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The q-state Potts-ferromagnet on d-dimensional hypercubic lattices

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Abstract. We use a high-temperature star-graph expansion to compute the free energy and the susceptibility of a q-state Potts-model for arbitrary q on d-dimensional hypercubic lattices. The series are to order O(10) in the expansion variable $v := (e^K - 1)/(e^K + (q-1))$. We show how to compute the expectation value of any operator on a finite graph for arbitrary number q of states of the Potts-model.

1. Introduction

The Potts-ferromagnet is defined by a simple Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \delta_{s_i s_j} \,. \tag{1.1}$$

The spins can be in q different states. It is possible to map the $q = 2$ case to the Ising-model. In contrast to the well known Ising-ferromagnet this model has no spin-inversion symmetry for general q. This enriches the model but also makes it far more complicated.

For the two-dimensional model critical properties are known exactly [1]. The model shows a first-order phase transition for $q > 4$. From the Ising-model ($q = 2$) it is known that the critical dimension d_c above which mean-field critical behaviour applies is $d_c = 4$. The critical dimension for the percolation limit $q = 1$ is 6. It is assumed that these points lie on a curve in the (d, q) plane which separates a region of first-order phase transitions from continuous phase transitions. This curve is not fully known [2]. It would be very interesting to study the exact location of this curve as accurately as possible. On the other hand a general formula for some thermodynamic functions, which are used to determine the order of a phase transition, as a function of q and d would open the possibility to study the dependency of the type of phase transition on these parameters. It would be possible to gain some insight on how a discontinuity in these thermodynamic functions arises.

Potts-models were studied by many authors, for a review see [1]. We know a lot of details about special cases especially on simple cubic lattices. The susceptibility in the cases $q = 3, 4, 5, 6$; $d = 2$ were studied by high temperature series expansions (HTE) up to O(8) [3]. The case $q = 2$ is the well known Ising-model [4], where recently a HTE with 15 terms for general dimension was published [5]. In four dimensions a HTE of the susceptibility is known up to O(17) [6]. The $q = 4$ Potts-model was also studied via series expansions, the free energy and the susceptibility were obtained for arbitrary dimensionality up to O(10) [7]. Very recently low-temperature series of the susceptibility for the Ising-model were extended up to O(24) and high-temperature series of the susceptibility were extended to O(22) [9]. In two dimensions, where the self-duality relation holds, we have for comparison a low-temperature expansion of the case $q = 8$ with 25 excited bonds for the susceptibility [10].

All of these results lack the possibility of studying the dependency on the parameters q and d. Some effort was put into the study of a large q expansion [11, 12].

We are able to present a method which is *exact* in q and d up to the achieved order of the HTE.

2. Method

The Helmholtz free energy A of the Ising-model has a star-graph expansion [13]. Therefore the *inverse* susceptibility which can be written as second derivative of A with respect to the magnetization M

$$\chi^{-1} = \left(\frac{\partial^2 A}{\partial M^2}\right)_T \tag{2.1}$$

also has this property. The proof for the Ising-model [13] can be extended to the general q-state Potts-model [8]. The partition function for a N-spin system can be written as

$$Z = \sum_{s_i=0}^{q-1} \cdots \sum_{s_N=0}^{q-1} \prod_{\langle i,j \rangle} \exp(K\delta_{s_i s_j}) \qquad K := \beta J\,. \tag{2.2}$$

The exponential function is rewritten as

$$\exp(K\delta s_i s_j) = \frac{e^K + (q-1)}{q}(1 + v(q\delta_{s_i s_j} - 1)) \tag{2.3}$$

with the expansion variable for the general q-state Potts-model

$$v := \frac{e^K - 1}{e^K + (q-1)} \tag{2.4}$$

which simplifies for $q = 2$ to $v = \tanh K/2$, the well known Ising case. The symmetry of the tanh is unique in this family of functions. This is the source of the problems one encounters when dealing with general q-state Potts-models.

