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LETTER TO THE EDITOR

Some simple solutions of the 16-vertex model

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Abstract. The 16-vertex model of ferroelectrics is shown to contain some special cases in which simple relationships among the vertex weights allow the partition function to be calculated by elementary methods. These models are essentially one-dimensional Ising chains except in a limiting case in which a rudimentary sort of phase transition may occur.

The transfer matrix for vertical bonds in the 16-vertex model can be written (Lieb and Wu 1972) in terms of spin operators at N sites as

$$\begin{aligned}
 T &= \text{Tr}_2 \prod_{j=1}^N \left\{ \begin{pmatrix} \omega_1 & \omega_{12} \\ \omega_{10} & \omega_4 \end{pmatrix} \sigma_j^+ \sigma_j^- + \begin{pmatrix} \omega_3 & \omega_{14} \\ \omega_{16} & \omega_2 \end{pmatrix} \sigma_j^- \sigma_j^+ + \begin{pmatrix} \omega_9 & \omega_5 \\ \omega_7 & \omega_{15} \end{pmatrix} \sigma_j^+ + \begin{pmatrix} \omega_{11} & \omega_8 \\ \omega_6 & \omega_{13} \end{pmatrix} \sigma_j^- \right\} \\
 &\equiv \text{Tr}_2 \prod_{j=1}^N (A \sigma_j^+ \sigma_j^- + B \sigma_j^- \sigma_j^+ + C \sigma_j^+ + D \sigma_j^-)
 \end{aligned}
 \tag{1}$$

where the ω_i ($i = 1, \dots, 16$) are weights (positive real numbers) for the vertices of figure 1 and Tr_2 means the trace taken over the products of 2×2 matrices A, B, C, D .

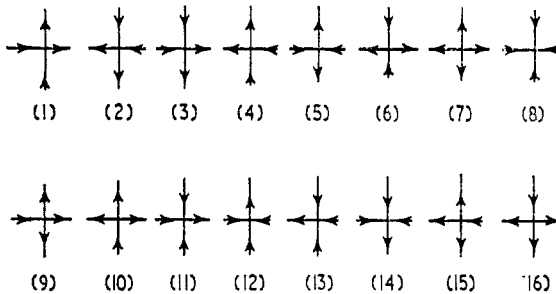


Figure 1. The 16 vertex configurations.

From an algebraic point of view T is very much simplified if the matrices A, B, C, D can be put simultaneously into upper (or lower) triangular form. A direct examination shows that this can be done by a (unitary) similarity transformation provided that either: (a) $\omega_i \neq 0$ for $i = 1, \dots, 16$ and there exists a real number z such that the equations

$$\begin{aligned}
 \omega_{10}z^2 + (\omega_4 - \omega_1)z - \omega_{12} &= 0 \\
 \omega_{16}z^2 + (\omega_2 - \omega_3)z - \omega_{14} &= 0 \\
 \omega_7z^2 + (\omega_{15} - \omega_9)z - \omega_5 &= 0 \\
 \omega_8z^2 + (\omega_{13} - \omega_{11})z - \omega_8 &= 0
 \end{aligned}
 \tag{2}$$

hold simultaneously; or (b) either

$$\begin{aligned} \text{or} \quad & \omega_{10} = \omega_{16} = \omega_7 = \omega_6 = 0 \\ & \omega_{12} = \omega_{14} = \omega_5 = \omega_8 = 0. \end{aligned} \tag{3}$$

(These can be regarded as limiting cases of (2) but are kept separate for the discussion below.)

When A, B, C, D satisfy conditions (a) or (b) the eigenvalues of any reasonable function $f = f(A, B, C, D)$ are $f(\lambda_i(A), \lambda_j(B), \lambda_k(C), \lambda_l(D))$ where the λ are eigenvalues of the four matrices in (1); in particular we have

$$\begin{aligned} T &= \prod_{j=1}^N (\lambda_1(A)\sigma_j^+ \sigma_j^- + \lambda_1(B)\sigma_j^- \sigma_j^+ + \lambda_1(C)\sigma_j^+ + \lambda_1(D)\sigma_j^-) \\ &\quad + \prod_{j=1}^N (\lambda_2(A)\sigma_j^+ \sigma_j^- + \lambda_2(B)\sigma_j^- \sigma_j^+ + \lambda_2(C)\sigma_j^+ + \lambda_2(D)\sigma_j^-) \\ &= E_1 \otimes E_1 \otimes \dots \otimes E_1 + E_2 \otimes E_2 \otimes \dots \otimes E_2 \equiv T_1 + T_2 \end{aligned} \tag{4}$$

where in the tensor product the matrices

$$E_i = \begin{pmatrix} \lambda_i(A) & \lambda_i(C) \\ \lambda_i(D) & \lambda_i(B) \end{pmatrix} \tag{5}$$

are formed from corresponding eigenvalues of A, B, C, D and are repeated N times.

