

REFERENCES

1. Ya. G. Sinai, *Theory of Phase Transitions. Rigorous Results* (Acad. Kiado, Budapest, 1982).
2. S. E. Burkov, *J. Phys. (Paris)* **46**:317-327 (1985).
3. R. L. Dobrushin, *Teor. Veroyat. Primenenie* **17**(4):619-639 (1972).
4. M. Aizenman, *Commun. Math. Phys.* **73**:83-94 (1980).
5. Y. Higuchi, *Random Fields, Colloquium Math. Soc. Janos Bolyai* **27** 1:517-534 (1981).
6. R. L. Dobrushin and B. B. Shlosman, *Sov. Sci. Rev. Ser. C* **5** (1985).
7. R. L. Dobrushin, *Teor. Mat. Fiz.* **12**(1):115-134 (1972).
8. V. A. Malyshev, *Uspekhi Mat. Nauk* **50**(3):3-53 (1970).
9. E. I. Dinaburg and Ya. G. Sinai, in *International Symposium on Selected Topics in Statistical Mechanics* (Dubna, 1984, Vol. 1, pp. 255-289 [in Russian]).
10. J. Brémont, K. Kuroda, and J. L. Lebowitz, *Commun. Math. Phys.* **101**:501-538 (1985).
11. A. E. Mazel, *Teor. Mat. Fiz.* **68**(1):128-140; **68**(2):287-300 (1986).
12. R. A. Minlos and Ya. G. Sinai, *Trudy Mosk. Mat. Obshch.* **17**:213-242 (1967).
13. H. van Beijeren, *Commun. Math. Phys.* **40**:1-7 (1975).

Potts Model and Graph Theory

F. Y. Wu¹*Received December 15, 1987*

Elementary exposition is given of some recent developments in studies of graph-theoretic aspects of the Potts model. Topics discussed include graphical expansions of the Potts partition function and correlation functions and their relationships with the chromatic, dichromatic, and flow polynomials occurring in graph theory. It is also shown that the Potts model realization of these classic graph-theoretic problems provides alternate and direct proofs of properties established heretofore only in the context of formal graph theory.

KEY WORDS: Potts model; partition function; correlation function; graph theory; chromatic function; flow polynomial.

1. INTRODUCTION

Studies of the Potts model⁽¹⁾ are often facilitated by the use of graphical terms and graphical analyses. The connection of the Potts model with graph theory was first formulated by Kasteleyn and Fortuin,^(2,3) who treated the bond percolation, resistor network, spanning trees, and other problems of graph-theoretic nature as a Potts model. Conversely, graph-theoretic considerations have led to formulations of the Potts model leading to results in statistical mechanics otherwise difficult to see. (For reviews of the Potts model see Wu.^(4,5)) More recently, Essam and Tsallis⁽⁶⁾ uncovered the connection of the Potts model with the flow polynomial in graph theory,^(7,8) and this consideration has since been extended to multisite correlation functions⁽⁹⁾ and their applications⁽¹⁰⁾ and the associated duality relations.⁽¹¹⁾ However, many of these findings are presented in formal mathematical language and often rely on theorems established in graph

¹Department of Physics, University of Washington, Seattle, Washington 98195. Permanent address for reprint requests: Department of Physics, Northeastern University, Boston, Massachusetts 02115.

theory. As a result, the significance of these developments does not appear to have been generally appreciated.

In this paper we present a self-contained, albeit elementary, exposition of these recent developments. While most of the results presented here are not new, our derivations are less formal and in many instances more direct than those previously given, thus shedding new light to the role played by these classic graph-theoretic problems in statistical physics.

Definitions useful to our discussions are given in Section 2. In Section 3 we describe high-temperature expansions of the Potts partition function and their associated graphical representations, and show that they lead to the chromatic, dichromatic, and flow polynomials in graph theory. In Section 4 we discuss properties of the flow polynomial and show that the Potts model formulation leads to alternate and simple proofs of these properties. In Section 5 graphical considerations are extended to correlation functions.

2. DEFINITIONS

Consider a standard Potts model on a graph G of N sites and E edges (we assume that G does not contain single-edge loops). The spin at the i th site can take on q distinct values $\sigma_i = 1, 2, \dots, q$, and the Hamiltonian is

$$-\beta\mathcal{H} = K \sum_{e \in G} \delta_{\kappa_r}(\sigma_i, \sigma_j) \quad (1)$$

where the summation extends to all edges in G . It should be noted that, while we have assumed the same interaction K along all edges, our discussions and results can be extended to include edge-dependent interactions. We chose not to consider this generalization, however, for the sake of retaining clarity of discussions. A concise summary of results in the general case can be found in ref. 10.

