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LETTER TO THE EDITOR

Proof of long range order for a class of ferroelectric vertex models

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Abstract. A class of ferroelectric models on a square lattice, including some models used for studying the phase transitions in crystals of squaric acid, is shown to exhibit long range order at low enough temperatures. This is accomplished by taking into account the property of reflection positivity and using a modified Peierls argument.

In the present work we use a method proposed by Fröhlich and Lieb (1978) to prove the existence of long range order for a class of ferroelectric vertex models on a square lattice. As a particular case, we include a 12-vertex model which has recently been used to study the phase transition in squaric acid (Stilck and Salinas 1981). The well known Peierls (1936) argument, which was made rigorous by Griffiths (1964) and Dobrushin (1965), leads to an inequality for the magnetisation of discrete spin systems submitted to fixed boundary conditions. At low enough temperatures, this inequality establishes the existence of spontaneous magnetisation. On the other hand, the approach of Fröhlich and Lieb (1978) relies on the property of reflection positivity (Osterwalder and Schrader 1973, 1975) to show that the pair correlations of some spin models will not decay to zero at infinite distances, provided the temperature is sufficiently low.

Let us consider the 16-vertex model on the square lattice, and number the configurations according to the notation of Lieb and Wu (1972). Since we are concerned with energy levels which are invariant under the inversion of all arrows, we make $e_1 = e_2 = E_1$, $e_3 = e_4 = E_2$, $e_5 = e_6 = E_3$, $e_7 = e_8 = E_4$, $e_9 = e_{13} = E_5$, $e_{10} = e_{14} = E_6$, $e_{11} = e_{15} = E_7$, $e_{12} = e_{16} = E_8$. Following Suzuki and Fisher (1970), this vertex model may be transformed into an Ising model with nearest-neighbour, next-nearest-neighbour and four-spin interactions on the medial square lattice. If we associate an Ising spin with each link of the original lattice, such that $\sigma = 1$ if the arrow points up or rightwards, and $\sigma = -1$ if it points down or leftwards, the energy of every vertex may be written as a function of the four incident Ising spins (see figure 1). We thus have

$$E(\sigma_1, \sigma_2, \sigma_3, \sigma_4) = -J_0 - (J_1\sigma_1\sigma_2 + J_2\sigma_2\sigma_3 + J_3\sigma_3\sigma_4 + J_4\sigma_4\sigma_1) - (J_5\sigma_1\sigma_3 + J_6\sigma_2\sigma_4) - J_7\sigma_1\sigma_2\sigma_3\sigma_4, \tag{1}$$

where

$$J_0 = -\tfrac{1}{8}\sum_{i=1}^{8} E_i, \qquad J_1 = \tfrac{1}{8}[(E_2 + E_3 + E_7 + E_8) - (E_1 + E_4 + E_5 + E_6)],$$

$$\begin{aligned}
J_2&=\tfrac{1}{8}[(E_2+E_4+E_5+E_8)-(E_1+E_3+E_6+E_7)],\\
J_3&=\tfrac{1}{8}[(E_2+E_3+E_5+E_6)-(E_1+E_4+E_7+E_8)],\\
J_4&=\tfrac{1}{8}[(E_2+E_4+E_6+E_7)-(E_1+E_3+E_5+E_8)],\\
J_5&=\tfrac{1}{8}[(E_3+E_4+E_5+E_7)-(E_1+E_2+E_6+E_8)],\\
J_6&=\tfrac{1}{8}[(E_3+E_4+E_6+E_8)-(E_1+E_2+E_5+E_7)],\\
J_7&=\tfrac{1}{8}[(E_5+E_6+E_7+E_8)-(E_1+E_2+E_3+E_4)].
\end{aligned}\tag{2}$$

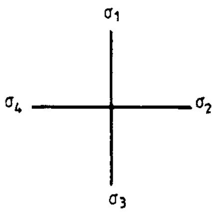

Figure 1. A vertex and the four links where the Ising spins are located.

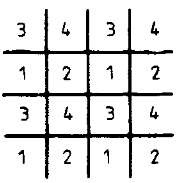

Figure 2. Numbering scheme for the elementary squares of the lattice.

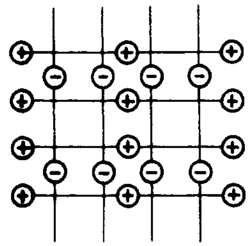

Figure 3. A pictorial description of the projection operator P_Ω.