If the weights ω_i satisfy conditions (2) above we may derive the partition function by the following argument. All the entries in matrices A, B, C, D are real and positive so each matrix has two eigenvalues one of which is positive (say λ_+) and exceeds in magnitude the other (λ_-) which may be positive or negative. The eigenvector corresponding to λ_+ may be taken with all positive entries whereas that of λ_- must have one positive and one negative (the Perron-Frobenius theorem). But as A, B, C, D can be made simultaneously triangular they have a common eigenvector and the (1,1) element of the triangular matrix is the corresponding eigenvalue. It follows that in the triangular form the λ_+ for A, B, C, D occupy corresponding positions and likewise the λ_- . Thus we may take $\lambda_1(A), \lambda_1(B), \lambda_1(C), \lambda_1(D)$ to be of λ_+ type and all the λ_2 to be of λ_- type. A straightforward induction argument now shows that the (i, j) th element of any product of E_1 and E_2 with M factors is less in magnitude than the (i, j) th element of E_1^M and hence that

$$\text{Tr}_2^N(T^M) = \sum_{\substack{\text{all products} \\ \text{with } \sum k + \sum l = M}} \{\text{Tr}_2(E_1^{k_1} E_2^{l_1} E_1^{k_2} \dots)\}^N \sim (\text{Tr}_2 E_1^M)^N$$

for large N . As the entries of E_1 are real and positive its eigenvalue of greatest magnitude is always

$$\Lambda = \frac{1}{2}(\lambda_1(A) + \lambda_1(B)) + \frac{1}{2}\{(\lambda_1(A) - \lambda_1(B))^2 + 4\lambda_1(C)\lambda_1(D)\}^{1/2} \tag{6}$$

and the result for the partition function as $N, M \rightarrow \infty$ is

$$Z = \text{Tr}_2^N(T^M) \sim \Lambda^{MN}. \tag{7}$$

If we wish to interpret the vertex weights as Boltzmann weights in terms of a vertex energy e_i and inverse temperature β as $\omega_i = \exp(-\beta e_i)$ the equations (2) cannot hold at all temperatures without further restriction. This leads to essentially two

cases

$$\omega_1 = \omega_4, \quad \omega_2 = \omega_3, \quad \omega_5 = \omega_7, \quad \omega_6 = \omega_8, \quad (8)$$

and

$$\begin{aligned} \omega_{10} = \omega_{12}, \quad \omega_{11} = \omega_{13}, \quad \omega_9 = \omega_{15}, \quad \omega_{14} = \omega_{16} \\ \omega_1 = \omega_{10}, \quad \omega_4 = \omega_{12}, \quad \omega_3 = \omega_{16}, \quad \omega_2 = \omega_{14}, \\ \omega_7 = \omega_9, \quad \omega_5 = \omega_{15}, \quad \omega_6 = \omega_{11}, \quad \omega_8 = \omega_{13}. \end{aligned} \quad (9)$$

(From symmetry properties of Z (Lieb and Wu 1972) there are a few other pairings of weights which lead to the same thermodynamics as these two.) In both cases (8) and (9) the eigenvalues λ_1 , and hence Λ of (6), become analytic functions of β so there is here no possibility of a phase transition. If the states of the four bonds at a vertex are labelled clockwise round the vertex by classical ‘spin’ variables s_1, s_2, s_3, s_4 (each $s_i = \pm 1$) the method of Suzuki and Fisher (1971) gives the equivalent Ising models as follows.

In case (9) the partial Ising hamiltonian for ‘spins’ round vertex r becomes

$$H_r = -J_0 - J_1s_1 - J_2s_2 - J_3s_4 - J_4s_1s_2 - J_5s_1s_4 - J_6s_2s_4 - J_7s_1s_2s_4 \quad (10)$$

with eight independent parameters J . By drawing the Ising lattice it is easy to see that (10) corresponds to a set of decorated one-dimensional Ising chains. The decoration spin s_1 can be summed out in the usual way (Green and Hurst 1964) so that the Ising equivalent of (9) is basically a one-dimensional chain with nearest-neighbour interactions and a magnetic field.

