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The partition function of the XY chain

J S Denbigh†

Wheatstone Physics Laboratory, King's College, Strand, London WC2R 2LS

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Abstract. A new form of solution to the XY chain is found which bears a remarkable similarity to the Onsager solution. It is used to examine the analyticity of the thermodynamic limit. This solution has transfer matrix like properties and the question of some form of universality of eigenvalue distribution is examined.

1. Introduction

1.1. The XY chain

The Hamiltonian H_N for the closed anisotropic XY chain with N sites in field B is given by

$$H_N \equiv -J \sum_{i=1}^{N} [(1+\gamma)\sigma_{xi}\sigma_{xi+1} + (1-\gamma)\sigma_{yi}\sigma_{yi+1}] - B \sum_{i=1}^{N} \sigma_{zi}, \tag{1.1}$$

the $(N+1)$th site being the same as the first site. The partition function Z_N for this Hamiltonian was originally found by Lieb et al (1961) and Katsura (1962). In this paper the existing solution for Z_N is taken and re-expressed in a different form. This leads to a new expression for $A = \lim_{N\to\infty} Z_N^{1/N}$ as an infinite product and not as an integral as before.

This new solution is shown to have a remarkable similarity to the Onsager solution, suggesting the possibility of close relations between other one-dimensional models and higher-dimensional models. In § 3 the new expression is used to find the zeros and singularities of A. This may shed some light on what functions make good approximants to the thermodynamic functions of other systems. It is well known that the XY chain has critical points at zero temperature where $B = \pm 2J$ and Suzuki (1971) related the critical exponents of this model to those of the Ising square lattice. Below it is found that A has an infinite number of singular surfaces intersecting at the critical points.

1.2. The transfer matrix form

This paper will also deal with the way in which Z_N depends on N. This dependence is examined in detail for the XY model because it may be an important prototype for other models. We discuss how this may lead to a numerical solution for one-dimensional models which cannot be solved analytically. Those one-dimensional

† Present address: Physics Department, Imperial College, Prince Consort Road, London SW7 2BZ.

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models which have transfer matrices can normally be dealt with by diagonalising the transfer matrix. For such models the partition function is given by

$$Z_N = \sum_{j=0}^{K} g_j \lambda_j^N \tag{1.2}$$

where the λ_j are the eigenvalues of the transfer matrix and K is its order. Even models which do not have transfer matrices may have this property, although K may now be infinite. If K is infinite some restriction on the λ_j, g_j is necessary since without restriction it may be shown that any sequence $\{Z_N\}$ can be expressed by the right-hand side of equation (1.2). Let us assume that equation (1.2) is satisfied for each Z_N for $N \geq N_0$, $\Sigma_j |g_j \lambda_j^{N_0}|$ is bounded and the λ_j have no limit point other than zero. Then it will be said (Denbigh 1974) that the sequence $\{Z_N\}$ is a transfer matrix form of order K beyond N_0. The λ_j will be called its 'eigenvalues' and the $-g_j$ its 'residues'. It is normally assumed that $|\lambda_{j-1}| \geq |\lambda_j|$ for each j. Let $\mathscr{Z}(w)$, the grand partition function, be defined as $\Sigma_{N=N_0}^{\infty} Z_N w^{N-1}$. Equation (1.2) and the conditions on the λ_j, g_j ensure that

$$\mathscr{Z}(w) = -\sum_j g_j (w\lambda_j)^{N_0 - 1} (w - \lambda_j^{-1})^{-1}. \tag{1.3}$$

The only singularities of $\mathscr{Z}(w)$ are first-order poles which occur at the λ_j^{-1}.

Unpublished analytical work carried out by J L Martin and the author suggests a rigorous proof exists that the transfer matrix form applies to a variety of systems which do not have transfer matrices. Denbigh (1974) proved that the XY chain yields a transfer matrix form. This is also shown by an easier method. For models soluble by a transfer matrix the inverse correlation length is normally $\ln(\lambda_0/\lambda_1)$ (Fisher and Burford 1967). Martin's theory suggests the same may be true of the XY chain and other models which do not have ordinary transfer matrices.

For short chains of many models the eigenvalues of the Hamiltonian can be evaluated (e.g. Bonner and Fisher 1964) and from these the Z_N for small N at various temperatures may be obtained. The Padé approximant (Baker 1965, Gaunt and Guttmann 1974) has simple poles and can be fitted to $\mathscr{Z}(w)$. Since the coefficients of $\mathscr{Z}(w)$ are the Z_N Padé analysis can be used to obtain estimates of the largest eigenvalues and their residues for various temperatures. This method has been successfully used by the author in unpublished work on the closed isotropic field free spin-$\frac{1}{2}$ Heisenberg chain. It gives accurate and convincing results except at very low temperatures where the Padé estimates become inaccurate. His work shows that the partition function is given by

$$Z_{\text{Heis}\, N} = \lambda_0^N + 3\lambda_1^N + O(\lambda_4^N) \qquad \text{where } \lambda_1 = 2\beta - \tfrac{2}{3}\beta^2 + O(\beta^3).$$

At low temperatures it is found that the dominant eigenvalue λ_0 is no longer much greater than $|\lambda_1|$, $|\lambda_2|$ etc, and this makes it difficult to obtain reliable estimates of λ_0 using Padé analysis. It may be shown (Denbigh 1974 and below) that in the XY chain the eigenvalues behave in a similar fashion and this behaviour is expected for other models as a critical point is approach. In the summary we discuss how, if it may be assumed that the eigenvalue distribution of a model under examination is similar to that of the XY chain, the known results for the XY chain can be used to improve the Padé estimates. It is also shown that the open isotropic XY chain has far fewer eigenvalues than the closed chain and reasons are given why open chains for other models are probably more suitable for Padé analysis than closed ones.

In § 4 the eigenvalue distributions of various models are compared and one seeks to show that there are basic similarities. There is a detailed comparison between the Onsager solution and the Ising chain in a transverse magnetic field. The results suggest that for most models as temperature tends to zero, the eigenvalues become very dense apart from the few largest which may stand out from the rest. If, however, there is a critical magnetic field, then the number of eigenvalues lying in any neighbourhood of λ_0 tends to infinity as the temperature tends to zero.

