \lambda_k^{N_0}|$ is convergent and the λ_k are bounded and have no limit point other than zero it may be shown that

$$\mathscr{z}(w) = -\sum_k \frac{g_k (w\lambda_k)^{N_0-1}}{w - \lambda_k^{-1}}.$$

Any sequence $\{Z_N\}$ satisfying the conditions above will be called a 'transfer matrix form'.

The work described in this paper was undertaken with the possibility in mind that the transfer matrix form may apply to many systems which do not have transfer matrices of a conventional kind. There would clearly be advantages if this were the case. The variation of the partition function with the size of the system would be easy to visualize. The grand partition function would have simple poles at the λ_k^{-1} with residues equal to $-g_k$. If the Z_N were evaluated numerically for small N by direct evaluation of the eigenvalues (eg Bonner and Fisher 1964), Padé analysis could be applied to obtain λ_0, λ_1 etc. By this method one could obtain both the behaviour of finite systems and of the infinite system. Unpublished numerical work of this kind by the author strongly suggests that the partition function of the closed field-free anisotropic Heisenberg chain is a transfer matrix form.

J L Martin (private communication) has proposed a form of transfer matrix of infinite size applicable to various models including the open XY and open Heisenberg chains. His work as yet has not been proved fully rigorously. The elements of the vectors on which his matrices act are not related to the states of the last site and have no obvious physical significance.

1.2. Layout of the paper

In §2 the XY model is defined and the formula for its partition function in a form similar to that obtained by Katsura (1962) is stated. There is a brief derivation and discussion of the result. The partition function consists of four terms and the way in which each depends on N is not very obvious. In § 3 each term is re-expressed in the form

$$A^N \prod_{k=1}^{\infty} (1-\xi_k^{-N}),$$

A and the ξ_k being independent of N. From here it follows fairly easily that the solution has the form $\lambda_0^N + \Sigma_{k=1}^{\infty} g_k \lambda_k^N$. In § 4 the position of all the ξ_k and their behaviour with temperature and external field are discussed. The positions of the poles of the grand partition function are examined. In the final section all the results obtained are briefly stated. There is a discussion of the XY model with slightly different boundary conditions.

2. The partition function of the XY model

2.1. Introduction to the XY model

The Hamiltonian for the model under consideration is given by

$$H_N = -J \sum_{i=1}^{N} (1+\gamma)\sigma_{xi}\sigma_{xi+1} + (1-\gamma)\sigma_{yi}\sigma_{yi+1} - B \sum_{i=1}^{N} \sigma_{zi}. \tag{2.1}$$

Here $\sigma_{xi}, \sigma_{yi}, \sigma_{zi}$ are Pauli operators for the ith site. The $(N+1)$th site is taken to be the same as the 1st site, thus effectively arranging the sites in a closed loop. J, B, γ are arbitrary parameters representing the strength of interaction, the external field and the degree of anisotropy between the X and Y interactions.

The problem of finding the partition function was essentially solved by Lieb *et al* (1961). They solved the problem for infinite N and pointed out how it could be solved for finite N. Katsura (1962) obtained the partition function for an even number of sites and discussed the thermodynamic properties of the model and compared them with those for other models. In the next subsection a more general result is stated for an odd number of sites as well. The method of derivation is similar to that used by Katsura.

2.2. Statement and method of the solution

Suppose that $Z_N(\beta)$ is the partition function for H_N as given by equation (2.1) and $\beta = (kT)^{-1}$. Then

$$Z_N \times 2^{1-N} = \prod_{q\in\mathscr{L}_+} \cosh v_q + \prod_{q\in\mathscr{L}_-} \cosh v_q + S_1^N \prod_{q\in\mathscr{L}_+} \sinh v_q + S_0 S_1^N \prod_{q\in\mathscr{L}_-} \sinh v_q. \tag{2.2}$$

Here the following definitions apply:

$$S_0 \equiv \begin{cases} 1, 4J^2 - B^2 > 0 \\ 0, 4J^2 - B^2 = 0, \\ -1, 4J^2 - B^2 < 0 \end{cases} \qquad S_1 \equiv \begin{cases} 1, \beta(2J+B) > 0 \\ 0, \beta(2J+B) = 0 \\ -1, \beta(2J+B) < 0 \end{cases}$$

$$v_q \equiv |\beta[(B-2J\cos q)^2 + (2J\gamma \sin q)^2]^{1/2}|. \tag{2.3}$$

$\mathscr{L}_+$ is the set $\{(\pi/N)+(2\pi/N)j\}$ and $\mathscr{L}_-$ the set $\{(2\pi/N)j\}$. Here j must be an integer and the elements of $\mathscr{L}_+$ and $\mathscr{L}_-$ are *modulo* 2π.