In case (8) the Suzuki-Fisher method leads to a partial hamiltonian at the r th vertex.

$$H_r = -J_0 - J_1s_2 - J_2s_4 - J_3s_1s_3 - J_4s_2s_4 - J_5s_1s_2s_3 - J_6s_1s_3s_4 - J_7s_1s_2s_3s_4 \quad (11)$$

where again the eight J are independent. In (11) the variables s_1 and s_3 occur only in the combination s_1s_3 ; the introduction of $t = s_1s_3$ as a new independent random variable immediately reduces (11) to (10) so that the discussion above again applies.

If the weights ω_i satisfy (3) the argument is no longer valid because the Perron-Frobenius theorem does not apply in the form used above. We may however go back to equation (4) which now holds with

$$E_1 = \begin{pmatrix} \omega_1 & \omega_9 \\ \omega_{11} & \omega_3 \end{pmatrix} \quad E_2 = \begin{pmatrix} \omega_4 & \omega_{15} \\ \omega_{13} & \omega_2 \end{pmatrix}. \quad (12)$$

Since all the elements of E_1 and E_2 are positive we have in the notation used earlier (extended so that $\lambda_{\pm}(T)$ mean the largest and smallest eigenvalues of the $2^N \times 2^N$ matrix T)

$$\lambda_+(E_1) > |\lambda_-(E_1)|, \quad \lambda_+(T_1) = \lambda_+^N(E_1) \quad (13)$$

$$\lambda_-(T_1) = \lambda_-^N(E_1) \quad \text{if } \lambda_-(E_1) \geq 0 \quad (14)$$

$$\lambda_-(T_1) = \lambda_+^{N-1}(E_1)\lambda_-(E_1) \quad \text{if } \lambda_-(E_1) < 0$$

and corresponding results for T_2 . Suppose now that $\lambda_+(E_1) > \lambda_+(E_2)$. By using the minimax principle (Bellman 1960) we can write

$$\begin{aligned} \lambda_+(T_1) + \lambda_-(T_2) &= \max(x, T_1x) + \min(x, T_2x) \\ &\leq \max(x, (T_1 + T_2)x) = \lambda_+(T_1 + T_2) \\ &\leq \max(x, T_1x) + \max(x, T_2x) \\ &= \lambda_+(T_1) + \lambda_+(T_2). \end{aligned} \quad (15)$$

Here the max and min are taken over all normalized 2^N dimensional vectors x . On inserting (13) and (14) into (15) and taking N to be large there results immediately

$$\lambda_+(T) \sim \max(\lambda_+^N(E_1), \lambda_+^N(E_2))$$

and so

$$Z \sim \max(\lambda_+^{MN}(E_1), \lambda_+^{MN}(E_2)). \quad (16)$$

If one of $\lambda_+(E_1)$, $\lambda_+(E_2)$ remains greater than the other as the weights in (12) vary with temperature the thermodynamic behaviour is again that of (6) and (7). However, in the present case we have the additional possibility that as temperature varies $\lambda_+(E_1)$ and $\lambda_+(E_2)$ may cross one or more times. For example, the case with vertex energies $e_1 = e_3 = 1$, $e_2 = e_4 = 2$, $e_9 = e_{11} = 8$, $e_{13} = e_{15} = 4$ has a phase transition at $\beta \sim 1/10$. Since $\lambda_+(E_1)$ and $\lambda_+(E_2)$ are two distinct analytic functions of temperature each such crossing point constitutes a first-order phase transition. The lattice interpretation of the transition can be seen at once from figure 1. The effective elimination of vertices 5, 6, 7, 8, 10, 12, 14, 16 from the problem means that on a given row all horizontal arrows point in the same direction; the partial transfer matrices T_1 and T_2 correspond to right- and left-pointing rows respectively. For a large lattice the 'average' configuration has all rows pointing in the same direction and the reversal of this universal direction constitutes the phase transition. Between transitions the partition function behaves again like (7). The columns of vertical bonds behave independently one from another and the 2×2 matrices E_1 and E_2 play the role of transfer matrices along the columns. Thus the thermodynamics and correlations along a column are again those of a one-dimensional Ising chain.

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