2. The reduction of $\{Z_N\}$ to a transfer matrix form

2.1. *The solution of the XY model*

The partition function corresponding to the Hamiltonian of equation (1.1) is given by

$$2^{1-N}Z^N = \prod_{q\in\mathcal{Q}_+} \cosh \nu_q + \prod_{q\in\mathcal{Q}_-} \cosh \nu_q + S_1^N \prod_{q\in\mathcal{Q}_+} \sinh \nu_q + S_0 S_1^N \prod_{q\in\mathcal{Q}_-} \sinh \nu_q. \tag{2.1}$$

Here the following definitions apply for real β, J, γ, B:

$$\begin{aligned} S_1 &\equiv \begin{cases} 1, & \beta(B+2J)\geq 0 \\ -1, & \beta(B+2J)<0, \end{cases} \\ S_2 &\equiv \begin{cases} 1, & \beta(B-2J)\geq 0 \\ -1, & \beta(B-2J)<0, \end{cases} \\ S_0 &\equiv -S_1S_2, \qquad K\equiv 2\beta J, \qquad t\equiv \tfrac{1}{2}J^{-1}B, \\ \nu_q &\equiv |K[(t-\cos q)^2+\gamma^2 \sin^2 q]^{1/2}|, \end{aligned} \tag{2.2}$$

$\mathcal{Q}_+$ is the set $\{\pi/N+(2\pi/N)j\}$ and $\mathcal{Q}_-$ is the set $\{(2\pi/N)j\}$, here j must be an integer and the elements of $\mathcal{Q}_+$ and $\mathcal{Q}_-$ are modulo 2π. The expressions for S_0 and S_1 correct an error in the solution published by Denbigh (1974) which occurs when $B=\pm 2J$.

2.2. *An infinite product*

From Copson (1935, p 179, example 7) one may deduce that

$$\cosh \nu = \prod_{k=1}^{\infty} [1+4\pi^{-2}\nu^2(2k-1)^{-2}], \qquad \sinh \nu = \nu \prod_{k=1}^{\infty} (1+\pi^{-2}\nu^2k^{-2}). \tag{2.3}$$

Let $p=\cos q$, $z=e^{iq}$ so that $2p=z+z^{-1}$ and ν_q may be regarded as $\nu(z)$.

One may say that for $k\geq 1$

$$1+4\pi^{-2}\nu^2k^{-2} = a_k(1-\xi_{k1}^{-1}z)(1-\xi_{k1}^{-1}z^{-1})(1-\xi_{k2}^{-1}z)(1-\xi_{k2}^{-1}z^{-1}). \tag{2.4}$$

Here z is one of ξ_{k1}, ξ_{k1}^{-1}, ξ_{k2}, ξ_{k2}^{-1} when

$$-\tfrac{1}{4}\pi^2k^2=\nu^2. \tag{2.5}$$

The $\xi_{k\alpha}$ may be obtained from

$$\xi_{k\alpha}+\xi_{k\alpha}^{-1}=2p_{k\alpha} \tag{2.6}$$

where p_{k1} and p_{k2} are the solutions of

$$-\tfrac{1}{4}\pi^2k^2=\nu^2=K^2[t^2+\gamma^2-2tp+(1-\gamma^2)p^2]. \tag{2.7}$$

If $\xi_{k\alpha}$ is a root, so also is $\xi_{k\alpha}^{-1}$ and $\xi_{k\alpha}$ is usually chosen so that $|\xi_{k\alpha}| \geq 1$. If both $|\xi_{k\alpha}| > 1$ then (ξ_{k1}, ξ_{k2}) will be said to be the principal pair of values. ξ_{01}, ξ_{02} and a_0 are defined by

$$\nu^2 = a_0(1-\xi_{01}^{-1}z)(1-\xi_{01}^{-1}z^{-1})(1-\xi_{02}^{-1}z)(1-\xi_{02}^{-1}z^{-1}). \tag{2.8}$$

Since each $\xi^{-1}\,\mathrm{e}^{2\pi \mathrm{i}j/N}$ is a root of ξ^{-N}

$$\begin{aligned}
&\prod_{j=1}^{N}(1-\xi^{-1}\,\mathrm{e}^{2\pi\mathrm{i}j/N}) = 1-\xi^{-N}.\\
&\prod_{q\in\mathscr{Q}_+}(1-\xi^{-1}z) = \prod_{q\in\mathscr{Q}_+}(1-\xi^{-1}z^{-1}) = 1+\xi^{-N}\\
&\prod_{q\in\mathscr{Q}_-}(1-\xi^{-1}z) = \prod_{q\in\mathscr{Q}_-}(1-\xi^{-1}z^{-1}) = 1-\xi^{-N}.
\end{aligned} \tag{2.9}$$

From equations (2.3), (2.4) and (2.9)

$$\prod_{q\in\mathscr{Q}_+}\cosh\nu_q = \prod_{k=1}^{\infty}[a_{2k-1}^{N}(1+\xi_{2k-11}^{-N})^2(1+\xi_{2k-12}^{-N})^2]. \tag{2.10}$$

If p, q are both integers such that $p \leq q$, let

$$\prod_{k=p-\frac{1}{2}}^{q+\frac{1}{2}}{}' b_k \equiv \prod_{k=p}^{q} b_k, \qquad \prod_{k=p-1}^{q+1}{}' b_k \equiv b_{p-1}^{1/2} b_{q+1}^{1/2} \prod_{k=p}^{q} b_k.$$

Applying results like equation (2.10) to equation (2.1) one obtains

$$\begin{aligned}
2^{1-N}Z_N = {}& \prod_{\substack{(k\alpha)\\k=1/2}}^{\infty}{}' [a_{2k-1}^{N/2}(1+\xi_{2k-1\alpha}^{-N})^2] + \prod_{\substack{(k\alpha)\\k=1/2}}^{\infty}{}' [a_{2k-1}^{N/2}(1-\xi_{2k-1\alpha}^{-N})^2]\\
&+S_1^N \prod_{\substack{(k\alpha)\\k=0}}^{\infty}{}' [a_{2k}^{N/2}(1+\xi_{2k\alpha}^{-N})^2] + S_0 S_1^N \prod_{\substack{(k\alpha)\\k=0}}^{\infty}{}' [a_{2k}^{N/2}(1-\xi_{2k\alpha}^{-N})^2].
\end{aligned} \tag{2.11}$$

If K, t, γ are real and $\gamma \neq 0$ and $t \neq \pm 1$, then for real q ν_q^2 is positive by equation (2.2). The principal values of (ξ_{k1}, ξ_{k2}) lie outside the unit circle since otherwise equation (2.5) cannot be satisfied. Clearly ξ_{k1} and ξ_{k2} are complex conjugates of each other or else both real. By continuation when $t = \pm 1$ or $\gamma = 0$ this is still true although they may now lie on the unit circle. By applying equations (2.4) and (2.8) when z takes an arbitrary value on the unit circle it follows that a_0 is non-negative real and every other a_k is positive real.