It is often convenient to regard the spin σ_i as being represented by a unit vector \hat{s}_i pointing in one of the q symmetric directions of a hyper-tetrahedron in $q-1$ dimensions. The connection to (1) is then made by using

$$\delta_{\kappa_r}(\sigma_i, \sigma_j) = \frac{1}{q} [1 + (q-1) \hat{s}_i \cdot \hat{s}_j] \quad (2)$$

The partition function is

$$Z_G = \text{Tr} e^{-\beta\mathcal{H}} \quad (3)$$

where the spin sum $\sum_{\sigma_i=1,2,\dots,q}$ has been denoted by taking the trace. When $K = -\infty$, all pairs of neighbors connected by edges must be in different

states. Then in this limit the partition function becomes the chromatic function,

$$Z_G|_{e^{\kappa=0}} = P(q, G) \quad (4)$$

which gives the number of q -colorings of G , i.e., the number of ways that the N vertices of G can be colored with q colors such that two vertices connected by an edge always bear different colors.

The m -spin correlation function for spins at sites $1, 2, \dots, m$ is the probability that vectors $\hat{s}_1, \dots, \hat{s}_m$ point in the same direction. This probability is given by

$$\Gamma_{12\dots m} \equiv Z_G^{-1} \text{Tr} [s_{1\alpha} s_{2\alpha} \cdots s_{m\alpha} \exp(-\beta\mathcal{H})] \quad (5)$$

$$\equiv \langle s_{1\alpha} s_{2\alpha} \cdots s_{m\alpha} \rangle^T$$

where the superscript T denotes the thermal average dictated by taking the trace. Here $s_{i\alpha} \equiv \hat{s}_i \cdot \hat{e}_\alpha$, and \hat{e}_α is a unit vector pointing in the direction α of the hypertetrahedron. In particular, the one-spin correlation function

$$\Gamma_1 = \langle s_{i\alpha} \rangle^T = \frac{1}{q-1} \langle q\delta(\sigma_i, \alpha) - 1 \rangle^T \quad (6)$$

is the order parameter of the ferromagnetic Potts model, whose numerical value lies between 0 and 1.

More generally, one defines a *partitioned* m -spin correlation function⁽⁹⁾ as the probability that spins at vertices $1, 2, \dots, m$ are partitioned into b ($\leq q$) blocks such that (i) all spins within a block are in the same spin state, and (ii) the spin states of the b blocks are all distinct. For each block partition $P(m)$ of the m integers $1, 2, \dots, m$, the corresponding partitioned correlation function is

$$\Gamma_{P(m)} = \left\langle \prod_{B \in P} \prod'_{i \in B} s_{i\alpha_B} \right\rangle^T \quad (7)$$

where B is a block index and the prime of the second product indicates the restriction (ii), namely, spin states of the b blocks are all different. Clearly, (7) becomes (5) when there is only one block, so that $b=1$ and $P(m) = (12 \dots m)$.

Graphical representations that we shall encounter are derived on the basis of the Mayer expansion,⁽¹²⁾ which converts a product of edge factors into a summation of products over subgraphs. The basic identity, which we shall use repeatedly, is

$$\prod_{e \in G} (1 + h_{ij}) = \sum_{G' \subseteq G} \prod_{e \in G'} h_{ij} \quad (8)$$

Here, the edge factor connecting vertices i and j is written as $1 + h_{ij}$, and the summation of the rhs of (8) is taken over all subgraphs $G' \subseteq G$ covering the same vertex set.

It is convenient to introduce a "percolation" average as follows: Consider subgraphs $G' \subseteq G$, which we regard as representing percolation configurations with bond occupation probability p . Then, the percolation average of any quantity $X(g)$ considered as a function of the subgraph g is defined to be

$$\langle X \rangle_p \equiv \sum_{g \subseteq G} X(g) p^{b(g)} (1-p)^{E-b(g)} \tag{9}$$

where $b(g)$ is the number of edges in g .

