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Ferroelectric ice model on a triangular lattice

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Abstract. A ferroelectric ice model or KDP model, after the Slater KDP model for a square lattice, is formulated on a triangular lattice and solved for all temperatures. It is found that this system undergoes a phase transition of the first order into a frozen ferroelectric state.

1. Introduction

In this paper we solve exactly a lattice model in statistical mechanics that can be regarded as the analogue for the triangular lattice of the KDP model on the square lattice.

An 'ice-type' model is one in which arrows are placed on the bonds of a lattice of even coordination number so that at each vertex there are as many arrows in as out. Energies are associated with the various possible arrangements of arrows at each vertex. We attempt to calculate the partition function and free energy for this type of model.

Lieb (1967a, b) and Sutherland (1967) have shown that such models can be solved exactly on a square lattice. They exhibit two types of phase transition: an infinite-order transition to an ordered antiferroelectric phase (the F model; Lieb 1967a), and a first-order transition to a frozen ferroelectric phase (the KDP model; Lieb 1967b).

Baxter (1969, 1972) has considered a rotationally-invariant ice-type model on a triangular lattice. This turns out to be soluble only when a temperature-dependent algebraic relation is satisfied by the Boltzmann weights. If the Boltzmann weights are varied so as to satisfy this relation then the model undergoes an F-model type of transition in the sense that an infinite-order singularity occurs in the free energy.

Here we consider another triangular ice-type model which turns out to be soluble for all temperatures. It has a phase transition similar to the square lattice KDP model.

Arrows are placed on the bonds of a triangular lattice so that there are three entering and three leaving each vertex. There are twenty possible vertex configurations. If configurations in which all arrows are reversed are identified then there are the ten distinct configurations shown in figure 1. With the vertices are associated the energies: $e_1 = 0$, $e_i = \epsilon > 0$ $(i = 2, 3, \ldots, 10)$.

We consider a triangular lattice of M rows, each row having $N/2$ vertices and with cyclic boundary conditions as indicated in figure 2. The partion function is

$$Z = \sum \exp\left(\frac{-p\epsilon}{kT}\right) \tag{1}$$

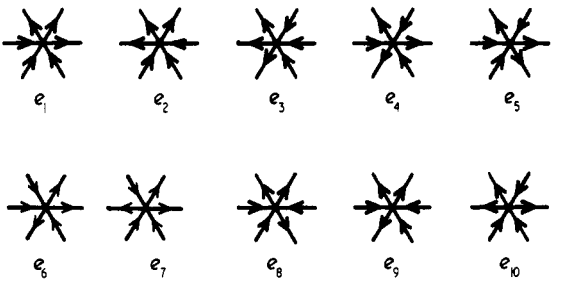

Figure 1. Ten possible reversal-symmetric vertex configurations with corresponding energies.

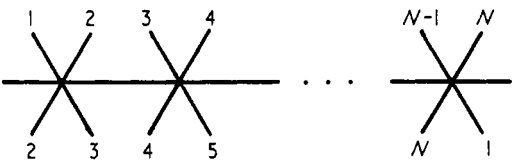

Figure 2. Numbering of the bonds on a specific row of the lattice.

where p is the number of vertices of types $2, 3, \ldots, 10$, and the sum extends over all allowable configurations on the lattice. The free energy per vertex $\mathscr{F}$ is given by

$$-\beta\mathscr{F} = \lim_{\substack{N\to\infty \\ M\to\infty}} \frac{2}{MN} \ln Z. \tag{2}$$

Set $u = \exp(-\epsilon/kT)$. We find that there is a phase transition when $u = \frac{1}{3}$, which corresponds to a critical temperature

$$T_c = \frac{\epsilon}{k \ln 3}.$$

When $T < T_c$ the free energy is zero. When $T > T_c$ the free energy is given by the principal value integral

$$-\beta\mathscr{F} = \mathrm{P}\int_{-\infty}^{\infty} \frac{16 \sinh(\pi-\phi)m \cosh^3(\pi-\phi)m}{m(e^{2\phi m}+1)(1-e^{-2\pi m})}\,dm \tag{3}$$

where

$$2\cos\phi = -\sqrt{1+u^{-1}}, \qquad \tfrac{3}{4}\pi < \phi < \pi \tag{4}$$

(see figure 3). The behaviour of the free energy near and above T_c is given by

$$-\beta\mathscr{F} = \frac{3\ln 3}{4}\left(\frac{T}{T_c}-1\right) + \frac{\sqrt{3}}{4\pi}(\ln 3)^{3/2}\left(\frac{T}{T_c}-1\right)^{3/2} + \ldots. \tag{5}$$

The internal energy at the transition is $\frac{3}{4}\epsilon$, and the leading behaviour of the specific heat is

$$C_v \simeq \frac{3\sqrt{3}}{16\pi}(\ln 3)^{3/2}\left(\frac{T}{T_c}-1\right)^{-1/2}. \tag{6}$$

The critical exponent α is therefore $\frac{1}{2}$.