Computing the trace means one has to know all states of the system. In the case of the q-state Potts-model this is related to the chromatic function of the graph [1]. But one does not have to compute the full chromatic function, if one looks at the Hamiltonian in (1.1) the delta-function is the essential ingredient. One only has to know the different classes of colourings, which are defined by the same energy content. It does not matter in exactly what state a spin and its neighbour are. It is only interesting if both are in the same state or in *different* states. This is a significant simplification of the problem of finding all states of the system. Furthermore, it is noticeable that a graph of N vertices can have at most N different colours attached to them. By means of this it is easy to generate all classes of

Table 1. All states of the graph p3 in a three-state Potts-model.

		3 equal vertices			
AAA	BBB	CCC			
		2 equal vertices			
AAB	AAC	BBA	BBC	CCA	CCB
ABA	ACA	BAB	BCB	CAC	CBC
ABB	ACC	BAA	BCC	CAA	CBB
		3 different vertices			
ABC	BCA	CAB	CBA	BAC	ACB

different colourings of the graph which belong to the same energy. Consider the triangle graph p3. Table 1 shows all different *colourings* of the graph with three colours.

If one looks at the first column these entries define a *pattern* of all the configurations in the corresponding line. This means the symbols A, B, C are reinterpretated as *possible* colours. Different symbols mean different colours but it is not specified which colour is meant. So it is sufficient to know all different patterns of N vertices and q possible colours to generate all different colourings. The number of all colourings associated to a certain pattern can be computed by means of simple combinatorics. One finds that the number of realizations of a pattern with n different symbols out of a set of q elements is simply

$$C(q,n) = \prod_{i=0}^{n-1} (q-i) . \tag{2.5}$$

An example will show how this can be used to compute the partition function of the triangle graph p3:

$$\begin{aligned}
Z(\mathrm{p3}) &= \mathrm{Tr} \prod_{(i,j)} \frac{\mathrm{e}^K + (q-1)}{q} (1 + v(q\delta_{i,j} - 1)) \\
&= \left(\frac{\mathrm{e}^K + (q-1)}{q} \right)^3 \\
&\quad \times \left[(1 + v(q-1))^3 \cdot q \right. && \text{AAA} \\
&\quad + (1 + v(q-1))(1-v)^2 \cdot q(q-1) && \text{AAB} \\
&\quad + (1 + v(q-1))(1-v)^2 \cdot q(q-1) && \text{ABA} \\
&\quad + (1 + v(q-1))(1-v)^2 \cdot q(q-1) && \text{ABB} \\
&\quad \left. + (1-v)^3 \cdot q(q-1)(q-2) \right] && \text{ABC} \\
&= \left(\frac{\mathrm{e}^K + (q-1)}{q} \right)^3 q^3 (1 + (q-1)v^3) .
\end{aligned} \tag{2.6}$$

One can evaluate the delta functions very comfortably by using a pattern-matching procedure on the patterns and therefore it is not necessary to compute the Boltzmann-weight for each pattern. It is sufficient to compute the (here three) possible weights and collect the patterns with their combinatorial factors which possess the same weightfactor. By this means it is possible to compute the expectation value of any function $\mathcal{F}$ by simply generating all patterns, computing their combinatorical factors and applying a pattern matching if the functions $\mathcal{F}$ contains deltas.

In contrast to the Ising-model where computing the trace can be transformed into a 'graphical' rule which says 'use all polygon-graphs' one has to use all *closed* graphs in the general q-state Potts-model. Even worse, they carry different multiplicities depending on the topology of the graph. The result in (2.6) translated in a graphical picture is up to a factor $(1 + (q-1)\text{p3})$, p3 being the only closed graph among the subgraphs of p3. The prefactor is $(q-1)$, in the Ising-case this simplifies to 1. A general 'graphical' rule for computing these factors is not known. However, one finds that this factors solely depend on the topology of the subgraphs. The factors for the first topologies arising are shown in figure 1. With the help of this table it is possible to write down the partition function for all graphs which contain no other star-subgraphs than such with these topologies without explicitly computing the trace. One only has to generate all star-subgraphs of the given graph and determine their topology, e.g. the first graph with an α topology, which is embeddable in a cubic lattice. One of its realizations is drawn in figure 3 in the second column of the last row. One has to look for closed subgraphs, find out their topology and look up their factor in the table.

