

LETTER TO THE EDITOR

Polychromatic Potts model: a new lattice-statistical problem and some exact results

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Abstract. We propose a generalisation of the q -state Potts model in which two neighbouring spins in states s and s' have a coupling $-J_s\delta(s, s')$, and develop an exact graphical expansion of the partition function where each cluster in the graph can be coloured in one of $C \leq q$ colours. This spin model reduces to the standard Potts model (one colour) when $J_s = J$; it also encompasses many new applications including *correlated* polychromatic bond percolation, the dilute *branched* polymer problem, and *weighted* clusters in the standard Potts model.

The Potts model (for a review see Wu 1982) is a natural generalisation of the lattice-gas or Ising model in which each spin can exist in more (and fewer!) than two states. This model has attracted considerable recent attention, because the extra degree of freedom exhibited by q , the number of states, permits the model to encompass a wide range of physical phenomena of recent interest. These range from surface adsorption (Alexander 1975) and structural phase transitions (Aharony *et al* 1977) to percolation (Kasteleyn and Fortuin 1969), biophysics, and diffusion in porous media (Stephen 1983). The purpose of this letter is to propose, and present exact results for, a generalisation of the standard Potts model; we call this the polychromatic Potts model. Special cases of this model are of considerable current interest. These include the problem of the dilute *branched* polymers, a *correlated* polychromatic percolation process[¶], and weighted clusters in the standard Potts model.

Consider a lattice of N sites and E edges. Associate with the i th site a spin variable $s_i = 1, 2, \dots, q$ such that two neighbouring spins in spin states s and s' interact with a Potts interaction $-J_s\delta(s, s')$. There is also an external field H_s applied to spins in state s . Thus the reduced Hamiltonian is

$$-\mathcal{H}/kT = \sum_{(ij)} K_s \delta(s_i, s_j) + \sum_{i=1}^N L_{s_i}. \quad (1)$$

where $K_s = J_s/kT$, $L_s = H_s/kT$ and the first summation is over all nearest-neighbour pairs. This defines a polychromatic Potts model which reduces to the standard

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[¶] This is not to be confused with *random* site polychromatic percolation, introduced by Zallen (1977).

'monochromatic' Potts model upon taking $J_s = J$ for all s and $H_s = 0, s > 1$. Following Baxter (1973) we write

$$e^{K_s \delta(s, s')} = 1 + v_s \delta(s, s'), \tag{2}$$

where $v_s = e^{K_s} - 1$. Then the partition function defined by (1),

$$Z_N(q; \{K_s\}; \{L_s\}) = \sum_{s_1=1}^q \dots \sum_{s_N=1}^q \prod_{(ij)} [1 + v_s \delta(s_i, s_j)] \prod_i \exp(L_{s_i}), \tag{3}$$

can be conveniently expressed in terms of a graphical expansion. There are 2^E terms that arise when the product in (3) is expanded. Each term of the expansion is placed in a 1:1 correspondence with a graph G embedded on the lattice if we draw a bond on the edge of the lattice for each factor $v_s \delta(s, s')$. After carrying out the sums over the q^N states of the system, we are left with a single sum over the 2^E graphs G :

$$Z_N(q; \{K_s\}; \{L_s\}) = \sum_G \prod_c [v_1^{b_c} \exp(L_1 s_c) + v_2^{b_c} \exp(L_2 s_c) + \dots + v_q^{b_c} \exp(L_q s_c)]. \tag{4}$$

Here the product is taken over all connected clusters in G , including isolated points; $b_c = 0, 1, 2, \dots$ and $s_c = 1, 2, 3, \dots$ are, respectively, the numbers of bonds and sites in each cluster. When $K_s = K$, and $L_s = L \delta(s, 1)$, equation (4) reduces to the known expansion for the monochromatic Potts model (Wu 1978),

$$Z_N(q; K; L) = \sum_G v^b \prod_c [\exp(L s_c) + q - 1]. \tag{5}$$

Here $b = \sum_c b_c$ is the total number of bonds in G . In the case of the standard Potts model the graphical formulation (5) forms the basis of developing an exact enumeration approach as well as relating the Potts model to other lattice-statistical problems. Here we shall use the graphical formulation (4) to relate the polychromatic Potts model to further problems of interest.

In the standard or monochromatic Potts model we can regard the bonds as being coloured in, say, black. Then the logarithmic derivative of (5) at $q = 1$ is related to the bond percolation process. The polychromatic generalisation in (4) regards the bonds in each cluster to be coloured in one of q different colours. Generally, some of the interactions ('colours') may be identical (degenerate). Let the interaction K_α , $\alpha = 1, 2, \dots, C$, be m_α -fold degenerate where $C \leq q$ is the number of distinct colours, and $\sum_\alpha m_\alpha = q$. Also assume the L_α have the same m_α -fold degeneracy†. Then (4) becomes

$$Z_N(q; \{K_\alpha\}; \{L_\alpha\}, \{m_\alpha\}) = \sum_{\text{config}} \prod_{\alpha=1}^C [v_\alpha^{b_\alpha} m_\alpha^{n_\alpha} \exp(L_\alpha s_\alpha)]. \tag{6}$$

Here b_α, n_α and s_α are, respectively, the numbers of bonds, clusters and sites of colour α , and the summation is taken over all graphs G and over all C^n colouring configurations of each graph, where $n = \sum_\alpha n_\alpha$ is the total number of clusters including isolated points.

