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1983 J. Phys. A: Math. Gen. 16 353

(http://iopscience.iop.org/0305-4470/16/2/018)

J. Phys. A: Math. Gen. 16 (1983) 353-367. Printed in Great Britain

Some analytical consequences of the inverse relation for the Potts model

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Received 28 June 1982, in final form 13 August 1982

Abstract. We present some analytical results for the Potts model, using the symmetry group (acting on its parameters) generated by the inverse relation and other symmetries of this model. In particular, we find the critical manifolds and we study the relationship between this group and the Lee–Yang singularities in the complex plane. For those cases where the symmetry group is finite, we look at the possible consequences for some colouring problems in graph theory and more specifically for chromatic polynomials.

1. Introduction

Recently, an exact functional relation which holds for the partition function of different models in statistical mechanics has been derived, in particular for the Potts model (Jaekel and Maillard 1982a). It is called an inverse relation. This symmetry together with obvious geometrical symmetries generates an infinite discrete group acting on the parameters of the corresponding models. In this paper we study some properties resulting from this group structure, using the specific case of the Potts model. In particular, we study three main points. Firstly, we generalise the duality argument (Kramers and Wannier (1941), to be referred to as KW) in order to find the critical manifold, even in the case where the model is not self-dual. Secondly, we show the relationship between the Lee–Yang singularities (Lee and Yang 1952) of the partition function and the group structure. Finally, we consider the particular case when the group becomes finite, showing some connections with different map colouring problems in graph theory as well as with other problems of mathematical physics.

In all these three parts, we compare our results obtained using the group structure successively with exact known results, conjectured results and already known or new numerical studies.

The main results of this paper are as follows. Using the automorphy group we propose a new method to localise the critical manifold of a given lattice model. In particular we recover all known (or conjectured) results for Potts models on various two-dimensional lattices. For the three-dimensional Potts model we observe the non-algebraic character of the critical manifold with regard to the parameters of the model. The automorphy group allows us to obtain, in a unified way, the partition

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0305-4470/83/020353+15$02.25

function for the ferromagnetic and antiferromagnetic Potts model. When expressed in the natural variables associated with the automorphy group, the Lee–Yang circle theorem (at $q \geq 4$) takes a simple form. Using new numerical results on the square lattice, we check a possible extension of this theorem at $q < 4$.

2. Critical manifolds

2.1. Square lattice

2.1.1. The group structure for the Potts model. Let us consider the q-state two-dimensional anisotropic Potts model for a square lattice (for a recent review of the Potts model see Wu (1982)). If the two spins σ_i and σ_j belonging to $\boldsymbol{Z}_q$ are in the same state, the statistical weight associated with this vertical (horizontal) bond will be c (b); if they are not, it will be $+1$.

Therefore the partition function is

$$Z = \sum_{\{\sigma\}} \prod_{\langle ij\rangle} c^{\delta\sigma_i,\sigma_j} \prod_{\langle jk\rangle} b^{\delta\sigma_j,\sigma_k} \tag{1}$$

where the products are to be taken over all the vertical and horizontal bonds. The sum is to be taken over all the configurations of spins $\{\sigma\}$.

The inverse relation (I) on this partition function takes the form (Jaekel and Maillard 1982a)

$$Z(b, c)Z(1/b, 2-q-c) = (c-1)(1-q-c) \tag{2}$$

$$\text{I}: (b, c) \to (1/b, 2-q-c) \tag{3a}$$

and can be combined with the obvious geometrical symmetry (S):

$$Z(b, c) = Z(c, b) \tag{4}$$

$$\text{S}: (b, c) \to (c, b). \tag{5a}$$

These two involutions can be viewed as the generators of a discrete symmetry group G, which has the structure

$$0 \to \boldsymbol{Z} \to G \to \boldsymbol{Z}_2 \to 0.$$

G possesses a special element

$$(\text{SI})^2: (b, c) \to \left(2-q-\frac{1}{b}, \frac{1}{2-q-c}\right) \tag{6a}$$

for which the transformations act separately on b and c. These two transformations have the same fixed points:

$$q_\pm = 1 - \tfrac{1}{2}q \pm \tfrac{1}{2}[q(q-4)]^{1/2}. \tag{7}$$

It is then convenient to consider new variables x and y:

$$x = (b-q_+)/(b-q_-) \qquad y = (c-q_+)/(c-q_-) \tag{8}$$

for which the actions of the elements of G take the simple forms

$$\text{I}: (x, y) \to (1/x, q_+^2/y) \tag{3b}$$

$$\text{S}: (x, y) \rightarrow (y, x) \tag{5b}$$

$$(\text{SI})^2: (x, y) \rightarrow (q_+^2 x, y/q_+^2). \tag{6b}$$

Note that in terms of these new variables, the duality transformation becomes

$$\text{D}: (x, y) \rightarrow (-q_+/y, -q_+/x). \tag{9}$$

D does not belong to G, but commutes with all its elements.

2.1.2. Critical manifold. It is well known that it is possible to localise the critical temperature, when it is unique, as the stable point of KW duality. Thus it is natural to extend this line of argument, by taking other symmetries into account in the cases when no self-dual property is available. It can be seen that if (x_0, y_0) is a singularity of the partition function, then the automorphic properties associated with the group G imply that the images of this point under G are also singularity points. Therefore the critical manifold has to be stable under the action of the group G. In general, manifolds which are stable under such a discrete infinite group are very complicated. We still assume that the critical manifold $f(x, y) = 0$ is an algebraic variety. Such an assumption is supported by almost all the exactly known critical manifolds. (It is not clear if this algebraic property comes from the dimensionality or the complete integrability of these problems or any other reason.)