The subgraphs stand for $v^{\#\text{bonds}}$. The result of the example is

$$Z(\alpha 13132) = 1 + (q-1)(3v^4 + 2v^6 + v^8) + 2(q-1)(q-2)(v^7 + v^9) + (q-1)^2 v^8 + (q-1)(q-2)^2 v^{10}\,.$$

This computation of the partition function corresponds to a 'graphical' computation as shown in figure 2.

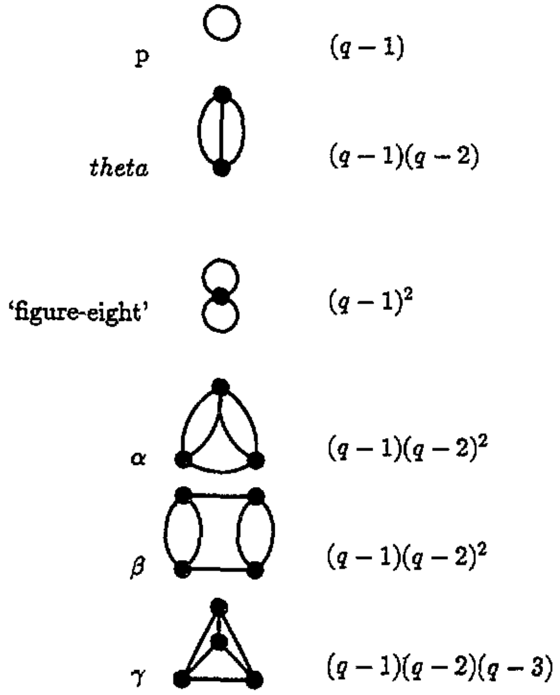

Figure 1. Multiplicities of the subgraphs in the computation of the partition function of the q-state Potts-model.

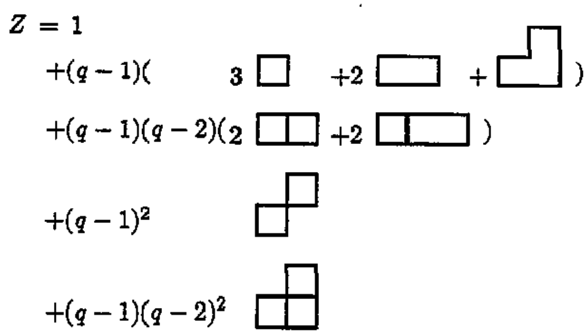

Figure 2. Computation of the partition function of the α 13132-graph.

Notice that all the factors for graphs which contain odd vertices vanish in the Ising-case $q = 2$. In the example here only polygons and so-called 'figure-eight' graphs survive.

We computed the partition function and all two-point correlations of all star-graphs up to O(10) for simple cubic lattices. The contributing graphs are listed in figure 3.

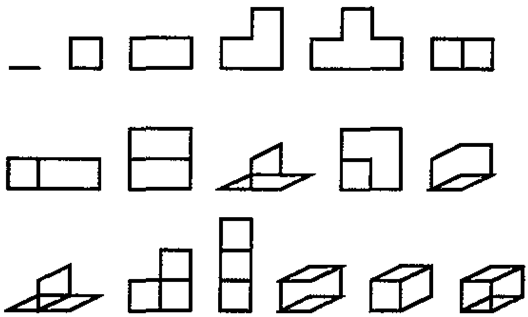

Figure 3. Star graphs up to O(10) on simple cubic lattices.

