

Univerzita Karlova v Praze  
Matematicko-fyzikální fakulta

## BAKALÁŘSKÁ PRÁCE



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### **Pottsův antiferromagnet**

Ústav teoretické fyziky

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Prohlašuji, že jsem svou bakalářskou práci napsal samostatně a výhradně s použitím citovaných pramenů. Souhlasím se zapůjčováním práce.

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Abstrakt: Cieľom práce bolo zoznámiť sa s Pottsovým modelom a klastrovými rozvojmí. Táto práca môže slúžiť ako úvod k týmto zaujímavým témam a tiež ako prezentácia základných výsledkov, ako aj možných aplikácií a súvislostí s ďalšími oblasťami štatistickej fyziky. Získané poznatky sa následne využili na výpočet nízkoteplotného rozvoja voľnej energie Pottsovho antiferromagnetu na tzv. "diced" mriežke.

Klíčová slova: štatistická fyzika, Pottsov model, diced mriežka, klastrové rozvoje.

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Abstract: The purpose of this work was to familiarize oneself with the Potts model and cluster expansions. This work can serve as an introduction into these intriguing themes and also as a presentation of the basic results, applications and relations to other areas of statistical physics. The acquired knowledge was then applied to the calculation of the low-temperature expansion of the free energy of the Potts antiferromagnet on the diced lattice.

Keywords: statistical physics, Potts model, diced lattice, cluster expansion.





# 1. INTRODUCTION

Potts model – a generalization of Ising model – plays an important role in statistical physics, especially in the study of critical phenomena. It is also related to a number of important condensed matter systems and outstanding problems.

In chapter two we will provide definition and history of Potts model and then review some of the most important results. After that we will turn our attention to the antiferromagnetic model.

In chapter three we will explore an useful tool called cluster expansion which provides a systematic way for calculation of thermodynamics quantities for a certain class of statistical models. We will first give an informal overview. Then we will make the statements more precise by providing a rather general and rigorous mathematical treatment. To illustrate the method, we will also provide a simple application to the Ising ferromagnet on the square lattice.

In chapter four we will introduce Potts antiferromagnet on diced lattice and finally apply the knowledge obtained in chapters two and three to the calculation of low-temperature free energy of this model.

## 2. POTTS MODEL

### 2.1. Definition and history

Potts model is a generalization of Ising model to more than 2 spin states. Of course, Ising models can be generalized in a number of ways and it is of interest that the model first considered in the Ph.D. thesis of Renfrey B. Potts [1] was actually what is now called planar Potts model. This generalization relies on noticing that Ising model spin states can be interpreted as 2 unit vectors lying in the plane and pointing in the opposing directions. For a  $q$ -state planar Potts model we get  $q$  unit vectors pointing to equally spaced directions differing by angle  $2\pi/q$  and with Hamiltonian that only depends on the angle between the spins.

Another possible generalization is to the following Hamiltonian for  $q$  spin states

$$H(\sigma) = \sum_{\langle i,j \rangle} -J\delta(\sigma_i, \sigma_j) \quad (2.1)$$

which can alternatively be interpreted as a system of  $q$  vectors pointing in the directions given by the vertices of the  $(q-1)$ -dimensional simplex [2]. This, incidentally, coincides with the planar Potts model in dimensions  $q=2$  and  $q=3$  but for the higher  $q$  they differ. It is this second model – now called standard Potts model, or simply just Potts model –, which has received so much attention.

### 2.2. Mean-field solution

The Potts model can be investigated in a number of ways, but the most straightforward one would be to apply mean-field approximation. It was shown by Mittag and Stephen [3] that  $(d=2)$ -dimensional Potts model has a first-order phase transition for all  $q > 4$  and the mean-field approximation is valid. More generally, it is expected that there exists  $q_c(d)$  for all dimensions, such that for all  $q > q_c(d)$  the mean-field approximation is valid. Likewise, there should exist  $d_c(q)$  such that for  $q$ -state model for all  $d > d_c$  will the approximation again hold. The known points therefore are  $q_c(2) = 4$  and  $d_c(2) = 4$  (this is of course the old result for Ising model). Monte Carlo simulations carried out by Kirkpatrick [4] suggest that  $d_c(1) = 6$ . Also  $q_c(d) = 2$  for  $d > 4$  [5].

### 2.3. Re-expressing the partition function

There exist various forms of the Potts model partition function. Often the Peierls contour argument [6] can be applied and we will make use of contours several times in this article (see sections 3.1, 3.3 and 4.2). Here we will illustrate another useful form that comes from combinatorics and graph theory [2].

Begin with the Hamiltonian (3.1) multiplied by  $-\beta$

$$-\beta H(\sigma) = K \sum_{\langle i,j \rangle} \delta(\sigma_i, \sigma_j) \quad (2.2)$$

where  $K \equiv -\beta J$  and rewrite its partition function

$$Z_G(q, K) = \sum_{\sigma} \exp(-\beta H) \quad (2.3)$$

where the sum is over all the possible spin configurations in the following form

$$Z_G(q, K) = \sum_{\sigma} \prod_{\langle i, j \rangle} (1 + v\delta(\sigma_i, \sigma_j)) \quad (2.4)$$

with  $v \equiv e^K - 1$ . This is possible because the exponential for each term only takes on the values of 1 and  $e^K$ . Now expand the product to obtain sum over all the subgraphs of the lattice  $G$  the model was defined on

$$Z_G(q, K) = \sum_{\sigma} \sum_{G' \subset G} \prod_{\langle i, j \rangle} v\delta(\sigma_i, \sigma_j) \quad (2.5)$$

Notice that the product terms survive only if all the components of the graph carry the same spin state. Also, every surviving term will be equal to  $v^{b(G')}$  where  $b(G')$  is the number of edges of the graph  $G'$ . There will be precisely  $q^{n(G')}$  such terms (one for each possible choice of spin state for a given component) where  $n(G')$  is a number of components of the graph  $G'$ . So we arrive to

$$Z_G(q, K) = \sum_{G' \subset G} v^{b(G')} q^{n(G')} \quad (2.6)$$

For zero-temperature antiferromagnet this gives

$$P_G(q) = \sum_{G' \subset G} -1^{b(G')} q^{n(G')} \quad (2.7)$$

where  $P_G(q)$  is a chromatic function counting number of ways the graph  $G$  can be colored with  $q$  colors. Physical interpretation is that this gives a number of ground states and therefore is connected to zero-temperature entropy for the given Potts model.