We make the following change of variables: $u = xy$ and $v = x/y$. We are now concerned with an algebraic variety $g(u, v) = 0$ stable under G and in particular under the action of $(\text{SI})^2$:

$$(\text{SI})^2: (u, v) \rightarrow (u, q_+^4 v). \tag{6c}$$

Hence, the function g must be stable under the transformation $v \rightarrow q_+^4 v$. However, this property (periodicity up to a multiplicative factor) is in contradiction with the algebraic character of g, unless g does not depend on v. Then the critical variety is necessarily of the form $g(u) = 0$, i.e. $u = C$ where C is a constant depending only on q. This constant can be determined by using the invariance under the action of I:

$$\text{I}: (u, v) \rightarrow (q_+^2/u, 1/q_+^2 v). \tag{3c}$$

We find $C^2 = q_+^2$, which leads to two critical manifolds: $xy = -q_+$ and $xy = +q_+$. The first is the well known equation for the critical temperature of the anisotropic ferromagnetic Potts model, usually written in the form $(b-1)(c-1) = q$ (Baxter 1973). The second relation $xy = q_+$ identifies exactly with the equation recently obtained by Baxter (1982a) for the critical temperature of the anisotropic antiferromagnetic case: $(b+1)(c+1) = 4 - q$. (Note that these two varieties are stable under the duality transformation D.)

The automorphic properties can also be used to obtain very quickly the expression for the partition function at the ferromagnetic critical temperature (Jaekel and Maillard 1982a):

$$Z(x, -q_+/x) = (-qq_+)^{1/2} \frac{A(x)A(-q_+/x)}{A(-q_+x)A(q_+^2/x)} \tag{10}$$

where

$$A(x) = \prod_{n=0}^{\infty} (1 + q_+^{2n-1}x)/(1 - q_+^{2n}x). \tag{11}$$

The same reasoning can be applied to the antiferromagnetic critical case *mutatis mutandis*: the inverse relation, as well as its automorphy factor $(c-1)(1-q-c)$, remain the same; the only change is in the symmetry (s) which becomes $x \to y = +q_+/x$ instead of $x \to y = -q_+/x$. In other words, we see that to obtain the partition function in the antiferromagnetic case, we have to replace q_+ by $-q_+$ formally (this can indeed be checked on the exact solution (Baxter 1982a)).

This approach unifies the ferromagnetic and antiferromagnetic expressions of the partition function, despite differences suggested by physical considerations (entropy, etc) (Berker and Kadanoff 1980).

2.2. *Triangular and simple cubic lattice*

2.2.1. The group structure. Let us consider in parallel the anisotropic Potts model on the triangular and on the simple cubic lattice. In contrast to the preceding case, these two models are described by three variables denoted respectively by x, y and z, and corresponding to the couplings in the three different directions. The corresponding functional relations take the following forms, which are the same for the two lattices:

$$Z(x, y, z)Z\left(\frac{1}{x}, \frac{q_+^2}{y}, \frac{q_+^2}{z}\right) = -qq_+ \frac{(1+x/q_+)(1+1/xq_+)}{(1-x)(1-1/x)} \tag{12}$$

$$\text{I}: (x, y, z) \to \left(\frac{1}{x}, \frac{q_+^2}{y}, \frac{q_+^2}{z}\right) \tag{13}$$

$$Z(\tau(x, y, z)) = Z(x, y, z) \tag{14}$$

where τ denotes an arbitrary element of the permutation group of three elements $\mathfrak{S}_3$. The inverse I and the group $\mathfrak{S}_3$ generate a group G, the structure of which is given elsewhere (Jaekel and Maillard 1982b). For our present discussion, we shall need only the following property: G has a normal subgroup, denoted by H, generated by the transformations

$$h_1: (x, y, z) \to (q_+^2 x, x/q_+, z) \tag{15a}$$

$$h_2: (x, y, z) \to (q_+^2 x, y, z/q_+^2). \tag{16}$$

As can be seen, this subgroup is isomorphic to $\boldsymbol{Z} \times \boldsymbol{Z}$.

2.2.2. Critical manifold. Once again we try to find the critical manifold as an algebraic variety which is stable under the group G, and which will be given by the equation $f(x, y, z) = 0$. Letting $u = xy$, $v = x/y$, we re-express the equation of this variety in terms of these new variables: $\varphi(u, v, z) = 0$. The action of the element h_1:

$$h_1: (u, v, z) \to (u, q_+^4 v, z) \tag{15b}$$

implies that φ must be periodic up to a multiplicative factor when considered as a function of v. This can occur if, and only if, φ does not depend on v, leading to $\varphi_1(u, z) \equiv \varphi_1(x, y, z) = 0$.

