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1979 J. Phys. A: Math. Gen. 12 L275

(http://iopscience.iop.org/0305-4470/12/10/007)

J. Phys. A: Math. Gen., Vol. 12, No. 10, 1979. Printed in Great Britain

LETTER TO THE EDITOR

A modified antiferroelectric six-vertex model

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Received 11 July 1979

Abstract. A modified antiferroelectric model (MF-model) is introduced. It is shown that the general solution of this model, whose basic ingredients are two energies ϵ_1 and ϵ_2, includes as special cases the F-model ($\epsilon_1=\epsilon_2=\epsilon$) and the Ising model ($\epsilon_1=\epsilon$, $\epsilon_2=\infty$). The MF-model has a polymer equivalent in which a polymer bond can assume one of three available states, one *trans* state (energy zero) and two *gauche* states with energies ϵ_1 and ϵ_2.

The partition function of the six-vertex model on a square lattice with N points can be written

$$Z_N=\sum_{\mathrm{C}}\prod_{i=1}^{N}\omega_{\xi(i)}. \tag{1}$$

The summation is extended over all possible arrow configurations, C, on the square lattice, $\xi(i)$ indicates the type of vertex configuration at the ith lattice point, and $\omega_\xi\equiv\exp(-\beta e_\xi)$ is the Boltzmann weight of a vertex having energy e_ξ. The six different kinds of vertices (ice rule) are shown in figure 1 ($\xi=1,2,\ldots,6$). Consider the case $\omega_1=\omega_2=\omega_3=\omega_4=\exp(-\beta\epsilon)<1$, $\omega_5=\omega_6=1$. This is the well-known antiferroelectric F-model (Rys 1963) solved by Lieb (1967). It undergoes an infinite-order transition (Lieb 1967, Lieb and Wu 1972). The ground state consists of alternating vertices (5) and (6), and so has no spontaneous polarisation.

Suppose that the lattice is divided into two sublattices A and B (figure 2) with N_A and N_B ($N_\mathrm{A}=N_\mathrm{B}$) points respectively. We generalise (1) to

$$Z_N=\sum_{\mathrm{C}}\Big(\prod_{i=1}^{N_\mathrm{A}}\omega_{\xi(i)}\Big)\Big(\prod_{j=1}^{N_\mathrm{B}}\omega'_{\xi(j)}\Big), \tag{2}$$

where $\omega'_\xi\equiv\exp(-\beta e'_\xi)$. We introduce a modified antiferroelectric model, which we shall call the MF-model, as follows:

$$\omega_1=\omega_2=\omega'_3=\omega'_4=\exp(-\beta\epsilon_1)<1,\qquad \omega_3=\omega_4=\omega'_1=\omega'_2=\exp(-\beta\epsilon_2)<1,$$
$$\omega_5=\omega_6=\omega'_5=\omega'_6=1. \tag{3}$$

The partition function of the MF-model depends on two energies ϵ_1 and ϵ_2, i.e. $Z_N^{\mathrm{MF}}(\epsilon_1,\epsilon_2)$. The F-model is the special case $\epsilon_1=\epsilon_2=\epsilon$, i.e.

$$Z_N^{\mathrm{MF}}(\epsilon,\epsilon)\equiv Z_N^{\mathrm{F}}(\epsilon). \tag{4}$$

The zero-field Ising model is also a special case of the MF-model, deriving from the case $\epsilon_1>0$ and $\epsilon_2=\infty$; something far from obvious. This is the main result of this Letter.

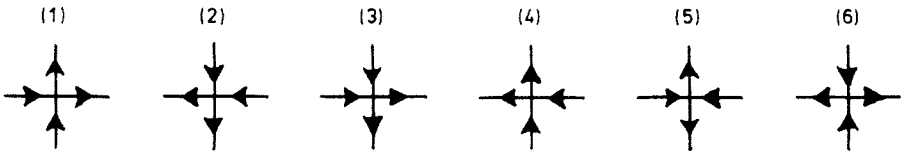

Figure 1. The six ice rule vertex configurations.