At the conclusion we note that the form (2.6) leads to a nice duality

$$Z_G(q, K) = v^{b(G)} q^{1-N_D} Z_D(q, K^*) \quad (2.8)$$

where  $D$  is a dual graph to  $G$ ,  $N_D$  is the number of vertices in  $D$  and  $(e^K - 1)(e^{K^*} - 1) = q$ .

## 2.4. Relation to other models

Potts model is related to various other problems. This can give useful into Potts model's properties by analyzing other models and the Potts model results can be applied to study these related models. We already noted in section 3.1 that standard and planar Potts models are equivalent for  $q = 2$  and  $q = 3$  spin states. Let us now mention few non-trivial relations.

### 2.4.1. Percolation model

Start with a graph  $G$ . Bond-percolation model assigns probability  $p$  that a given edge will be occupied (and correspondingly  $1 - p$  that it will not be). Two vertices are said to be in the same cluster if there exists a path between them through occupied edges. Then one can investigate various properties of the clusters.

It can be shown that this is related is related to the  $q = 1$  Potts model on  $G$  [7]. To make sense of the  $q = 1$  limit one has to use the (2.6) re-expression of the partition function or similar.

To illustrate the connection one can for example show that [8]

$$c(\mathbf{r}, p) = \left[ \frac{\partial}{\partial q} \Gamma_{\alpha\alpha}(\mathbf{0}, \mathbf{r}) \right]_{q=1} \quad (2.9)$$

where  $c(\mathbf{r}, p)$  is the probability that vertices at the origin and at  $r$  belong to the same cluster and  $\Gamma_{\alpha\alpha}$  is the two-point correlation function of the corresponding Potts model.

These results can be generalized to site-percolation and mixed-percolation models where not only edges, but also vertices have a probability to be vacant.

#### 2.4.2. Vertex model

It can be shown that the two-dimensional Potts model is equivalent to ice-rule vertex model [9, 10]. To define the vertex model take a graph  $H$  where each vertex has precisely four neighbors. Then for each vertex consider the set oriented edges incident to it. Vertex model assigns a weight to each set that contains precisely two ingoing edges and two outgoing edges. There are six distinct possibilities for such sets. This model can be regarded as a crude model of ice, which is where the name comes from.

Now for a given graph  $G$  on which we would like to investigate the Potts model there exists a (non-unique) graph  $G'$  such that the vertex model formulated on  $G'$  is related to the Potts model on  $G$  by the following relation

$$Z_{Potts} = q^{N/2} Z_{Vertex} \quad (2.10)$$

where  $N$  is the number of vertices in  $G$ .

### 2.5. Potts antiferromagnet

Consider Potts model Hamiltonian as in (2.1) and take  $J$  negative. Then it is favorable for neighbors to carry different spin values. This behavior is called antiferromagnetic and it leads to many interesting properties. As already noted in the discussion of equation of (2.7), at zero temperature this model is equivalent to the problem of graph coloring. Usually (when  $q$  is high enough) there will be very many ways to color the graph and correspondingly a non-zero entropy at the zero temperature.

To qualitatively investigate the antiferromagnetic properties, it is useful to first recall the behavior of the ferromagnetic model. At low temperatures there is a tendency to form clusters of the same spin value. So in this class of models there usually appears a (energetically-driven) long-range order.

Compare this with the antiferromagnetic case. If one takes  $q$  high enough then there will be no long range order as there is no preference for any spin values at low temperatures, so it essentially behaves as in the high temperature case. However when  $q$  is small, there will be zero entropy at zero temperature. For example, take Ising model on square lattice. There at the zero temperature the spins on even sublattice will take one value and the spins on the odd the other. These sublattices will each behave as a ferromagnetic one, so we do not get anything new.

But for some special values of  $q$  – imagine  $2 < q < 4$  – there could appear interesting entropy-driven long-range order. And indeed, already in 1980 there were some indications [11] for the existence of the ordered low-temperature phase. One expects that for a given

graph  $G$  there should exist a value  $q_c(G)$  such that for all  $q > q_c(G)$  the model on  $G$  is unordered at all temperature, at  $q = q_c(G)$  the model will have a critical point at zero temperature.

Note that this long-range order depends strongly on the underlying graph structure and therefore it is very hard to analyze generally and to find all the universality classes [12]. We will return to these considerations in chapter 4 where we will investigate  $q = 3$  Potts antiferromagnet on a diced lattice.

### 3. CLUSTER EXPANSION

#### 3.1. Prelude

Cluster expansion is a useful tool for computing the free energy of a given system. The general idea behind this mechanism is that while partition function and free energy both contain the same amount of information about the system, in some instances it is much harder to compute the partition function because, as we will see, lot of terms in the free energy expansion will vanish.

Because general cluster expansion in abstract setting is not an entirely trivial matter, we will defer the formal treatment until the next section. Here we will just informally illustrate the method on a concrete example.

Consider an Ising model on a square lattice with ferromagnetic interaction between nearest neighbors. We will also enforce a homogeneous boundary condition to remove degeneracy of the ground state. To employ the cluster expansion, we first note a well-known Peierls duality between spin configuration and a set of mutually non-intersecting contours over the dual lattice. From the point of view of the spin model, contour is a boundary separating regions of different spin. <sup>1)</sup> Which means a contour must be non-intersecting closed line.