From equation (2.7)

$$p_{k\alpha} = \{t \pm [\gamma^2 t^2 - (1-\gamma^2)(\gamma^2 + \tfrac{1}{4}\pi^2 K^{-2} k^2)]^{1/2}\}(1-\gamma^2)^{-1}. \tag{2.12}$$

From equation (2.6)

$$\xi_{k\alpha} = p_{k\alpha} \pm (p_{k\alpha}^2 - 1)^{1/2}. \tag{2.13}$$

If $\gamma \neq \pm 1$ when $(k/K) \to \infty$

$$p_{k\alpha} = [t \pm \tfrac{1}{2}\mathrm{i}\pi(1-\gamma^2)^{1/2}K^{-1}k + \mathrm{O}(K/k)](1-\gamma^2)^{-1}, \tag{2.14}$$

$$\xi_{k\alpha} = 2p_{k\alpha} + \mathrm{O}(p_{k\alpha}^{-1}) = [2t \pm \mathrm{i}\pi(1-\gamma^2)^{1/2}K^{-1}k + \mathrm{O}(K/k)](1-\gamma^2)^{-1}. \tag{2.15}$$

For large k the $\xi_{k\alpha}$ approximately lie on a straight line at equal intervals going off to infinity in both directions. The distribution of the $\xi_{k\alpha}$ is discussed in greater detail by Denbigh (1974).

2.3. *A further reduction of the partition function*

Because of the way ξ_k behaves as $k \to \infty$ $\Pi_{(k\alpha)}(1-\xi_{k\alpha}^{-N})$ is absolutely convergent for $N \geq 2$. From equation (3.3) $\Pi_{k=0}^{\infty} a_k$ is absolutely convergent. Hence each of the infinite products of equation (2.11) is absolutely convergent for $N \geq 2$. Let

$$A \equiv 2 \prod_{k=1/2}^{\infty}{}' a_{2k-1}, \qquad C \equiv 2 \prod_{k=0}^{\infty}{}' a_{2k}. \tag{2.16}$$

Then for $N \geq 2$

$$\begin{aligned} 2Z_N = {} & A^N \prod_{\substack{(k\alpha)\\ k=1/2}}^{\infty}{}' (1+\xi_{2k-1\alpha}^{-N})^2 + A^N \prod_{\substack{(k\alpha)\\ k=1/2}}^{\infty}{}' (1-\xi_{2k-1\alpha}^{-N})^2 \\ & + S_1^N C^N \prod_{\substack{(k\alpha)\\ k=0}}^{\infty}{}' (1+\xi_{2k\alpha}^{-N})^2 + S_0 S_1^N C^N \prod_{\substack{(k\alpha)\\ k=0}}^{\infty}{}' (1-\xi_{2k\alpha}^{-N})^2. \end{aligned} \tag{2.17}$$

If $\Pi_{k=1}^{\infty}(1+x_k^N)$ is absolutely convergent for $N \geq N_0$ then the sequence of such infinite products as $N \to \infty$ is a transfer matrix form beyond N_0, Denbigh (1974). When $|t| < 1$ so that $S_0 = 1$, by expanding equation (2.17) for $N \geq 2$

$$\begin{aligned} Z_N = {} & A^N[1+(\xi_{11}^2)^{-N}+(\xi_{12}^2)^{-N}+4(\xi_{11}\xi_{12})^{-N}+\ldots] \\ & + S_1^N C^N[1+(\xi_{01}\xi_{02})^{-N}+2(\xi_{01}\xi_{21})^{-N}+2(\xi_{01}\xi_{22})^{-N}+\ldots]. \end{aligned} \tag{2.18}$$

When $|t| > 1$ so that $S_0 = -1$

$$\begin{aligned} Z_N = {} & A^N[1+(\xi_{11}^2)^{-N}+(\xi_{12}^2)^{-N}+4(\xi_{11}\xi_{12})^{-N}+\ldots] \\ & + S_1^N C^N(\xi_{01}^{-N}+\xi_{02}^{-N}+2\xi_{21}^{-N}+2\xi_{22}^{-N}+\ldots). \end{aligned} \tag{2.19}$$

It is clear from the cancellation or duplication of terms that $\{Z_N\}$ is a transfer matrix form beyond 2. For $|t| < 1$ the eigenvalues of the transfer matrix form are A, S_1C, $A\xi_{11}^{-2}$, $S_1C\xi_{01}^{-1}\xi_{02}^{-1}$, etc, and for $|t| > 1$ they are A, $S_1C\xi_{01}^{-1}$, $S_1C\xi_{02}^{-1}$, $A\xi_{11}^{-2}$, etc. In both cases, the degeneracy of each eigenvalue is a positive integer.

A and C may be obtained from equations (2.16). The a_k may be obtained by equating the coefficients of z^2 in equations (2.4) and (2.8):

$$\begin{aligned} a_0 &= \tfrac{1}{4}\xi_{01}\xi_{02}(1-\gamma^2)K^2 \\ a_k &= \pi^{-2}\xi_{k1}\xi_{k2}(1-\gamma^2)K^2k^{-2} \qquad \text{for } k \neq 0 \end{aligned} \tag{2.20}$$

From equations (2.16) and (2.20) one obtains

$$A = \lim_{l\to\infty}\left((2\pi)^{-2l+1}(\Gamma(l+\tfrac{1}{2}))^{-2}(1-\gamma^2)^l K^{2l} \prod_{k=1/2}^{l+\frac{1}{2}}{}' (\xi_{2k-1\,1}\xi_{2k-1\,2})\right) \tag{2.21}$$

$$C = \lim_{l\to\infty}\left((2\pi)^{-2l+1}(l^{1/2}\Gamma(l))^{-2}(1-\gamma^2)^l K^{2l} \prod_{k=0}^{l}{}' (\xi_{2k1}\xi_{2k2})\right). \tag{2.22}$$

These are new expressions for A and C which may be compared with

$$\ln(\tfrac{1}{2}A) = (2\pi)^{-1} \int_{q=0}^{2\pi} \ln\cosh\nu_q \, dq \tag{2.23}$$

$$\ln(\tfrac{1}{2}C) = (2\pi)^{-1} \int_{q=0}^{2\pi} \ln\sinh\nu_q \, dq. \tag{2.24}$$

These equations were obtained by Lieb *et al* (1961) and Katsura (1962) from equation (2.1) by letting $N \to \infty$ so that q becomes a continuum.