Let us now define horizontal and vertical reflection lines on the original N-site lattice Ω. We assume toroidal boundary conditions, each reflection line separating the lattice Ω into two congruent parts, Ω_+ and Ω_-. It should be noticed that there will be a set of spins on the reflection line. We will call this set $\Omega_\pm$. If we define the reflection of a spin,

$$\theta_l(\sigma_i)\equiv\sigma_{\theta_l i},\tag{3}$$

and the reflection of an arbitrary function of the spins,

$$\theta_l F(\{\sigma_i\})\equiv F(\{\theta_l\sigma_i\}),\tag{4}$$

it is easy to see that in order to make

$$E(\sigma_1,\sigma_2,\sigma_3,\sigma_4)=\theta_l E(\sigma_1,\sigma_2,\sigma_3,\sigma_4)\tag{5}$$

for all vertices and reflection lines, we must have $J_1=J_2=J_3=J_4$, or, alternatively,

$$E_3=E_4,\qquad E_5=E_7,\qquad E_6=E_8.\tag{6}$$

From equation (5) we may write the 16-vertex model Hamiltonian in the form

$$\mathscr{H}=\mathscr{H}_++\theta_l\mathscr{H}_+,\tag{7}$$

where $\mathscr{H}_+$ comprises the contribution of vertices belonging to Ω_+. Following Fröhlich and Lieb (1978), it is not difficult to show that, given an arbitrary function $F(\{\sigma_i\})$, with $\sigma_i\in\Omega_+,\Omega_\pm$, we have the inequality

$$\langle F\theta_l F\rangle\equiv\sum_{\{\sigma_i\}}F\theta_l F\,\mathrm{e}^{-\beta\mathscr{H}}\Big/\sum_{\{\sigma_i\}}\mathrm{e}^{-\beta\mathscr{H}}\geqslant 0.\tag{8}$$

From this last property, which is the so-called reflection positivity, we may set up a

Schwarz inequality,

$$\langle F\theta_l G\rangle^2 \leq \langle F\theta_l F\rangle + \langle G\theta_l G\rangle, \tag{9}$$

where F and G are functions of $\sigma_i \in \Omega_+, \Omega_\pm$.

Our aim is to show that, under some restrictions, $\langle\sigma_0\sigma_i\rangle > 0$ at sufficiently low temperatures and independent of the localisation of σ_i. We start by defining projection operators P_i, which act on the spin configurations $\{\sigma_i\}$,

$$P_i^+ \equiv \tfrac{1}{2}(\sigma_i^+ + 1), \qquad P_i^- \equiv 1 - P_i^+. \tag{10}$$

Therefore

$$\langle\sigma_0\sigma_i\rangle = \langle P_0^+P_i^+\rangle + \langle P_0^-P_i^-\rangle - \langle P_0^-P_i^+\rangle - \langle P_0^+P_i^-\rangle, \tag{11}$$

and the invariance of the model under the inversion of arrows ensures that

$$\langle P_0^+P_i^+\rangle = \langle P_0^-P_i^-\rangle \qquad \text{and} \qquad \langle P_0^+P_i^-\rangle = \langle P_0^-P_i^+\rangle. \tag{12a, b}$$

Since we may write $\langle P_0^+P_i^+\rangle = \langle P_0^+\rangle - \langle P_0^+P_i^-\rangle$, and the toroidal boundary conditions, as well as the arrow inversion invariance, give $\langle P_0^+\rangle = \frac{1}{2}$, equation (11) may then be rewritten as

$$\langle\sigma_0\sigma_i\rangle = 1 - 4\langle P_0^+P_i^-\rangle. \tag{13}$$

To obtain an inequality for $\langle P_0^+P_i^-\rangle$ we followed the steps outlined in §§ I.C–I.E of Fröhlich and Lieb (1978). Therefore, we omit here most of the details. Let us define γ to be a closed contour on the medial lattice of Ω, which separates the link 0 from the link i. We may thus write the inequality

$$\langle P_0^+P_i^-\rangle \leq \sum_\gamma \left\langle \prod_{\langle i,j\rangle\in\gamma} P_i^+P_j^- \right\rangle, \tag{14}$$

where the symbols $\langle i, j\rangle$ label pairs of nearest-neighbour links which define the contour γ. Now we may number the elementary squares of the original lattice from 1 to 4, according to the scheme depicted in figure 2. The set of nearest-neighbour links γ may be split into eight subsets $\gamma_{\alpha\beta}$, with $\alpha = 1, 2, 3, 4$, and $\beta = h, v$. The value of α corresponds to the number of the square in whose sides the links are located. β is given by $h(v)$ if the + link of the pair is horizontal (vertical). The second member of the inequality (14) satisfies

$$\left\langle \prod_{\langle i,j\rangle\gamma} P_i^+P_j^- \right\rangle \leq \prod_{\substack{\alpha=1,2,3,4\\ \beta=h,v}} \left\langle \prod_{\langle i,j\rangle\in\gamma_{\alpha\beta}} P_i^+P_j^- \right\rangle^{1/8}. \tag{15}$$