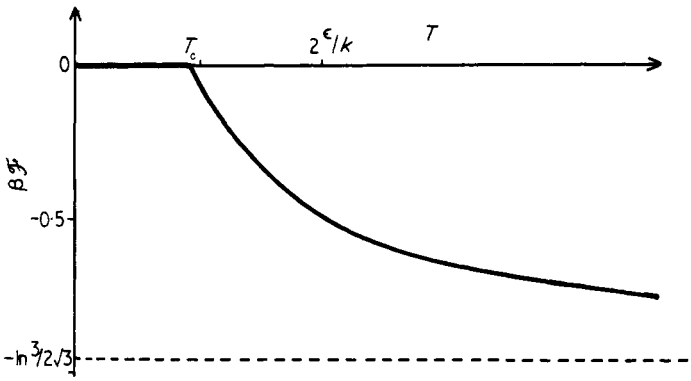

Figure 3. Plot of the free energy with temperature showing the behaviour at the critical temperature.

2. The transfer matrix

We solved this problem by the transfer matrix method. The numbering of the bonds is shown in figure 2. The lower row of non-horizontal bonds will be regarded as the incoming row and the upper row of non-horizontal bonds as the outgoing row. The number n, of down arrows in each row of bonds, is conserved, ie is the same for the outgoing row as the incoming row.

Proceeding in the usual way (Lieb 1967a, b, Sutherland 1967, Baxter 1972), let $X = \{x_1, \ldots, x_n\}$ be the positions of the down arrows in a row. Further let $f(X)$ be the element of the eigenvector of the transfer matrix corresponding to the configuration X, and Λ the eigenvalue. Then the eigenvalue equation for Λ and f is

$$\Lambda f(X) = \sum_{y_1=1}^{x_1'} \sum_{y_2=x_1'}^{x_2'} \cdots \sum_{y_n=x_{n-1}'}^{x_n'} f(Y) D_1(X, Y) + \sum_{y_1=x_1'}^{x_2'} \sum_{y_2=x_2'}^{x_3'} \cdots \sum_{y_n=x_n'}^{N} f(Y) D_2(X, Y) + C_n \tag{7}$$

where

$$D_1(X, Y) = c(0, y_1)c(x_1, y_2) \ldots c(x_{n-1}, y_n)c(x_n, N+1) \tag{8a}$$

$$D_2(X, Y) = c(x_1, y_1)c(x_2, y_2) \ldots c(x_n, y_n) \tag{8b}$$

$$c(x, y) = u^{(y''-x'+2)/2} \tag{8c}$$

$$x' = \begin{cases} x-1 & (x \text{ even}) \\ x-2 & (x \text{ odd}) \end{cases} \qquad y'' = \begin{cases} y-1 & (y \text{ even}) \\ y & (y \text{ odd}) \end{cases} \tag{9}$$

The term C_n is a correction term which removes the double counting of some configurations.

3. The Bethe ansatz

We try a modified Bethe-type ansatz (Lieb 1967a, b)

$$f(X) = \sum_P A(P) \exp\left(\sum_{j=1}^{n} \mathrm{i} k_{P(j)} x'_j \right) \tag{10}$$

where the sum is over all permutations $P = \{P(1), P(2), \ldots, P(n)\}$ of the n integers $1, 2, \ldots, n$. When (10) is substituted into the right-hand side of (7) we obtain as usual three types of terms: *wanted terms* of same form as the left-hand side, *internal unwanted* terms containing factors of the form $\exp[\mathrm{i} k_{P(j)}(x'_j + x'_{j+1})]$, and *boundary terms* independent of either x'_1 or x'_n.