The method of solution used was by first expressing the Hamiltonian in terms of Fermi operators, P_k, Q_k as described by Lieb *et al* (1961) and Katsura (1962). A proper orthogonal transformation creating a new set of Fermi operators was performed as follows:

$$Q_k = \frac{1}{\sqrt{N}} \sum_{q \in \mathscr{L}_\pm} [\cos(qk + \tfrac{1}{4}\pi)Q'_q - \sin(qk+\tfrac{1}{4}\pi)P'_q]$$

$$P_k = \frac{1}{\sqrt{N}} \sum_{q \in \mathscr{L}_\pm} [\sin(qk + \tfrac{1}{4}\pi)Q'_q + \cos(qk+\tfrac{1}{4}\pi)P'_q].$$

H_N becomes

$$\tfrac{1}{2}(I+U)\tfrac{1}{4}\mathrm{i} \sum_{q\in\mathscr{L}_+} [(B-2J\cos q)X_q + 2\gamma J \sin q Y_q] + \tfrac{1}{2}(I-U)\tfrac{1}{4}\mathrm{i} \sum_{q\in\mathscr{L}_-} [(B-2J\cos q)X_q + 2\gamma J \sin q Y_q].$$

Here

$$U \equiv \prod_{k=1}^{N} \sigma_{zk},$$

$$X_q \equiv Q'_q P'_q - P'_q Q'_q + Q'_{-q} P'_{-q} - P'_{-q} Q'_{-q}$$

$$Y_q \equiv Q'_q P'_{-q} - P'_{-q} Q'_q + P'_q Q'_{-q} - Q'_{-q} P'_q.$$

By a further set of proper orthogonal transformations on the P'_q, Q'_q

$$(B-2J\cos q)X_q + 2\gamma J \sin q\ Y_q \quad \text{becomes} \quad 2\mathrm{i}c_q(\sigma_{zq} + \sigma_{z-q}).$$

Here

$$c_q = |(B-2J\cos q)^2 + (2J\gamma \sin q)^2|^{1/2} \qquad \text{if } q \neq 0 \text{ or } \pi$$

$$= B - 2J\cos q \qquad \text{if } q = 0 \text{ or } \pi$$

and $\sigma_{zq} = \mathrm{i}P_q Q_q$. Hence

$$H_N = -\tfrac{1}{2}(I+U) \sum_{q\in\mathscr{L}_+} c_q \sigma_{zq} - \tfrac{1}{2}(I-U) \sum_{q\in\mathscr{L}_-} c_q \sigma_{zq}. \tag{2.4}$$

It can be shown since all the transformations are proper orthogonal ones that $U = \Pi_{q\in\mathscr{L}_\pm} \sigma_{zq}$ and that the P_q, Q_q for $q \in \mathscr{L}_\pm$ are a set of Fermi operators obtainable from the P_k, Q_k by a similarity transformation. Using the fact that $\tfrac{1}{2}(I+U)$ and $\tfrac{1}{2}(I-U)$ are projection operators whose product is zero one may deduce the partition function from equation (2.4).

2.3. Discussion of the above solution

Since the proof of the above formula has only been sketched several points will be made in corroboration.

(i) This formula agrees with that obtained by Katsura (1962) when N is even.

(ii) It is possible to show that Z is unaltered by changing the sign of the external field. When N is even each of the four components of Z is unaltered when B is reversed. When N is odd reversing the field causes the 1st and 2nd components and the 3rd and 4th components to be interchanged.

(iii) Letting $B = 0$ and $\gamma = 1$, the Ising case for zero field is obtained. Each v_q becomes $|2J\beta|$, $S_0 = 1$, $S_1 = \mathrm{sgn}(2J\beta)$ and $Z \times 2^{1-N}$ becomes $\cosh^N(2J\beta) + \sinh^N(2J\beta)$ which agrees with the well known result (eg Stanley 1971, p 133).