We may rewrite (9) as a power series in p . Expanding $(1-p)^{E-b(g)}$ in (9), we obtain

$$\langle X \rangle_p = \sum_{g \subseteq G} X(g) p^{b(g)} \sum_{g'} (-p)^{b(g')} \tag{10}$$

where g' is a set of edges not in g . The union of the two edge sets g and g' constitutes a subgraph of G . Call this subgraph $G' \subseteq G$, so that

$$b(G') = b(g) + b(g') \tag{11}$$

and regard g as a subgraph of G' . It follows that (10) can be rewritten as

$$\begin{aligned} \langle X \rangle_p &= \sum_{G' \subseteq G} p^{b(G')} \sum_{g \subseteq G'} (-1)^{b(G')-b(g)} X(g) \\ &= \sum_{G' \subseteq G} p^{b(G')} Q(X, G') \end{aligned} \tag{12}$$

where the expansion coefficient in the p series is

$$Q(X, G) \equiv \sum_{g \subseteq G} (-1)^{b(G)-b(g)} X(g) \tag{13}$$

Relations (12) and (13) hold for any $X(G')$, which may describe, e.g., connectivity properties of G' .

We can obtain an inverse of (13) if $X(G)$ is expressible as the trace over a product of edge factors, i.e.,

$$X(G) = \text{Tr} \prod_{e \in G} h_{ij} \tag{14}$$

In this case it is easily verified² that

$$Q(X, G) = \text{Tr} \prod_{e \in G} (h_{ij} - 1) \tag{15}$$

Writing in (14) $h_{ij} = 1 + (h_{ij} - 1)$ and again expanding the resulting expression using (8), we obtain the following inverse of (13):

$$X(G) = \sum_{G' \subseteq G} Q(X, G') \tag{16}$$

This is one example of the Möbius inversion,⁽¹³⁾ which generally inverts summations over partially ordered sets⁽¹⁴⁾ and follows as a consequence of the principle of inclusion and exclusion.⁽¹⁵⁾

3. HIGH-TEMPERATURE EXPANSIONS OF THE PARTITION FUNCTION

It is most natural to obtain expansions of the Potts partition function using the Mayer expansion. This is done by writing the edge Boltzmann factor in (3) as a sum of two terms and expanding using (8). This leads to different expansions when the Boltzmann factor is split differently.

The most often used expansion,^(2,3) which forms the basis of relating the Potts model to the bond percolation problem, involves rewriting the partition function (3) as

$$Z_G = \text{Tr} \prod_{e \in G} [1 + (e^K - 1) \delta_{\mathbf{K}r}(\sigma_i, \sigma_j)] \tag{17}$$

Using (8) with $h_{ij} = (e^K - 1) \delta_{ij}$, one finds for the partition function (17) the simple form after taking the trace:

$$Z_G \equiv Z(q, e^K - 1) = \sum_{G' \subseteq G} (e^K - 1)^{b(G')} q^{n(G')} \tag{18}$$

where $n(G')$ is the number of components, including isolated points, in G' . This is a high-temperature expansion, since $e^K - 1 \rightarrow 0$ at high temperatures. The function $Z(x, y)$ is the dichromatic polynomial in graph theory [cf. ref. 8, (IX.1.12)] and the function $x^N Z(x, y/x)$ is known as the Whitney rank polynomial.^(16,17) It is also known that the dichromatic polynomial, hence the Potts partition function, generates spanning trees⁽³⁾ and forests⁽¹⁸⁾ by taking appropriate $q=0$ limits. See ref. 4 for a description of these connections.

² Expand (15) as in (8) and compare with (13). Note the extra minus signs.

One immediate consequence of (18) is, upon using (4),

$$P(q, G) = \sum_{G' \subseteq G} (-1)^{b(G')} q^{n(G')} \quad (19)$$

This is the Birkhoff⁽¹⁹⁾ formula for the chromatic function, establishing the fact that $P(q, G)$ is a polynomial of q .

The quantity $(-1)^{b(G)} Z_G$ given by (17) is of the form of (15) with $h_{ij} = -(e^K - 1)\delta_{ij}$. It follows from (14) and (16) that the inverse of (18) is

$$(1 - e^K)^{b(G)} q^{n(G)} = \sum_{G' \subseteq G} (-1)^{b(G')} Z_{G'} \quad (20)$$