Equating wanted terms gives

$$\Lambda = u^{N/2} \prod_{i=1}^{n} \lambda_i + \prod_{i=1}^{n} \mu_i \tag{11}$$

where λ_i and μ_i are given by

$$\lambda_i = \frac{(z_i + 1)[(1 + z_i)u - 1]}{(uz_i - 1)z_i} \tag{12}$$

$$\mu_i = \frac{(z_i + 1)u}{(uz_i - 1)z_i} \tag{13}$$

$$z_i = \mathrm{e}^{2\mathrm{i}k_i}. \tag{14}$$

The internal unwanted terms in (7) vanish if

$$B(k_i, k_j) = \frac{A(\ldots, i, j, \ldots)}{A(\ldots, j, i, \ldots)} = -\frac{z_i z_j + z_j - u^{-1} z_i + 1}{z_i z_j + z_i - u^{-1} z_j + 1}. \tag{15}$$

Equation (15) is actually four equations which arise by requiring the internal unwanted terms in (7) to cancel. Fortunately in this model, as in the F model, the equations are identical. The vanishing of the boundary terms imposes the condition

$$\mathrm{e}^{\mathrm{i}k_i N} = \prod_{\substack{j=1 \\ j \neq i}}^{n} B(k_i, k_j). \tag{16}$$

We now have n equations to solve for the n k_i and by using equations (11), (12), (13) and (14) we can calculate Λ in the n subspace.

4. The model in the limit $N \to \infty$

We are interested in the behaviour of the model as $N \to \infty$ and the corresponding limiting maximum eigenvalue Λ. We obtain the free energy per vertex from Λ by

$$-\beta \mathscr{F} = \lim_{N \to \infty} \frac{2}{N} \ln \Lambda. \tag{17}$$

4.1. Low temperature ($T < T_c$)

When the temperature is below the critical temperature it is particularly easy to calculate the maximum value of Λ.

Since $0 < u < 1$ it is clear from equations (12) and (13) that $|u\lambda_i| < |\mu_i|$. When $T < T_c$ we have $u < \frac{1}{3}$ which implies, by (13), that $|\mu_i| < 1$. Therefore in the low temperature region $|\Lambda|$ is a non-increasing function of n. The maximum value is therefore attained at $n = 0$; ie $\Lambda = u^{N/2} + 1$. In the limit of N large $\Lambda \simeq 1$ and

$$\mathscr{F} = 0. \tag{18}$$

4.2. High temperature ($T > T_c$)

The solution in this region is not so straightforward. Guided by previous solutions (Lieb 1967a, b, Southerland 1967), we assume that as we increase N keeping n/N fixed the k_i will be continuously distributed in some real interval $(-a, a)$ with the density function $\rho(k)$. In order to put the problem into the form of an integral equation with a difference kernel we make the transformation

$$e^{2ik} = \frac{e^{2i\phi} + e^{2\alpha}}{e^{2i\phi + 2\alpha} + 1} \tag{19}$$

from k to α. The parameter ϕ is given by $2\cos\phi = -\sqrt{1+u^{-1}}$, $\frac{3}{4}\pi < \phi < \pi$. In the limit of N and n large the equations (15) and (16) then imply

$$R(\alpha) = \xi(\alpha) - \int_{-b}^{b} K(\alpha - \beta) R(\beta)\, d\beta \tag{20}$$

$$n = N \int_{-b}^{b} R(\alpha)\, d\alpha \tag{21}$$

where

$$\xi(\alpha) = \frac{-2\sin 2\phi}{\cosh 2\alpha + \cos 2\phi} \tag{22a}$$

$$K(\alpha) = \frac{2\sin 2\phi}{\cosh 2\alpha - \cos 2\phi}. \tag{22b}$$

$R(\alpha)$ is the density function of the α_i such that $\rho(k)\, dk = R(\alpha)\, d\alpha$. We wish to solve (20) for $R(\alpha)$. This can be done by Fourier transforms when $b = \infty$, giving

$$R(\alpha) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\cos(\pi - \phi)m}{\cosh \phi m} e^{2i\alpha m}\, dm \tag{23}$$

and $n = \frac{1}{2}N$. Following Yang and Yang (1966) and Lieb (1967b) we expect this value of n to correspond to the maximum eigenvalue. The k_i occupy the interval $(\phi - \pi, \pi - \phi)$. When $\frac{1}{3} < u < 1$, $|u\lambda_i| < |\mu_i|$ and therefore $\Lambda = \Pi_{i=1}^{n} \mu_i$ for large N. We can therefore write

$$\ln \Lambda \simeq N \int_{-\infty}^{\infty} R(\alpha) \ln \mu(\alpha)\, d\alpha. \tag{24}$$

Substituting expression (23) for $R(\alpha)$, performing the integration with respect to α, and using (13), (14) and (17) we obtain the result stated in equation (3) for the free energy.

5. Extension to more general vertex energies

We have considered the general case of arbitrary energies $\epsilon_1, \epsilon_2, \ldots, \epsilon_{10}$ for the ten reversal-symmetric pairs of vertex configurations represented in figure 1. We find that an appropriate Bethe-type ansatz works only if certain conditions are satisfied. Unfortunately these conditions are, in general, temperature dependent. We intend to present these results in a subsequent paper.

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