+	+	+	+	+	+	+	+
+	+	+	+	+	+	+	+
+	+	-	-	-	-	+	+
+	+	-	-	+	-	-	+
+	+	-	+	+	-	-	+
+	+	-	-	-	-	+	+
+	+	-	+	+	+	+	+
+	+	+	+	+	+	+	+

Image 3.1: *Contours for the Ising model on a square lattice*

The duality is as follows. We start from the boundary of the lattice, assigning to the lattice spins the value determined by the boundary condition. Every time we cross some contour, we flip the spin value we are assigning. Conversely, if we are given a spin configuration, we can easily determine the contours because these are just boundaries of regions having the same spin. This is illustrated in the image 3.1 where the spin values are denoted by + and -. There are two contours separating three regions.

Now the only thing remaining to establish the duality is to determine the energy cost of a given contour so that we can give a Boltzmann weight to every contour set. By definition, there is a spin flip at every line of the contour, so that total energy of the system will be proportional to the sum of lengths of the contours plus the energy of the ground state. The proportionality constant obviously depends only on the strength of the neighboring spin interaction and will not be important for the rest of this discussion.

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1) \*

We have thus reformulated the problem of ferromagnetic Ising model to the problem of a set of mutually non-intersecting contours with energy proportional to their length. The term *non-intersecting* is precisely what makes the cluster expansion work. This is so because free energy of such a system can be shown to be equal to the sum over mutually *intersecting* contours. Now, to see why this can be useful, consider  $N$  contours on a lattice with  $L$  sites,  $L$  being much larger than the size of any contour. In the partition function there are approximately  $L^N$  terms because on a big lattice we are relatively free to position small contours anywhere just keeping in mind they must not intersect. This is not so with free energy. There we need contours to be intersecting, so the number of terms will be proportional to  $L$  as now we only get to position contour system around as a whole. This, as a nice by-product, also shows that free energy in large  $L$  limit is proportional to the number of sites, as required for any well-behaved thermodynamic system.

### 3.2. Abstract treatment

In previous section we tried to illustrate the significance of the cluster expansion, but it is not yet clear how to formalize our statements nor is it obvious how to carry out an actual expansion for a given model. To elucidate these points, let us introduce an abstract formalism in the language of graph theory (for more details see [13]). In this view, previously mentioned contours will correspond to vertices, while the property of mutual intersection of two such vertices will be modeled by edges. Let us begin then by giving a few key definitions and proving the loosely stated statements in the previous section.

**Definition 3.1.** A *graph*  $G$  is a set of vertices  $V$  together with a binary relation  $E \subset V \times V$ . In the following, we will always require  $V$  to be countable and  $E$  to be non-reflexive and symmetric. We write  $G = (V, E)$ . We call the graph  $G$  *connected* (or *cluster*) if there exists a path connecting every pair of vertices. We will use a notation  $G(V')$  to denote a *restriction to a subgraph*  $(V', (V' \times V') \cap E)$ . When we will need to refer to the edge set of a given graph  $G$ , we will use notation  $E(G)$ . We denote by  $N(v) \equiv \{v' \in V | \exists (v, v') \in E\}$  the *neighbors* of  $v$ .

**Definition 3.2.** Let  $G = (V, E)$  be a graph. Set  $I \subset V$  is called *independent with respect to  $G$*  if  $\forall v_1, v_2 \in I \quad (v_1, v_2) \notin E$ . Let  $w : V \rightarrow \mathbb{C}$  be a complex function on the vertices of  $V$ . For all finite  $L \subset V$  we define the *partition function on  $L$*

$$Z_L(w) = \sum_{I \subset L} \prod_{v \in I} w(v) \quad (3.1)$$

where the sum runs over independent sets of  $L$  with respect to  $G$ .

**Definition 3.3.** Let  $S$  be a set. A *multiindex*  $X$  on  $S$  is any function  $X : S \rightarrow \mathbb{N}$ .<sup>1)</sup> We denote by  $\mathcal{X}(S)$  the *set of all multiindices on  $S$* . When there will be no risk of confusion which set we are working with, we will simply denote this set as  $\mathcal{X}$ . When the multiindex  $X$  is defined on a set of vertices of a graph  $G$ , we say  $X$  is a *cluster* whenever the graph  $G(\text{supp}(X))$  is a cluster.

Observe that  $Z_L(w)$  is a finite sum of real polynomials in  $w(v)$  taken as a vector in  $\mathbb{C}^L$ . Therefore it is analytic in  $w(v)$ . Moreover  $Z_L(0) = 1$  because the only contribution to the sum is from the empty set. Therefore we have the following result

---

1) \*

**Lemma 3.4.** *There exists  $U \subset \mathbb{C}^L$ , a neighborhood of 0, such that*

$$\forall w \in U \quad \log Z_L(w) = \sum_{X \in \mathcal{X}(L)} a_L(X) w^X \quad (3.2)$$

where  $w^X \equiv \prod_{v \in L} w(v)^{X(v)}$ .

**Proof:** Considering above remarks,  $\forall \varepsilon > 0$  there exists a neighborhood of 0,  $U_\varepsilon$ , such that  $\forall w \in U_\varepsilon \quad |Z_L(w) - 1| < \varepsilon$ . Therefore  $\log Z_L(w)$  is analytic on  $U_\varepsilon$  for any  $\varepsilon < 1$  and it agrees with its Taylor expansion which is precisely what the formula says.  $\square$

**Lemma 3.5.** *Coefficients  $a_L(X)$  have the following properties*

i)  $a_L(X) = a_{\text{supp}(X)}(X)$ , so that the coefficients  $a_L(X)$  are independent of the set  $L$ . From now on we therefore write just  $a(X)$ .

ii)  $a(X) = 0$  whenever induced subgraph  $G(\text{supp}(X))$  is not connected.