(iv) Suppose $|B| < |2J|$. Then $S_0 = 1$ and $S_1 = \mathrm{sgn}(\beta J)$. In the antiferromagnetic case the last two terms combine to give a quantity which is always positive when N is even and negative when N is odd. This corresponds to the physical argument that in the antiferromagnetic case alternating spins try to orientate themselves in opposite directions. When N is odd they do not match up round the ring and this gives rise to a larger free energy and a smaller partition function. When N is even the spins match up and the partition function is larger. In the ferromagnetic case the spins tend to point in the same direction and always match up leading to a greater partition function. This corresponds to the fact that since now both S_0 and S_1 equal 1 the last two terms always combine to give a positive quantity. Bonner and Fisher (1964) showed numerically that for the closed Heisenberg chain this alternating effect exists in the antiferromagnetic case.

(v) If $|B| > |2J|$, $S_0 = -1$ and the last two terms of the partition function tend to cancel. Physically this might correspond to supposing that the transverse field is now so large that the spins tend to orientate themselves towards it anyway, and the matching or antimatching effect does not take place.

(vi) The formula agrees with that obtained by Thompson (1972) apart from the signs of the four terms. In his proof Thompson does not appear to have properly considered the cases when $q = 0$ or π.

3. Reduction of the partition function to transfer matrix form

3.1. Introduction

In this section each of the four components of the partition function just obtained is first re-expressed in the form $A^N \prod_{k=1}^{\infty} (1-\xi_k^{-N})$. Taking the first component as typical the method used is essentially as follows: putting $\cos q = \frac{1}{2}(z+1/z)$, $\cosh v_q$ can be nearly expressed as an infinite product of terms, $(1-z/\xi_k)$. The terms of $\prod_q \cosh v_q$ will be recombined to form $\prod_k \prod_q (1-z_q/\xi_k)$ times some simple function. $\prod_q (1-z_q/\xi_k)$ is simplified with the aid of a lemma stated below to become $(1-\xi_k^{-N})$.

Having achieved the form $A^N \prod_{k=1}^{\infty} (1-\xi_k^{-N})$, this can without much difficulty be re-expressed as $A^N(1+\sum_{j=1}^{\infty} g_j \lambda_j^{-N})$.

3.2. Re-expressing cosh v_q in terms of functions derived from its zeros

Let $z \equiv e^{iq}$ so that $\cos q = \frac{1}{2}(z+z^{-1}) \equiv p$, say. Let v_q be called $v(z)$.

From equation (2.3)

$$v_q^2 = \beta^2[B^2 + 4J^2\gamma^2 - 4BJ\cos q + 4J^2(1-\gamma^2)\cos^2 q]. \tag{3.1}$$

Since $\cosh \nu$ is an analytic function of ν^2 everywhere and $\nu^2(z)$ is an analytic function of z except at $z = 0$, $\cosh \nu(z)$ is an analytic function of z everywhere except at $z = 0$.

Let us now consider the zeros of $\cosh \nu(z)$. These occur when $\nu(z) = (k+1/2)\mathrm{i}\pi$ for some integer k. Inverting (3.1) one obtains

$$p = \frac{B \pm [\gamma^2 B^2 - (1-\gamma^2)(4J^2\gamma^2 - \nu_q^2/\beta^2)]^{1/2}}{2J(1-\gamma^2)} \tag{3.2}$$

and $z = p \pm (p^2-1)^{1/2}$. Using these equations all the zeros of $\cosh \nu(z)$ may be obtained. Each such z yields a zero of order one since $\mathrm{d}\cosh \nu/\mathrm{d}\nu = \sinh \nu \neq 0$ whenever $\nu = (k+1/2)\mathrm{i}\pi$.

If $|z| = 1$, p is real and by equation (2.3) $\nu^2(z)$ is real and positive so $\cosh \nu(z)$ is non-zero. Therefore, no zeros lie on the unit circle. Since $p = \frac{1}{2}(z+z^{-1})$ if z_1 is a zero so also is z_1^{-1}. Let the zeros outside the unit circle be ordered in some way to give ξ_1, ξ_2, etc. They may be ordered so that $|\xi_{k+1}| \geqslant |\xi_k|$ or so that ξ_{2k+1}, ξ_{2k+2} correspond to $\nu(z) = (k+1/2)\mathrm{i}\pi$. When k becomes large

