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The self-avoiding domain problem and generalised Potts models

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Abstract. Hilhorst's result that the self-avoiding domain problem can be related to a slight generalisation of the Potts problem, of which it is the limiting case as $n \to 0$, is rederived by a different method. It is also shown that a further set of such models exist whose transition points can be located exactly by developing Potts's original argument and it is shown to be a numerically reasonable hypothesis that the number of self-avoiding domains could be determined from the limiting case of these models as $n \to 0$. Unfortunately, as we only possess the data for integral values of n, it is not entirely clear how to do this extrapolation.

1. Introduction

Hilhorst (1977) has pointed out a connection between the generating function for self-avoiding domains on the square lattice and the limit as $n \to 0$ of a slight generalisation of the Potts problem with $2n$ colours. For the new model we arrange the $2n$ colours on a circle or polygon (the colour chart) and give a weight e^{nH} to each pair of neighbouring sites that are coloured alike, a weight e^{-nH} for a pair of neighbouring sites with complementary colours (at opposite points on the circle or polygon) and a weight of unity for all other types of pair. For $n = 1$ we have just the Ising model, for $n = 2$, we can represent the four colours by the possible configurations of two spins on each site, and it is easily seen that the partition function factorises into the square of an Ising partition function. However, this information is insufficient to enable us to extrapolate to $n = 0$ and for $n \geqslant 3$ we do not even know how to locate the transition. We shall show that the cases $n = 1$ and $n = 2$ can also be regarded as the first two of a series of more general models whose transitions can be precisely located by Potts's (1952) transformation, and that these models also have a symmetry enabling us to conclude that the self-avoiding domain problem again appears as their limit as $n \to 0$. In particular we can try to extrapolate the transition point data for finite n to determine the number of self-avoiding domains, the results being consistent with the accepted value of the 'connective constant' for the plane square lattice.

2. An alternative derivation of Hilhorst's results

Baxter (1973) pointed out that the generating function for the ordinary Potts model can be written as a Whitney–Tutte polynomial, that is to say as a sum over all subgraphs of

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the lattice obtained by deleting one or more lines from it. If, in the Potts model, we give a weight of $1+f$ to each pair of neighbouring sites coloured alike and a weight of 1 for each unlike pair of neighbouring sites, the generating function for any lattice can be written

$$\sum q^c f^l \tag{1}$$

where the sum is over subgraphs obtained by removing lines from the lattice, q is the number of possible colours, c is the number of connected components of the subgraphs and l is the number of lines it contains. (An isolated point is counted as a component.) If two or more sites are connected by an f factor (line) in a subgraph these two sites are coloured alike in that subgraph. (1) is actually true for any lattice, regular or irregular, and is easily proved by induction on the numbers of points and lines.

For the Hilhorst model, we have $q = 2n$. We can split the graph into subgraphs as before, but this time a line between two sites can mean either that they are coloured alike or that they are coloured with complementary colours. For example, the generating function for a 'lattice' consisting of two points connected by a line is

$$(2n)(2n-2)+2n\,\mathrm{e}^{nH}+2n\,\mathrm{e}^{-nH} \tag{2}$$

the second and third terms corresponding to the two sites coloured alike, and the two sites coloured with complementary colours, respectively. This may be written

$$(2n)^2+2n(\mathrm{e}^{nH}-1)+2n(\mathrm{e}^{-nH}-1). \tag{3}$$

No extra terms are needed to take account of the two sites being coloured in two different but non-complementary colours because we are assigning a weight of unity to all such colourings. By analogy with (1) we may write (3) as

$$(2n)^2+2n(f_1+f_2). \tag{4}$$

We can easily show by induction that a connected subgraph of l lines without cycles induces a factor $2n(f_1+f_2)^l$, made up of the factor $2n$ for the connected component and f_1+f_2 for each of the l lines. Choosing an f_1 means that two adjacent points are coloured alike, choosing an f_2 means that they are coloured in complementary colours.

If, however, we have a subgraph of l lines containing cycles we can no longer have a factor $(f_1+f_2)^l$ but we must remove some of these terms. For example, for a simple cycle the factor is

$$n[(f_1+f_2)^l+(f_1-f_2)^l] \tag{5}$$

because there must be an even number of f_2's in the cycle in order to obtain a permissible colouring of it.

