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Generalised percolation probabilities for the self-dual Potts model

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Abstract. A set of generalised percolation probabilities P_n are defined for the dichromatic polynomial formulation of the Potts model. A generating function for these P_n is calculated at the self-dual temperature. P_1 and P_2 are explicitly given and the behaviour of P_n is investigated.

1. Introduction

It is known that the two-dimensional q-state Potts model has a first-order transition for $q>4$ at a self-dual temperature T_d (Baxter 1973). For an anisotropic q-state Potts model on a square lattice the partition function Z is given by

$$Z=\sum \exp\left[\left(J\sum_{\langle ij\rangle}\delta(\sigma_i,\sigma_j)+J'\sum_{\langle ih\rangle}\delta(\sigma_i,\sigma_h)\right)(kT)^{-1}\right] \tag{1}$$

where σ_i, σ_j, σ_h are the neighbouring Potts spins, the $\langle ij\rangle$ sum is over all horizontal edges of the lattice $\mathscr{L}$, the $\langle ih\rangle$ sum is over all vertical edges, and the outer sum is over the values $1,\ldots,q$ of the spins. The self-dual temperature is determined by

$$[\exp(J/kT_d)-1][\exp(J'/kT_d)-1]=q. \tag{2}$$

Defining a local magnetisation as in equation (11) of Baxter (1982) (hereafter equations of that paper will be preceded by B), it was shown that for $q>4$ there is a jump discontinuity in $M(T)$ (Cardy *et al* 1980, Kim 1981, Baxter 1982). This was calculated by Baxter (1982) as

$$\Delta M=M(T_d)=\lim_{T\to T_d^-}M(T)=\prod_{j=1}^{\infty}\{1-\exp[-(4j-2)\theta]\}/[1+\exp(-4j\theta)] \tag{3}$$

where $q^{1/2}=2\cosh\theta$, $\theta>0$, in the thermodynamic limit of $\mathscr{L}$ large.

Following Kasteleyn and Fortuin (1969), Baxter (1982) wrote Z as a dichromatic polynomial:

$$Z=\sum_G q^c v^l w^m \tag{4}$$

where $K=J/kT$, $L=J'/kT$, $v=e^K-1$ and $w=e^L-1$. The dichromatic polynomial is a sum over all graphs G on the lattice $\mathscr{L}$: c is the number of connected clusters of G, l and m are the number of horizontal and vertical lines respectively. On these graphs there are always a set of boundary sites that are linked to form a 'boundary cluster'. The central spin of lattice is known as site 0. Each graph of the sum is made up of clusters of spins (including isolated spins as primitive clusters). Baxter defined a percolation probability P via (B31) that site 0 belongs to the boundary cluster (Kelland 1976). This is a weighted sum over only graphs with that property. Baxter showed that this P is the same as the magnetisation M of the Potts model (B30) and (B31). He then used the six-vertex equivalence to the dichromatic polynomial (Baxter *et al* 1976) to express P in terms of the corner transfer matrices of the six-vertex model. This expression could be evaluated (in the thermodynamic limit) when the self-dual condition (2) is satisfied. He thus obtained the result (B2) for $M(T_d)$.

In recent work on other models (to be published), we have found the need to generalise P to the set of probabilities $\{P_n : n = 0, 1, \ldots\}$ where the P_n are related to how 'deep' within the graph the cluster containing site 0 does lie. Here we calculate these P_n as coefficients of a generating function similar to (3).

In the following §§ 2-5 we consider the limit $T \to T_d^-$. In this case the graphs G that contribute to (4) (in the thermodynamic limit) each contain an infinite cluster, so on finite lattices it is appropriate to impose the condition that all the boundary sites be linked. This 'boundary cluster' becomes the infinite cluster in the thermodynamic limit. In § 6 we extend the work to the limit $T \to T_d^+$ when there is no infinite (or boundary) cluster.

2. Generalised percolation probabilities

We define P_n as the probability that the given site 0 belongs to a cluster which is surrounded completely by just n clusters (one of them being the boundary cluster). P_0 is then just the probability that no clusters surround site 0 and so site 0 must be in the boundary cluster, giving $P = P_0$. We define the set of graphs G_n as those having n clusters around the cluster of site 0. In figure 1 we show a typical graph of G_2, in which the site 0 is surrounded by two clusters (including the boundary cluster).