$$p \simeq \frac{B \pm (1-\gamma^2)^{1/2}\nu/\beta}{2J(1-\gamma^2)}$$

$$z \simeq \frac{B \pm (1-\gamma^2)^{1/2}\nu/\beta}{J(1-\gamma^2)}. \tag{3.3}$$

Since $\nu = (k+1/2)\mathrm{i}\pi$ it is clear from (3.3) that the number of ξ_k in the circle

$$|z| < R \rightarrow \text{constant} \times R$$

as $R \rightarrow \infty$. $\Sigma_k |\xi_k|^{-\tau}$ is convergent if $\tau > 1$. This means that the infinite product,

$$W(z) \equiv \prod_{k=1}^{\infty} (1 - z/\xi_k)\, \mathrm{e}^{z/\xi_k}$$

is convergent. $W(z)$ is called the canonical product of genus 1 (Copson 1935, § 7.5, § 7.51). $W(z)$ is analytic everywhere and has zeros at the ξ_k. Let $U(z)$ be such that

$$\cosh \nu(z) = W(z)W(z^{-1})U(z). \tag{3.4}$$

Because the zeros of $W(z)W(z^{-1})$ coincide with those of $\cosh \nu(z)$, $U(z)$ is analytic everywhere except possibly at the origin and infinity and it has no zeros.

3.3. *Examination of* $U(z)$

Let us imagine what happens to the arguments of the above functions as z passes right round the unit circle. As has been said above, $\nu(z)$ remains real and positive and so does $\cosh \nu(z)$. Hence $\arg \cosh \nu(z)$ remains unchanged. Since $W(z)$ is analytic and has no zeros inside or on the unit circle $\arg W(z)$ is also unchanged by passing round the unit circle. Hence the same is true for $\arg W(z^{-1})$ and likewise for $\arg U(z)$. Let $V(z) = \ln U(z)$. $V(z)$ is analytic everywhere except possibly at the origin and infinity. Because $\arg U(z)$ is unaltered by passing round the unit circle, $V(z)$ is unchanged by passing round it. Hence $V(z)$ is uniquely defined. Because of these properties $V(z)$ has a Laurent expansion and can be expressed as $v_0 + V_1(z) + V_2(z^{-1})$ everywhere except at the origin. $V_1(z)$ is analytic everywhere and can be expressed as $\Sigma_{k=1}^{\infty} v_k z^k$. Because $\nu(z) = \nu(z^{-1})$, $U(z) = U(z^{-1})$ and $V_2(z) = V_1(z)$.

It is now necessary to consider the behaviour of $U(z)$ as $|z| \to \infty$. By a theorem by Borel (Copson 1935), for any radius ρ, there is a circle, $|z| = R$, outside it such that $W(z) > \exp(-R^{(1+\epsilon)})$ on it for any $\epsilon > 0$. If R is large enough then

$$|\cosh v(z)| < \exp R^{(1+\epsilon)}$$

on it. Let this circle be labelled Γ. On Γ, $|\cosh v(z)/W(z)| < \exp(2R^{(1+\epsilon)})$.

It is possible to choose two contours, α_1 and α_2, close to Γ, one just outside it and the other just inside it, such that $|\cosh v(z)| > 0{\cdot}5$ everywhere on α_1 and α_2. This is done by avoiding the zeros, ξ_k, and remembering that for large $|z|$, $v(z) \simeq \beta J(1-\gamma^2)^{1/2}z$. For sufficiently large R, using another theorem by Borel, it is possible to say that

$$|W(z)| < \exp(R^{(1+\epsilon)})$$

on α_1 and α_2. Hence $|W(z)/\cosh v(z)| < 2\exp(R^{(1+\epsilon)})$ on α_1 and α_2. Since this function is analytic between α_1 and α_2 and applying the maximum modulus theorem

$$\left|\frac{\cosh v(z)}{W(z)}\right| > 0{\cdot}5\exp(-R^{(1+\epsilon)})$$

on Γ.

Because $W(z)$ is analytic everywhere and has no zeros inside the unit circle it is possible to say that if $|z| \geqslant 2$ then $l_1 < |W(z^{-1})| < l_2$ for some positive l_1, l_2. Putting $U(z) = (\cosh v(z)/W(z))W(z^{-1})$ and combining the above results it is possible to say that for any positive ϵ and ρ, there is an $R > \rho$ such that on $|z| = R$,

$$\exp(-R^{(1+\epsilon)}) < |U(z)| < \exp(R^{(1+\epsilon)}).$$

Hence $-R^{(1+\epsilon)} < Rl\,V(z) < R^{(1+\epsilon)}$ on this circle and likewise for $Rl\,V_1(z)$.