Equation (20) is a peculiar sum rule for the Potts partition function,³ which does not appear to have been previously noted. In the special case of $K = -\infty$, (20) becomes, after introducing (4), the following inversion for the chromatic polynomial:⁽¹⁶⁾

$$q^{n(G)} = \sum_{G' \subseteq G} (-1)^{b(G')} P(q, G') \quad (21)$$

The partition function Z_G can now be written as a power series in p . Using (9) and (12) with $X = q^n$, $Q = (-1)^b P$, we obtain

$$\begin{aligned} Z_G &= e^{EK} \langle q^n \rangle_p \\ &= e^{EK} \sum_{G' \subseteq G} P(q, G') (-p)^{b(G')} \end{aligned} \quad (22)$$

where we have introduced (19) and

$$p = 1 - e^{-K} \quad (23)$$

Generally, any splitting of the edge Boltzmann factor (into a sum of two terms) other than that in (17) will lead to a different expansion equivalent to a resummation of the p series. A particularly useful splitting is to write

$$1 + (e^K - 1)\delta_{ij} = A[(1 - t) + qt\delta_{ij}] = A(1 + qtf_{ij}) \quad (24)$$

where

$$A = \frac{1}{q} (e^K + q - 1) \quad (25)$$

$$t = \frac{1 - e^{-K}}{1 + (q - 1)e^{-K}} \quad (26)$$

$$f_{ij} = \delta_{ij} - q^{-1} = \frac{q - 1}{q} \hat{s}_i \cdot \hat{s}_j \quad (27)$$

³ If G is a connected graph such as a lattice, then $b(G) = E$, $n(G) = 1$.

For two-dimensional systems the variable t is the corresponding Boltzmann factor e^{-K} in the dual space, but more generally t is the thermal transmissivity arising in renormalization group treatments⁽²⁰⁾ of the Potts model. The substitution of the first identity in (24) into (17) now leads to the expression

$$\begin{aligned} Z_G &= A^E \langle q^{b+n} \rangle_t \\ &= q^N A^E \langle q^c \rangle_t \end{aligned} \quad (28)$$

Here, use has been made of the Euler relation

$$b(G') + n(G') = N + c(G') \quad (29)$$

where $c(G')$ is the number of independent circuits in G' . The advantage of introducing the t variable becomes apparent when we write Z_G as a power series in t . This is done by identifying q^c and F as, respectively, X and Q in (12) and (13). This leads to

$$Z_G = q^N A^E \sum_{G' \subseteq G} F(q, G') t^{b(G')} \quad (30)$$

where

$$F(q, G) \equiv \sum_{g \subseteq G} (-1)^{b(G) - b(g)} q^{c(g)} \quad (31)$$

The expansion coefficient $F(q, G)$ in the t series is precisely the flow polynomial occurring in graph theory.^(7,8)

An alternate expression for the flow polynomial can now be formulated using the Potts model realization. Substituting the second identity of (24) into (17) and comparing the resulting expression with (30), we obtain the expression⁴

$$F(q, G) = q^{b(G) - N} \text{Tr} \prod_{e \in G'} f_{ij} \quad (32)$$

valid for any $G' \subseteq G$. Now, (32) is of the form of (15) with $h_{ij} = 1 + qf_{ij}$; it follows that we can use (16) and (14) to obtain an inverse of (31). This leads to

$$\begin{aligned} \sum_{G' \subseteq G} F(q, G') &= q^{-N} \text{Tr} \prod_{e \in G} (1 + qf_{ij}) \\ &= q^{-N} \text{Tr} \prod_{e \in G} (q\delta_{ij}) \\ &= q^{-N + b(G) + n(G)} \\ &= q^{c(G)} \end{aligned} \quad (33)$$

⁴ Direct evaluation of (32) using the first identity in (27) for f_{ij} again leads to (31). (Cf. ref. 6.)

If G is planar, then consider its dual D and the associated subgraph $D' \subseteq D$ complementing g ; we then have $b(g) + b(D') = b(G)$, $c(g) = n(D') - 1$ and, after introducing (19), (31) becomes

$$F(q, G) = q^{-1} P(q, D) \quad (34)$$

A general high-temperature expansion, which encompasses both the p and t expansions described above, is obtained by writing, in place of (24),

$$1 + (e^K - 1)\delta_{ij} = A_\mu[(1 - t_\mu) + \mu t_\mu \delta_{ij}] = A_\mu[1 + \mu t_\mu f_{ij}(\mu)] \quad (35)$$

where

$$A_\mu = (e^K + \mu - 1)/\mu \quad (36)$$

$$t_\mu = (1 - e^{-K})/[1 + (\mu - 1)e^{-K}] \quad (37)$$

$$f_{ij}(\mu) = \delta_{ij} - \mu^{-1} \quad (38)$$

and μ is a parameter which can be chosen at our disposal. By taking $\mu = 1$ and $\mu = q$, e.g., (35) generates the p and t expansions, respectively.