**Proof:**

i) Define  $w_0 : V \rightarrow \mathbb{C}$  such that  $\forall v \in \text{supp}(X) \quad w_0(v) \equiv w(v)$  and  $w_0(v) \equiv 0$  otherwise. Then we can see that  $Z_L(w_0) = Z_{\text{supp}(X)}(w)$  and  $\log Z_L(w_0) = \log Z_{\text{supp}(X)}(w)$  so that by Lemma 3.4 these functions have identical Taylor expansions and the claim follows.

ii) Suppose  $G(\text{supp}(X))$  is not connected. Then there must exist sets  $L_1, L_2 \subset V$  such that  $E(G(\text{supp}(X))) = E(G(L_1)) \cup E(G(L_2))$  and  $E(G(L_1)) \cap E(G(L_2)) = \emptyset$ . But then to any independent subset of  $L_1$  we can append any independent subset of  $L_2$  to get an independent subset of  $L$  which means that  $Z_{\text{supp}(X)}(w) = Z_{L_1}(w)Z_{L_2}(w)$  so that  $\log Z_{\text{supp}(X)}(w) = \log Z_{L_1}(w) + \log Z_{L_2}(w)$ . From this it is clear that there are no non-zero  $a(Y)$  terms in  $\log Z_{\text{supp}(X)}$  if  $Y$  contains vertices of both  $L_1$  and  $L_2$ . This is of course true for  $Y = \text{supp}(X)$ .  $\square$

Now we can see that the only terms contributing to the  $\log Z_L(w)$  come from connected components of  $G$  which is of course where the name *cluster* comes from. However, there is still one step left to perform. Until now, we have been restricting ourselves to finite subgraphs of the original graph  $G$ . To compute the true partition function (or its logarithm) for the whole graph  $G$ , we need to perform a limit with  $L \subset V$  arbitrary large. Given that the following convergence condition is satisfied, this can indeed be done.

**Definition 3.6.** Let  $R : V \rightarrow \mathbb{R}$ . We say it satisfies a *convergence condition* if

$$\exists r : V \rightarrow [0, 1) \quad \forall v \in V \quad R(v) \leq r(v) \prod_{v' \in N(v)} (1 - r(v')) \quad (3.3)$$

**Definition 3.7.** Let  $R : V \rightarrow \mathbb{R}$  and  $L$  a finite subset of  $V$ . We call the set

$$\mathcal{D}_{L,R} \equiv \{w : L \rightarrow \mathbb{C} \mid \forall v \in L : |w(v)| \leq R(v)\} \quad (3.4)$$

a *polydisc*.

Now we have everything in place to formulate the key result of this theory



**Theorem 3.8. Cluster expansion.** *There exists a function  $a : \mathcal{X} \rightarrow \mathbb{R}$  such that  $a(X) = 0$  whenever  $X$  is not a cluster. For every  $R$  satisfying a convergence condition (3.3) it holds that*

*i) For every finite  $L \in V$  and for all  $w \in \mathcal{D}_{L,R}$   $Z_L(w) \neq 0$  and*

$$\log Z_L(w) = \sum_{X \in \mathcal{X}(L)} a(X)w^X \quad (3.5)$$

*ii)*

$$\forall v \in V \quad \sum_{X \in \mathcal{X}, v \in \text{supp}(X)} |a(X)w^X| \leq -\log(1 - r(v)) \quad (3.6)$$

We will not prove this theorem. For more information see e.g. [13] and references therein. For the proof of this theorem with slightly weaker (but easier to work with) convergence condition, see [14].

Whenever the model under investigation enjoys the translational invariance (as is the case with all the models defined on a lattice) there will be about  $L$  identical terms in the cluster expansion that correspond to the cluster of the same shape, just translated. But this is precisely what we need to make the free energy  $F$  an extensive variable. Therefore, using an intensive free energy  $f$  we can write

$$-\beta f = \lim_{|L| \rightarrow \infty} \frac{1}{|L|} \log Z_L(w) = \lim_{|L| \rightarrow \infty} \sum_{X \in \mathcal{X}} a(X)w^X \quad (3.7)$$

where in the last summation it is understood that we sum only over one cluster from each translational orbit.

We will now compute few of the lowest order expansion coefficients as these will be essential for our following work. For this we will need a definition

**Definition 3.9.** Let  $X$  be a multiindex and  $G = (V, E)$  a graph. We define a graph  $\theta(X) \equiv (V', E')$  where the vertex set is  $V' \equiv \{v_i | \forall v \in V, 1 \leq i \leq X(v)\}$  and the edge set has the following property  $\forall v, w \in V, 1 \leq i \leq X(v), 1 \leq j \leq X(w) \quad (v_i, w_j) \in E' \leftrightarrow (v, w) \in E$ . Also  $\forall i, j \quad 1 \leq i < j \leq X(v) \quad (v_i, v_j) \in E'$ .

and the following result [15]

**Lemma 3.10.**

$$a(X) = \frac{1}{X!} \sum_{G \in \mathcal{G}_{|X|}, G \subset \theta(X)} (-1)^{|E(G)|} \quad (3.8)$$

where  $X! \equiv \prod_{v \in V} X(v)!$  and  $\mathcal{G}_n$  is a set of all connected subgraphs having  $n$  vertices.

As stated in lemma 3.5, the coefficients  $a(X)$  only depend on the  $\text{supp}(X)$ , not the whole graph. Therefore, the easiest way to compute these for small  $\text{supp}(X)$  seems to be direct expansion of the partition function  $Z_{\text{supp}(X)}$ . To simplify the notation a little bit, let us write  $w_i = w(v_i)$ . Let's start with a graph containing a single vertex. For such a graph we have

$$Z_1 = 1 + w_1 \quad (3.9)$$

$$\log Z_1 = \sum_{k=1}^{\infty} (-1)^{k+1} \frac{w_1^k}{k} \quad (3.10)$$

$$a_1(n) \equiv a(\{n\}) = \frac{(-1)^{k+1}}{k} = \frac{(-1)^{k+1}(k-1)!}{k!} \quad (3.11)$$

Thanks to lemma 3.10, we can immediately derive the following result

$$a(X) = \frac{1}{X!} \sum_{G \in \mathcal{G}_{|X|}, G \subset \theta(X)} (-1)^{|X|+1} (|X| - 1)! \quad (3.12)$$

whenever  $G(\text{supp}(X))$  is a complete graph. This is so because  $\theta(X)$  will then also be a complete graph and the summation in (3.8) will give the same result regardless of the exact form of  $X$ .