It is now necessary to use the fact that if $w(z) = \Sigma_{j=0}^{\infty} w_j z^j$ and has a radius of convergence greater than r, then for $k \geqslant 1$

$$w_k = \frac{1}{\pi}\int_{\theta=0}^{2\pi} Rl\,w(r\,e^{i\theta})r^{-k}\,e^{-ik\theta}\,d\theta.$$

This can be deduced by putting the right-hand side equal to

$$\frac{1}{2\pi}\sum_{j=0}^{\infty}\int_{\theta=0}^{2\pi}(w_j r^j\,e^{ij\theta}+w_j^* r^j\,e^{-ij\theta})r^{-k}\,e^{-ik\theta}\,d\theta = w_k.$$

Applying this result to $V_1(z)$, one obtains

$$|v_k| \leqslant \frac{1}{\pi}\int_{\theta=0}^{2\pi}|Rl\,V_1(R\,e^{i\theta})|R^{-k}\,d\theta.$$

Letting $R \to \infty$ one deduces that $v_k = 0$ if $k > 1$. Hence

$$V(z) = v_0 + v_1 z + v_1 z^{-1}.$$

3.4. Obtaining the first two components of Z_N

Two lemmas which can easily be proved are now stated. Suppose we have the set $z_0, z_1 \ldots z_{N-1}$ where $z_j = z_0\,e^{2\pi ij/N}$, j being an integer.

Lemma 1.

$$\frac{1}{N}\sum_{j=0}^{N-1} z_j^k = z_0^k \qquad \text{if } k = Nl \text{ for some integer } l$$
$$= 0 \qquad \text{otherwise}$$

Lemma 2.

$$\prod_{j=0}^{N-1} (1-z_j) = 1-z_0^N.$$

This follows from the fact that the Nth roots of z_0^N are the z_j.

The set $\mathscr{L}_-$ corresponds to z_j when $z_0 = 1$ and the set $\mathscr{L}_+$ to z_j when $z_0 = e^{\pi i/N}$. From equation (3.4)

$$\prod_{q\in\mathscr{L}} \cosh v_q = \prod_j W(z_j) \prod_j W(z_j^{-1}) \ \exp\left(\sum_j V(z_j)\right).$$

Using Lemma 1,

$$\sum_j V(z_j) = Nv_0 \qquad \text{if } N \geqslant 2$$

$$\prod_{j=0}^{N-1} W(z_j) = \prod_{k=1}^{\infty}\prod_{j=1}^{N} (1-z_j/\xi_k)\exp(z_j/\xi_k) \ = \prod_{k=1}^{\infty} [1-(z_0/\xi_k)^N]$$

using lemmas 1 and 2 and assuming that $N \geqslant 2$. Now if $z_j \in \{z_j\}$ then so also is z_j^{-1}. Hence

$$\prod_{j=0}^{N-1} W(z_j^{-1}) = \prod_{j=0}^{N-1} W(z_j)$$

$$\prod_{q\in\mathscr{L}_-} \cosh v_q = \prod_{k=1}^{\infty} (1-\xi_k^{-N})^2 \, e^{Nv_0}$$

$$\prod_{q\in\mathscr{L}_+} \cosh v_q = \prod_{k=1}^{\infty} (1+\xi_k^{-N})^2 \, e^{Nv_0} \qquad \text{for } N \geqslant 2. \tag{3.5}$$