2.4. *When $\gamma = \pm 1$*

When $\gamma = \pm 1$ we have the Ising interaction. But the magnetic field is now perpendicular to the spins and not parallel to them as in the problem solved by Ising. As $t \to 0$ the $|\xi_{k\alpha}| \to \infty$ so that all but two eigenvalues tend to zero. This is to be expected from Ising's solution. Suppose now t is not very small and γ is very close to ± 1. From equation (2.7) and taking p_{k1} as the smaller of the two solutions

$$p_{k1} = (t^2 + \gamma^2 + \tfrac{1}{4}\pi^2 k^2 K^{-2})(2t)^{-1} + O(1-\gamma^2). \tag{2.25}$$

If $\gamma = \pm 1$ by equation (2.6)

$$\xi_{k1} + \xi_{k1}^{-1} = t + t^{-1} + \tfrac{1}{4}\pi^2 k^2 K^{-2} t^{-1}. \tag{2.26}$$

From equation (2.7)

$$p_{k1} p_{k2} = (t^2 + \gamma^2 + \tfrac{1}{4}\pi^2 k^2 K^{-2})(1-\gamma^2)^{-1}.$$

Applying equations (2.25) and (2.6)

$$\xi_{k2} = 4t(1-\gamma^2)^{-1} + O(1). \tag{2.27}$$

From equations (2.21) and (2.22) when $\gamma = \pm 1$

$$\begin{aligned} A &= \lim_{l\to\infty} \left(2\pi^{-2l+1} (\Gamma(l+\tfrac{1}{2}))^{-2} K^{2l} t^l \prod_{k=1/2}^{l+\frac{1}{2}}{}' \xi_{2k-1\,1} \right) \\ C &= \lim_{l\to\infty} \left(2\pi^{-2l+1} (l^{1/2}\Gamma(l))^{-2} K^{2l} t^l \prod_{k=0}^{l}{}' \xi_{2k\,1} \right). \end{aligned} \tag{2.28}$$

Later these equations will be compared with Onsager's solution.

3. An analysis of the solution

3.1. *The behaviour of the a_k*

Let J_x, J_y be respectively the strengths of the OX, OY interactions, so that

$$J_x = J(1+\gamma), \qquad J_y = J(1-\gamma).$$

The case where $J_y = -J_x$ and $\gamma = \pm\infty$ is no longer exceptional using these parameters as equation (2.12) might suggest. From equations (2.6) and (2.7)

$$\begin{aligned} 0 &= \tfrac{1}{4}\pi^2 k^2 + \beta^2 [B^2 + J_x^2 + J_y^2 - (J_x + J_y) B (\xi_{k\alpha} + \xi_{k\alpha}^{-1}) + J_x J_y (\xi_{k\alpha}^2 + \xi_{k\alpha}^{-2})] \\ &\equiv \xi_{k\alpha}^2 P(\xi_{k\alpha}^{-1}), \quad \text{say}. \end{aligned} \tag{3.1}$$

P as defined above is a quartic polynomial except when β, J_x or J_y is zero. Points in β, B, J_x, J_y space where all the coefficients of P are zero will be said to be of type L or simply labelled L. It is shown in the appendix that a_k is zero at and only at points of type L. The zeros of A and C may be obtained this way. At L at least two of J_x, J_y and B must be zero. It may be of significance that in such cases the problem is soluble by an ordinary transfer matrix. It is shown in the appendix that each a_k is continuous everywhere. It is also shown that if $\xi_{k\alpha}$ takes its principal value $\xi_{k\alpha}^{-1}$ is continuous everywhere except at L where it may take any value.

Let us consider what happens to the a_k as $k \to \infty$. Suppose that β, B, J_x, J_y lie in any bounded domain D. If $|\xi_{k\alpha}| \geq 1$ it follows from equation (3.1) that for some A' independent of k

$$\tfrac{1}{4}\pi^2 k^2 < A' + |\beta^2|(|J_x + J_y|\,|B| + |J_x J_y|)|\xi_{k\alpha}^2|.$$

Thus, there exist positive A'', k'' independent of k such that for β, B, J_x, $J_y \in$ D and $k > k''$

$$|\xi_{k\alpha}| > A''k. \tag{3.2}$$

Equating the coefficients of z^0 in equation (2.4)

$$1 + 4\pi^{-2}\beta^2(B^2 + J_x^2 + J_y^2)k^{-2} = a_k(1 + \xi_{k1}^{-2} + \xi_{k2}^{-2} + 2\xi_{k1}^{-1}\xi_{k2}^{-1} + \xi_{k1}^{-2}\xi_{k2}^{-2}).$$

Equation (3.2) shows that there exist A''', k''', independent of k, such that for β, B, J_x, $J_y \in D$ and $k > k'''$

$$|a_k - 1| < A'''k^{-2}. \tag{3.3}$$

Let is be said that when (ξ_{k1}, ξ_{k2}) take their principal pair of values a_k, A and C take their principal values and lie on the principal Riemann surface and will be labelled a_{kp}, A_p and C_p respectively. From equation (3.3) $\Pi_{k=1}^{l} a_{kp}$ converges absolutely and uniformly in any finite domain as $l \to \infty$. Hence by Copson (1935, p 94) A_p and C_p exist and are analytic in β, B, J_x, J_y except where any a_{kp} has a singularity. The uniformity of convergence combined with the continuity of the $\xi_{k\alpha}^{-1}$ show that each eigenvalue of $\{Z_N\}$, is continuous everywhere in β, B, J_x, J_y.