In analogy to (28) and (30), we now have

$$\begin{aligned} Z_G &= \mu^N A_\mu^E \langle \mu^c (q/\mu)^n \rangle_{t_\mu} \\ &= \mu^N A_\mu^E \sum_{G' \subseteq G} F(\mu, q, G') t_\mu^{b(G')} \end{aligned} \quad (39)$$

where

$$F(\mu, q, G) \equiv \sum_{G' \subseteq G} (-1)^{b(G) - b(G')} \mu^{c(G')} \left(\frac{q}{\mu}\right)^{n(G')} \quad (40)$$

which becomes $(-1)^{b(G)} P(q, G)$ and $F(q, G)$, respectively, for $\mu = 1$ and $\mu = q$. One can also write, as in (32),

$$F(\mu, q, G') = \mu^{b(G') - N} \text{Tr} \prod_{e \in G'} f_{ij}(\mu) \quad (41)$$

from which one obtains the inverse of (40) by following (33):

$$\mu^{c(G)} \left(\frac{q}{\mu}\right)^{n(G)} = \sum_{G' \subseteq G} F(\mu, q, G') \quad (42)$$

Similarly, using arguments leading to (34), one derives for planar G the following duality relation:

$$\mu F(\mu, q, G) = (-1)^E \frac{q}{\mu} F\left(\frac{q}{\mu}, q, D\right) \quad (43)$$

The p expansion (22) of the Potts partition function is well known from its connection with the bond percolation.^(2,3) Consideration of the t expansion (28) and (30) also has a long history. Nagle⁽²¹⁾ considered the special case of $t = -(q-1)^{-1}$ in a numerical evaluation of the chromatic function for a lattice. Domb⁽²²⁾ analyzed the case of general t and explicitly evaluated what is equivalent to (31) for small star graphs. The expression (34) for planar graphs was observed by Wu,^(4,23) who also expressed $F(q, G)$ in the form of a recursion relation of the Potts partition function. However, it was only recently that Essam and Tsallis⁽⁶⁾ explicitly obtained (31) and pinpointed its connection with the flow polynomial in graph theory. The formulation in terms of the variable t_μ and the associated generalized coefficients $F(\mu, q, G)$ is due to de Magalhães and Essam.⁽⁹⁾

4. FLOW POLYNOMIAL

The flow polynomial (31) is known to possess a number of graph-theoretic properties. While many of these properties follow intuitively from the concept of "flow" of the polynomial (see description below), their derivations have so far appeared only as theorems in formal graph theory.^(7,8) The formulation of the flow polynomial as expansion coefficients in the t expansion of the Potts partition function, particularly the representation (32) for $F(q, G)$, now provides alternate proof of these properties, which can be more easily visualized.

We first state some of the more important properties.⁵

1. $F(q, G) = 0$ if G has a vertex of degree one or an isthmus (an articulation edge).
2. $F(q, G)$ is topologically invariant.
3. If G has components (which may have articulation vertices in common), then $F(q, G)$ is equal to the product of the flow polynomials of individual components.
4. Contraction-deletion rule:

$$F(q, G) = F(q, G^\gamma) - F(q, G^\delta) \quad (44)$$

where G^γ is G with one edge contracted and G^δ is G with the same edge deleted.

⁵ See ref. 8 for a complete list and formal proofs of all properties of the flow polynomial.

The above (and other) properties of $F(q, G)$ can be established by using the representation (32) for the flow polynomial and the readily verified identities

$$\text{Tr}_j f_{ij} = 0 \quad (45)$$

$$\text{Tr}_j f_{ij} f_{jk} = f_{ik} \quad (46)$$

where $f_{ij} = \delta_{ij} - q^{-1}$.

Consider first property 1. If G has a vertex of degree one, then, upon using (45), $F(q, G)$ vanishes identically by tracing over the spin variable of this spin. If G has an isthmus, we use the spin symmetry, which states that the trace over a cluster of spins except one is independent of the spin state of the untraced spin. Thus, we trace over all spins located in an isthmus except the one at the articulation point. Due to the spin symmetry, this gives rise to a common factor, irrespective of the spin state of the remaining spin. The remaining spin can therefore be treated as a vertex of degree one, and its trace now gives $F(q, G) = 0$.