Now we repeatedly apply the Schwarz inequality (9) to each factor on the right-hand side of (15), for different reflection lines l, and obtain

$$\left\langle \prod_{\langle i,j\rangle\gamma_{\alpha\beta}} P_i^+P_j^- \right\rangle \leq \langle P_\Omega\rangle^{|\gamma_{\alpha\beta}|/N}, \tag{16}$$

where $|\gamma_{\alpha\beta}|$ is the number of pairs of links in $\gamma_{\alpha\beta}$ and P_Ω is a 'universal' projection operator which covers the whole lattice and is defined in figure 3. Expressions (15) and (16) lead to

$$\langle P_0^+P_i^-\rangle \leq \sum_\gamma \langle P_\Omega\rangle^{|\gamma|/8N}. \tag{17}$$

Now let us obtain an inequality for the expectation value,

$$\langle P_\Omega \rangle \equiv \sum_{\{\sigma\}} P_\Omega \, e^{-\beta \mathscr{H}} \Big/ \sum_{\{\sigma\}} e^{-\beta \mathscr{H}}. \tag{18}$$

The denominator may be replaced by the Boltzmann factor corresponding to the ground state energy $\mathscr{H}_0$. Supposing that $E_1 = 0$ is the minimum value of the energies E_i, it follows that

$$\mathscr{H}_0 = -N(J_0 + 4J_1 + J_5 + J_6 + J_7). \tag{19}$$

The evaluation of the numerator of equation (18) leads to

$$\langle P_\Omega \rangle \leqslant \left[\sum_{i-1}^{9} a_i \exp[-4\beta f_i(\{E\})] \right]^{N/4}, \tag{20}$$

where $a_1 = 4$, $a_2 = a_3 = a_4 = a_5 = 2$, $a_6 = a_7 = a_8 = a_9 = 1$; and $f_1 = \frac{1}{4}[E_2 + E_3 + E_5 + E_6]$, $f_2 = \frac{1}{2}[E_2 + E_6]$, $f_3 = \frac{1}{2}[E_2 + E_5]$, $f_4 = \frac{1}{2}[E_3 + E_5]$, $f_5 = \frac{1}{2}[E_3 + E_6]$, $f_6 = E_2$, $f_7 = E_6$, $f_8 = E_5$, $f_9 = E_3$. Let us call f^* the minimum value of f_i, for all i. Then

$$\langle P_\Omega \rangle \leqslant [2 \, e^{-\beta f^*}]^N, \tag{21}$$

and equation (17) may be rewritten in the form

$$\langle P^+ P_i^- \rangle \leqslant \sum_{\gamma} e^{-K|\gamma|}, \tag{22}$$

where

$$K \equiv \tfrac{1}{8}(\beta f^* - \ln 2). \tag{23}$$

Using a type of Peierls argument the summation over contours in (22) may be bounded, and at low enough temperatures we have

$$\langle P_0^+ P_i^- \rangle \leqslant 18 e^{-4K}/(1 - 9e^{-2K})^2. \tag{24}$$

Thus there is ferroelectric long range order if $f^* > 0$, or alternatively, if

$$E_2, E_3, E_5, E_6 > 0. \tag{25}$$

Therefore, the 16-vertex model orders ferroelectrically at low temperatures, provided that there are only two vertex configurations (1 and 2) in the ground state. It is worth remarking that Abraham and Heilmann (1976) presented an argument supporting the idea that a model with a fourfold degenerate ground state (configurations 1, 2, 3 and 4) would not display ferroelectric ordering at finite temperatures.

The ferroelectric 12-vertex model (Stilck and Salinas 1981) is defined by $E_1 = 0$, $E_2 = E > 0$, $E_5 = E_6 = E_7 = E_8 = E' < E$ and $E_3 = E_4 \to \infty$. It fulfils conditions (6), and ferroelectric ordering should exist for $E > 0$. If we consider a 16-vertex model with $E_3 = E_4 = E'' > E'$ this conclusion still holds. As a matter of fact, this model may be solved for $E = 0$, with an analytic free energy (Stilck and Salinas 1981). A ferroelectric 8-vertex model, with $E_1 = 0$, $E_2 > 0$, $E_3 = E_4 > 0$, $E_5, E_6, E_7, E_8 \to \infty$ is also included in the class of models we consider.

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