In a similar way, using h_2 and another element of G, one is led to write the critical variety equation in the form $\varphi_2(xz, y) = 0$ and $\varphi_3(yz, x) = 0$. The only way for these three forms to be compatible is for f to reduce to the equation $xyz = C$, where C is a function of q. C is determined, as in the square lattice case, by the action of $\text{I} \in G$. We find $C^2 = q_+^4$, leading to the two varieties: $xyz = q_+^2$ and $xyz = -q_+^2$. The first is the relation conjectured by Wu (1979a, b) for the critical temperature of the ferromagnetic Potts model on the triangular lattice. The pertinence of the second as a possible equation for the critical temperature of the antiferromagnetic Potts model on the triangular lattice is not obvious (see § 3). As in the square lattice case, the automorphy group leads to the following expression for the partition function at the ferromagnetic critical temperature:

$$Z(x, y, z) = (-qq_+)^{1/2} \frac{A(x)A(y)A(z)}{A(q_+^2/x)A(q_+^2/y)A(q_+^2/z)} \tag{17}$$

when $xyz = q_+^2$. (As can be verified, expression (17) is nothing other than the exact solution for the triangular lattice obtained by Baxter *et al* (1978)).

As can be seen, the preceding analysis on the group structure is common to the two lattices. However, the predicted critical varieties $xyz = \pm q_+^2$ are excluded by precise numerical estimates for the simple cubic lattice (Ditzian and Kadanoff 1979, Blöte and Swendsen 1979). This leads to the conclusion that in this case the critical manifold is definitely not an algebraic one (*a fortiori*, (17) cannot represent the solution at T_c). This suggests that some profound differences seem to occur on that model between $d = 2$ and $d = 3$.

2.3. Generalisation

Other regular lattices can also be considered. For instance, in the case of the honeycomb lattice, the inverse relation, expressed with natural variables x, y, z, takes the form

$$\text{I}: (x, y, z) \to \left(\frac{1}{x}, \frac{1}{y}, \frac{q_+^2}{z}\right). \tag{18}$$

Similar analysis leads to the critical varieties $xyz = C$ where $C^2 = q_+^2$, giving $xyz = -q_+$ and $xyz = q_+$. The former was conjectured (in another form) by Hintermann *et al* (1978) as the critical manifold for the anisotropic ferromagnetic Potts model on the honeycomb lattice. In addition, it can be checked that it is the dual image $(x, y, z) \to (-q_+/x, -q_+/y, -q_+/z)$ of the critical variety on the triangular lattice. More generally, the whole analysis (the group structure, the critical partition function, the critical manifold, etc) can be deduced by duality from that done for the triangular lattice.

As a natural extension of the lattices considered above, the same considerations apply to the Potts generalisation of the Utiyama model (see figure 1(a)) (Utiyama 1951). For this model, we obtain the following results. The inverse relation takes the form

$$\text{I}: (x, y, z, t) \to \left(\frac{1}{x}, \frac{q_+^2}{y}, \frac{1}{z}, \frac{q_+^2}{t}\right) \tag{19}$$

and the partition function satisfies

$$Z(x, y, z, t) Z\left(\frac{1}{x}, \frac{q_+^2}{y}, \frac{1}{z}, \frac{q_+^2}{t}\right) = -qq_+\left(\frac{(1+x/q_+)(1+1/q_+x)(1+z/q_+)(1+1/q_+z)}{(1-x)(1-1/x)(1-z)(1-1/z)}\right)^{1/2} \tag{20}$$

where x, y, z and t are defined as in equation (8).

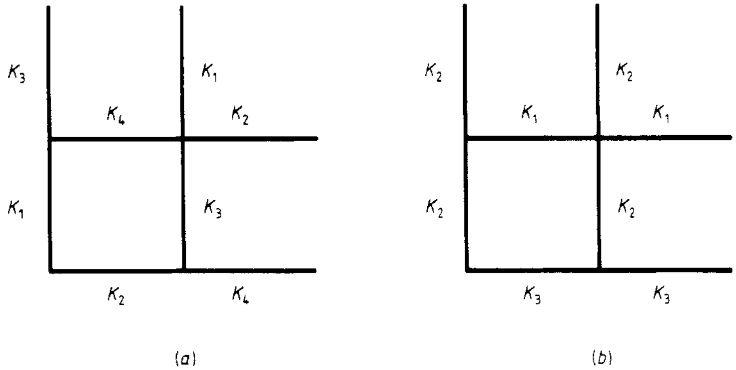

Figure 1. (*a*) Elementary cell of the generalised Utiyama model: $n_1=n_2=n_3=n_4=1$. (*b*) Elementary cell of the Ising model, discussed in the text: $n_1=n_3=1$, $n_2=2$.

In addition, Z is invariant under the action of the Klein group (isomorphic to the square group C_{4v}), acting on its arguments x, y, z and t). The structure of the corresponding symmetry group G generated by all symmetry elements is: $0\to \boldsymbol{Z}\to G\to \boldsymbol{Z}_2\times\boldsymbol{Z}_2\to 0$.

We will not be surprised to obtain the critical varieties $xyzt=q_+^2$ (conjectured in another form by Wu (1979a, b)) and $xyzt=-q_+^2$. It should be noted that the symmetry group G here is smaller than that corresponding to previous lattices. Many other algebraic varieties exist which are stable under the action of G, but the proposed varieties $xyzt=\pm q_+^2$ are the only ones consistent with the limiting cases of the square lattice ($z\to x$, $t\to y$), triangular lattice ($t\to 1$) and honeycomb lattice ($t\to -q_+$). In particular, in the Ising limit ($q=2$), we can check that $xyzt=q_+^2$ is a natural extension of the well known formula

$$gd(2K_1)+gd(2K_2)+gd(2K_3)+gd(2K_4)=\pi \qquad \text{(Syosi 1972)}.$$

(It should be noticed that the critical manifold for this Potts model cannot be deduced in general from the heuristic argument of Svrakic (1980), which is thus valid only at $q=2$.)