We now give examples of applications of this new model that follow from the formulation (4) and (6).

Connection with the dilute branched polymer (bond lattice animal) problem. A special case of the polychromatic Potts model was introduced by one of us (Wu 1978) and shown (Harris and Lubensky 1981) to reduce to the bond animal generating function.

† In general, the fields L_s may have a different degeneracy from the interactions K_s , (examples are (5) and (13)); the most general incommensurate case will not be discussed further.

This result can be obtained by setting $C = 2, m_1 = q - 1, m_2 = 1$ in (6),

$$f(q) \equiv Z_N(q; K_1, K_2; L_1, 0; q - 1, 1) = \sum_{\text{config}} v_1^{b_1} (q - 1)^{n_1} \exp(L_1 s_1) v_2^{b_2}, \tag{7}$$

where, without loss of generality, we have taken $L_2 = 0$. Motivated by the relationship of (5) with bond percolation, consider now the logarithmic derivative of (7) evaluated at $q = 1$. The presence of the factor $(q - 1)^{n_1}$ in (7) means that only those graphs with $n_1 = 0$ make a contribution in (7) at $q = 1$ so that $f(1) = (1 + v_2)^E$. Similarly, only those graphs with $n_1 = 1$ will contribute in the derivative of (7) and we find

$$f'(1) = \sum_{\text{config}} {}^{(1)}v_1^{b_1} \exp(L_1 s_1) v_2^{b_2}, \tag{8}$$

where the summation is over all graphs containing a single cluster of colour 1. Next we sum those terms in (8) having the same single cluster. A factor $1 + v_2$ arises for each edge other than those inside the cluster or on its perimeter. Thus we obtain

$$(1/N)[(d/dq) \ln f(q)]_{q=1} = \sum_A p^b Q^t y^s = Q^z y + z p Q^{2(z-1)} y^2 + \dots \tag{9}$$

where $p = v_1/(1 + v_2), Q = (1 + v_2)^{-1}, y = e^{L_1}$ and $b \geq 0, t \geq z, s \geq 0$ are, respectively, the numbers of bonds, perimeter bonds, and sites of the single cluster (bond animal), z being the coordination number of the lattice. The summation (9), which is taken over all bond animals that are topologically different, is the generating function for bond animals ($Q = 1$), percolation ($p + Q = 1$), and perimeter bond animals ($p = y = 1$). Note that $Q = 1$ corresponds to $K_2 = 0$.

Spin clusters in the Potts model. As a generalisation of (9) let $C = 2, m_1 = q - t, m_2 = t$ and $L_2 = 0$. We obtain

$$N^{-1}[(\partial/\partial q) \ln Z_N(q; K_1, K_2; L_1, 0; q - t, t)]_{q=t} = \sum_G s_0^{-1} (v_1/v_2)^{b_0} \exp(L_1 s_0) t^n v_2^{b_1} / \sum_G t^n v_2^{b_2}, \tag{10}$$

where b_0, s_0 are the numbers of bonds and sites of the cluster containing a given point, say, the origin. Clearly, the expression (10) generates percolation clusters weighted by a factor t^n . Our Hamiltonian formulation thus produces the spin clusters arising in the t -state Potts model, a problem studied recently using Monte Carlo finite-size scaling (Sweeny 1983). Note that when $v_2 = K_2 = 0$, the denominator of (10) is simply t^N and (10) again reduces to (9) with $p = v_1, Q = 1$.

Connection with a correlated polychromatic bond percolation. As another example of an application of the expansions (4) and (6), we consider a bond percolation process in which each lattice edge can be either covered by a bond in one of C different colours, or be left empty. However, the coloured bonds are strongly correlated in that no two bonds of different colours may touch each other. Thus for $C = 1$ we have standard *random* bond percolation, but for $C > 1$ we have a more general *correlated* polychromatic bond percolation problem.

If each bond of colour α carries a fugacity v_α , then the usual questions regarding percolation processes can be asked. In particular, one wishes to compute the mean number of clusters and the mean cluster size for a particular colour. One wishes also to compute the percolation probability that clusters of particular colours will percolate. We now show that these quantities can be generated from (6). Consider first $L_\alpha = 0$

and start from (4) for $C + 1$ colours:

$$Z_N(q; \{K_\alpha\}; \{0\}; \{m_\alpha\}) = \sum_{\text{config}} q^I \prod'_{\alpha=1}^{C+1} (v_\alpha^{b_\alpha} m_\alpha^{n_\alpha}), \tag{11}$$

where we have rewritten (4) slightly by singling out the clusters of single points. Here I is the number of isolated points and the prime denotes that the product is taken over all remaining clusters having at least one bond. Note that now *only* the bond clusters are coloured. Further let $K_{C+1} = v_{C+1} = 0$ so that the summation in (11) is over the configurations of C colours, not $C + 1$. Thus Z_N is independent of m_{C+1} and we can assign *arbitrary* values for q, m_1, \dots, m_C . It follows that

$$\langle n_\alpha \rangle = N^{-1} [(\partial/\partial m_\alpha) \ln Z_N]_{q=m_1=\dots=m_C=1}, \quad \alpha = 1, \dots, C, \tag{12}$$

is the (per site) mean number of bond clusters of colour α . Here the average $\langle \rangle$ is taken over all configurations of correlated bond percolation of C colours.