To prove property 2, we see from (46) that a sequence of edges can be combined into a single one without affecting $F(q, G)$. Furthermore, the exponent $b(G') - N = c(G') - n(G')$ in (32) is also unchanged when a sequence of edges is combined. This establishes the fact that $F(q, G)$ is topologically invariant.

Property 3 is self-evident when the components are disjoint. When there are articulation vertices, decompose G into disjoint clusters by separating at the articulation points. The extra q factors thus introduced in (32) from the trace of the extra vertices (created in the decomposition process) cancel exactly with the q factors introduced by the increase of N , the number of vertices. Thus, the flow polynomial (32) is given by the product of those of its components as if they were disjoint. This establishes property 3.

Property 4 can be established as follows: Let the contracted and deleted edge be (1, 2) and rewrite (32) as

$$F(q, G) = q^{b(G) - N} \text{Tr} \left[f_{12} \prod_{e \neq (1, 2)} f_{ij} \right] \quad (47)$$

Now both the contraction and deletion of a single edge decrease the total number of edges by 1, implying

$$b(G) - N = b(G^\gamma) - (N - 1) = b(G^\delta) + 1 - N \quad (48)$$

Using (48) and by observation, we see⁶

$$F(q, G^\gamma) = F(q, G)|_{f_{12} = \delta_{12}} \quad (49)$$

$$F(q, G^\delta) = q^{-1} F(q, G)|_{f_{12} = 1} \quad (50)$$

Property 4 is now established by substituting $f_{12} = \delta_{12} - q^{-1}$ into (47) and splitting (47) into two terms as in f_{12} .

For completeness, we now describe the graph-theoretic meaning of $F(q, G)$ in the context of a flow. Orient all edges of G . A given orientation of G defines an $N \times N$ incidence matrix whose elements are

$$\begin{aligned} D_{ij} &= -D_{ji} = 1 && \text{if edge } ij \text{ is directed from } i \text{ to } j \\ &= 0 && \text{if no edge connects } i \text{ and } j \end{aligned} \quad (51)$$

A flow on G is specified by assigning to each edge a number Φ_e satisfying the flow condition

$$\sum_j D_{ij} \Phi_{ij} = 0 \quad (52)$$

at all vertices i . If one visualizes G as a network with electric currents Φ_e flowing along its edges, then (52) is the mere statement of the first Kirchhoff law, that the net outgoing current is zero at all nodes. Clearly, the reversal of the orientation of one particular edge corresponds to the negation of the associated Φ_e , hence does not create a new flow configuration.

A mod- q flow is a flow specified by integral $\Phi_e = 0, 1, \dots \pmod{q}$. A proper mod- q flow is one for which none of the Φ_e is zero. The counting of the number of proper mod- q flows is a highly nontrivial problem. Tutte^(7,8) showed that this number is given precisely by $F(q, G)$. The correctness of this counting can also be verified by applying the following argument:⁽¹⁴⁾ First, (33) states that the total number of mod- q flows is $q^{c(G)}$.⁷ To obtain the number of proper mod- q flows, we must subtract the number of flows with some zero Φ_e . We do this by applying the principle of inclusion and exclusion,⁽¹⁵⁾ i.e., by deleting those flows with exactly one branch carrying zero current, including those with exactly two branches carrying zero current, etc. This leads to (31). See ref. 6 for a table of flow polynomials for all graphs with five or fewer independent circuits.

⁶ In writing down (49) we use the fact that the contraction of an edge reduces the number of vertices by 1.

⁷ This fact is implicit in the Kirchhoff law, when one assigns loop currents to a network to describe its current configuration.

5. SPIN CORRELATION FUNCTIONS

In this section we show that correlation functions of the Potts model can also be represented by graph expansions.⁽⁹⁾ To keep our presentation simple and concise, we confine it to essential results. See ref. 9 for more general discussions.