3.5. Evaluating the second two components

Let $\mathrm{sh}(v) \equiv \sinh(v)/v$. Since $\mathrm{sh}(v)$ is an analytic function of v^2, and v^2 is an analytic function of z, $\mathrm{sh}\, v(z)$ is analytic everywhere except at the origin. The zeros of $\mathrm{sh}\, v(z)$ occur when $v_q = ik\pi$ for k equal to any integer except 0. Let the zeros outside the unit circle be arranged in some order and labelled η_1, η_2, etc. Just as with $\cosh v(z)$, $\mathrm{sh}\, v(z)$ must also have as zeros η_1^{-1}, η_2^{-1}, etc. $\mathrm{sh}(v)$ is positive real on the unit circle so it has no zeros on it and passing round it causes no change in the argument. The arguments that were applied to $\cosh v(z)$ can equally well be applied to $\mathrm{sh}\, v(z)$ and the corresponding results are listed below:

$$\prod_{q\in\mathscr{L}_-} \mathrm{sh}(v_q) = \prod_{k=1}^{\infty} (1-\eta_k^{-N})^2\, \mathrm{e}^{Nu_0}$$

$$\prod_{q\in\mathscr{L}_+} \mathrm{sh}(v_q) = \prod_{k=1}^{\infty} (1+\eta_k^{-N})^2\, \mathrm{e}^{Nu_0}$$

for some u_0.

It now remains to evaluate $\Pi_{q\in\mathscr{L}}\, v_q$ which equals $(\Pi_{q\in\mathscr{L}}\, v_q^2)^{1/2}$. The right-hand side of (3.1) can be factorized and re-expressed to give

$$v^2(z) = A(1-z\zeta_1^{-1})(1-z^{-1}\zeta_1^{-1})(1-z\zeta_2^{-1})(1-z^{-1}\zeta_2^{-1}).$$

$\zeta_1, \zeta_1^{-1}, \zeta_2, \zeta_2^{-1}$ are the zeros of $v^2(z)$ and they may lie on the unit circle. It can be assumed that $1 \leqslant |\zeta_1| \leqslant |\zeta_2|$. Applying lemma 2

$$\prod_{j=0}^{N-1} v^2(z_j) = A^N(1-z_0^N\zeta_1^{-N})(1-z_0^{-N}\zeta_1^{-N})(1-z_0^N\zeta_2^{-N})(1-z_0^{-N}\zeta_2^{-N}).$$

Hence

$$\prod_{q\in\mathscr{L}_-} v_q = A^{N/2}(1-\zeta_1^{-N})(1-\zeta_2^{-N})$$

$$\prod_{q\in\mathscr{L}_+} v_q = A^{N/2}(1+\zeta_1^{-N})(1+\zeta_2^{-N}). \tag{3.6}$$

Finally, whenever $N \geqslant 2$

$$\begin{aligned} Z\times 2^{1-N} = {} & \mathrm{e}^{Na}\left(\prod_{k=1}^{\infty}(1+\xi_k^{-N}) + \prod_{k=1}^{\infty}(1-\xi_k^{-N})^2\right) \\ & + S_1^N\, \mathrm{e}^{Nb}\left((1+\zeta_1^{-N})(1+\zeta_2^{-N})\prod_{k=1}^{\infty}(1+\eta_k^{-N})^2\right. \\ & \left. + S_0(1-\zeta_1^{-N})(1-\zeta_2^{-N})\prod_{k=1}^{\infty}(1-\eta_k^{-N})^2\right). \end{aligned} \tag{3.7}$$

It is easy to show from equation (2.2) that

$$a = (2\pi)^{-1}\int_{q=0}^{2\pi} \ln\cosh(v_q)\,\mathrm{d}q \tag{3.8}$$

$$b = (2\pi)^{-1}\int_{q=0}^{2\pi} \ln\sinh(v_q)\,\mathrm{d}q. \tag{3.9}$$

All that remains is to prove that the above can be re-expressed in transfer matrix form. Now

$$\prod_{k=1}^{\infty}(1+x_k^N) = 1 + \sum_{k=1}^{\infty} x_k^N + \sum_{\{k_1k_2\}} (x_{k_1}x_{k_2})^N + \sum_{\{k_1k_2k_3\}} (x_{k_1}x_{k_2}x_{k_3})^N + \text{etc},$$

if $\Sigma_{k=1}^{\infty} |x_k^N|$ is convergent. Here $\Sigma_{\{k_1k_2\ldots k_r\}}$ means that the summation is taken over every possible unordered set $\{k_1k_2\ldots k_r\}$.

It has already been stated that $\Sigma|\xi_k^{-N}|$ and $\Sigma|\eta^{-N}|$ are convergent for $N \geqslant 2$. Hence Z_N must be a transfer matrix form.