Therefore we can write

$$a_2(n, m) \equiv a(\{n, m\}) = \frac{(-1)^{n+m+1}(n+m-1)!}{n!m!} \quad (3.13)$$

$$a_3(n, m, k) \equiv a(\{n, m, k\}) = \frac{(-1)^{n+m+k+1}(n+m+k-1)!}{n!m!k!} \quad (3.14)$$

for the complete graph on two and three vertices respectively.

These simple closed forms only arise because the corresponding graph  $\theta(X)$  has very little structure. For generic clusters, one has to compute the coefficients one by one and the calculation can be tedious. That being said, for the purposes of this article it is enough to compute one more coefficient – the one whose cluster has three vertices and two edges –  $a_{3-2} \equiv a(\{1, 1, 1\})$ . For such a multiindex,  $\theta(X) = G(\text{supp}(X))$  and the only connected subgraph on three vertices is the graph itself. Therefore, according to (3.8) we have

$$a_{3-2} = 1 \quad (3.15)$$

### 3.3. Application to Ising model on square lattice

We will now formally reproduce statements about the ferromagnetic Ising model on a square lattice given in section 3.1 and compute few first terms of the free energy. Given a square lattice  $L$ , the energy of the configuration  $\sigma : L \rightarrow \{-1, 1\}$ <sup>1)</sup> We will refer to the range of values as spins is defined to be

$$H(\sigma) = -J \sum_{\langle i, j \rangle} \sigma_i \sigma_j \quad (3.16)$$

where  $J > 0$  is a coupling constant and the summation is over the nearest neighbors of the lattice. We will also assume a homogeneous boundary condition of the lattice. Partition function for this model will be

$$Z = \sum_{\sigma} \exp(-\beta H(\sigma)) = \sum_{\sigma} \exp(K \sum_{\langle i, j \rangle} \sigma_i \sigma_j) \quad (3.17)$$

---

1) \*

where we have used a dimensionless coupling  $K \equiv \beta J$ .

Now to establish Peierls duality, note that arbitrary configuration can be seen as a family of regions of the same spin. Contour is then defined to be a loop on a dual lattice that separates the regions of unequal spin. Because of the boundary condition, every spin configuration is in one-to-one correspondence to a set of contours which represent border lines (see image 3.1). Now, denote by  $\sigma_0$  a configuration that minimizes  $H$ . Such a configuration must be clearly homogeneous and with the same spin as is required by boundary condition. The corresponding contour set will therefore be empty. For every other configuration there will be some contours present and for every line of such a contour this will introduce an energy cost of  $2J$  when compared with the  $\sigma_0$ . We can thus re-express the partition function  $Z$  by summing over all the possible sets of mutually non-intersecting contours (denoted by  $\Gamma$ )

$$Z = \sum_{\Gamma} \exp(-\beta(H(\sigma_0) + \sum_{\gamma \in \Gamma} 2J|\gamma|)) \quad (3.18)$$

$$Z = Z_0 \sum_{\Gamma} \prod_{\gamma \in \Gamma} \exp(-2K|\gamma|) \quad (3.19)$$

where the  $Z_0 \equiv \exp(-\beta H(\sigma_0))$  is an unimportant prefactor that can't change the physics, so we can safely omit it from now on.

As we can see, we obtained a partition function in a form that we investigated in the previous section. The summation here is over independent sets of a graph that has a set of all possible contours as a set of vertices and where there is an edge between two such vertices precisely when they are intersecting. The weight for a given contour is  $w(\gamma) = \exp(-2K|\gamma|)$ .

Let us now discuss first few summands of the cluster expansion. There is only one (taking into regard the talk in section 3.2 about translational invariance) possibility for the contour of length four (encircling one square in the lattice). There are two possibilities for contours of length six (encircling two squares either vertically or horizontally). As for the length eight, there are the following clusters with one contour – one possibility of a contour encircling four squares, two possibilities for contours encircling three squares in a row and four contours encircling three squares that remain when one one square is removed from the above mentioned contour around four squares. As for the cluster on two contours, we have one possibility for two contours of length four one above each other. The other choice if the contours are touching on the side. This gives us two inequivalent possibilities. We could continue, but this is enough for illustration purposes. According to result (3.7) we can thus write

$$\begin{aligned} -\beta f &= a_1(1)(\exp(-8K) + 2 \exp(-12K) + 7 \exp(-16K)) \\ &\quad + a_1(2) \exp(-8K)^2 + a_2(1, 1) \exp(-8K)^2 + \dots \\ &= \exp(-8K) + 2 \exp(-12K) + \frac{11}{2} \exp(-16K) + \dots \end{aligned} \quad (3.20)$$

where we have used that  $a_1(1) = 1$ ,  $a_1(2) = -\frac{1}{2}$ ,  $a_2(1, 1) = -1$ .

## 4. POTTS ANTIFERROMAGNET ON A DICED LATTICE

### 4.1. Definition

To define diced lattice we have to start with a couple of definitions

**Definition 4.1.** *Medial graph*  $M(G) = (V', E')$  of a graph  $G = (V, E)$  is obtained by taking  $V' = E$  and taking  $(e_1, e_2) \in E'$  whenever edges  $e_1 \neq e_2 \in E$  have a common vertex and belong to the same face.

**Definition 4.2.** Let  $V''$  equal to the set of faces of  $G$  and let there be an edge  $(f_1, f_2 \in E'')$  whenever the faces  $f_1, f_2$  are adjacent.