Consider first the m -spin correlation function $\Gamma_{12\dots m}$ defined by (5), which is the probability that spins at sites $1, 2, \dots, m$ all point in the same direction α . By spin symmetry, this correlation is independent of α . It is then convenient to sum over α , which can be regarded as replacing \hat{e}_α by a spin \hat{s}_0 . This leads to the consideration of a graph G^+ derived from G by adding an extra vertex numbered 0, the ghost vertex, connected to vertices $1, 2, \dots, m$. Thus, upon introducing (24) and (27), (5) becomes

$$\begin{aligned} \Gamma_{12\dots m} &= (qZ_G)^{-1} A^E \left(\frac{q}{q-1}\right)^m \text{Tr}^+ \left[f_{10} \cdots f_{m0} \prod_{e \subseteq G} (1 + qt f_{ij}) \right] \\ &= (qZ_G)^{-1} A^E \left(\frac{q}{q-1}\right)^m \sum_{G' \subseteq G} (qt)^{b(G')} \text{Tr}^+ \left[f_{10} \cdots f_{m0} \prod_{e \subseteq G'} f_{ij} \right] \end{aligned} \tag{53}$$

where we have used (8), and Tr^+ denotes that the trace is being taken over G^+ .

Let

$$g' = G' \cup g_1 \cdots \cup g_m \tag{54}$$

where g_i is the edge linking vertices i and 0. Compared to G' , g' has m more edges and one more vertex. Then, by (32), the flow polynomial on g' is

$$F(q, g') = q^{b(G') + m - (N+1)} \text{Tr}^+ \left[f_{10} \cdots f_{m0} \prod_{e \subseteq G'} f_{ij} \right] \tag{55}$$

The substitution of (55) and (30) for Z_G into (53) now leads to the following expression for the m -spin correlation function:

$$\Gamma_{12\dots m} = \left(\frac{1}{q-1}\right)^m \frac{\sum_{G' \subseteq G} F(q, g') t^{b(G')}}{\sum_{G' \subseteq G} F(q, G') t^{b(G')}} \tag{56}$$

To obtain an expression similar to (56) for the partitioned correlation function $\Gamma_{P(m)}$ defined by (7), consider first a partitioned correlation without the restriction (ii) described in Section 2. That is, a partitioned

correlation for which spin states in different blocks are not necessarily distinct. This "modified" partitioned correlation is given by

$$\Gamma_{P(m)}^0 = \left\langle \prod_{B \in P} \prod_{i \in B} s_{i\alpha_B} \right\rangle^T \tag{57}$$

which is (7) with the prime over the second product removed. Following the same reasoning as in the above, it is straightforward to verify that $\Gamma_{P(m)}^0$ is also given by the rhs of (56), provided that a ghost vertex is introduced for each block of $P(m)$, and that the i th vertex is connected to its block ghost spin via the edge g_i .

It is not difficult to see that $\Gamma_{P(m)}^0$ can be written as a linear combination of $\Gamma_{P(m)}$. Write (57) as

$$\Gamma_{P(m)}^0 = (Z_G)^{-1} \text{Tr} \left[\left(\prod_{B \in P} \prod_{i \in B} s_{i\alpha_B} \right) e^{-\beta \mathcal{H}} \right] \tag{58}$$

and recall that the trace in (58) is taken without the restriction (ii), so that spin states of different blocks may or may not be equal. We can therefore expand this trace into a summation of traces for which spin states of different blocks are always distinct. A moment's reflection shows that this leads to the expression

$$\Gamma_{P(m)}^0 = \sum_{P' \geq P} c(q, b') \Gamma_{P'(m)} \tag{59}$$

where the summation is taken over all block partitions $P'(m)$ of the m integers $1, 2, \dots, m$ such that every block of P is contained in a block of P' , b' is the number of blocks in P' , and $c(q, b')$ is the number of q colorings of the b' blocks such that they all bear different colors. This number is given by

$$c(q, b') \equiv q(q-1) \cdots (q-b'+1) \tag{60}$$

Now (59) is a sum over a partially ordered set of the partition $P(m)$, and therefore has a Möbius inverse. The inverse is⁽¹⁴⁾

$$\Gamma_{P(m)} = \frac{1}{c(q, b)} \sum_{P' \geq P} \mu(P, P') \Gamma_{P'(m)}^0 \tag{61}$$

with the Möbius function

$$\mu(P, P') = (-1)^{b-b'} (2!)^{a_3} (3!)^{a_4} \cdots [(m-1)!]^{a_m} \tag{62}$$

Here, a_i specifies the class of P' , i.e., $a_i = 0, 1, \dots, b'$ is the number of blocks in P' (which are in the same block of P) having i elements.

ACKNOWLEDGMENTS

I am indebted to J. W. Essam for calling my attention to the importance of the t expansion. I have also benefited from discussions with A. C. N. de Magalhães, who explained to me the essence of her work with J. W. Essam. I would also like to thank M. Schick and D. Thouless for the hospitality kindly extended to me at the University of Washington, where this research was carried out. Work has been supported in part by National Science Foundation grants DMR-8219254, DMR-8613598, and DMR-8702596.