We can simplify some of the subgraph contributions as follows. If a subgraph has any vertex of degree unity we can remove it and again introduce a factor f_1+f_2 to allow for the possible colourings of this vertex and in this way we can progressively remove all tree-like portions, which we call 'whiskers', the subgraph contribution having a factor f_1+f_2 for every line that is part of a 'whisker'. If we are left with a cycle expression (5) applies, while the addition of bridges in general introduces further factors f_1+f_2. The fundamental reason why this model incorporates a preference for cycle graphs can be seen from (4) and (5). As n becomes smaller, $f_1-f_2 = 2\sinh nH$ becomes progressively

larger than $f_1+f_2=4\sinh^2\frac{1}{2}nH$. Since we are giving a weight smaller than unity to a complementary colouring of a pair of neighbouring sites f_2 is negative. Thus as $n\to 0$ the 'whiskers' and bridge graphs drop out. Hilhorst (1977) arrived at the same conclusion by another route.

3. The Potts transformation

Potts (1952) located the transition temperature of his model by an argument of which the following is a slight expansion, and his result has been confirmed by many later workers. Define operators as follows, a pair for each site: S_A introduces a factor ω^r if site A is of colour r; t_A: if site A is of colour r, site A′ is of colour $r+1$, where $\omega=\exp(2i\pi/2n)$. It is easily shown that the following operator selects configurations in which sites A and B are coloured alike

$$(1+S_AS_B^{2n-1}+S_A^2S_B^{2n-2}+\ldots+S_A^{2n-1}S_B)/2n \tag{6}$$

and the operator (6′) which selects configurations in which sites A and B are of complementary colours is obtained by changing the sign of the terms with odd powers of S_A in (6). The operator describing the interaction between sites A and A′ according to Hilhorst's model is

$$1+t_A+t_A^2+\ldots+t_A^{2n-1}+(e^H-1)+(e^{-H}-1)t_A^n. \tag{7}$$

Potts's transformation (1952) is a natural generalisation of Onsager's (1944). It is equivalent to the one-step replacements of operators as follows

$$\begin{aligned}&t_A\to S_AS_B^{2n-1}\to t_B^{2n-1}\to S_B^{2n-1}S_C\to t_C\to\ldots\\&t_A^2\to S_A^2S_B^{2n-2}\to t_B^{2n-2}\to S_B^{2n-2}S_C^2\to t_C^2\to\ldots\text{ etc}\\&\ldots\end{aligned} \tag{8}$$

which can be done without any effect on the eigenvalues of the transfer matrix, because all these operators are $2n$th roots of unity and each commutes with all the others except the two neighbours in its subseries in (8). (The commutation relation between any two neighbours in a given subseries is the same.)

We now generalise the Hilhorst model. For the completely general Potts model, we give a weight a_0 to a nearest neighbour pair coloured alike, a_1 to a nearest neighbour pair coloured with colours s, $s+1$ (any s) . . . and a_r to a nearest neighbour pair coloured with colours s, $s+r$ (any s). Such a model will transform into itself under the Potts transformation if

$$\begin{aligned}\sqrt{2}na_0&=a_0+a_1+a_2+\ldots+a_{2n-1}\\\sqrt{2}na_1&=a_0+\omega a_1+\omega^2a_2+\ldots+\omega^{2n-1}a_{2n-1}\\\sqrt{2}na_r&=a_0+\omega^ra_1+\omega^{2r}a_2+\ldots\end{aligned} \tag{9}$$

where $\omega=e^{\pi i/n}$.

It is easily found that these equations are not independent, and that they are always satisfied by the critical values for the Potts model itself:

$$a_0=1+\sqrt{2}n \qquad a_1=a_2=\ldots=1. \tag{10}$$

We also find (e.g. multiplying the a_1 equation by ω^2, the a_r equation by ω^{2r} and adding) that $a_r = a_{2n-r}$. Thus the equations become

$$\begin{aligned}
\sqrt{2}na_0 &= a_0 + 2a_1 + 2a_2 + \ldots + a_n \\
\sqrt{2}na_1 &= a_0 + 2a_1\cos\phi + 2a_2\cos 2\phi - \ldots - a_n \\
\sqrt{2}na_n &= a_0 - 2a_1 + 2a_2 - \ldots + a_n
\end{aligned} \tag{11}$$

where $\phi = \pi/n$. These equations are still not independent.

