Graph parameters and invariants of the orthogonal group

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Chapter 3

Partition functions of edge- and vertex-coloring models

In this chapter we give formal definitions of edge- and vertex-coloring models and their partition functions. We will also discuss the action of the orthogonal group on edge-coloring models and explain why this action leaves the partition function invariant.

Whereas our intention in this thesis is for example to characterize partition functions of edge-coloring models and study connections between invariant theory of the orthogonal group, partition functions of edge-coloring models have also been studied in different contexts. We will briefly say a few things about that in this chapter.

3.1 Graph parameters from statistical models

The graph parameters that we study in this thesis were introduced by de la Harpe and Jones [28] in 1993 and are motivated by statistical models. Although we will not discuss any relation of our work to statistical mechanics, it makes sense to say a few words about the origin of these graph parameters. Statistical physics is a huge area of research and we will not make any attempt to say much about it. We refer to [2, 29] for an introduction to statistical physics and its connections to graph theory.

We will now introduce the Ising model and show how it can be generalized to obtain interesting graph parameters. This introduction is based on [40].
The Ising model
Let $H$ be a finite lattice; for example the $n \times n$ grid. We can think of the vertices of $H$ as the atoms of some crystal, where each of the atoms can have an up or down spin. This will be modeled by a 1 and a $-1$ respectively. An assignment of spins to the vertices of $H$ is called a state. This is described by a map $\sigma : V(H) \rightarrow \{-1,1\}$. Two vertices that are adjacent in $H$ have an interaction energy, which, in the Ising model, is equal to some real number $-J$, if the atoms have the same spin and which is equal to $J$, if the atoms have opposite spin. For a state $\sigma \in \{-1,1\}^{V(H)}$, the total energy of this state is given by

$$H(\sigma) = -\sum_{uv \in E(H)} J\sigma(u)\sigma(v). \quad (3.1)$$

The probability of a system to be in state $\sigma$ is proportional to $e^{-H(\sigma)/kT}$, where $T$ denotes the temperature, and $k$ the Boltzmann constant. As probabilities add up to one, these values need to be normalized; the normalizing factor $Z$ is the partition function of the system:

$$\sum_{\sigma : V(H) \rightarrow \{-1,1\}} e^{-H(\sigma)/kT} = \sum_{\sigma : V(H) \rightarrow \{-1,1\}} \exp \left( \frac{1}{kT} \sum_{uv \in E(H)} J\sigma(u)\sigma(v) \right). \quad (3.2)$$

The physical behavior of the system depends very much on the signature of $J$, but we will however not discuss this. Instead we will show how we can obtain interesting graph parameters from partition functions of generalizations of the Ising model.

The spin model
Let

$$S := \begin{pmatrix} \exp(J/kT) & \exp(-J/kT) \\ \exp(-J/kT) & \exp(J/kT) \end{pmatrix}. \quad (3.3)$$

This allows to rewrite (3.2) as follows:

$$Z = \sum_{\sigma : V(H) \rightarrow \{1,2\}} \prod_{uv \in E(H)} S_{\sigma(u),\sigma(v)}. \quad (3.4)$$

From a mathematical point of view, the parameters $k$, $T$ and $J$ are just constants; so we might as well replace $S$ by an arbitrary symmetric $2 \times 2$ matrix. Then (3.4) might not have any physical interpretation, but it still assigns a number to the graph $H$. Of course we can calculate (3.4) for any graph $H$, it need not represent any crystal structure. In other words (3.4) describes a graph parameter.

The next step is to generalize it to symmetric $n \times n$ matrices for arbitrary $n$. We then end up with what de la Harpe and Jones [28] call a spin model. The
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The partition function of a spin model is a similar expression as (3.4), except that the sum is now taken over all maps from $V(H)$ to $[n]$.

From a physical point of view it is natural to equip the Ising model with an external magnetic field. In the simplest case we just need to add $-\sum_{v \in V(H)} h \sigma(u)$ to (3.4), for some number $h$, to obtain the total energy of the state $\sigma$. For (3.4) this implies we would, for each $\sigma$, have to multiply $\prod_{uv \in E(G)} S_{\sigma(u), \sigma(v)}$ by the term $\prod_{v \in V(H)} \exp(-h \sigma(v)/kT)$ to obtain the partition function of the model. Again, this can be generalized by replacing the vector $(\exp(-h/kT), \exp(h/kT))$ by any nonnegative vector (or even any complex one). See Section 3.2 for the formal definition.