To compute the percolation probability and the mean cluster size of, say, colour 1, introduce an external field L to *one* of the m_α states of colour $\alpha, \alpha = 1, 2, \dots, C$. Again taking $v_{C+1} = K_{C+1} = 0$, one obtains

$$Z_N = \sum_{\text{config}} [C e^L + q - C]^I v_1^{b_1} \dots v_C^{b_C} \prod_c (e^{L s_c} + m_\alpha - 1), \tag{13}$$

where the product is taken over all bond clusters coloured in $\alpha = 1, 2, \dots, C$. Thus one obtains the generating function for bond clusters of colour 1

$$g(L) \equiv N^{-1} [(\partial/\partial m_1) \ln Z_N]_{m_1=\dots=m_C=1, q=1+C(1-e^L)} = N^{-1} \left\langle \sum_c^{(1)} e^{-L s_c} \right\rangle. \tag{14}$$

The summation in (14) extends to all bond clusters of colour 1. For $L = 0, g(0) = \langle n_1 \rangle$ (cf (12)), while the derivatives of $g(L)$ generate the percolation probability and the mean cluster size for colour 1,

$$P(K_1, \dots, K_C) = 1 + g'(0+), \tag{15}$$

$$S(K_1, \dots, K_C) = g''(0+). \tag{16}$$

Exact results. In the formulations of branched polymers as well as the correlated bond percolation it is necessary to consider the case for which $K_s = 0$ for m of the q spin states (for example, $m = 1$ for bond animals and $m = m_{C+1}$ for the correlated bond percolation). We now show that the case of arbitrary m is always reducible to $m = 1$. Consider $K_s = 0$ for $s = 1, 2, \dots, m$. Since the m spin states have zero interaction with *all* states, they can be grouped together and referred to as a single state. Naming this single state $s = 1$, then each site is associated with a Boltzmann factor $(e^{L_1} + \dots + e^{L_m}) \delta(s, 1)$. Thus the q -state model with $K_s = 0$ for m states is completely equivalent with a $(q - m + 1)$ -state model with $K_s = 0$ for one state having an effective external field $L = \ln \sum_{\alpha=1}^m e^{L_\alpha}$.

An immediate consequence of this equivalence is that in some cases we can completely determine the critical properties of the model (1) whenever $K_s = 0$ for all states except one, i.e. $m = q - 1$. Following the procedure described above we see that the problem is identical to that of a lattice gas and, hence, an Ising model in an external magnetic field. It is then straightforward to deduce that a first-order transition occurs in this model at $zK = \ln \sum_{\alpha=1}^m e^{L_\alpha}$ for $K > \frac{1}{4} K_c^1$, where K_c^1 is the corresponding Ising critical parameter and K is the only non-vanishing K_s in the Potts model. This result

holds in any dimension. If all interactions $K_s = 0$, except for two of the q states, then the same procedure reduces the Hamiltonian (1) to that of the Blume–Emery–Griffiths model (Blume *et al* 1971).

In summary, we have proposed a generalisation of the standard q -state Potts model, and developed an exact graphical expansion of the partition function valid for arbitrary external field and arbitrary ‘degeneracy’ of the interaction parameters J_s between neighbouring pairs of spins. This polychromatic model is shown to encompass, as special cases, many interesting physical systems, including the dilute *branched* polymer problem, *correlated* bond percolation problem, and the problem of *weighted* clusters in the conventional Potts model. After this work was completed, we learned that our polychromatic model is also applicable to the biophysical problem of cholesterol–lipid phase separation (Zuckermann 1983). We are currently exploring further applications.

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References

- Aharony A, Müller K A and Berlinger W 1977 *Phys. Rev. Lett.* **38** 33
Alexander S 1975 *Phys. Lett. A* **54** 353
Baxter R J 1973 *J. Phys. C: Solid State Phys.* **6** L445
Blume M, Emery V J and Griffiths R B 1971 *Phys. Rev. A* **4** 1071
Harris A B and Lubensky T C 1981 *Phys. Rev. B* **24** 2656
Kasteleyn P W and Fortuin C M 1969 *J. Phys. Soc. Japan* **26** (suppl) 11
Stephen M J 1983 *Preprint*
Sweeny M 1983 *Phys. Rev. B* **27** 4445
Wu F Y 1978 *J. Stat. Phys.* **18** 115
— 1982 *Rev. Mod. Phys.* **54** 235
Zallen R 1977 *Phys. Rev. B* **16** 1426
Zuckermann M J 1983 *Private communication*