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LETTER TO THE EDITOR

Chromatic and thermodynamic limits

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Abstract. Simple arguments about graph colouring yield existence proofs for a limit analogous to the thermodynamic limit. This approach also explains a difficulty in the ice model, concerning the equality of limits for free and periodic boundary conditions.

Questions concerning the existence of the thermodynamic limit are of considerable importance in statistical mechanics, and it has been noticed that several models dealt with in such questions can be reformulated as colouring problems on graphs; the ice model is a notable example. At the recent SRC Rencontre in Aberdeen I posed the general problem of the existence of the required limit in a graph-theoretical context, and several of the participants (in particular, P Erdös and E H Lieb) made helpful suggestions. On reflection, it seems that the methods involved in the theory of the 'chromatic limit' may illuminate some studies of the thermodynamic limit, and conversely. In this letter I shall show that a general approach, by means of colourings of the square lattice, results in a neat proof for the special case of the ice problem, and that it explains the reason for a difficulty encountered by Lieb and Wu (1972).

Let $C(\Gamma; u)$ denote the number of ways of colouring the vertices of a finite graph Γ with u colours available; a colouring is always understood to satisfy the condition that adjacent vertices have different colours. The function $C(\Gamma; u)$ is a polynomial function of u, and it is called the 'chromatic polynomial' of Γ. An account of some of its properties may be found in Biggs (1974). For an infinite graph G we are interested in the existence of the 'chromatic limit'

$$\lim_{m \to \infty} [C(G_m; u)]^{1/v_m}$$

where $\{G_m\}$ is a sequence of graphs, with v_m vertices, whose limit is G.

For the infinite plane square lattice graph S, a suitable choice for S_m is the graph induced by an $m \times m$ set of vertices of S; S_m has m^2 vertices and $2(m^2-m)$ edges. The crucial fact is that

$$C(S_{m+n}; u) \geqslant C(S_m; u)C(S_n; u) \qquad (u \geqslant 3).$$

To see this, we imbed S_m and S_n disjointly in S_{m+n} by putting S_m in the bottom left corner and S_n in the top right corner. In this situation S_m and S_n may be coloured independently, and the resulting partial colouring of S_{m+n} can always be extended to all the vertices by means of the following 'diagonal' construction. Let us denote a vertex by (i, j), where $1 \leqslant i, j \leqslant m+n$, and write $k = i+j$, so that the vertices with a fixed value of k lie on a diagonal line. The colour $c(i, j)$ which is to be assigned to an uncoloured vertex (i, j) is given by

$$c(i,j) = \begin{cases} c(k-m, m) & \text{if } k \leqslant 2m, i < m; \\ c(m, k-m) & \text{if } k \leqslant 2m, i > m; \\ c(m+1, k-m-1) & \text{if } k \geqslant 2m+2, i < m+1; \\ c(k-m-1, m+1) & \text{if } k \geqslant 2m+2, i > m+1. \end{cases}$$

Finally, if $k = 2m+1$ then $c(i, j)$ can be any colour except $c(m, m)$ or $c(m+1, m+1)$, so that we must have at least three colours available. It is easy to check that this does indeed yield a colouring of S_{m+n}, and since there is one such for every pair of colourings of S_m and S_n, we have the stated inequality.

Furthermore, the sequence $\{\ln C(S_n; u)/n^2\}$ is bounded above, because the number of colourings of S_n is not more than u^{n^2}. It follows that a well known result in analysis (see Pólya and Szegö 1972) can be applied, with suitable modifications, to show that the sequence converges. Thus the chromatic limit exists for the sequence $\{S_n\}$, for each $u \geqslant 3$; in particular it exists in the case $u = 3$, corresponding to the ice model.

Effective methods for calculating limits of this kind are based on the transfer matrix technique, and in order to apply this technique one must work with a slightly different sequence of graphs. Let T_m denote the $m \times m$ toroidal square lattice graph, formed by identifying opposite sides of S_{m+1}; T_m has m^2 vertices and $2m^2$ edges. It is desirable to prove that the chromatic limit for the sequence $\{T_n\}$ exists and is the same as that for $\{S_n\}$; I shall show that this can be done very simply, provided that $u \geqslant 4$.

We begin by remarking that the number $C_p(S_m; u)$ of colourings of S_m which satisfy the 'periodic boundary conditions'

$$c(1, i) = c(m, i), \qquad c(i, 1) = c(i, m) \qquad (1 \leqslant i \leqslant m),$$

is the same as the number $C(T_{m-1}; u)$, and that

$$C(S_m; u) \geqslant C_p(S_m; u).$$

In order to obtain an opposite inequality, consider S_n imbedded as the central $n \times n$ portion of S_{n+4}, and suppose that this copy of S_n is coloured. Let the boundary vertices of S_{n+4} be given any periodic colouring which satisfies the restriction that $c(1, 2)$ and $c(2, 1)$ are the same. Then the vertices not yet coloured lie on the sides of an $(n+2) \times (n+2)$ square; we shall colour these vertices in clockwise order, beginning at $(2, 3)$. The vertex $(2, 3)$ is adjacent to two vertices which are already coloured, and so it can be assigned a different colour, provided $u \geqslant 3$. The next vertex $(2, 4)$ is adjacent to three vertices already coloured, and so it can be assigned a different colour, provided $u \geqslant 4$; the same is true for all the remaining vertices, except the last one, $(2, 2)$. Although this vertex is adjacent to four vertices which are already coloured, the restriction that $c(1, 2) = c(2, 1)$ means that it too can be coloured if $u \geqslant 4$. Thus any colouring of S_n can be extended to a colouring of S_{n+4} with periodic boundary conditions, and

$$C_p(S_{n+4}; u) \geqslant C(S_n; u) \qquad (u \geqslant 4).$$

In terms of the toroidal graphs, we have the inequalities

$$C(S_{n+1}; u) \geqslant C(T_n; u) \geqslant C(S_{n-3}; u),$$

from which it follows that the chromatic limit for $\{T_n\}$ exists and is equal to that for $\{S_n\}$, provided that $u \geqslant 4$.

Lieb and Wu (1972) were unable to establish this fact for the ice model case, $u = 3$. The simple approach given above makes it clear that the difficulty is due to the valency of the graph being four, which exceeds the number of colours available in the ice model. Of course, it is possible that more complicated colouring arguments may settle this case as well.

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