3.2. The analyticity of the eigenvalues

The eigenvalues and $\xi_{k\alpha}$ may be regarded as functions of the variables K, t, γ. A brief exposition of the theory of functions of several complex variables may be found in chapters 1 of Narasimhan (1971) or Hervé (1963). By equation (2.6) $\xi_{k\alpha}$ may have a branch-point singularity on the surfaces $p_{k\alpha} = \pm 1$ for if K, t, γ vary in such a way that $p_{k\alpha}$ makes a small contour round this value $\xi_{k\alpha}$ is deformed into $\xi_{k\alpha}^{-1}$. Inserting $p_{k\alpha} = 1$ into equation (2.7) one obtains

$$t = 1 \pm \mathrm{i}\tfrac{1}{2}\pi k K^{-1}. \tag{3.4}$$

Provided one does not have

$$\frac{\partial p_{k\alpha}}{\partial K} = \frac{\partial p_{k\alpha}}{\partial t} = \frac{\partial p_{k\alpha}}{\partial \gamma} = 0$$

at $p_{k\alpha} = 1$ then $\xi_{k\alpha}$ is a two-valued function in a small neighbourhood of this surface. Differentiating equation (2.7) shows that $\partial p_{k\alpha}/\partial t \neq 0$ if $k \neq 0$ so that $\xi_{k\alpha}$ is two valued where $p_{k\alpha} = 1$. It can, however, be shown that on passing round the surface $t = 1$ $p_{0\alpha}$

makes two contours round 1 so that $\xi_{0\alpha}$ is not singular in this neighbourhood. Inserting $p_{k\alpha} = -1$ into equation (2.7) one obtains the family of singular surfaces

$$t = -1 \pm \mathrm{i}\tfrac{1}{2}\pi k K^{-1} \qquad \text{for } k = 1, 2, 3, \ldots. \tag{3.5}$$

$p_{k\alpha}$ and $\xi_{k\alpha}$ are also singular on the surface where p_{k1} equals p_{k2} for on making a contour round this surface p_{k1} is deformed into $p_{k\alpha}$. By equation (2.12) the surface is where

$$\gamma^2 t^2 - (1-\gamma^2)(\gamma^2 + \tfrac{1}{4}\pi^2 K^{-2} k^2) = 0. \tag{3.6}$$

If ξ_{k1} and ξ_{k2} both take their principal values they exchange values on making a small contour round this surface so that a_{kp} by equation (2.20) is unaltered. Each a_k has four possible values since $\xi_{k\alpha}$ can be replaced by $\xi_{k\alpha}^{-1}$ and if k is non-zero all these values may be otained from a_{kp} by analytic continuation. A singularity in a_k where equation (3.6) is satisfied may occur on some Riemann surfaces but not others.

The singularities of A occur where one of equations (3.4), (3.5) or (3.6) is satisfied for odd k. In the neighbourhood of most points on these singular surfaces A is a two valued function. It has already been shown that A is continuous everywhere. Katsura and Ohminami (1972) assumed that A is singular if the integrand of equation (2.23) is infinite for some value of q. This we believe to be incorrect for by substituting $q = \mathrm{e}^{\mathrm{i}z}$ the integral may be turned into a contour integral and by deforming the contour it is often possible to avoid this infinity. The singularities obtained from equations (3.4) and (3.5) form two families of surfaces which all meet at $t = \pm 1$ and zero temperature. These are critical points (Suzuki 1971).

Analytic continuation of A_p round a contour leads to a new value of the form $A_p \Pi_{(k\alpha)} \xi_{2k-1\alpha}^{-n_{2k-1\alpha}}$ where each $n_{2k-1\alpha}$ is 0 or 2. This is also an eigenvalue of the transfer matrix form. Not all eigenvalues can be generated from A_p in this way as for example $A_p \xi_{11}^{-1} \xi_{12}^{-1}$ to be found in equation (2.18). Those eigenvalues involving C cannot be generated from A_p either. The eigenvalues of the transfer matrix of the Ising spin-$\frac{1}{2}$ chain in the absence of a magnetic field are $2\cosh\beta J$ and $2\sinh\beta J$ which cannot be analytically continued into each other. If a longitudinal magnetic field is allowed to vary, however, the eigenvalues (Stanley 1971, p 133) can be analytically continued into each other. We conjecture that for the XY model in a general magnetic field all the eigenvalues can be generated from A_p by analytic continuation.

3.3. *The behaviour as temperature $T \to \infty$ and 0*

It follows from equation (2.7) that $\xi_{0\alpha}$ is independent of temperature T. If $\gamma \neq \pm 1$ and $k \neq 0$, then from equation (2.15) each $\xi_{k\alpha}$ varies as T as $T \to \infty$. As $T \to \infty$, $A_p \to 2$ but by equations (2.24) and (2.2) C_p varies like T^{-1}. It is clear from equations (2.18) and (2.19) that the largest eigenvalue of the transfer matrix form is approximately 2, the next two largest vary as T^{-1} and after that there are an infinity of eigenvalues which vary as T^{-2}. This is true whether $t \lesseqgtr \pm 1$. For $\gamma = \pm 1$ by equation (2.26) each ξ_{k1} varies as T^2 *for* $k \neq 0$ and each $\xi_{k2} = \infty$. Hence, after the largest eigenvalue there is only one eigenvalue $S_1 C$ or $S_1 C \xi_{01}^{-1}$ which varies as T^{-1} and after that an infinity of eigenvalues vary as T^{-3}. For the Heisenberg chain numerical evidence (§ 1.1) suggests that after the largest eigenvalue there are three eigenvalues which vary as T^{-1}.

As $T \to 0$ it follows from equations (2.23), (2.24) and (2.2) that $C/A \to 1$ and from equations (2.12) and (2.25) that $|\xi_{k+1\alpha} - \xi_{k\alpha}| \to 0$ for any k. If some $|\xi_{k\alpha}| \simeq 1$ then from equations (2.18) and (2.19) there must be many eigenvalues whose moduli are close to A_p. For real physical parameters this can happen only if $t=\pm 1$ or if $\gamma=0$ and $|t|<1$. When $t=\pm 1$, $\xi_{01}=\pm 1$ but in the other case where $\gamma=0$ and $|t|<1$, ξ_{01} and ξ_{02} are complex conjugates and lie on the unit circle. The two situations are different, the first being critical points. For $|t|<1$ as $T\to 0$ the two largest eigenvalues are A_p and C_p which are nearly equal. For $|t|>1$, A_p remains greater than all the other eigenvalues as $T\to 0$ since by equation (2.19) C_p is no longer an eigenvalue. This situation very closely resembles the Onsager solution. t in the XY chain roughly corresponds to temperature in the Ising square lattice. The relationship between the two models is particularly remarkable in the case where $\gamma=\pm 1$ and will be discussed in detail below.