Then P_n is given by

$$P_n = Z^{-1} \sum_{G_n} q^c v^l w^m \tag{5}$$

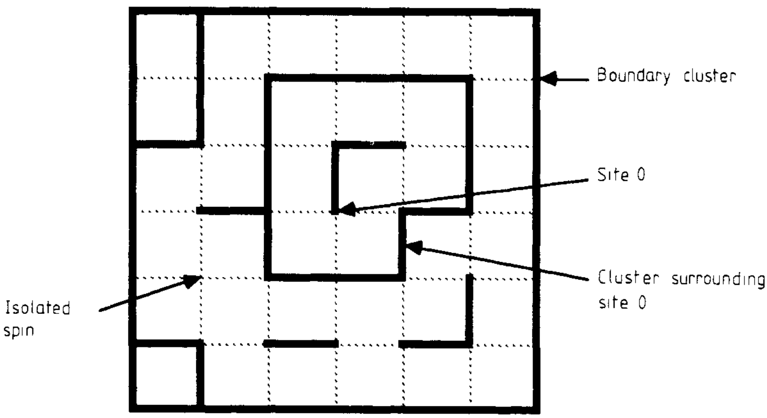

Figure 1. A graph of type G_2 where heavy lines are the links of the graph and the vertices are sites of the Potts lattice.

where c, l and m are as defined before. From (4), the sum of $P_0, P_1, \ldots,$ must be one, and hence the P_n are properly normalised probabilities.

We now generalise the method of Baxter (1982) so that we can calculate a generating function for the P_n. That method converted the dichromatic polynomial problem to a six-vertex model via the known method (Baxter *et al* 1976) of placing arrows on the edges of an associated medial lattice $\mathscr{L}'$ (see figure 1 of Baxter (1982)). A device of Kelland (1975) was used to express the percolation probability in terms of this six-vertex model. It was shown that the expectation values of a function $s(\alpha)$ defined on an 'arrow spin' set $\{\alpha_1, \ldots, \alpha_m\}$ that lay on a row E of edges from site 0 to the boundary site gives P as

$$P = \langle s(\alpha)\rangle \tag{6}$$

where $\langle s(\alpha)\rangle$ is given by (B39) and $s(\alpha)$ by (B38). We now generalise $s(\alpha)$ to $s(\alpha, \phi)$ by

$$s(\alpha, \phi) = \exp[-\phi(\alpha_1 + \ldots + \alpha_{m-1})] \qquad \phi \in \mathbb{C}. \tag{7}$$

We shall now argue that the expectation value of $s(\alpha, \phi)$ gives a generating function for the P_n.

As in Baxter (1982) we use the result that the dichromatic polynomial can be written as a sum over polygon decompositions of $\mathscr{L}'$. The six-vertex arrows follow each other around these polygons. A weight e^{θ} is given to a set of anticlockwise arrows on each polygon and a weight $e^{-\theta}$ for a clockwise set. We write the expectation value of $s(\alpha, \phi)$ as

$$\langle s(\alpha, \phi)\rangle = Z_{6V}^{-1} \sum_{\mathrm{AC}} s(\alpha, \phi) \prod \text{weights} \tag{8}$$

where AC refers to arrow configurations and the product is over all sites of $\mathscr{L}'$. We convert this sum to one over polygon decompositions of $\mathscr{L}'$. There is a one-to-one correspondence between polygon decompositions of $\mathscr{L}'$ and cluster graphs G on $\mathscr{L}$ (Baxter *et al* 1976). We therefore can split this sum into a series of sums over the polygon decompositions of each of the G_n. We now examine these sums separately.

Each cluster of G is surrounded by a polygon, and so is each circuit of G. Here we shall ignore the polygon surrounding the outside of the boundary cluster B: thus all polygons lie inside B. When site 0 is connected to B there is no polygon surrounding it. We can think of a circuit as a 'hole' surrounded by a cluster. Thus each polygon is either external or internal to just one cluster.

If one cluster surrounds site 0 the cluster will be B. Therefore two polygons will surround site 0: one of them external to the cluster containing 0, the other internal to B.