The other interesting particular case corresponds to the percolation limit $q\to 1$. In this case, $q_+=-j$ where $j^3=1$, and one recovers the critical thresholds which are known for bond percolation on square, triangular and honeycomb lattices (Sykes and Essam 1964). Of course, the obvious generalisation to anisotropic bond percolation can also be considered.

As in previous cases, we can use the automorphy property of the partition function to find its expression at criticality. This problem will be discussed elsewhere (Rammal and Maillard 1983).

2.4. *Discussion*

The critical variety obtained for the generalised Utiyama model invites us to extend this kind of result to more general periodic two-dimensional lattices. Such periodic lattices can be viewed as a repetition of an elementary cell having n coupling constants K_i, $i=1,2,\ldots,n$. The expected critical manifolds would have the equation

$$\prod_{i=1}^{n} x_i^{n_i}=C \tag{21}$$

where C denotes some power of q_+, n_i is a sequence of integers such that $n_i/\Sigma_i n_i$ is the concentration of bonds K_i in the elementary cell and x_i is defined as in equation (8).

However, this assumption can be ruled out by the example of an Ising model ($q=2$) having the elementary cell shown in figure 1(b). In fact, a direct calculation gives the following equation for the critical temperature: $K_1+K_3=2K_2^*$, where K_2^* denotes the dual of K_2. In terms of the variables x_i, this can be written

$$\frac{x_1+x_3}{1+x_1x_3}=\mathrm{i}\,\frac{2x_2}{1-x_2^2}. \tag{22}$$

Clearly, this critical variety is stable with respect to the two inverse transformations

$$(x_1,x_2,x_3)\rightarrow\left(-\frac{1}{x_1},\frac{1}{x_2},-\frac{1}{x_3}\right) \quad \text{or} \quad \left(\frac{1}{x_1},-\frac{1}{x_2},\frac{1}{x_3}\right) \tag{23}$$

and the only geometrical symmetry

$$(x_1,x_2,x_3)\rightarrow(x_3,x_2,x_1). \tag{24}$$

The symmetry group generated by equations (23) and (24) is not rich enough to force the critical manifold to have the form (21).

This last example should not be considered as a serious limitation of the systematic study based on the group structure. Each case must be considered separately. The method proposed to obtain critical manifolds does not involve any duality or star-triangle symmetries (see for instance Burkhardt and Southern 1978). Thus it has to be distinguished from all other methods using such arguments. In addition, it must be distinguished from the heuristic, interface free energy method, based on the SOS approximation (Müller-Hartmann and Zittartz 1977): this approach gives algebraic critical varieties in all cases and requires knowledge of interface configurations at zero temperature (degeneracy problems, etc).

3. Lee–Yang singularities of the partition function

As analyticity properties seem to be deeply involved in the action of the automorphy group, it is tempting to look at the relationship between the group structure and the Lee–Yang singularities of the partition function.

3.1. Lee–Yang theorem for the Potts model, for $q \geqslant 4$

The circle theorem of Lee and Yang (1952) for the Ising model in the presence of a magnetic field has been generalised to include some vertex models (Suzuki and Fisher 1971). This result has been extended to the staggered six-vertex model (Hintermann *et al* 1978) which is known to be equivalent to the Potts model (Temperley and Lieb 1971). It was then possible to localise the Lee–Yang singularities for $q \geqslant 4$, for the square, triangular and honeycomb lattices. The singularities are located, using our variables x, y and z, at

$$|xy/-q_+|=1 \qquad \text{for the square lattice} \tag{25}$$

$$|xyz/(q_+)^2|=1 \qquad \text{for the triangular lattice} \tag{26}$$

$$|xyz/-q_+|=1 \qquad \text{for the honeycomb lattice.} \tag{27}$$

As can be seen, the equations of these varieties are extremely simple when expressed in these variables. Moreover, these expressions should then reflect the existence of a relationship between the group G and the statement of the Lee–Yang theorem. The restriction of (25), (26) and (27) to the real axis recovers, for $q \geqslant 4$, the critical manifolds which were obtained in § 2, as it should. A natural extension of the above results would then suggest that the Lee–Yang singularities for the generalised Utiyama model lie on the following variety (for $q \geqslant 4$):

$$|xyzt/(q_+)^2| = 1. \tag{28}$$

The 'fugacity' variables for the different Potts models are $xy/-q_+$ (square), $xyz/(q_+)^2$ (triangular) and $xyz/-q_+$ (honeycomb). Hence the conjugate variable of this 'fugacity' identifies with the internal energy. In this scheme (see table 1) the jump of the internal energy in the Potts model (or the latent heat ΔQ) corresponds to the discontinuity of the magnetisation ΔM at zero field ($H = 0$) below the critical temperature in the ferromagnetic model. With g denoting the density of zeros on the unit circle, the partition function, for the square lattice for instance, can be written

$$\ln Z = \int_{-\pi}^{\pi} d\theta \ln\left(\frac{xy}{-q_+} - e^{i\theta}\right) g(\theta, x/y) \tag{29}$$

where g should depend *a priori* on the anisotropy x/y.