4. Comparison between the eigenvalue distributions of various models

4.1. *The Ising square lattice and the Ising chain with transverse magnetic field*

Suppose we have a square lattice with m columns and N rows joined up to form a torus and a Hamiltonian given by

$$H=J_x\sum_{(ij)\in S_x}\sigma_{zi}\sigma_{zj}+J_y\sum_{(ij)\in S_y}\sigma_{zi}\sigma_{zj}. \tag{4.1}$$

Here $(ij)\in S_x$ means that j is the right-hand neighbour of site i. S_y is the same in the vertical direction. Let

$$\phi=2\beta J_x, \qquad \psi=2\beta J_y, \qquad \theta=2\tanh^{-1}(e^{-2\beta J_y})$$

$$\eta_k+\eta_k^{-1}=e^{\phi-\theta}+e^{\theta-\phi}+(e^{\phi+\theta}+e^{-\phi-\theta}-e^{\phi-\theta}-e^{\theta-\phi})\sin^2(\pi k/2m). \tag{4.2}$$

For real J_x and J_y it is assumed that $\eta_k\geqslant 1$ except that $\eta_0<1$ when $\theta>\phi$. From Kaufmann (1949, equation (39)) it may be shown that the partition function is given by

$$2Z_{mN}=F^N\prod_{k=1/2}^{(m+1)/2}{}'(1+\eta_{2k-1}^{-N})^2+F^N\prod_{k=1/2}^{(m+1)/2}{}'(1-\eta_{2k-1}^{-N})^2$$

$$+G^N\prod_{k=0}^{m/2}{}'(1+\eta_{2k}^{-N})^2+G^N\prod_{k=0}^{m/2}{}'(1-\eta_{2k}^{-N})^2. \tag{4.3}$$

where

$$F=(2\sinh\psi)^{m/2}\prod_{k=1/2}^{(m+1)/2}{}'\eta_{2k-1}, \qquad G=(2\sinh\psi)^{m/2}\prod_{k=0}^{m/2}{}'\eta_{2k}. \tag{4.4}$$

If one considers the limit as $m\to\infty$ the eigenvalue distribution for the Ising square lattice bears a very close resemblance to that of the Ising chain with transverse magnetic field if the parameters are correctly chosen. If equation (2.26) is matched with equation (4.2)

$$t=e^{\theta-\phi}, \qquad K^{-2}=(e^{\phi+\theta}+e^{-\phi-\theta}-t-t^{-1})tm^{-2}. \tag{4.5}$$

As m and $K\to\infty$, $\eta_k\to\xi_{k1}$, $G/F\to 1$ for $\theta<\phi$ and $C_p/A_p\to 1$. The similarity between equations (2.17) and (2.28) and equations (4.3) and (4.4) is obvious. If the eigenvalues of the two matching models are $\lambda_{0I}, \lambda_{0XY}, \lambda_{1I}, \lambda_{1XY}$ etc, taken in order of decreasing magnitude, then as $m\to\infty$

$$\lambda_{iI}/\lambda_{0I}\to\lambda_{iXY}/\lambda_{0XY}. \tag{4.6}$$

Where $\theta > \phi$ and $|t| > 1$

$$G \simeq \eta_0 F, \qquad C \simeq \xi_{01} A_p,$$

since η_{01}, ξ_{01} are replaced by η_0^{-1}, ξ_{01}^{-1}. Since η_0 and ξ_{01} are nearly equal equation (4.6) still holds.

4.2. *The replacement of an interaction by a mean field*

The result above means that one of the interactions of the Ising square lattice can in a sense be replaced by a mean field while preserving the eigenvalue distribution. Below one of the interactions of the isotropic field free XY chain is replaced by a mean field and the eigenvalue distributions compared.

Let us consider models A, B, C, D with Hamiltonians H_{AN}, H_{BN}, H_{CN}, H_{DN} defined below, and their partition functions Z_{AN}, Z_{BN}, Z_{CN}, Z_{DN}.

$$H_{AN} = -J \sum_{j=1}^{N} \sigma_{zj}, \qquad Z_{AN} = [2\cosh(\beta J)]^N$$

$$H_{BN} = -J \sum_{j=1}^{N} \sigma_{zj}\sigma_{zj+1}, \qquad Z_{BN} = [2\cosh(\beta J)]^N + [2\sinh(\beta J)]^N$$

$$H_{CN} = -2J \sum_{j=1}^{N} \sigma_{xj}\sigma_{xj+1} - 2Jt \sum_{j=1}^{N} \sigma_{zj}$$

$$H_{DN} = -J' \sum_{j=1}^{N} (\sigma_{xj}\sigma_{xj+1} + \sigma_{yj}\sigma_{yj+1}).$$

Systems A and B are thermodynamically equivalent, although $\{Z_{AN}\}$ has only one eigenvalue and $\{Z_{BN}\}$ has two. It can be shown from equations (2.2) and (2.23) that systems C and D are thermodynamically equivalent when $2J = J'$ and $t = \pm 1$. Inspection shows that the eigenvalue distributions are again different. In both cases an interaction is replaced by a mean field.

However, let us compare systems C and D when $t = -1$, $J' = J$ and $K \equiv 2\beta J$ is positive. $S_0 = S_1 = 1$ in both cases. Applying equation (2.26) to system C one obtains

$$\xi_{k1}^{1/2} + \xi_{k1}^{-1/2} = \pm \tfrac{1}{2} \mathrm{i} \pi K^{-1} k. \tag{4.7}$$

Applying equation (2.12) to system D one obtains

$$\xi_{k\alpha} + \xi_{k\alpha}^{-1} = \pm \mathrm{i} \pi K^{-1} k.$$

If one considers system D with two sites as the basic unit, the correct partition function is obtained if each $\xi_{k\alpha}$ is replaced by $\xi'_{k\alpha} \equiv \xi_{k\alpha}^2$:

$$\xi_{k\alpha}'^{1/2} + \xi_{k\alpha}'^{-1/2} = \pm \mathrm{i} \pi K^{-1} k. \tag{4.8}$$

It must be remembered that here there is both ξ'_{k1} and ξ'_{k2} which are both equal, whereas in equation (4.7) there is just ξ_{k1}. The factor of $\frac{1}{2}$ in equation (4.7) approximately doubles the density of the ξ_{k1} and compensates for this. Thus, $\{Z_{CN}\}$ and $\{Z_{D2N}\}$ have similar eigenvalue distributions.