Now begin with a triangular lattice. Apply the above construction to obtain its medial graph. This is called Kagome lattice. Diced lattice is then a dual of the Kagome lattice. This lattice is bipartite meaning that the vertices can be divided in two disjoint sets such that there is no edge between the vertices of the same set. This can be seen in the image 4.1.

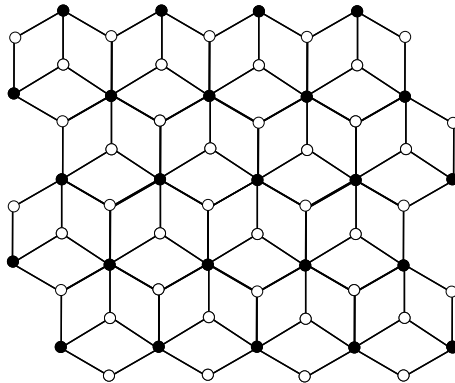


Image 4.1: *Diced lattice*

Kotecký, Salas, and Sokal [12] showed that on such a lattice, 3-states Potts antiferromagnet will have a phase transition at a non-zero temperature.

### 4.2. Low temperature expansion

The Hamiltonian for Potts antiferromagnet is

$$\beta H = \sum_{\langle i,j \rangle} +K \delta(\sigma_i, \sigma_j) \quad (4.1)$$

where the sum is over nearest neighbors and  $K = -\beta J > 0$  is the dimensionless coupling. Partition function for this Hamiltonian is

$$Z = \sum_{\sigma} \exp(K \sum_{\langle i,j \rangle} \delta(\sigma_i, \sigma_j)) \quad (4.2)$$

where the first sum is over all spin configurations.

Following [12], we integrate the spins on the hexagonal sublattice and obtain model on triangular lattice with triangle Boltzmann weights  $(w_1, w_2, w_3)$

$$\begin{aligned} w_1 &= e^{-3K} + 2 \\ w_2 &= e^{-2K} + e^{-K} + 1 \\ w_3 &= 3e^{-K} \end{aligned} \quad (4.3)$$

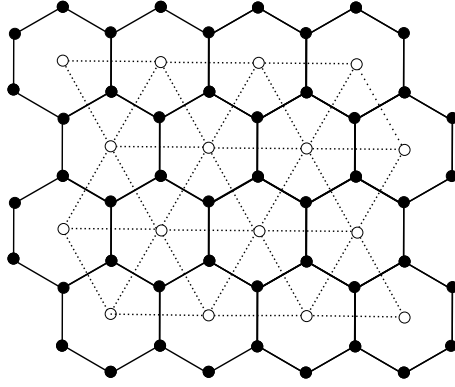


Image 4.2: *Hexagonal and triangular lattices*

depending on how many distinct spin values given triangle has.

In the image 4.2 one can see the remaining triangular lattice (shown with white vertices and dotted edges) as well as its dual – the hexagonal lattice (black vertices and full edges). It is this dual hexagonal lattice that will play the main role in the following, because Peierls correspondence always passes from the graph to its dual. <sup>1)</sup>Note that we did not discuss this in the square lattice case because there the dual is again a square lattice. However, the notion of contour is slightly more complex this time because of the three spin states. In particular, because contour separates the domains of different spins it will have to carry a notion of two inner spin values. Therefore the contour will also have to have inner structure that denotes distribution of these two spins. There will always be two ways how to assign spin values to a given contour (see image 4.3 and note that the values 2 and 3 can be swapped), so this does not give us an isomorphism, but it suffices for the purpose of computing partition function.

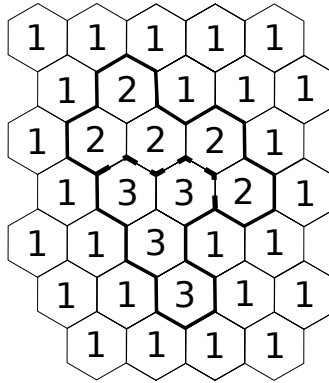


Image 4.3: *Peierls contour on a hexagonal lattice*

The partition function – in the contour form – thus becomes

$$Z = 3 \sum_{\Gamma \in \delta_{hex}} 2^{|\Gamma|} \prod_{v \in hex} \begin{cases} w_1 & \forall \gamma \in \Gamma v \notin \gamma \\ w_2 & \deg(v) = 2 \\ w_3 & \deg(v) = 3 \end{cases} \quad (4.4)$$

where  $\Gamma$  is a contour set,  $\delta_{hex}$  denotes the set of all contour sets on the hexagonal sublattice and  $hex$  denotes hexagonal sublattice itself. We can carry out the production on the

---

<sup>1)</sup> \*

hexagonal sublattice and we obtain

$$Z = 3w_1^N \sum_{\Gamma \in \delta_{hex}} 2^{|\Gamma|} x^{\Gamma_2} y^{\Gamma_3} \quad (4.5)$$

where  $N \equiv |hex|$  is the number of sites of the hexagonal sublattice,  $x \equiv w_2/w_1$ ,  $y \equiv w_3/w_1$  and  $\Gamma_i$ ,  $i = 2, 3$  denotes the number of vertices of degree  $i$  in the contour set. We can already see that the partition function is in the form required by cluster expansion. If we denote

$$w(\gamma) \equiv 2x^{\gamma_2} y^{\gamma_3} \quad (4.6)$$

then the partition function will have the form

$$Z = 3w_1^N \sum_{\Gamma \in \delta_{hex}} \prod_{\gamma \in \Gamma} w(\gamma) \quad (4.7)$$

and we can apply cluster theorem to obtain the free energy. But first, let us investigate the zero temperature entropy.

#### 4.2.1. Zero temperature entropy

We start with zero temperature computations because – as can be seen from (4.3) –  $w_3$  and  $y$  terms are zero. This is just a restatement of a simple fact that at zero temperature it is forbidden for the antiferromagnet to have nearest neighbors in the same state. Thanks to this observation contours will have simple form that we have already encountered in the previous chapter.