Table 1. Correspondence between the Potts model and the ferromagnetic model.

Potts model	Ferromagnetic model
$q - 4 \geqslant 0$	$T_c - T \geqslant 0$
ΔQ	ΔM
$z = xy/-q_+$	$z = e^H$

Known exact results for the Potts model can be used to provide information on the density g. For instance, the expression for the latent heat ΔQ (Baxter 1973) is directly related to the density of zeros at $\theta = 0$:

$$\Delta Q = 2\pi g(0, x/y) = \prod_{n=1}^{\infty} \left(\frac{1 - (-q_+)^n}{1 + (-q_+)^n}\right)^2. \tag{30}$$

Equation (30) shows that the density of zeros at $\theta = 0$ is independent of x/y, and this is the counterpart of the magnetisation being independent of the anisotropy in ferromagnetic models. This exact expression (30) shows that $g(0, x/y)$ has an essential singularity at $q = 4$. On the other hand, knowledge of the partition function at the critical point $xy = -q_+$ (Baxter 1973) provides the sum rule

$$\int_{-\pi}^{\pi} d\theta \ln(1 - e^{i\theta}) g(\theta, x/y) = \ln Z(x, -q_+/x) \tag{31}$$

where $Z(x, -q_+/x)$ is given by equation (10).

The inverse relation obeyed by Z, equation (2), together with the symmetry relation, equation (4), can be re-expressed in terms of equations for the density g, and one could think of using them to determine the function g. Unfortunately this task is very delicate as can already be seen by considering the simpler example of the one-dimensional Ising model with a magnetic field. (In this case an inverse relation occurs, the circle theorem holds and the density of zeros g is known exactly.)

3.2. *Lee–Yang theorem for the Potts model, for $q < 4$*

Let us consider first the case of a square lattice. In general, the relation

$$xy/-q_+ = (v - q_+)/(1 - vq_+) \tag{32}$$

where

$$v = (bc - 1)/(b + c + q - 2) \tag{33}$$

leads to the equivalence, when $q \geq 4$, between

$$|xy/-q_+| = 1 \qquad \text{and} \qquad |v| = 1. \tag{34, 35}$$

However, this equivalence fails to hold for $q < 4$. We limit ourselves, in the first place, to the isotropic case. Equation (34) can be written as $|x| = 1$ (because $|q_+| = 1$), which can be identified with the real axis in the b complex plane. Obviously, this cannot be the location of Lee–Yang singularities for $q < 4$. On the other hand, equation (35) is equivalent at $q = 2$ to $|b \pm 1| = \sqrt{2}$, which is just the equation of the Fisher circles (Fisher 1964) for the Ising model. These two circles can be viewed as a 'reappearance' of the Lee–Yang circle occurring at $q \geq 4$. In general, equation (35) can be seen to be, in the isotropic case, that of the two circles:

$$|b - 1| = \sqrt{q} \qquad \text{and} \qquad |b + 1| = \sqrt{4 - q}. \tag{36}$$

The first is called the ferromagnetic circle, and is the only one present for $q \geq 4$. On the other hand, the second circle is new, and is a natural extension for $q < 4$ of the so called antiferromagnetic Fisher circle.

Let us remark that each of these two circles is stable with respect to duality symmetry $b \to (b + q - 1)/(b - 1)$. Then an approach based on the stability by duality can also be used to obtain (36), and in particular the second circle. This second circle gives again the correct antiferromagnetic critical temperature $v = -1$ (Baxter 1982a) in contradiction with Ramshaw's (1979) analysis.

Let us consider now the anisotropic case and the Ising limit $q = 2$. The locus of singularities is given by the equation

$$\left(\frac{bc - 1}{b + c}\right)^2 + 1 - \left(\frac{bc - 1}{b + c}\right)(\cos\omega_1 + \cos\omega_2) - \left(\frac{bc + 1}{b + c}\right)\left(\frac{b - c}{b + c}\right)(\cos\omega_1 - \cos\omega_2) = 0 \tag{37}$$

where $0 \leq \omega_1,\ \omega_2 \leq 2\pi$. This locus is stable by duality, as well as by the symmetry group. On the other hand, equation (37) reduces trivially to equation (35) in two special cases: the isotropic case ($b = c$) and for $\cos\omega_1 = \cos\omega_2$ in the anisotropic case. Hence equations (37) and (35) are not equivalent and represent, in general, two distinct overlapping sets of points.

An analogous situation occurs on the triangular lattice even for an isotropic Ising model. Figure 2 shows the location of the zeros of the partition function, in the complex plane $\tanh K$. This locus contains an arc of the unit circle ($e^{i\theta}$, $|\theta| < \frac{1}{3}\pi$) and an algebraic curve.