4.3. *The open XY chain*

The open isotropic XY chain with $N-1$ sites and $N-2$ bonds, solved by Matsubara and Katsura (1973) has a partition function given by

$$Z_{\text{op}N-1} = 2^{N-1} \prod_{j=1}^{N-1} \cosh [\beta B - 2\beta J \cos (j\pi/N)]$$

$$= 2^{N-1} \left(\prod_{q \in \mathcal{Q}_-} \cosh \nu_q \right)^{1/2} \{\cosh [K(t-1)] \cosh [K(t+1)]\}^{-1/2}. \qquad (4.9)$$

Here $\mathcal{Q}_-$ is the set $\{\pi j/N\}$ for integral $j = 1$ to $2N$, and in accordance with equation (2.2) $\nu_q = K(t - \cos q)$. Just as equation (2.17) was obtained from equation (2.1)

$$Z_{\text{op}N-1} = 2^{-1} A^N \prod_{\substack{(k\alpha) \\ k=1/2}}^{\infty}{}' (1 - \xi_{2k-1\alpha}^{-2N})\{\cosh [K(t-1)] \cosh [K(t+1)]\}^{-1/2}. \qquad (4.10)$$

This can be expanded to give a transfer matrix form as before, but the residues are now no longer integers.

For an open system with a conventional transfer matrix Z_N is of the form $a \,.\, T^N \,.\, b$, while for a closed system Z_N is of the form tr (T^N). Thus for the closed system all the eigenvalues of T are present in the transfer matrix form, and the residues must be negative integers depending on the degeneracy of the eigenvalues. For the open system the eigenvalues must be the same as before, but the residues depend on a and b and no longer need be integers. Since they may be zero, some eigenvalues present for the closed system may be absent for the open system, but not vice versa. This is clearly borne out in the comparison between the closed and open isotropic XY chains. It was observed by Denbigh (1974) that the c-cyclic problem, an XY chain with unusual boundary conditions, has eigenvalues not common to those of the ordinary XY chain. However, one of the bonds involves the spins of every site and one would not expect transfer-matrix-like behaviour to occur anyway.

If the temperature of the open system is halved K is replaced by $2K$. Because the $\xi_{k\alpha}$ are now twice as dense as before the N-dependent factor of $Z_{\text{op}N-1}$ is now approximately

$$\prod_{\substack{(k\alpha) \\ k=1/2}}^{\infty}{}' (1 - \xi_{2k-1\alpha}^{-2N})^2.$$

This yields an eigenvalue distribution rather similar to that of $\{Z_{2N}\}$ for the closed XY chain as can be seen by examination of equation (2.17).

The Padé analysis method, described in § 1, for obtaining A numerically is least effective at low temperatures where the eigenvalues crowd together. The above result shows that the open chain is much more suitable for Padé analysis than the closed one, and this is probably true for other models. For antiferromagnetic systems the spins of neighbouring sites tend to orientate themselves in opposite directions, and if N is odd and the chain is closed they do not match up. For this reason $\{Z_{2N}\}$ is a somewhat different sequence from $\{Z_{2N-1}\}$ as observed by Bonner and Fisher (1964) for the closed Heisenberg chain. This results in the generation of important eigenvalues which do not exist for the open chain. It can also be shown by the transfer matrix method that in the partition function of the open field free Ising chain the coefficient of the smaller eigenvalue vanishes. This is no longer true when a longitudinal magnetic field is introduced and the second eigenvalue is now present.

5. Summary and discussion

The new form of solution to the XY chain that has been obtained shows a remarkable similarity to the Onsager solution, especially in the case where $\gamma = \pm 1$. This suggests that solutions of one-dimensional problems may lead to solutions of higher-dimensional problems. In particular, the Ising chain in a general field may be related to the Ising square lattice in a longitudinal field. Suzuki (1971, equations (4.23*a*)–(4.25*b*)) proved several relations between the critical exponents of the two models. He showed the susceptibility with respect to a small field parallel to the X axis of the XY chain at zero temperature varies as $(B-2J)^{-7/4}$ just as the susceptibility of the Ising model in two dimensions varies as $(T-T_c)^{-7/4}$.

The singularities of $A = \lim_{N\to\infty} Z_{XYN}^{1/N}$ have been studied. It is shown that A is singular where

$$B = \pm 2J \pm \mathrm{i}\tfrac{1}{2}\pi k k_{\mathrm{B}} T \qquad \text{for odd } k,$$

T being temperature. Each singular surface passes through one of the two critical points $B = \pm 2J$, $T = 0$. It is also found that if T, B, J, γ are arbitrary analytic functions of some parameter z then most of the singularities of A are twofold branch-point singularities like $(z-z_0)^{1/2}$. If higher-dimensional models also have an infinite number of singular surfaces intersecting at the critical points this possibly suggests that two-variable rational approximants (Chisholm 1973) would give poor results.

It is shown in § 4 that there is a similarity between the eigenvalue distributions of the Ising square lattice and the Ising chain with transverse field and also between the isotropic XY chain and the Ising chain with transverse field. In both cases an interaction has been replaced by a mean field. The Heisenberg chain has a critical point at $T = 0$, $B = 0$ where the susceptibility tends to infinity. Numerical studies mentioned in § 1.2 indicate that as this point is approached the moduli of many eigenvalues approach the dominant eigenvalue. At high temperatures all spin-$\frac{1}{2}$ chains must have their largest eigenvalue approximately two since $Z_N \simeq 2^N$. Numerical results indicate that after this the Heisenberg chain has three eigenvalues of order T^{-1}. Exact results above show that the XY chain with $\gamma \neq \pm 1$ has two eigenvalues of order T^{-1} and the Ising chain in transverse or longitudinal field has one eigenvalue of order T^{-1}. It appears that the number of eigenvalues of order T^{-1} is the same as the dimensionality of the interaction.