The vertex model

By viewing the edges of the graph $H$ as particles or atoms and thinking of the vertices of $H$ as the interaction between them, we get a different physical model. Since a vertex can be incident with an arbitrary large number of edges, a symmetric matrix does not suffice to describe the energy of a system. If we allow each particle to be in $k$ possible states, we need for each multiset of colors $\{c_1, \ldots, c_d\}$, with $c_1, \ldots, c_d \in \{1, \ldots, k\}$, a real number. That is we have a map $h : \mathbb{N}^k \to \mathbb{R}$. De la Harpe and Jones call $h$ a vertex model. The partition function of $h$ is a similar expression as (3.4), but the role of edges and vertices is interchanged (cf. (1.1)). See section 3.3 for the formal definition.

Edge-and vertex-coloring models

As the partition functions of the respective generalizations of the Ising model generalize graph and linegraph coloring (cf. Sections 3.2 and 3.3 below), we choose to call them vertex-coloring models instead of spin models and edge-coloring models instead of vertex models to emphasize their combinatorial interpretation. This is consistent, at least for edge-coloring models, with the book by Lovász [40], but in the literature (including the work of the author) both terminologies have been used.

3.2 Partition functions of vertex-coloring models

Let $a \in (\mathbb{F}^*)^n$ and let $B \in \mathbb{F}^{n \times n}$ be a symmetric matrix. We call the pair $(a, B)$ an $n$-color vertex-coloring model over $\mathbb{F}$. We think of $n$ as the number of colors of the model (or states from the physical point of view). When talking about a vertex-coloring model, we will sometimes omit the number of colors or the field of definition. In case $(a, B)$ is defined over $\mathbb{F} = \mathbb{R}$ and $a_i > 0$ for each $i = 1, \ldots, n$, we will call $(a, B)$ a real vertex-coloring model. The partition function
of an $n$-color vertex coloring model $(a, B)$ is the graph invariant $p_{a,B} : \mathcal{G} \to \mathbb{F}$ defined by

$$p_{a,B}(H) := \sum_{\phi : V(H) \to [n]} \prod_{v \in V(H)} a_{\phi(v)} \cdot \prod_{uv \in E(H)} B_{\phi(u), \phi(v)}$$

for $H \in \mathcal{G}$. Clearly, $p_{a,B}$ is multiplicative.

If one takes $a = 1$, the all ones vector, and $B$ the adjacency matrix of a graph $G$, then $p_{1,B}(H) = \text{hom}(H, G)$, the number of homomorphisms from $H$ to $G$ (adjacency preserving maps from $V(H)$ to $V(G)$). In particular, for $G = K_n$, the complete graph on $n$ vertices, $\text{hom}(H, G)$ counts the number of proper vertex-colorings of $H$ with $n$ colors.

For general $(a, B)$, we can view $p_{a,B}$ in terms of weighted homomorphisms. Let $G(a, B)$ be the complete graph on $n$ vertices (including loops) with vertex weights given by $a$ and edge weights given by $B$. Then $p_{a,B}(H)$ can be viewed as counting the number of weighted homomorphisms of $H$ into $G(a, B)$. In this context $p_{a,B}$ is denoted by $\text{hom}(\cdot, G(a, B))$. In this thesis we will use both $p_{a,B}$ and $\text{hom}(\cdot, G(a, B))$ to denote the same graph parameter.

**Twins**

Let $(a, B)$ be an $n$-color vertex-coloring model. We say that $i, j \in [n]$ are twins of $(a, B)$ if $i \neq j$ and the $i$th row of $B$ is equal to the $j$th row of $B$. If $(a, B)$ has no twins we call the model twin free. Suppose now $i, j \in [n]$ are twins of $(a, B)$. If $a_i + a_j \neq 0$, let $B'$ be the matrix obtained from $B$ by removing row and column $i$ and let $a'$ be the vector obtained from $a$ by setting $a'_j := a_i + a_j$ and then removing the $i$th entry from it. In case $a_i + a_j = 0$, we remove the $i$th and the $j$th row and column from $B$ to obtain $B'$ and we remove the $i$th and the $j$th entry from $a$ to obtain $a'$. Then $p_{a',B'} = p_{a,B}$. So for every vertex-coloring model with twins, we can construct a vertex-coloring model with fewer colors which is twin free and which has the same partition function.

At several points in this thesis we will assume that an $n$-color vertex-coloring model is twin free. By the above we do not lose any graph parameters in this way.