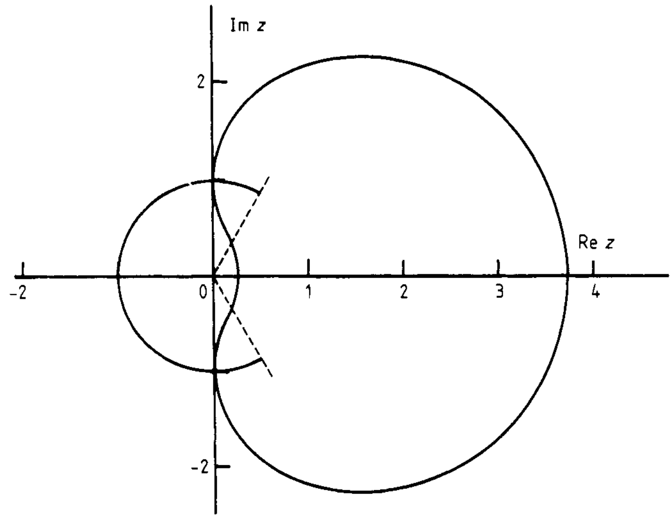

Figure 2. Zeros in the complex plane tanh K $(=z)$ for the triangular lattice for $q=2$.

In general, as for the square lattice, we have equivalence (for $q \geqslant 4$) between

$$|xyz/q_{+}^{2}|=1 \qquad \text{and} \qquad |w|=1 \tag{38, 39}$$

where

$$w=\frac{(q-2)abc+(ab+bc+ca)-1}{(ab+bc+ca)+(q-2)(a+b+c)+(q-2)^2-1}. \tag{40}$$

It is easy to see that the locus represented by figure 2 is definitely different from the $q=2$ limit of equation (39) in the isotropic case.

In conclusion, despite its stability with respect to the action of the symmetry group, the locus of singularities for $q<4$ seems to be quite complicated. So it is natural to investigate first of all the 'easy' case of the isotropic square lattice. For this particular case, the question is whether or not the singularities actually lie on circles (36) for $q<4$.

3.3. *Numerical studies*

We have studied the zeros of the Potts partition function on finite square lattices $N \times N$ $(N \leqslant 5)$. Using a transfer matrix formalism (Temperley and Lieb 1971, Blöte *et al* 1981), it was possible to give a polynomial expression†, in the variables $u=b-1$ and q, for the partition function, with free boundary conditions. In this case, the calculation of zeros in the complex u plane, for different real values of q, was not conclusive. The scatter of the results obtained was certainly due to small values of N $(N \leqslant 5)$ and also to the boundary conditions. The formalism used in this calculation also seems to suffer some fundamental difficulties, especially in the antiferromagnetic case.

In parallel, we used the standard $q^N \times q^N$ transfer matrix formalism (q is now an integer) with periodic boundary conditions on finite lattices $N \times N, N \leqslant 6, q \leqslant 4$. Figure 3 shows the location of zeros in the b complex plane, at $q=2$ and $N=6$. Already

† These formal calculations have been performed using AMP computer language, at CEN-Saclay.

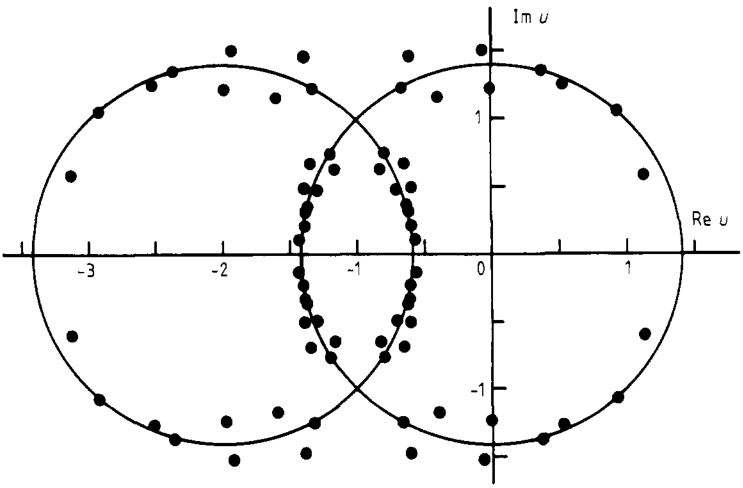

Figure 3. Location of the zeros in the complex plane b, for $q=2$, on a square $N\times N$; $N=6$ with periodic boundary conditions. We have drawn the Fisher circles $|b\pm 1|=\sqrt{2}$.

for lattices of this small size, the close approach to the expected asymptotic Fisher circles can be seen clearly. Figures 4 and 5 allow a comparison of the results obtained for $N=4$ at $q=2$ and $q=3$, respectively. The closeness of the set of zeros to the asymptotics circles (equation (36)) is comparable in these two cases. This non-negative result suggests an extension of the numerical calculations to more important sizes ($N\geqslant 6$).

