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2009 J. Phys. A: Math. Theor. 42 385004

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Some exact results on the Potts model partition function in a magnetic field

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Received 13 July 2009

Published 7 September 2009

Online at stacks.iop.org/JPhysA/42/385004

Abstract

We consider the Potts model in a magnetic field on an arbitrary graph G . Using a formula by F Y Wu for the partition function Z of this model as a sum over spanning subgraphs of G , we prove some properties of Z concerning factorization, monotonicity and zeros. A generalization of the Tutte polynomial is presented that corresponds to this partition function. In this context, we formulate and discuss two weighted graph-coloring problems. We also give a general structural result for Z for cyclic strip graphs.

PACS numbers: 05.20.-y, 05.50.+q, 75.10.H

The q -state Potts model has served as a valuable system for the study of phase transitions and critical phenomena [1–3] and has interesting connections with mathematical graph theory [4–6]. On a lattice or, more generally, on a graph G , at temperature T and in an external magnetic field H , this model is defined by the partition function

$$Z = \sum_{\{\sigma_i\}} e^{-\beta\mathcal{H}}, \quad (1)$$

with the Hamiltonian

$$\mathcal{H} = - \sum_{\langle ij \rangle} J_{ij} \delta_{\sigma_i, \sigma_j} - H \sum_i \delta_{\sigma_i, 1}, \quad (2)$$

where $\sigma_i = 1, \dots, q$ are classical spin variables on each vertex (site) $i \in G$, $\beta = (k_B T)^{-1}$, $\langle ij \rangle$ denote pairs of adjacent vertices, and J_{ij} are the associated spin–spin couplings. The graph $G = G(V, E)$ is defined by its vertex set V and its edge (bond) set E ; we denote the number of vertices of G as $n = n(G)$ and the number of edges of G as $e(G)$. With no loss of generality, we take G to be connected and the external field to pick out the value $\sigma_i = 1$ from the q possible values. We first consider the case of a single spin–spin coupling $J_{ij} = J$ and use the notation

$$K = \beta J, \quad h = \beta H, \quad y = e^K, \quad v = y - 1, \quad w = e^h. \quad (3)$$

From (7), it follows that Z is a polynomial in q, v and w , so we write $Z = Z(G, q, v, w)$ and, for the zero-field ($w = 1$) case, we set $Z(G, q, v) \equiv Z(G, q, v, 1)$. Positive H gives a weighting that favors spin configurations in which σ_i have the value 1, while negative H disfavors such configurations. In the limit $h \rightarrow -\infty$, configurations in which any $\sigma_i = 1$ make no contribution to Z , so that the model reduces to the zero-field case with q replaced by $q - 1$:

$$Z(G, q, v, 0) = Z(G, q - 1, v, 1). \tag{4}$$

The original definition of the Potts model, (1) and (2), requires q to be a positive integer, $q \in \mathbb{N}_+$. This restriction is removed for the zero-field Potts model by the Fortuin–Kasteleyn representation [7]:

$$Z(G, q, v) = \sum_{G' \subseteq G} v^{e(G')} q^{k(G')}, \tag{5}$$

where $G' = (V, E')$, $E' \subseteq E$ is a spanning subgraph of G , and $k(G')$ denotes the number of (connected) components of G' . Equation (5) has the crucial property that $Z(G, q, v)$ is expressed in a manner that does not make any explicit reference to the spins $\{\sigma_i\}$ or summation over spin configurations, $\sum_{\{\sigma_i\}}$. This enables one to define the zero-field Potts model partition function for any real $q \geq 0$. For the ferromagnetic case, $v > 0$, so $Z(G, q, v) > 0$ for $q > 0$ and hence (5) defines a Gibbs measure. For the antiferromagnetic case, since v is negative ($-1 \leq v \leq 0$), (5) does not, in general, yield a positive definite Z with Gibbs measure if $q \notin \mathbb{N}_+$. Equation (5) also establishes the equivalence of the zero-field Potts partition function to the Tutte polynomial $T(G, x, y)$, a function of major importance in graph theory:

$$T(G, x, y) = \sum_{G' \subseteq G} (x - 1)^{k(G') - k(G)} (y - 1)^{c(G')}, \tag{6}$$

where $c(G') = e(G') + k(G') - n(G')$ is the number of independent cycles on G' [4–6, 8–10]. The equivalence is $Z(G, q, v) = (x - 1)^{k(G)} (y - 1)^{n(G)} T(G, x, y)$, where $x = 1 + (q/v)$.

The Fortuin–Kasteleyn cluster formula (5) was generalized to the case of a nonzero external magnetic field by Wu [2, 11]. Denote each of the connected components of G' as $G'_i, i = 1, \dots, k(G')$. Wu’s result is [2, 11]

$$Z(G, q, v, w) = \sum_{G' \subseteq G} v^{e(G')} \prod_{i=1}^{k(G')} (q - 1 + w^{n(G'_i)}). \tag{7}$$

We first use the Wu formula (7) to prove a number of properties of $Z(G, q, v, w)$ concerning factorization, monotonicity and zeros. Combining (5), which shows that $Z(G, q, v)$ contains a factor of q , with (4), we deduce that $Z(G, q, v, 0)$ contains a factor of $(q - 1)$. Substituting $q = 0$ in (7) and using the factorization $w^{n(G'_i)} - 1 = \tilde{w} \sum_{\ell=0}^{n(G'_i)-1} (\tilde{w} + 1)^\ell$, where $\tilde{w} = w - 1$, we prove that $Z(G, 0, v, w)$ contains a factor of $(w - 1)$. Setting $w = q - 1$ in (7) yields the result that $Z(G, q, v, q - 1)$ has $(q - 1)$ as a factor. Substituting $w = 0$ in (7) is another way to derive (4). Two elementary results are $Z(G, 1, v, w) = (v + 1)^{e(G)} w^{n(G)}$ and $Z(G, q, 0, w) = (q - 1 + w)^{n(G)}$.

We can write $Z(G, q, v, w)$ in several equivalent ways:

$$\begin{aligned} Z(G, q, v, w) &= \sum_{r,t=0}^{n(G)} \sum_{s=0}^{e(G)} a_{rst} q^r v^s w^t = \sum_{r,t=0}^{n(G)} \sum_{s=0}^{e(G)} b_{rst} q^r y^s w^t \\ &= \sum_{r,t=0}^{n(G)} \sum_{s=0}^{e(G)} c_{rst} \tilde{q}^r v^s w^t = \sum_{r,t=0}^{n(G)} \sum_{s=0}^{e(G)} d_{rst} q^r v^s \tilde{w}^t, \end{aligned} \tag{8}$$