We used a program especially written to compute the expectation values in the manner described above. These results were used to compute the free energy and the inverse susceptibility as follows:

$$A = \ln(Z) \tag{2.7}$$

$$\frac{1}{\beta}\chi = \sum_{\langle i,j\rangle}\left\langle \frac{1}{q-1}(q\delta_{s_i s_j} - 1)\right\rangle. \tag{2.8}$$

The right-hand side of (2.8) can be seen as the sum of some matrix elements M_{ij}. The inverse of the matrix M is computed to generate the correct weight function for the star-graph expansion. The star-graph weight of a graph g is defined as

$$\Psi(g) = \sum_{ij}(M^{-1})_{i,j} - \dim(M) - \sum_{g_s \subseteq g}\Psi(g_s)\,. \tag{2.9}$$

The sum to be subtracted runs over all star-subgraphs of g. By using the symmetry of each graph the number of matrix elements to be computed can significantly be reduced.

3. Results

The free energy of the q-state Potts-model for arbitrary dimension d of a simple cubic lattice is

$$F = ((28\,d_2 + 2328\,d_3 + 23\,136\,d_4 + 47\,616\,d_5)(q-1) + (12\,d_2 + 288\,d_3 + 768\,d_4)$$
$$\times(-q^2 + 2q - 1) + 24\,d_3(-2q^2 + 4 - 2)$$
$$+ (4\,d_2 + 312\,d_3 + 1728\,d_4)(q^2 - 3q + 2) + (2\,d_2 + 252\,d_3 + 1152\,d_4)$$
$$\times(q^2 - 3q + 2) + (2\,d_2 + 12\,d_3)(-2q^2 + 4q - 2) + 24\,d_3(q^3 - 6q^2 + 11q - 6)$$
$$+ (12\,d_3 + 32\,d_4)(-6 - 7q^2 + 12q + q^3) + (2\,d_2 + 48\,d_3 + 96\,d_4)(-4 - 5q^2 + 8q + q^3)$$
$$+ 6\,d_3(-4 - 5q^2 + 8q + q^3) + (4\,d_2 + 72\,d_3 + 192\,d_4)(-4 - 5q^2 + 8q + q^3))\,v^{10}$$
$$+ ((12\,d_2 + 288\,d_3 + 768\,d_4)(q^2 - 3q + 2)$$
$$+ (20\,d_3 + 32\,d_4)(q^2 - 3q + 2) + 8\,d_3(q^3 - 6q^2 + 11q - 6))\,v^9$$
$$+ ((7\,d_2 + 186\,d_3 + 648\,d_4)(q-1) + d_2(q^2/2 + q - 1/2)$$
$$+ (2\,d_2 + 12\,d_3)(-q^2 + 2q - 1) + 24\,d_3(q^2 - 3q + 2))\,v^8$$
$$+ (2\,d_2 + 12\,d_3)(q^2 - 3q + 2)\,v^7 + (2\,d_2 + 16\,d_3)(q-1)\,v^6 + d_2(q-1)\,v^4$$

where d_i stands for the binomial coefficients $\binom{d}{i}$. This reduces for $q = 2$, $d = 2, 3$ to the well known Ising free energy. Notice that in the Ising-case the odd terms v^{2n+1} vanish.

The series of the susceptibility for general q and d are too lengthy to be written down. For documentation the special cases $d = 2$–7 are shown in the appendix.

4. Discussion

It should be possible to extend the series without too much additional labour by two terms. The series analysis of some special cases in which longer series and exact results are known showed us that where a second-order transition occur we can achieve a precision up to one decimal place in the critical temperature and the exponents as well. This encourages us to extend the analysis to try to evaluate the critical line which separates the region of first-order and second-order phase transitions in the (q, d) plane in a more accurate way than it is known. This analysis of the series will be presented elsewhere.