One can envisage more complicated boundary conditions (self-dual lattices for instance) in order to reduce the scatter of data. Such a situation occurs at $q=2$ (Branscamp and Kunz 1974), but this kind of boundary condition could damage the antiferromagnetic behaviour for $q\neq 2$. More generally, it seems that the convergence

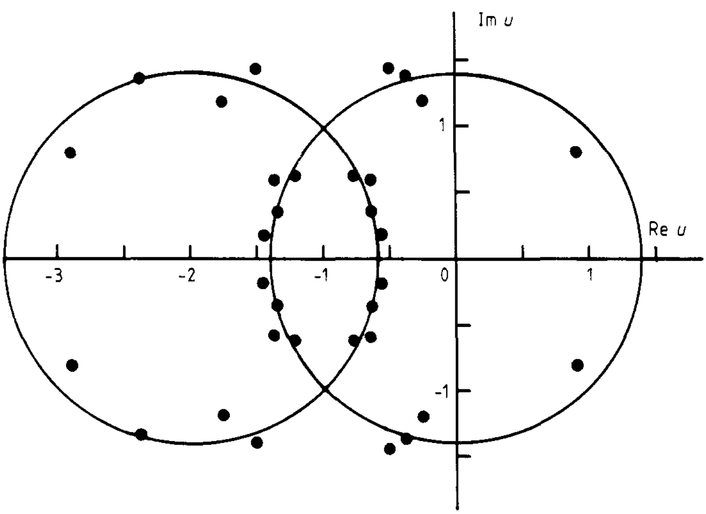

Figure 4. Same as figure 3 but for $N=4$, $q=2$.

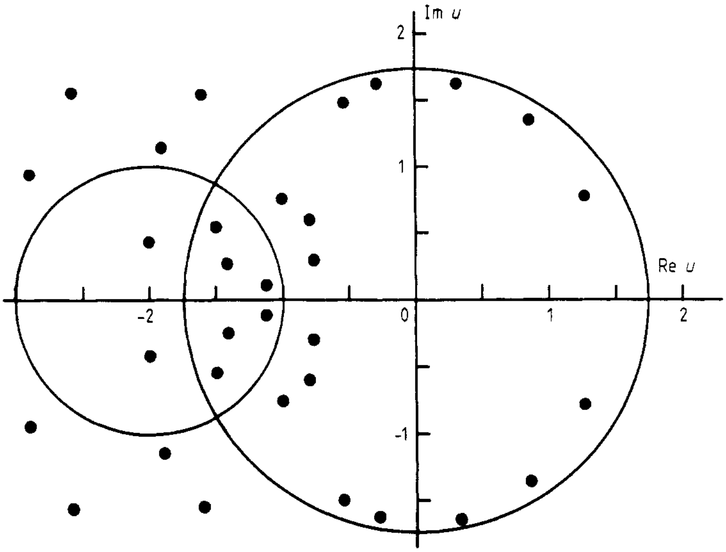

Figure 5. Same figure as figure 3 but for $N=4$, $q=3$. The two circles drawn are $|b-1|=\sqrt{q}$ and $|b+1|=\sqrt{4-q}$.

toward the ferromagnetic circle is plausible and probably correct. If it is true, then this calls for some formal proof (as for $q \geqslant 4$) of a 'partial' circle theorem, in some domain of the b complex plane. On the numerical level, the discussion must be devoted to the nature of the asymptotic locus of zeros in the antiferromagnetic region: line, surface, etc, and then to its comparison with the proposed circle $|b+1|=\sqrt{4-q}$.

4. Degeneracy of the group and Tutte–Beraha numbers

4.1. Degeneracy of the group

In the general case, the representation of the group G for $q>4$ leads to an infinite discrete group, allowing in particular an infinite product representation of the critical partition function. For $q \leqslant 4$, the effect of G is to multiply the variables $x, y, z, \ldots$ by numbers $(q_+)^i$ of unit modulus. The group remains infinite in general, but the expression of the partition function at the critical temperature becomes a formal one. Using an appropriate integral representation of the gamma function, one can then recover the known expression at $q \leqslant 4$ (Baxter *et al* 1978), which can be considered as an analytical continuation of the $q>4$ expression. However, for $q \leqslant 4$, G can degenerate, becoming a finite group for special values of q. This situation occurs if an integer n exists such that $q_+^n = 1$, i.e. $q = q_{n,k} \equiv 2+2\cos(2\pi k/n)$, $k = 1, 2, \ldots, n$.

For instance, G becomes isomorphic to $\boldsymbol{Z}_2 \oplus \boldsymbol{Z}_{2n}$ in the square lattice case. For these particular values of q, the natural question is whether the expression of the critical partition function could be given by a finite product implied by the new structure of G. In fact, it is really the case, as can be seen through the identification of the critical partition function of the Potts model, with the partition function of the six-vertex model (Temperley and Lieb 1971).

It can also be noted that the formal identification of the latter partition function with the quantum sine–Gordon S matrix in $1+1$ dimension allows the same reduction to be recovered (Korepin *et al* 1975). Indeed, for the sine–Gordon model, there exist particular values of the parameter $\gamma(\gamma = 2\pi/n$, n integer, in correspondence with some $q_{n,k})$ for which the S matrix becomes a finite product. These special values of γ also correspond to the appearance of new bound states in the theory.

Recently Baxter (1982b) has shown that the critical hard-hexagon model corresponds to the critical Potts model for $q = q_{5,1} = \frac{1}{2}(3+\sqrt{5})$. The degeneracy of the group G thus casts some lights on the simple expression (finite product of rational terms) that can be given to the partition function, when the elliptic uniformisation seemed to provide a more complicated result. The same phenomena occur in the three-colouring problem (Baxter 1970a, b). These $q_{n,k}$ numbers (or their equivalent) occur in different domains of mathematical physics such as the XXZ model (Yang and Yang 1966).

Another manifestation of these $q_{n,k}$ in the Potts model is that, according to den Nijs (1979) and Nienhuis *et al* (1980) critical exponents become rational numbers if, and only if, $q = q_{n,k}$; this seems to be strongly supported by numerical analysis.