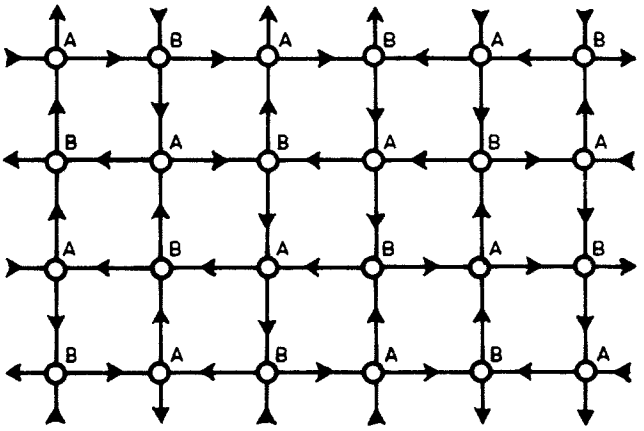

Figure 2. The square lattice and the two sublattices A and B. Arrows specify a C' configuration on the square lattice.

Indeed, we shall show that

$$Z_N^{\mathrm{MF}}(\epsilon_1, \epsilon_2 = \infty) = \exp(-N\beta\epsilon_1/2) Z_{N/2}^{\mathrm{I}}(\epsilon_1/2) \tag{5}$$

where $Z_{N/2}^{\mathrm{I}}(J)$ is the partition function of the zero-field Ising ferromagnet ($J > 0$) on a square lattice with $N/2$ points and diagonal periodic boundary conditions. The proof of (5), although very simple, requires two transformations which we proceed to describe.

We first show that $Z_N^{\mathrm{MF}}(\epsilon_1, \epsilon_2 = \infty)$ is the generating function for certain weighted self-avoiding polygons on the square lattice. We consider the Manhattan square lattice (MSL) shown in figure 3 (Kasteleyn 1963). A set of circuits (i.e. self-avoiding polygons following the orientation of the lattice) on the MSL, that cover all lattice points, is called a polygon (or polymer) configuration on the MSL (for an example see figure 4). Let t_{PC} be the number of polygonal corners of a polymer configuration on the MSL. The partition function

$$Z_{N,\mathrm{MSL}}^{\mathrm{P}}(\epsilon) \equiv \sum_{\mathrm{PC}} \exp(-t_{\mathrm{PC}}\beta\epsilon), \tag{6}$$

where the summation is extended over all possible polymer configurations, PC, on the MSL, defines a polymer model on the MSL in which a polymer bond can assume one of two available states: one *trans* state (energy zero) in which the bond is collinear with its preceding bond, and one *gauche* state (energy ϵ) in which the bond makes a corner with its preceding bond. We can show that

$$Z_N^{\mathrm{MF}}(\epsilon_1, \epsilon_2 = \infty) = Z_{N,\mathrm{MSL}}^{\mathrm{P}}(\epsilon_1). \tag{7}$$

Indeed, if $\epsilon_2 = \infty$, then vertices (3) and (4) do not occur on sublattice A, and vertices (1)

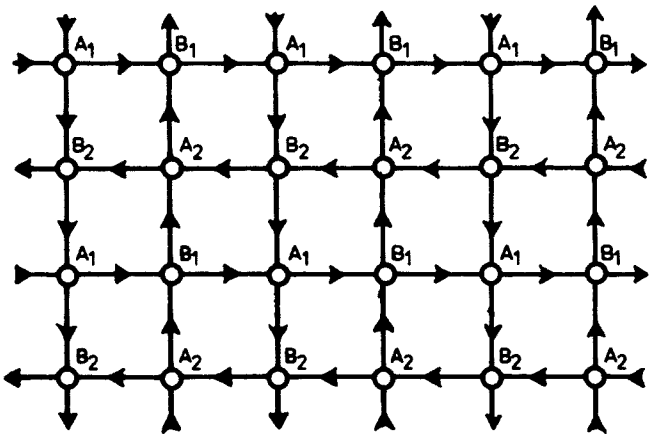

Figure 3. The Manhattan square lattice. The points are classified in four sublattices A_1, A_2, B_1 and B_2.