where $\tilde{w} = w - 1$ as before, $\tilde{q} = q - 1$, and the coefficients a_{rst} , b_{rst} , c_{rst} and d_{rst} are integers. Some a_{rst} and b_{rst} can be negative. In contrast, the Wu formula (7) shows that all of the nonzero c_{rst} are positive. This leads to three monotonicity and zero-free properties in the corresponding variables \tilde{q} , v and w , taken here as real: (i) for $\tilde{q} > 0$ and $v > 0$, $Z(G, q, v, w) \equiv Z$ is a monotonically increasing function (MIF) of $w > 0$ and has no zeros on the positive w -axis; (ii) for $v > 0$ and $w > 0$, Z is a MIF of $\tilde{q} > 0$ and has no zeros on the positive \tilde{q} -axis; (iii) for $w > 0$ and $\tilde{q} > 0$, Z is a MIF of $v > 0$ and has no zeros on the positive v -axis. We can also prove that all of the nonzero d_{rst} are positive by using (7) together with the relation used above, $w^{n(G'_i)} - 1 = \tilde{w} \sum_{\ell=0}^{n(G'_i)-1} (\tilde{w} + 1)^\ell$. Since each term in the expansion of $(\tilde{w} + 1)^\ell$ is positive for each G'_i , this shows that the nonzero d_{rst} are positive. This yields three more monotonicity and zero-free results (which have some overlap with (i)–(iii)): (iv) for $q > 0$ and $v > 0$, Z is a MIF of $\tilde{w} > 0$ and has no zeros on the positive \tilde{w} -axis, (v) for $v > 0$ and $\tilde{w} > 0$, Z is a MIF of $q > 0$ and has no zeros on the positive q -axis, (vi) for $\tilde{w} > 0$ and $q > 0$, Z is a MIF of $v > 0$ and has no zeros on the positive v -axis. Monotonicity relations for borderline cases are covered by our results above; e.g., for $q = 1$, $Z(G, 1, v, w)$ is a MIF of $v > -1$ for $w > 0$ and a MIF of $w > 0$ for $v > -1$, for $v = 0$, $Z(G, q, 0, w)$ is a MIF of $q - 1 + w > 0$, etc.

We define a rational function that generalizes the Tutte polynomial, namely

$$\begin{aligned}
 U(G, x, y, w) &= (x - 1)^{-k(G)} (y - 1)^{-n(G)} \sum_{G' \subseteq G} (y - 1)^{e(G')} \\
 &\times \prod_{i=1}^{k(G')} (xy - x - y + w^{n(G'_i)}). \tag{9}
 \end{aligned}$$

This function satisfies $U(G, x, y, w) = (x - 1)^{-k(G)} (y - 1)^{-n(G)} Z(G, q, v, w)$ and $U(G, x, y, 1) = T(G, x, y)$. Although $T(G, x, y)$ and $Z(G, q, v)$ satisfy deletion–contraction relations, we note that for w not equal to 1 or 0, the functions $U(G, x, y, w)$ and $Z(G, q, v, w)$ do not, in general, satisfy such deletion–contraction relations.

We define two types of graph-coloring problems and use special cases of (7) to describe these. Although graph coloring has been investigated intensively [4–6, 9, 10, 12], these two types of graph colorings have not, to our knowledge, been studied before. Recall that the chromatic polynomial $P(G, q)$ counts the number of ways of assigning q colors to the vertices of a graph G such that no adjacent vertices have the same color. This ‘proper q -coloring’ of the vertices of G is equivalent to Z for the zero-temperature, zero-field Potts antiferromagnet, $v = -1$: $P(G, q) = Z(G, q, -1)$. We generalize this to a weighted proper q -coloring of the vertices of G , as described by the polynomial $Ph(G, q, w) = Z(G, q, -1, w)$. For $H < 0$, i.e., $0 \leq w < 1$, we have a weighted graph-coloring problem in which one carries out a proper q -coloring of the vertices of G but with a penalty factor of w for each vertex assigned the color 1. For $H > 0$, we have a second type of weighted graph-coloring problem, namely a proper vertex q -coloring with a weighting that favors one color. Since this favoring of one color conflicts with the constraint that no two adjacent vertices have the same color, the range $w > 1$ involves competing interactions and frustration.

Both of these weighted graph-coloring problems have physical applications. For example, the weighted coloring problem with $0 < w < 1$ describes the assignment of frequencies to commercial radio broadcasting stations in an area such that (i) adjacent stations must use different frequencies to avoid interference, and (ii) stations prefer to avoid transmitting on one particular frequency, e.g., because it is used for data taking by a nearby radio astronomy antenna. The graph-coloring problem with $w > 1$ describes this frequency assignment process with a preference for one of the q frequencies, e.g., because it is most free of interference.