Considering more and more clusters surrounding site 0, one sees that each will contribute two polygons around site 0 as each cluster has its own inner and outer boundary. Generally for the cluster graphs containing n clusters surrounding site 0 there will be $2n$ polygons around site 0.

In addition to the weights $e^{\theta}(e^{-\theta})$ for an anticlockwise (clockwise) arrow covering, each polygon P acquires a weight $e^{-\phi}(e^{\phi})$ for a right-pointing (left-pointing) arrow on an edge of the set E. If P does not surround 0, it must cross E an equal number of times in each direction, so the total extra weight is unity.

If it does surround 0, there will be a net gain of just one extra edge weight factor. Summing over both the allowed arrow configurations for each polygon, it follows that a polygon that does not surround 0 has a total weight $e^{\theta} + e^{-\theta} = 2\cosh\theta$, as before.

However, if it does surround 0, its weight becomes $e^{\theta-\phi}+e^{-\theta+\phi}=2\cosh(\theta-\phi)$. Thus each polygon surrounding 0 acquires an extra factor $\cosh(\theta-\phi)/\cosh\theta$. Since each cluster surrounding 0 is associated with two such polygons, the numerator in (8) is the dichromatic polynomial (4), but with an extra factor $z=\cosh^2(\theta-\phi)/\cosh^2\theta$ for each cluster surrounding 0. From (5) it immediately follows that

$$\langle s(\alpha,\phi)\rangle=\sum_{n=0}^{(m-1)/2} z^n P_n. \tag{9}$$

Let us define $S_m(z)=\langle s(\alpha,\phi)\rangle$ so

$$S_m(z)=\sum_{n=0}^{(m-1)/2} z^n P_n. \tag{10}$$

3. Calculation of the generating function

Baxter used corner transfer matrices to evaluate his $\langle s(\alpha)\rangle$. We can do the same for $\langle s(\alpha,\phi)\rangle$ by simply replacing Baxter's $\theta+\mathrm{i}\pi/2$ by ϕ in (B45). We then obtain

$$S_m(z)=\mathrm{Tr}\,S(AB)^2/\mathrm{Tr}\,(AB)^2 \tag{11}$$

where A and B are the same matrices defined in Baxter (1982). Provided the self-dual condition (2) is satisfied, the same arguments as in § 6 of Baxter (1982) yield (analogously to (B59))

$$S_m(z)=\sum_{\{\alpha\}}\exp(\phi g(\alpha)+\theta h(\alpha))\left(\sum_{\{\alpha\}}\exp(\theta h(\alpha))\right)^{-1} \tag{12a}$$

where

$$g(\alpha)=-\sum_{j=1}^{m-1}\alpha_j \tag{12b}$$

and

$$h(\alpha)=-\sum_{j=1}^{m-2} j\alpha_j\alpha_{j+1}+(m-1)\alpha_{m-1} \tag{12c}$$

and the summation is over all values (+1 and −1, or simply + and −) of the arrow spin set $\{\alpha_1,\ldots,\alpha_{m-1}\}\equiv\{\alpha\}$. (We have discarded the α_m dependence (B58), since this comes simply from the outer polygon of B and cancels out of (12).)

In the thermodynamic limit we have

$$S(z)=\lim_{m\to\infty}S_m(z)=\lim_{m\to\infty}\langle s(\alpha,\phi)\rangle=\sum_{n=0}^{\infty}z^n P_n. \tag{13}$$

We will now calculate $S(z)$ and hence the generating function for P_n. Firstly let us define

$$x=e^{-2\theta} \qquad 0<x<1 \tag{14a}$$

$$y=e^{-2\phi}. \tag{14b}$$

If we define $R_{m-1}(\alpha_m,x,y)$ as

$$R_{m-1}(\alpha_m,x,y)=\sum_{\{\alpha\}}\prod_{j=1}^{m-1}(y^{\alpha_j/2}x^{j\alpha_j\alpha_{j+1}/2}) \tag{15}$$

then it can be shown that

$$S(z) = \lim_{m\to\infty} R_{m-1}(-, x, y)/R_{m-1}(-, x, +). \tag{16}$$

$R_{m-1}(\alpha_m, x, y)$ satisfies the following recurrence relations:

$$R_m(-, x, y) = y^{-1/2}x^{m/2}R_{m-1}(-, x, y) + y^{1/2}x^{-m/2}R_{m-1}(+, x, y) \tag{17a}$$

$$R_m(+, x, y) = R_m(-, x, y^{-1}) \tag{17b}$$

and

$$R_0(+, x, y) = R_0(-, x, y) = 1. \tag{17c}$$

Solving these recurrence relations lead us to

$$R_{m-1}(-, x, y) = y^{-(m-1)/2}x^{m(m-1)/4}\sum_{j=0}^{m-1}(y/x)^j\begin{bmatrix} m-1 \\ j \end{bmatrix}_{Q=x^{-2}} \tag{18}$$

where

$$\begin{bmatrix} n \\ j \end{bmatrix}_Q \tag{19}$$

is the Gaussian coefficient defined (Andrews 1976, p 35) as

$$\begin{aligned} \begin{bmatrix} n \\ j \end{bmatrix}_Q &= \prod_{k=1}^{j}\frac{1-Q^{n-j+k}}{1-Q^k} && 0 \leqslant j \leqslant n \\ &= 0 && \text{otherwise.} \end{aligned} \tag{20}$$

Therefore $S(z)$ is given by

$$S(z) = \lim_{m\to\infty} y^{-(m-1)/2}\sum_{j=0}^{m-1}(y/x)^j\begin{bmatrix} m-1 \\ j \end{bmatrix}_{Q=x^{-2}}\left(\sum_{j=0}^{m-1}x^{-j}\begin{bmatrix} m-1 \\ j \end{bmatrix}_{Q=x^{-2}}\right)^{-1}. \tag{21}$$

Let $t = y/x = \exp(2\theta - 2\phi)$, then the relationship

$$\begin{bmatrix} n \\ j \end{bmatrix}_{Q^{-1}} = Q^{-j(n-j)}\begin{bmatrix} n \\ j \end{bmatrix}_Q \tag{22}$$

may be used to obtain

$$\begin{aligned} S(z) = \lim_{m\to\infty}\Bigg[&\sum_{j=0}^{m-1} t^{j-(m-1)/2}x^{-2j(m-1-j)}\begin{bmatrix} m-1 \\ j \end{bmatrix}_{Q=x^2} \\ &\times\left(\sum_{j=0}^{m-1} x^{-[j-(m-1)/2]}x^{-2j(m-1-j)}\begin{bmatrix} m-1 \\ j \end{bmatrix}_{Q=x^2}\right)^{-1}\Bigg]. \end{aligned} \tag{23}$$

(From now on we take $Q = x^2 = e^{-4\theta}$.)

Let $m-1 = 2p$ and $j - p = k$ (remembering that m is odd) so

$$S(z) = \lim_{p\to\infty}\sum_{k=-p}^{p} t^k Q^{k^2}\begin{bmatrix} 2p \\ k+p \end{bmatrix}_Q\left(\sum_{k=-p}^{p}(x^{-1})^k Q^{k^2}\begin{bmatrix} 2p \\ k+p \end{bmatrix}_Q\right)^{-1}. \tag{24}$$

Now since $0 < x < 1$ then

$$|Q| < 1 \qquad \text{and} \qquad Q^{k^2} \to 0 \qquad \text{as } k \to \pm\infty.$$

So these sums converge and we may use the Jacobi triple product (Goulden and Jackson 1983, Andrews 1976) and the result that for $|Q|<1$

$$\lim_{n,j\to\infty}\begin{bmatrix} n+j \\ j \end{bmatrix}_Q=\prod_{k=1}^{\infty}(1-Q^k)^{-1} \tag{25}$$

to give

$$S(z)=\prod_{j=1}^{\infty}[1+Q^{2j-1}(t+t^{-1})+Q^{4j-2}][1+Q^{2j-1}(x+x^{-1})+Q^{4j-2}]^{-1}. \tag{26}$$

Now as $t+t^{-1}=qz-2=\exp[2(\theta-\phi)]+\exp[-2(\theta-\phi)]$ we have

$$S(z)=\prod_{j=1}^{\infty}\frac{\{1+\exp[-(8j-4)\theta](4z\cosh^2\theta-2)+\exp[-(16j-8)\theta]\}}{\{1+\exp[-(8j-4)\theta](e^{2\theta}+e^{-2\theta})+\exp[-(16j-8)\theta]\}}. \tag{27}$$

This equation is the result analogous to equation (3) we have sought. From it we can obtain $P_0, P_1, P_2, \ldots,$ by expanding and using (13). In particular, noting that $M(T_d)=P=S(0)$, we can readily verify (3).