4.2. *Connection with colouring problems in graph theory—Tutte–Beraha numbers*

The $q_{n,k}$ numbers also seem to play a relevant role in the problem of the zeros of chromatic polynomials. The equivalence between Whitney polynomials and Potts partition functions is a well known property (Baxter *et al* 1976). A limit of the Whitney polynomial then gives the chromatic polynomial which corresponds to the antiferromagnetic Potts model at zero temperature. On a finite graph, the chromatic polynomial $P(q)$, where q is the number of colours, is the number of ways of colouring the vertices of the graph without having the same colour for two adjacent vertices. Historically, the investigation of zeros of chromatic polynomials was an analytical approach to the four-colour problem in graph theory (Tutte 1975). Investigations of the location of the zeros of special families of chromatic polynomials (Beraha *et al* 1980, Hall *et al* 1965) have shown up the occurrence of the numbers $q = B_n = 2+2\cos 2\pi/n$ (called Tutte–Beraha numbers) as special zeros of $P(q)$. Depending on the map studied, some B_n appear as isolated zeros or as real limits of complex zeros (non-isolated zeros) at the infinite graph limit. Up to now, B_n for $n = 1$–10 have been identified numerically or proved to occur (Tutte 1975).

The possible occurrence of the general numbers $q_{n,k}$ (including B_n) as non-isolated zeros of chromatic polynomials, on more general lattices, such as square, triangular or simple cubic, must be elucidated. Two distinct approaches can be used for this task. The first is identical to that discussed in § 3 and consists of calculating the chromatic polynomials on $N \times N$ square lattices. The results that we have obtained for $N \leqslant 5$ are very similar to those of Biggs *et al* (1972). The set of zeros seems to converge, by increasing N, toward a curve having the shape of a cardoid.

The second approach is based on the transfer matrix formalism used for strips. However, two such formalisms exist. The first is specific to chromatic polynomials and adapted to well behaved maps, called recursive maps (figure 6) (Beraha *et al* 1980). The other method (Biggs and Meredith 1976) is more general and also identical to that currently used in the context of the Potts model (Blöte *et al* 1981). In its actual form, this method has serious problems in the antiferromagnetic Potts model, and so is ill-adapted to study the chromatic polynomials. Thus it would be interesting to extend the preceding study to finite lattices of increasing size ($N > 5$), in order to

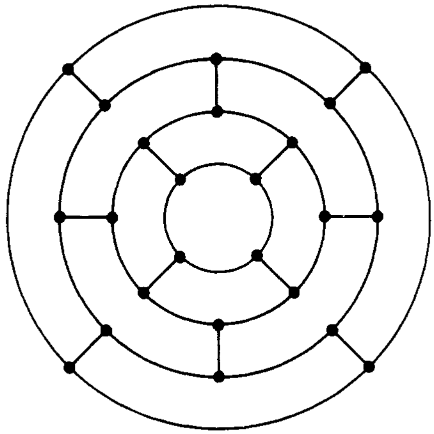

Figure 6. Example of map (called a four-ring) in a recursive family. The inner and outer regions are to be considered as proper regions.

look at the positions of limit zeros on the real axis. Such a study should also be extended to lattices in three dimensions, where B_n numbers could appear.

5. Conclusion

We now summarise the main points given in this paper. We have indicated some consequences of the existence of the symmetry group G for the Potts model. Using this new method, we are able to recover, in a systematic way, all exact or conjectured critical varieties in the literature without using duality or star–triangle arguments. In particular, we have indicated that the critical manifold cannot be algebraic for the three-dimensional Potts model. On the other hand, we have noticed the close connection between the ferromagnetic and antiferromagnetic partition functions on the square lattice.

We have also shed some light on the relationship between the Lee–Yang theorem, valid for $q \geqslant 4$, and the group structure of the Potts model. In the case of the square lattice the Fisher circle at $q = 2$ has been identified as a reappearance of the $q \geqslant 4$ Lee–Yang circle. This 'continuation' suggests that the Lee–Yang singularities for $q < 4$ could lie on two circles which are the generalisation of the Fisher circles for $q = 2$.

We have presented some physical implications associated with the degeneracy of the symmetry group, for special values of q, as well as the relevance of these numbers in colouring problems in graph theory (chromatic polynomials, Tutte–Beraha numbers, etc).

These ideas suggest further numerical and analytical investigations. It would be interesting to extend the numerical study of the Lee–Yang (in b) and Tutte–Beraha (in q) zeros to more general lattices, and in particular to three dimensions. Special attention should be given to the antiferromagnetic case (generalised Fisher circle ?). This approach is sufficiently general to treat other models (vertex models, etc) and lattices (Kagome, etc). The existence of some 'partial' Lee–Yang theorem at $q < 4$ could be elucidated. Finally, an open question is to know whether critical exponents could be calculated using the group structure of the Potts model.

Acknowledgments

We are grateful to Professor R J Baxter and Dr M T Jaekel for most helpful discussions, valuable comments and stimulating conversations. We are indebted to Professor T Lubensky and Dr J Vannimenus for criticisms of earlier drafts of this paper. The authors would like to thank Professor G Toulouse for hospitality in his group at École Normale Supérieure.

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