Taking the case when $|B| < 2|J|$, $S_0 = 1$ and expanding

$$Z \times 2^{-N} = e^{Na}[1+(\xi_1^2)^{-N}+4(\xi_1\xi_2)^{-N}+\text{etc}] + S_1^N e^{Nb}[1+(\zeta_1\zeta_2)^{-N}+2(\zeta_1\eta_1)^{-N}+\text{etc}]. \tag{3.10}$$

If one regards the quantities such as $(2e^a\xi_1^{-1}\xi_2^{-1})$ as the eigenvalues of some transfer matrix then most eigenvalues must have a high degree of degeneracy.

4. A more detailed study of the position of the zeros

4.1. A conformal mapping from p to z

Equation (3.2) makes it possible to say what the values of p are when $\cosh v(z)$ and $\sinh v(z)$ are zero. As v takes the values $ki\pi/2$ and k increases from 0 to ∞, v^2 travels along the negative real axis from 0 to $-\infty$. Equation (3.2) maps this line onto a curve, Ω, in the p plane. The zeros correspond to points on this curve and it is clear from equation (3.2) that as temperature tends to zero, Ω is unaltered but the points become closer together, forming a continuum in the limit.

Below, Ω will be examined in various cases and also its map, χ, in the z plane. Help is obtained from equation (3.3) as $z \to \infty$.

4.2. When $\gamma < 1$

This is when the X and Y interactions are both ferromagnetic or both antiferromagnetic. Typical Ω and χ are shown in figure 1. The arrows indicate the direction of travel as v^2 goes from 0 to $-\infty$. The multiplicity of directions is due to the two signs of

$$[\gamma^2B^2-(1-\gamma^2)(4J^2\gamma^2-v^2/\beta^2)]^{1/2}.$$

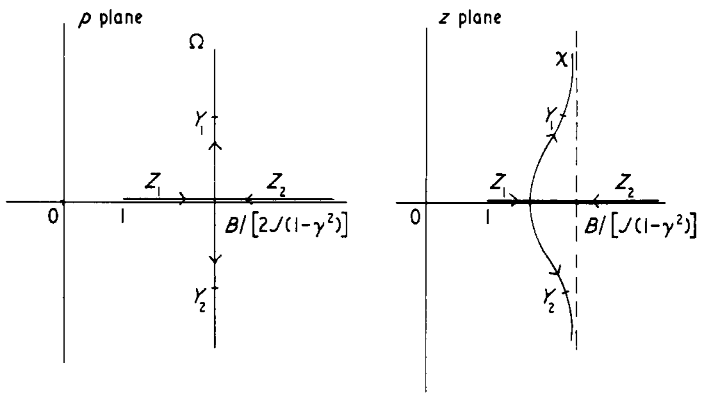

Figure 1. When $\gamma < 1$.

If $|B| < (1-\gamma^2)^{1/2}2|J|$ the path starts at points such as Y and all the ζ, ξ, η are complex. If $|B| > (1-\gamma^2)^{1/2}2|J|$, the path starts at points such as Z and some of the earliest ζ, ξ, η are real. Thus ζ_1, ζ_2 are Y_1, Y_2 or Z_1, Z_2 depending on which case. When the external field is zero all the zeros lie on the imaginary axis.

4.3. When $\gamma > 1$

This is when the X interaction is ferromagnetic and the Y interaction is antiferromagnetic or *vice versa*. p and z must obviously remain real on Ω and χ. Typical Ω and χ are given in figure 2. Whatever γ, p on Ω may not enter the region $-1 < p < 1$ because this would imply a real value of q, and if q is real $v^2 \geqslant 0$ by equation (2.3).

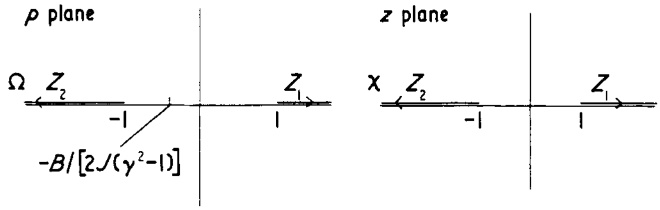

Figure 2. When $\gamma > 1$.

4.4. When $\gamma \simeq 1$

In this case the Y interaction nearly vanishes. If $B = 0$, then by equation (3.2)

$$p = \pm\left(\frac{(4J^2\gamma^2 - v^2/\beta^2)}{4J^2(\gamma^2-1)}\right)^{1/2}.$$

As $\gamma \to 1$, $p \to \infty$ and so do all ζ, ξ, η. Equation (3.10) degenerates into

$$Z = 2^N(\mathrm{e}^{Na} + S_1^N\,\mathrm{e}^{Nb})$$

which is the well known Ising solution.