Although it has not been proved formally, examination of the cases $n = 1$–6 shows that the problem becomes determinate if we impose the further conditions

$$a_0 a_n = a_1 a_{n-1} = a_2 a_{n-2} = 1 \tag{12}$$

which are a natural generalisation of Hilhorst's model, and it is easy to generalise the argument for Hilhorst's model to show that these models also produce the same type of preference for cycle graphs as $n \to 0$.

We treat the generalised model by expanding the generating function as a generalised Whitney–Tutte polynomial as before. In colouring the subgraphs, we assign a weight $a_0 - 1$ to two neighbouring sites joined by a line coloured alike, and $a_r - 1$ if they are coloured by two colours r steps apart. To describe the possible colourings of a cyclic subgraph of length p, we need the diagonal sum of the pth powers of the cyclic matrix

$$\begin{Vmatrix} a_0 - 1, & a_1 - 1, & a_2 - 1, & \ldots \\ a_1 - 1, & a_0 - 1, & a_1 - 1, & a_2 - 1 \\ \ldots & & & \end{Vmatrix} \tag{13}$$

that is, the sum of the pth powers of the eigenvalues of (13). But the eigenvalues of (13) are

$$\lambda_0 = a_0 - 1 + 2(a_1 - 1) + 2(a_2 - 1) + \ldots \qquad \text{where } \phi = \pi/n \tag{14}$$

$$\lambda_1 = a_0 - 1 + 2(a_1 - 1)\cos\phi + 2(a_2 - 1)\cos 2\phi + \ldots$$

$$\lambda_2 = a_0 - 1 + 2(a_2 - 1)\cos 2\phi + 2(a_2 - 1)\cos 4\phi + \ldots .$$

These, however, are known from (11). We have

$$\lambda_0 = \sqrt{2}na_0 - 2n \qquad \lambda_1 = \sqrt{2}na_1 \qquad \lambda_2 = \sqrt{2}na_2. \tag{15}$$

If, as is the case, all the a's are positive but decrease as r increases, the largest eigenvalue is λ_1. (λ_0 is smaller because of the term $2n$ resulting from subtracting 1 from all the weights.) This does not affect the other eigenvalues. Now, if we have a subgraph containing a whisker, we can colour each vertex of order 1 with any of the $2n$ colours, giving the total weight $a_0 - 1 + 2(a_1 - 1) + 2(a_2 - 1) \ldots = \lambda_0$, whereas the weight given to each line in a subgraph consisting of a long cycle is effectively λ_1.

Equations (11) and (12) have been solved for $n = 1$ to 6 with the following results (table 1).

Table 1.

n	a_0	a_1	a_2	a_3	a_4	a_5	a_6
1	1.55	0.64					
2	2.41	1.00	0.41				
3	3.42	1.77	0.565	0.29			
4	4.60	2.73	1.00	0.37	0.22		
5	5.85	3.85	1.58	0.63	0.26	0.17	
6	7.59	5.27	2.41	1.00	0.41	0.19	0.13

$n = 1$ and $n = 2$ are Hilhorst's cases. Note that for n even $a_{n/2}$ is unity because of (12) from which we deduce the following values of λ_0 and λ_1 (table 2).

Table 2.

n	1	2	3	4	5	6
λ_0	0.19	0.84	2.38	5.01	8.50	14.26
λ_1	0.90	2.00	4.30	7.70	12.20	18.20
λ_0/λ_1	0.21	0.42	0.55	0.65	0.70	0.78

These figures entirely confirm our expectations that as $n \to 0$ the model should favour cycles over 'whiskers', and that as n becomes large all lines should become of equal weight. The accepted value of the number of self-avoiding domains from series expansions is 2.639 . . . which means that λ_1 should extrapolate to about 0.379 and λ_0 to zero as $n \to 0$. These are quite consistent with the above values.

Clearly λ_0 and λ_1 must be definite functions of n, but since we only have them for integral values of n it is difficult to extrapolate accurately.

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