Also note that at zero temperature  $x = 1/2$  and  $\gamma_2 = |\gamma|$ . Therefore the longer the contour, the less it contributes to the free energy. For the purposes of this work, we will enumerate all the contours with number of vertices less than 22 (that gives us a rough precision estimate  $2^{-20} \approx 10^{-6}$ ).

Note that to correctly compute the cluster expansion, we have count each contour once and only once. But there can be many contours that differ only by rotation or reflection. We will consider this set as a single contour and write down the corresponding symmetry factor. This information – along with the length of the given contour – is shown in tables A.1, A.2 and A.3.

To save space, we show just a dual graph of a subgraph bounded by a given contour. The vertices of this graph belong to the triangular sublattice of the original diced lattice, as discussed above. Recall that each of these contours only correspond to single vertex cluster. One also has to consider the sets of mutually intersecting contours (these correspond to higher coefficients in cluster expansion  $a(2)$ ,  $a(1, 1)$ , etc.). Nevertheless, keeping in mind that we want our contours to have less than 22 vertices and that the smallest contours are of length 6 and 10, there are not so many possibilities left. All of these were accounted for.

To obtain the entropy, we note that

$$F = U - TS \quad (4.8)$$

At zero temperature there is zero energy. Putting this in (3.7) we obtain

$$s = k_B \lim_{|L| \rightarrow \infty} \frac{1}{|L|} \log Z_L(w) \quad (4.9)$$

Plugging in (4.7) and second equality in (3.7) we get

$$s = k_B \left( w_1 + \sum_{X \in \mathcal{X}} a(X) w^X \right) \quad (4.10)$$

which, using the results found in the tables and the knowledge of  $a(X)$  given in (3.11) through (3.15) evaluates to

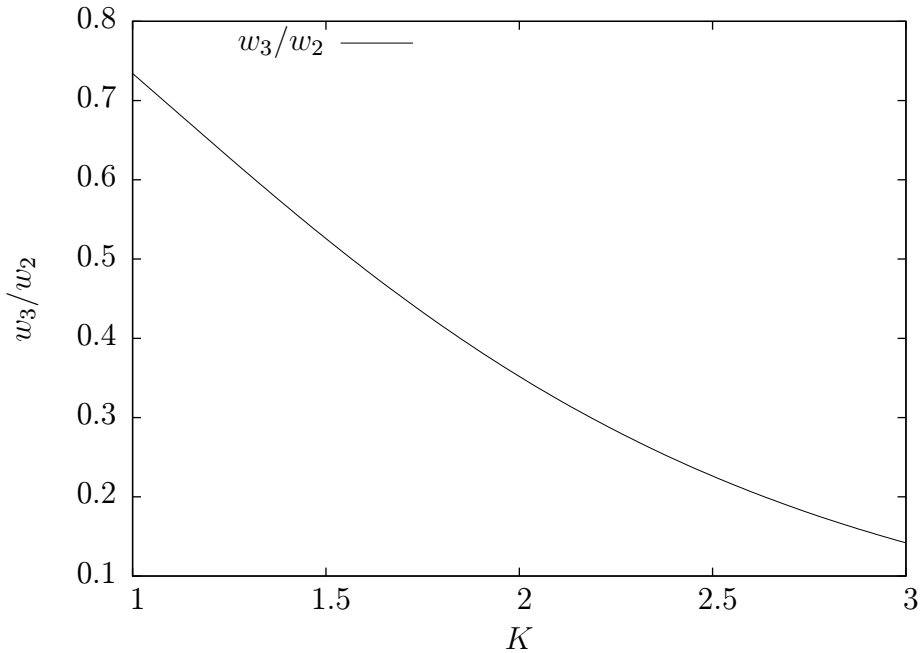
$$s = k_B \left( 2 - \frac{1}{3} (1836 x^{20} - 566 x^{18} + 252 x^{16} - 72 x^{14} + 66 x^{12} - 18 x^{10} - 6 x^6) + \dots \right) \quad (4.11)$$

$$s \approx 2.032 k_B \quad (4.12)$$

#### 4.2.2. Free energy at finite temperature

At finite temperature we also have to allow for more complex contours containing degree three vertices. These can be presented as contours in tables in the previous section, but now we allow for two colors of vertices (representing two possible spin values).

However, because near zero temperature  $w_3$  is almost zero, these contours will not change the situation much. We can make this statement more precise by looking at the graph 4.1



Graph 4.1:  $w_3$  decay

By requiring that  $K > 2$  (low-temperature condition) so that the ratio  $\frac{w_3}{w_2} = \frac{y}{x} < 2^{-3/2}$  we can usefully re-express the weight (4.6) as

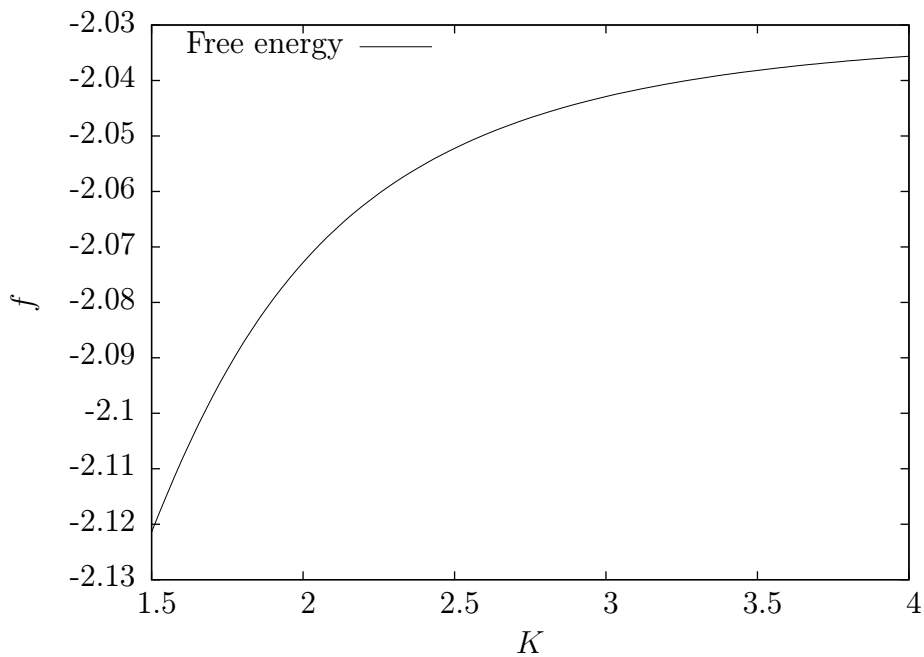
$$w = 2x^{|\gamma|} \left( \frac{y}{x} \right)^{\gamma_3} \quad (4.13)$$