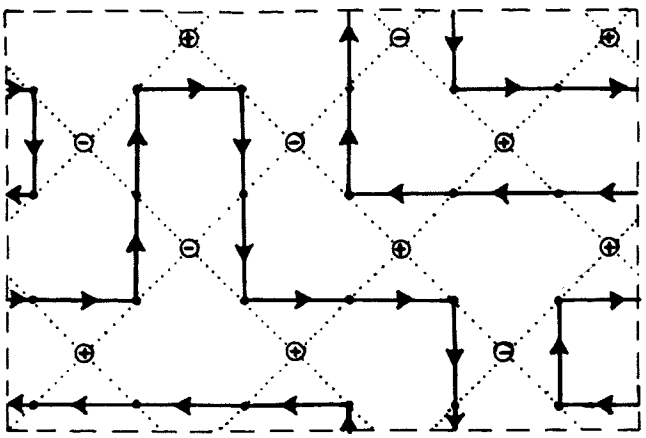

Figure 4. Open points and dotted lines show the underlying lattice of the Manhattan square lattice. + and − signs in these points specify a spin (Ising) configuration. Full oriented lines show the polymer configuration on the Manhattan square lattice (small full points) corresponding to the spin (Ising) configuration on the underlying square lattice as well as to the C′ configuration on the square lattice shown in figure 2.

and (2) do not occur on sublattice B. Let C′ denote the allowed six-vertex configurations on the square lattice when $\epsilon_2 = \infty$ (for an example see figure 2). Figure 5 shows how a C′ configuration can be converted into a polymer configuration on the MSL. The correspondence is one-to-one and the energies are completely matched if $\epsilon_1 = \epsilon$. This proves (7). Note that each sublattice A(B) is further divided into two sublattices A_1 and A_2 (B_1 and B_2) (see figure 3), so that the converted polygon configuration is compatible with the orientation of the MSL, under the rules specified in figure 5. The polymer configuration on the MSL shown in figure 4 corresponds to the C′ configuration on the square lattice shown in figure 2.

To prove (5) it remains to show that

$$Z^{\mathrm{P}}_{N,\mathrm{MSL}}(\epsilon) = \exp(-N\beta\epsilon/2) Z^{\mathrm{I}}_{N/2}(\epsilon/2). \tag{8}$$

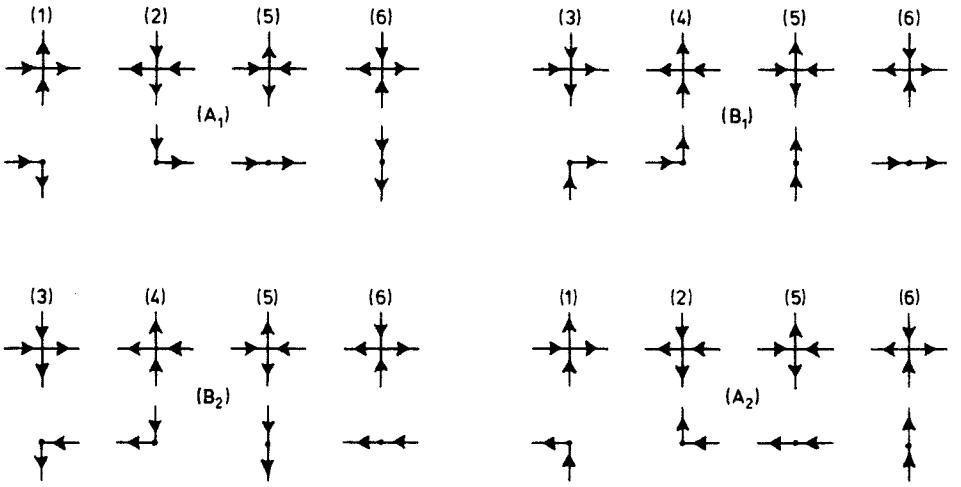

Figure 5. Below the four allowed vertex configurations on each sublattice A_1, B_1, B_2 and A_2, we show the bond arrangements by which we may convert a C′ configuration on the square lattice to a polymer configuration on the Manhattan square lattice.