Suppose $B \neq 0$. This corresponds to the Ising interaction with transverse magnetic field. From equation (3.2)

$$p \simeq \frac{B \pm \gamma B[1-(1-\gamma^2)(4J^2\gamma^2 - v^2/\beta^2)/(2\gamma^2B^2)]}{2J(1-\gamma^2)}.$$

If the positive sign is chosen $p \to \infty$ as $\gamma \to 1$, and the corresponding ζ, ξ, η make a neglibible contribution. Taking the negative sign,

$$p \simeq \frac{1}{2}\left(\frac{B}{2J} + \frac{2J}{B} - \frac{v^2}{2JB\beta^2}\right).$$

All the ζ, ξ, η are real and if B and J have the same sign they are positive, otherwise negative.

4.5. The grand partition function and its poles

N_0 may be taken as two in the definition of the grand partition function. The dominant pole is at $\frac{1}{2}\mathrm{e}^{-a}$ which is on the positive real axis. In the case where $\gamma \geqslant 1$ all the ζ, ξ, η are real and the poles are real. If $\gamma < 1$ and $B = 0$, then as has been shown, all the ζ, ξ, η are imaginary, and since the expansion (3.10) only involves even powers of ζ, ξ, η all the poles must be real. If $\gamma < 1$ and $B \neq 0$ then complex poles become possible. All the poles up to some number, μ, say, are real and it is seen from equation (3.2) and figure 2 that μ increases with B. It is also clear from equation (3.10) that as r increases the distribution of poles in the ring $r < |w| < r+\Delta$ becomes more uniform.

The second dominant pole is either at $\frac{1}{2}S_1\,e^{-b}$ or at $\frac{1}{2}\xi_1^2\,e^{-a}$. It can be shown that for small B and β that the first is the more important of the two.

5. Summary and discussion

5.1. Summary

In § 2 the partition function for the XY model was stated and discussed briefly. In § 3 this was re-expressed by the formula (3.7) where a and b are given by expressions (3.8) and (3.9). ζ, ξ, η are solutions of the equation

$$v_q^2 = \beta^2[B^2+4J^2\gamma^2-2BJ(z+z^{-1})+J^2(1-\gamma^2)(z+z^{-1})^2].$$

ζ_1, ζ_2 are the solutions when $v_q = 0$, the ξ_k are the solutions when $v_q = (k+1/2)\mathrm{i}\pi$ and the η_k are the solutions when $v_q = k\mathrm{i}\pi$ and $k \neq 0$. The equation has four solutions, two of which are reciprocals of the others, and those two chosen such that $|\xi_k| > 1$, $|\eta_k| > 1$, $|\zeta_k| \geqslant 1$.

Equation (3.7) can be expanded to give a transfer matrix form as in (3.10). A grand partition function was constructed which has only simple poles. It was shown that the poles move closer together as the temperature approaches zero and that for zero external field or $\gamma \geqslant 1$ they are all real.

5.2. The XY model with modified boundary conditions

A simpler problem than that above can be chosen by closing up the chain with a slightly different bond from the others with Hamiltonian equal to $-U(\sigma_{xN}\sigma_{x1}+\sigma_{yN}\sigma_{y1})$. The Hamiltonian for the whole system in terms of Fermi operators is now cyclic as it was not previously and it is no longer necessary to introduce projection operators. This problem is called by Lieb *et al* (1961) the c-cyclic problem as opposed to the a-cyclic problem which was solved in § 2. The partition function is simply $2^N \prod_{q\in\mathscr{S}_-} \cosh(v_q)$. This is also a transfer matrix form but the poles due to the ζ and η are entirely absent. On the other hand, there is no cancellation of odd powers of ξ_1, ξ_2, so there are many poles present which were previously absent. A similar problem has as partition function $2^N \prod_{q\in\mathscr{S}_+} \cosh(v_q)$.

The author does not know of a solution to the open XY chain. The question is raised as to if it has a transfer matrix form whether it would have many poles in common with the closed chain. It is well known that if there is any ordinary type of transfer matrix that the poles are independent of the boundary condition, although the residues are not.

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