to easily consider which contours to include in our calculation in order to satisfy the rough  $10^{-6}$  estimate using the fact that degree three vertex increases the precision about the same as  $3/2$  of degree two vertices (keeping in mind that  $x \approx 1/2$  near zero temperature). Also note that smallest contour that can contain a degree three vertex is the second one in the table A.1 and it is already of the order  $2^{-13}$ . Therefore it suffices to consider only single vertex clusters.

From (3.7), results from the previous section and accounting of the contours with degree three vertices we finally arrive at the expression for the free energy

$$\begin{aligned}
 f = -\frac{k_B T}{3} & \left( 3w_1 - 1836x^{20} + 566x^{18} - 252x^{16} + 72x^{14} - 66x^{12} + 18x^{10} + 6x^6 + \right. \\
 & + (666x^{16} + 288x^{15} + 126x^{14} + 36x^{13} + 108x^{12} + 36x^{11} + 18x^8) y^2 + \\
 & \left. + (18x^{12} + 54x^{10}) y^4 \right)
 \end{aligned}
 \tag{4.14}$$

This result with  $\beta = 1$  is plotted in graph 4.2. Note that there should be a critical point around  $K = 1.971$  [12], but of course this can not show up in cluster expansion which gives only analytical results.



Graph 4.2: *Free energy*



## 5. CONCLUSION

The purpose of this work was to get familiar with the Potts model. In chapter two we presented its definition and history. We reviewed the mean-field approximation, which is very useful for providing basic information about the model, although one has to be careful because this approximation often fails in the cases one is most interested in.

As is often the case in statistical physics and combinatorics, there exist various useful dualities between seemingly unrelated models and expressions. Thus we were able to conclude relation of Potts model to the graph coloring problems. We looked at percolation and ice-rule models and noted that Potts model can give useful insights into these models as well (or vice-versa). We have also qualitatively discussed the behavior of the Potts antiferromagnet. For the certain values of  $q$  there can appear an entropy-driven long-range order in this model. This behavior depends strongly on the microscopic structure of the lattice and still is not very well understood.

We have acquainted ourselves with the method of cluster expansion and in chapter three gave an informal introduction as well as a rigorous treatment of the subject. With the use of the famous Peierls duality we were then able to compute the low-temperature free energy of the Ising model on a square lattice.

In chapter four we turned to the main subject of this work – investigation of the Potts antiferromagnet on a diced lattice using the acquired knowledge of cluster expansion. We were again able to use Peierls-like duality and by enumerating all the possible low-temperature clusters were able to derive the zero-temperature entropy and low-temperature free energy.

# APPENDIX

In this section we present information on Peierls contours on a hexagonal lattice.




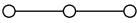
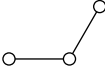
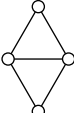
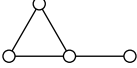
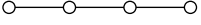
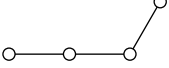
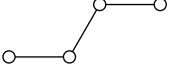
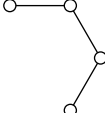
Contour	Symmetry factor	Length
	1	6
	3	10
	2	12
	3	14
	6	14
	3	14
	12	16
	3	18
	12	18
	6	18
	6	18

Table A.1: *Contours 1–11*

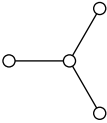
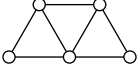
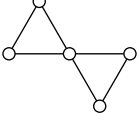
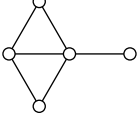
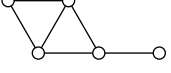
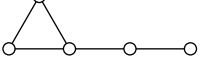
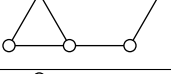
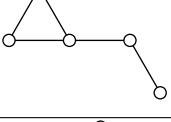
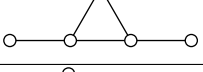
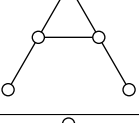
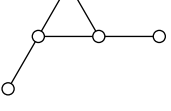
Contour	Symmetry factor	Length
	2	18
	6	16
	3	18
	6	18
	12	18
	12	20
	12	20
	12	20
	6	20
	6	20
	12	20

Table A.2: *Contours 12-22*

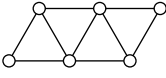
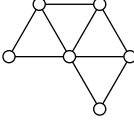
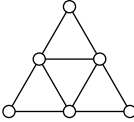
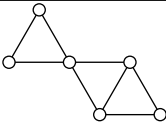
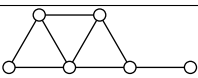
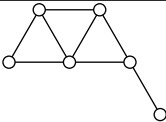
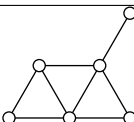
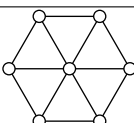
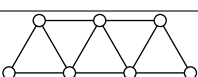
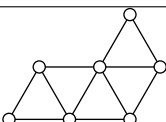
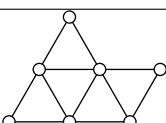
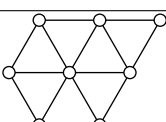
Contour	Symmetry factor	Length
	6	18
	6	18
	2	18
	3	20
	12	20
	12	20
	12	20
	1	18
	6	20
	12	20
	12	20
	6	20

Table A.3: *Contours 22–34*

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