This has been shown in Malakis (1979) for a MSL with diagonal periodic boundary conditions, and the proof for the present case is exactly the same. However, for completeness we shall briefly repeat the correspondence between polymer configurations on the MSL and Ising configurations on the underlying square lattice. The underlying lattice of the MSL is obtained by associating with every four-anticycle (which is an oriented four-cycle in which adjacent lines have opposite directions) of the MSL a new point. To form the underlying lattice, we then join these points by lines whenever the corresponding four-anticycles have a point in common. The underlying lattice of the MSL is shown in figure 4; it has the structure of the square lattice and obeys diagonal periodic boundary conditions. The one-to-one correspondence between spin configurations on the underlying square lattice and polymer configurations on the MSL may be seen from figure 4. A + sign (spin-up state) in any point P of the underlying lattice is associated with two horizontal bonds placed above and below the point P, whereas a − sign (spin-down state) is associated with two vertical bonds placed on the left and on the right of the point P. These bonds form a polymer configuration on the MSL, and one can see from figure 4 that a polygonal corner corresponds to a pair of neighbouring spins in opposite spin states. If the energies of such configurations are matched we obtain (8) (Malakis 1979).

In conclusion we have established an equivalence between the six-vertex and the Ising models. This is of theoretical interest, because up to now the only equivalence known between vertex and Ising models is derived from the eight-vertex model (Lieb and Wu 1972, Kasteleyn 1975). The ground state of the MF-model consists of alternating vertices (5) and (6), and so has no spontaneous polarisation like the F-model. However, unlike the F-model, the MF-model assumes that molecules placed on sublattices A and B may be different, and therefore the energies assigned to vertices with a net electric polarisation may be different for the two sublattices. Furthermore, even for a system with identical molecules on sublattices A and B, the real physical situation is undoubtedly more complicated than the picture described by such models; therefore it is important to investigate the effect of a different energy assignment. Since the

MF-model is a staggered-type model, we believe that its general solution cannot be obtained by a simple application of the existing methods for solving vertex models (Lieb and Wu 1972). However, the special case $\epsilon_1 = \epsilon$, $\epsilon_2 = \infty$, shown to be equivalent to the Ising model, does represent an antiferroelectric model in which molecules on sublattice A cannot assume polarisation on the northwest axis, whereas molecules on sublattice B cannot assume polarisation on the northeast axis. It is quite possible that the infinite-order transition is obtained only in the case $\epsilon_1 = \epsilon_2$, whereas the more general case $\epsilon_1 \neq \epsilon_2$ may yield an Ising-type transition with a logarithmic singularity in the specific heat. It should be pointed out that Wu (1969) considered a different modified F-model and found that it has an Ising-type transition. Wu's model is an eight-vertex model and consequently does not satisfy the 'ice constraint' which is supposed to account for local electrical neutrality (Slater 1941).

Finally, we note that the MF-model has an interesting polymer equivalent. The polymer equivalent of the F-model was discussed by Nagle (1974). In this model, a polymer bond can assume one of the three available states on the square lattice, one *trans* state (energy zero) in which the bond is collinear with its preceding bond, and two *gauche* states (energy ϵ) in which the bond makes a corner with its preceding bond. The polymer equivalent of the Ising model was the subject of a recent paper (Malakis 1979) and is essentially described by formulae (6) and (8) of this Letter. In this case one of the two *gauche* rotations is ruled out by the restrictions of the Manhattan orientation imposed on the square lattice. The polymer equivalent of the MF-model is obtained through the well-known equivalence between six-vertex configurations and polygon configurations on the square lattice (Lieb and Wu 1972, Nagle 1974). However, unlike Nagle's polymer model, the two *gauche* rotations available to each bond have different energies (ϵ_1 and ϵ_2). This would be a more realistic model than the previous two for the order–disorder transition in polymeric systems due to the rotational isomeric interaction (Flory 1956, Nagle 1974, Malakis 1979).

References

Flory P J 1956 *Proc. R. Soc.* A **234** 60
Kasteleyn P W 1963 *Physica* **29** 1329
—— 1975 *Proc. Wageningen Summer School, 1974: Fundamental Problems in Statistical Mechanics* vol III, ed. E G D Cohen (Amsterdam: North-Holland)
Lieb E H 1967 *Phys. Rev. Lett.* **19** 108
Lieb E H and Wu F Y 1972 *Phase Transitions and Critical Phenomena* vol 1, ed. C Domb and M S Green (London: Academic) p 331
Malakis A 1979 *J. Phys. A: Math. Gen.* **12** in the press
Nagle J F 1974 *Proc. R. Soc.* A **337** 569
Rys F 1963 *Helv. Phys. Acta* **36** 537
Slater J C 1941 *J. Chem. Phys.* **9** 16
Wu F Y 1969 *Phys. Rev.* **183** 604