4. Explicit formulae

We can rewrite $S(z)$ in terms of Jacobi theta functions (Abramowitz and Stegun 1965, Gradshteyn and Ryzhik 1980) as

$$S(z)=\frac{\Theta_1(u)}{\Theta_1(v)} \tag{28}$$

where u is defined via $z(u)=2[\cos(\pi u/K)+1]/q$ and v by $z(v)=1$. The nome is $Q=e^{-4\theta}$ and K is the quarter period. By performing a conjugate modulus transformation on $S(z)$ it can be shown that

$$S(z)=\exp[-(\pi^2/16\theta)(u/K)^2-\theta/4]\Theta_1(\mathrm{i}u)/\Theta_1(\mathrm{i}v) \tag{29a}$$

which has the product expansion

$$S(z)=\exp[-(\pi^2/16\theta)(u/K)^2-\theta/4]$$
$$\times\prod_{j=1}^{\infty}\frac{\{1+2\exp[-(2j-1)\pi^2/4\theta]\cosh(\pi^2u/4K\theta)+\exp[-(4j-2)\pi^2/4\theta]\}}{\{1+\exp[-(4j-2)\pi^2/4\theta]\}}. \tag{29b}$$

The nome and quarter period of the theta functions in (29a) are Q' and K', respectively: the conjugate nome and quarter period. They are related to Q and K by

$$Q'=\exp(-\pi^2/4\theta)=\exp(-\pi K/K') \qquad Q=\exp(-4\theta)=\exp(-\pi K'/K) \tag{30a}$$

and so

$$K'/K=4\theta/\pi. \tag{30b}$$

One can calculate $P_n(\theta)$ via the rule

$$P_n(\theta)=\frac{1}{n!}\left.\frac{\mathrm{d}^nS(z)}{\mathrm{d}z^n}\right|_{z=0}. \tag{31}$$

In particular $P_0 = P = M(T_d)$ is given by (3) and P_1, P_2 by

$$P_1(\theta) = \frac{q\,\Sigma_{n=1}^{\infty}(-1)^{n+1} n^2 \exp(-(4n^2\theta)}{1+2\,\Sigma_{n=1}^{\infty}(-1)^n \exp(-4n^2\theta)} P_0(\theta) \tag{32}$$

and

$$P_2(\theta) = \frac{(q^2/12)\,\Sigma_{n=1}^{\infty}(-1)^n (n-1)n^2(n+1)\exp(-4n^2\theta)}{1+2\,\Sigma_{n=1}^{\infty}(-1)^n \exp(-4n^2\theta)} P_0(\theta). \tag{33}$$

5. Behaviour of $P_n(\theta)$

5.1. Large θ behaviour

Baxter (1982) showed that $P_0(\theta)$ approaches 1 as θ approaches ∞. By examining (27) one can see the leading behaviour of the coefficients of z^n (which are the $P_n(\theta)$). $P_n(\theta)$ behaves as $\exp[-2n(2n-1)\theta]$ as θ becomes large. This is consistent with equations (32) and (33) where $P_1(\theta)$ behaves as $e^{-2\theta}$ and $P_2(\theta)$ as $e^{-12\theta}$ as θ becomes large. So $P_n(\theta)(n \geqslant 1)$ goes to zero as θ goes to infinity. This is expected as the sum of the $P_n(\theta)$ must be 1.