NOTE ADDED IN PROOF

After the completion of this work, Dr. de Magalhães has kindly pointed out to me that the relation (34) is an old result first obtained in W. T. Tutte, *Proc. Camb. Phil. Soc.* **43**:26 (1947).

REFERENCES

1. R. B. Potts, *Proc. Camb. Phil. Soc.* **48**:106 (1952).
2. P. W. Kasteleyn and C. M. Fortuin, *J. Phys. Soc. Jpn.* **26**(Suppl.):11 (1969).
3. C. M. Fortuin and P. W. Kasteleyn, *Physica* **57**:536 (1972).
4. F. Y. Wu, *Rev. Mod. Phys.* **54**:235 (1982).
5. F. Y. Wu, *J. Appl. Phys.* **55**:2421 (1984).
6. J. W. Essam and C. Tsallis, *J. Phys. A* **19**:409 (1986).
7. W. T. Tutte, *Can. J. Math.* **6**:80 (1954).
8. W. T. Tutte, *Encyclopedia of Mathematics and Its Applications*, Vol. 21, *Graph Theory* (Addison-Wesley, Reading, Massachusetts, 1984), Chapter 9.
9. A. C. N. de Magalhães and J. W. Essam, *J. Phys. A* **19**:1655 (1986).
10. A. C. N. de Magalhães and J. W. Essam, *J. Phys. A* **21**:473 (1988).
11. A. C. N. de Magalhães and F. Y. Wu, unpublished.
12. J. E. Mayer and M. G. Mayer, *Statistical Mechanics* (McGraw-Hill, New York, 1940).
13. A. F. Möbius, *J. R. A. Math.* **9**:105 (1832).
14. G.-C. Rota, *J. Wahrsch.* **2**:340 (1966).
15. H. Whitney, *Bull. Am. Math. Soc.* **38**:572 (1932).
16. H. Whitney, *Ann. Math.* **38**:688 (1932).
17. N. Biggs, *Interaction Models* (Cambridge University Press, Cambridge, 1977).
18. M. J. Stephens, *Phys. Lett. A* **56**:149 (1976).
19. G. D. Birkhoff, *Ann. Math.* **14**:42 (1912).
20. C. Tsallis and S. V. F. Levy, *Phys. Rev. Lett.* **47**:950 (1981).
21. J. F. Nagle, *J. Comb. Theory B* **10**:42 (1971).
22. C. Domb, *J. Phys. A* **7**:1335 (1974).
23. F. Y. Wu, in *Studies in Foundations and Combinatorics*, G.-C. Rota, ed. (1978).

Phase Diagrams of Lattice Systems with Residual Entropy

Christian Gruber¹ and András Sütő^{2,3}

Received July 6, 1987; revision received March 16, 1988

We introduce an equivalence relation on the family of ground states and generalize the Peierls and Pirogov-Sinai theory of phase transitions to systems with residual entropy. The idea consists in the replacement of the periodic ground states by equivalence classes together with an entropy factor. We apply these results to discuss the phase diagrams of diluted spin-1/2 systems.

KEY WORDS: Phase diagrams; first-order phase transitions; frustration; residual entropy; Pirogov-Sinai theory; spin-1 Ising models.

1. INTRODUCTION

The standard methods to prove the existence of phase transitions and to analyze the low-temperature phase diagrams are restricted either to ferromagnetic systems (Peierls' argument),^(1,2) to systems with a finite number of periodic ground states (Pirogov-Sinai theory,⁽³⁾ Slawny's asymptotic method⁽⁴⁾), or to systems with special properties (reflection positivity).

In the case of systems with an infinite number of periodic ground states no general results are known, although several models have been investigated. It appears that those systems, in particular the so-called frustrated models,⁽⁵⁾ present a large variety of phase diagrams. There are many systems (such as the ANNNI model,⁽⁶⁾) with an infinite number of periodic ground states but vanishing residual entropy (entropy per site). They display very complicated phase diagrams, but most of the results

¹ Institut de Physique Théorique, Ecole Polytechnique Fédérale de Lausanne, PHB-Ecublens, CH-1015 Lausanne, Switzerland.

² Institut de Physique Théorique, Université de Lausanne, BSP, CH-1015 Lausanne, Switzerland.

³ On leave of absence from the Central Research Institute for Physics, Budapest, Hungary.