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Appendix. Q-state Potts-model in d dimensions on hypercubic lattices high-temperature series expansion

$$\chi(q, d = 2, v) = 1 + 4\,v$$
$$+ 12\,v^2$$
$$+ 36\,v^3$$

$$
\begin{aligned}
&+(76+12q)\,v^4 \\
&+(196+40q)\,v^5 \\
&+(316+212q)\,v^6 \\
&+\left(932+400q+60q^2\right)v^7 \\
&+\left(780+1900q+148q^2\right)v^8 \\
&+\left(4420+1840q+1348q^2\right)v^9 \\
&+\left(-660+12848q+1788q^2+336q^3\right)v^{10} \\
&+O\left(v^{11}\right)
\end{aligned}
$$

$$
\begin{aligned}
\chi(q,d=3,v) = {}&1+6v \\
&+30v^2 \\
&+150v^3 \\
&+(654+36q)\,v^4 \\
&+(2982+264q)\,v^5 \\
&+(11790+2460q)\,v^6 \\
&+\left(51126+13104q+540q^2\right)v^7 \\
&+\left(189870+83076q+4788q^2\right)v^8 \\
&+\left(813702+373920q+51364q^2+336q^3\right)v^9 \\
&+\left(2826174+2076864q+307260q^2+12240q^3\right)v^{10} \\
&+O\left(v^{11}\right)
\end{aligned}
$$

$$
\begin{aligned}
\chi(q,d=4,v) = {}&1+8v \\
&+56v^2 \\
&+392v^3 \\
&+(2552+72q)\,v^4 \\
&+(16904+816q)\,v^5 \\
&+(105944+10296q)\,v^6 \\
&+\left(681224+87648q+1800q^2\right)v^7 \\
&+\left(4174328+799944q+24888q^2\right)v^8 \\
&+\left(26345096+6044256q+374456q^2+1344q^3\right)v^9 \\
&+\left(158933624+48252768q+3752008q^2+70240q^3\right)v^{10} \\
&+O\left(v^{11}\right)
\end{aligned}
$$

$$
\begin{aligned}
\chi(q,d=5,v) = {}&1+10v \\
&+90v^2 \\
&+810v^3 \\
&+(6970+120q)\,v^4 \\
&+(60490+1840q)\,v^5 \\
&+(510970+29000q)\,v^6 \\
&+\left(4359530+334240q+4200q^2\right)v^7 \\
&+\left(36471930+3932920q+78040q^2\right)v^8
\end{aligned}
$$

$$+ \left(308006410 + 40604800\,q + 1484440\,q^2 + 3360\,q^3\right) v^9$$
$$+ \left(2560931610 + 425372480\,q + 20129320\,q^2 + 232160\,q^3\right) v^{10}$$
$$+ O\left(v^{11}\right)$$

$$\chi(q, d = 6, v) = 1 + 12\,v$$
$$+ 132\,v^2$$
$$+ 1452\,v^3$$
$$+ (15492 + 180\,q)\,v^4$$
$$+ (166092 + 3480\,q)\,v^5$$
$$+ (1753812 + 65580\,q)\,v^6$$
$$+ \left(18606252 + 946800\,q + 8100\,q^2\right) v^7$$
$$+ \left(195530052 + 13576980\,q + 188460\,q^2\right) v^8$$
$$+ \left(2062580172 + 175852560\,q + 4296860\,q^2 + 6720\,q^3\right) v^9$$
$$+ \left(21613975332 + 2269255440\,q + 72618660\,q^2 + 579120\,q^3\right) v^{10}$$
$$+ O\left(v^{11}\right)$$

$$\chi(q, d = 7, v) = 1 + 14\,v$$
$$+ 182\,v^2$$
$$+ 2366\,v^3$$
$$+ (30086 + 252\,q)\,v^4$$
$$+ (383726 + 5880\,q)\,v^5$$
$$+ (4848326 + 128772\,q)\,v^6$$
$$+ \left(61411742 + 2226000\,q + 13860\,q^2\right) v^7$$
$$+ \left(773883110 + 37577820\,q + 386988\,q^2\right) v^8$$
$$+ \left(9769366670 + 582573600\,q + 10241308\,q^2 + 11760\,q^3\right) v^9$$
$$+ \left(122931701270 + 8910306048\,q + 206218628\,q^2 + 1215536\,q^3\right) v^{10}$$
$$+ O\left(v^{11}\right)$$

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