We note some other special cases. Just as the Tutte polynomial $T(G, 1 - q, 0)$ gives, up to a prefactor, $P(G, q)$, so $T(G, 0, 1 - q)$ determines the flow polynomial $F(G, q)$, which counts the number of nowhere-zero q -flows on G that satisfy flow conservation mod q at each vertex. The function $U(G, 0, 1 - q, w)$ then defines a weighted flow problem. With $0 < w < 1$, this could describe a discretized flow analysis in an electrical circuit or traffic flow situation in which one incorporates a finite penalization for one, say the maximal, flow, in order to minimize power dissipation in resistors in the circuit case or to minimize traffic jams in the traffic case.

For a planar G , $P(G, q)$ counts not just the number of proper q -colorings of G vertices but also, equivalently, the number of proper q -colorings of the faces of the dual graph G^* . Similarly, for planar G , $Ph(G, q, w)$ is a measure not only of the weighted proper q -colorings of G vertices, but also, equivalently, the weighted proper q -colorings G^* faces.

We have used (7) and combinatoric arguments of the type in [13] to obtain a general structural determination of $Z(G, q, v, w)$ for cyclic and Möbius strip graphs G_s of regular lattices of fixed width L_y vertices and arbitrary length as well as self-dual strips of the square lattice, extending [14]. This length is $L_x \equiv m$ ($L_x \equiv 2m$) for square and triangular (honeycomb) strips. For cyclic G_s we find

$$Z(G_s, q, v, w) = \sum_{d=0}^{L_y} \sum_{j=1}^{n_{Zh}(L_y, d)} \tilde{c}^{(d)}(q) [\lambda_{G_s, L_y, d, j}(q, v, w)]^m, \tag{10}$$

where Zh connotes Z for $h \neq 0$ and

$$\tilde{c}^{(d)} = \sum_{j=0}^d (-1)^j \binom{2d-j}{j} (q-1)^{d-j}. \tag{11}$$

We have $n_{Zh}(L_y, L_y) = 1$, $n_{Zh}(1, 0) = 2$ and $n_{Zh}(L_y, d) = 0$ for $d > L_y$; the other $n_{Zh}(L_y, d)$ are determined by the recursion relations $n_{Zh}(L_y+1, 0) = 2n_{Zh}(L_y, 0) + n_{Zh}(L_y, 1)$ and, for $1 \leq d \leq L_y + 1$:

$$n_{Zh}(L_y + 1, d) = n_{Zh}(L_y, d - 1) + 3n_{Zh}(L_y, d) + n_{Zh}(L_y, d + 1). \tag{12}$$

The form for Möbius strips involves switches of certain $\tilde{c}^{(d)}$ (generalizing switchings in the $w = 1$ case [13]), which are given in detail elsewhere [15]. For these cyclic (and Möbius) strip graphs of width L_y , the total number of different λ 's, $N_{Zh, L_y} = \sum_{d=0}^{L_y} n_{Zh}(L_y, d)$, is

$$N_{Zh, L_y} = \sum_{j=0}^{L_y} \binom{L_y}{j} \binom{2j}{j}. \tag{13}$$

It is straightforward to generalize (7) to the case where the spin-spin couplings J_{ij} depend on the edges e_{ij} . Let us define $K_{ij} = \beta J_{ij}$, $y_{ij} = e^{K_{ij}}$, $v_{ij} = y_{ij} - 1$, and the set of v_e for $e \equiv e_{ij} \in E$ as $\{v_e\}$. Then we have

$$Z(G, q, \{v_e\}, w) = \sum_{G' \subseteq G} \left[\prod_{e \in E'} v_e \right] \left[\prod_{i=1}^{k(G')} (q - 1 + w^{n(G'_i)}) \right]. \tag{14}$$

Acknowledgments

We thank F Y Wu for a valuable communication calling our attention to [11]. This research was partly supported by the grants NSC-97-2112-M-006-007-MY3, NSC-98-2119-M-002-001 (SCC), and NSF-PHY-06-53342 (RS).

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