5.2. Small θ behaviour

Baxter (1982) also showed that $P_0(\theta)$ tends to zero as $2\exp(-\pi^2/16\theta)$ as θ approaches zero. By examining (29) and making series expansions of the terms one can see that for θ small and $0 < z < 1$,

$$S(z) \sim 2\exp[-(\pi^2 + \varepsilon^2)/16\theta]\cosh(\pi\varepsilon/8\theta) \tag{34}$$

where $z = \sin^2(\varepsilon/2)$. Expanding in powers of z, it follows that for a given value of n $(n \geqslant 0)$

$$P_n \sim 2(\pi/4\theta)^{2n}\exp(-\pi^2/16\theta)/(2n)! \tag{35}$$

as $\theta \to 0$. Thus each P_n tends to zero. (To verify that their sum remains unity one needs to consider the limit when $\theta \to 0$ and $n \to \infty$, $n\theta$ remaining finite, for which the formula (35) does not apply: alternatively, and more easily, one can simply verify that (34) gives $S(1) = 1$ when $z = 1$ and $\varepsilon = \pi$.)

6. The case $T \to T_d^+$

Now let us consider the case $T \to T_d^+$. As remarked at the end of § 1, there is no longer an infinite cluster, so it is no longer appropriate to say that the centre site 0 is connected to the infinite (or boundary) cluster.

However, one can still ask how many finite clusters surround the cluster containing site 0. We can break up the graphs G' on the lattice into a series $G'_1, G'_2, \ldots,$ defined as follows: G'_n is the set of graphs where just $n-1$ clusters surround the cluster containing site 0. Any graph G' must be in one of the set G'_n, $n = 1, 2, \ldots$. We can define therefore $P'_1, P'_2, \ldots,$ as the probabilities that $G' \in G'_n$. If $G' \in G'_n$ then on the medial lattice $\mathscr{L}'$ there are $2n-1$ polygons surrounding site 0. We proceed in a similar way to that of §§ 2 and 3 to calculate a generating function for these P'_n. Equation (9) becomes

$$\langle s'(\alpha, \phi)\rangle = \sum_{n=1}^{m/2} z^{n-1/2} P'_n. \tag{36}$$

We still have

$$\lim_{m\to\infty} \langle s'(\alpha, \phi)\rangle = \lim_{m\to\infty} S_m(z) \tag{37}$$

where $S_m(z)$ is defined by (12), only now the boundary condition requires us to take the limit through *even* values of m. Using the result (23), but taking $m = 2p+2$, in place of (24) we obtain

$$S'(z) = \sum_{n=1}^{\infty} z^n P'_n = z^{1/2} \lim_{p\to\infty} \left[\sum_{k=-p}^{p+1} t^{k-1/2} Q^{(k-1/2)^2} \begin{bmatrix} 2p+1 \\ k+p \end{bmatrix}_{Q=x^2} \right.$$
$$\left. \times \left(\sum_{k=-p}^{p+1} (x^{-1})^{k-1/2} Q^{(k-1/2)^2} \begin{bmatrix} 2p+1 \\ k+p \end{bmatrix}_{Q=x^2} \right)^{-1} \right]. \tag{38}$$

Taking the limit term by term, it follows that

$$S'(z) = z^{1/2} \sum_{k=1}^{\infty} Q^{(k-1/2)^2} \cosh[2(k-1/2)(\theta-\phi)] \left(\sum_{k=1}^{\infty} Q^{(k-1/2)^2} \cosh[2(k-1/2)\theta] \right)^{-1}. \tag{39}$$

This expression is directly related to the ratio of two H_1 theta functions and by using their product expansion we obtain the analogous result to (27) as

$$S'(z) = z \prod_{j=1}^{\infty} \frac{[1+\exp(-8j\theta)(4z\cosh^2\theta - 2) + \exp(-16j\theta)]}{[1+\exp(-8j\theta)(e^{2\theta}+e^{-2\theta}) + \exp(-16j\theta)]}. \tag{40}$$

From (40) we can calculate the $P'_n(\theta)$. We see that as θ approaches infinity, $P'_n(\theta)$ approaches $\exp[-(4n-2)(n-1)\theta]$ and in particular $p'_{-1}(\theta) \to 1$.

7. Summary

In §§ 2-5 we have calculated the generalised percolation probabilities $P_n(\theta)$ for $\theta > 0$ ($q > 4$) in the thermodynamic limit, and for $T \to T_d^-$. They are given, via the generating function $S(z)$, by (13) and (27). In § 6 we give the corresponding results (equations (38) and (40)) for the limit $T \to T_d^+$. In both cases $P_n(\theta)$ and $P'_n(\theta)$ are the probabilities that a centre site is surrounded by $n-1$ finite clusters.

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