These results suggest that different models which have transfer matrices of infinite order may have basic similarities in their eigenvalue distribution. There are various schemes by which this idea could be used to improve the method of numerical examination outlined in § 1.2. For example, if U is a one-dimensional model consider the sequence

$$\{Z'_N\} = \left\{ Z_{\mathrm{U}N} - \mu Z_{XYN} + \mu \sum_{j=0}^{M} g_{XYj} \lambda_{XYj}^{N} \right\}.$$

Here $Z_{\mathrm{U}N}$ is the partition function of model U with N sites, Z_{XYN} is the partition function of the XY chain with suitably chosen T, B, J, γ, the λ_{XYj} are its eigenvalues in order of decreasing magnitude, the $-g_{XY}$ are the residues and μ, M are suitably chosen numbers. If the distribution of the smaller eigenvalues is similar for the two models then their contribution to the Z'_N nearly cancels itself. Only the first few eigenvalues of $\{Z_{\mathrm{U}N}\}$ make a significant contribution to the Z'_N making the generating function of this sequence easy to Padé analyse. The advantages of such a procedure must be greatest at low temperatures where $\{Z_{UN}\}$ is most likely to be hard to Padé analyse. The best values of μ, T, B, J, γ could be found by inspection. It has been shown in § 4.3 that the open isotropic XY chain has far fewer eigenvalues than the closed chain, suggesting that open chains are generally more suitable for numerical analysis than closed chains.

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Appendix. The continuity of the a_k and $\xi_{k\alpha}^{-1}$ and the zeros of the a_k

Let U be any point in β, B, J_x, J_y space and let $P(z)$ be the polynomial defined in equation (3.1). If $\xi_{k\alpha}$ is such that $P(\xi_{k\alpha}^{-1})$ is zero let Γ be any small circle in the z plane round $\xi_{k\alpha}^{-1}$ and let M be the greatest lower bound of $|P(z)|$ on Γ. Suppose that β, B, J_x, J_y are changed slightly so that $P(z)$ becomes $P(z)+Q(z)$. If $M>0$ there is a sufficiently small neighbourhood, D of U such that $|Q(z)|<M$ when β, B, J_x, $J_y$lies in D. By Rouché's theorem (Copson 1935, p 119) $P(z)+Q(z)$ has the same number of zeros within Γ as $P(z)$ when β, B, J_x, J_y likes in D. This means that $\xi_{k\alpha}^{-1}$ has not moved outside Γ as a result of a small change in β, B, J_x, J_y and hence $\xi_{k\alpha}^{-1}$ is continuous in β, B, J_x, J_y. Having chosen a suitable value of z, equations (2.4) and (2.8) show that a_{kp} is continuous in β, B, J_x, J_y and non-zero at U.

If M is zero for all Γ of sufficiently small radius, then the coefficient of each z^i in $P(z)$ is zero. Let such a U be labelled L and be β_L, B_L, J_{xL}, J_{yL}. (ξ_{k1}, ξ_{k2}) may take any values one likes at L. The left-hand side of equation (2.4) or (2.8) for relevant k is zero at L and there exists η such that it is of modulus less that

$$\eta(|\beta-\beta_L|+|B-B_L|+|J_x-J_{xL}|+|J_y-J_{yL}|)(1+|z^2|+|z^{-2}|)$$

in some neighbourhood of L. For any $(\xi_{k1}^{-1}, \xi_{k2}^{-1})$ a z on the unit circle may be found such that each $|1-\xi_{k\alpha}^{-1}z^{\pm 1}|>0{\cdot}1$. Equations (2.4) and (2.8) show that a_{kp} is zero and continuous at L.

The alternative values of a_{kp} are a_{kp}, $a_{kp}\xi_{k1}^{-2}$, $a_{kp}\xi_{k2}^{-2}$, $a_{kp}\xi_{k1}^{-2}\xi_{k2}^{-2}$ for $k>0$ and they must be continuous in β, B, J_x, J_y everywhere and zero at L. a_0 is similarly continuous and zero only at L.

It may further be shown that $\xi_{k\alpha}^{-1}$ is analytic in β, B, J_x, J_y except where $\xi_{k\alpha}^{-1}$ is a repeated solution of $P(z)=0$. For except at these points $\partial P/\partial z$ is non-zero so that

$$\frac{\partial \xi_{k\alpha}^{-1}}{\partial\beta}=-\frac{\partial P/\partial\beta}{\partial P/\partial\xi_{k\alpha}^{-1}}$$

is well defined. $\xi_{k\alpha}^{-1}$ must be an analytic function of β here and by similar arguments it is analytic in B, J_x, J_y. This means that all the eigenvalues of the transfer matrix form are analytic except where two are equal. Such behaviour is typical of the eigenvalues of a transfer matrix whose coefficients are analytic functions of the physical parameters.

References

Baker G A Jr 1965 *Adv. Theor. Phys.* **1** 1–58
Bonner J C and Fisher M E 1964 *Phys. Rev.* **135** A640–60
Chisholm J S R 1973 *Math. Comput.* **27** 841–8
Copson E T 1935 *Theory of Functions of a Complex Variable* (London: Oxford University Press) pp 170–4
Denbigh J S 1974 *J. Phys. A: Math., Nucl. Gen.* **7** 2161–72
Fisher M E and Burford R J 1967 *Phys. Rev.* **156** 583–622
Gaunt D S and Guttmann A J 1974 *Phase Transitions and Critical Phenomena* vol. 3, eds C Domb and M S Green (London: Academic) chap. 4
Hervé M 1963 *Several Complex Variables* (London: Oxford Univesity Press)
Katsura S 1962 *Phys. Rev.* **127** 1508–18
Katsura S and Ohminami 1972 *Phys. Lett.* **40A** 320–2
Kaufman B 1949 *Phys. Rev.* **76** 1232–52
Lieb E H, Schultz T D and Mattis D C 1961 *Ann. Phys., NY* **16** 407–66
Matsubara F and Katsura S 1973 *Prog. Theor. Phys.* **49** 367–8
Narasimhan R 1971 *Several Complex Variables* (Chicago, London: University of Chicago Press)
Stanley H E 1971 *Introduction to Phase Transitions and Critical Phenomena* (Oxford: Clarendon)
Suzuki M 1971 *Prog. Theor. Phys.* **46** 1337–59