### 3.3 Partition functions of edge-coloring models

Let

$$R(\mathbb{F}) := \mathbb{F}[x_1, \ldots, x_k]$$

denote the polynomial ring in $k$ variables. We will usually just write $R$ instead of $R(\mathbb{F})$. Note that there is a one-to-one correspondence between elements of $R^*$
and maps \( h : \mathbb{N}^k \to \mathbb{F} \); \( \alpha \in \mathbb{N}^k \) corresponds to the monomial \( x^\alpha := x_1^{\alpha_1} \cdots x_k^{\alpha_k} \in R \) and the monomials form a basis for \( R \). Moreover, \( \alpha \in \mathbb{N}^k \) corresponds to a multiset of \([k] \); \( \alpha_i \) is the multiplicity of \( i \).

We call any \( h \in R^* \) a \( k \)-color edge-coloring model over \( \mathbb{F} \). We think of \( k \) as the number of colors of the model (or states from the physical point of view). When talking about an edge-coloring model, we will sometimes omit the number of colors or the field of definition. In case \( h \) is defined over \( \mathbb{F} = \mathbb{R} \), we will sometimes call \( h \) a real edge-coloring model. The partition function of a \( k \)-color edge-coloring model \( h \) is the graph parameter \( p_h : \mathcal{G} \to \mathbb{F} \) defined by

\[
p_h(H) := \sum_{\phi : E(H) \to [k]} \prod_{v \in V(H)} h\left( \prod_{e \in \delta(v)} x_{\phi(e)} \right)
\]

for \( H \in \mathcal{G} \). Here \( \delta(v) \) is the multiset of edges incident with \( v \). Note that, by convention, a loop is counted twice. Moreover, observe that \( p_h(\emptyset) = k \), as the empty product is equal to 1 by definition. Clearly, \( p_h \) is multiplicative.

Many interesting graph parameters are partition functions of edge-coloring models. Let us give a few examples.

**Example 3.1** (Counting perfect matchings). Let \( k = 2 \). Define the the edge-coloring model \( h : \mathbb{F}[x_1, x_2] \to \mathbb{F} \) by \( h(x_1^{\alpha_1} x_2^{\alpha_2}) = \delta_{\alpha_1,1} \). Then \( p_h(H) \) is equal to the number of perfect matchings of \( H \). (A perfect matching in a graph \( H \) is a set of edges that covers each vertex exactly once.) To see this, note that for an assignment of the colors to the edges of \( H \) there is a contribution in the sum (3.7) if and only if at each vertex there is a unique edge which is colored with 1, that is, if and only if the edges colored with 1 form a perfect matching.

**Example 3.2** (Counting proper \( k \)-edge-colorings). Let \( k \in \mathbb{N} \). Define the \( k \)-color edge-coloring model \( h \) by

\[
h(x_1^{\alpha_1} \cdots x_k^{\alpha_k}) = \begin{cases} 
1 & \text{if } \alpha_i \leq 1 \text{ for all } i \in [k], \\
0 & \text{otherwise.}
\end{cases}
\]

(3.8)

Then \( p_h(H) \) is equal to the number of proper \( k \)-edge-colorings of \( H \).

**Example 3.3** (Counting linegraph homomorphisms). Let \( G = (V, E) \) be a simple graph with \( k \) edges. Identify \( E \) with \([k]\) and define the \( k \)-color edge-coloring model \( h \) by

\[
h(x_1^{\alpha_1} \cdots x_k^{\alpha_k}) = \begin{cases} 
1 & \text{if all } \alpha_i \leq 1 \text{ and if the edges } i \in [k] \text{ such that } \\
\alpha_i = 1 \text{ meet in a unique vertex in } G, \\
0 & \text{otherwise.}
\end{cases}
\]

(3.9)
Then $p_h(H)$ is equal to the number of homomorphisms from the linegraph of $H$ to the linegraph $L(G)$ of $G$.

We will see later that partition functions of vertex-coloring models over $\mathbb{C}$ are partition functions of edge-coloring models over $\mathbb{C}$ (cf. Lemma 7.1). So also the number of (ordinary) homomorphisms is the partition function of an edge-coloring model.

### 3.4 Tensor networks

We will introduce tensor networks in this section and show that they allow to give a more conceptual interpretation of the partition function of an edge-coloring model $h$.

Let $V$ be $k$-dimensional vectorspace over $\mathbb{F}$ equipped with a symmetric non-degenerate bilinear form $(\cdot, \cdot)$, i.e., $(\cdot, \cdot) : V \times V \to \mathbb{F}$ is a symmetric bilinear map such that for each nonzero $v \in V$ there exists $v' \in V$ such that $(v, v') \neq 0$. The bilinear form induces a nondegenerate symmetric bilinear form on the $l$-th tensor power, $V^\otimes l$, of $V$, via

$$(v_1 \otimes \cdots \otimes v_l, u_1 \otimes \cdots \otimes u_l) := \prod_{i=1}^{l} (v_i, u_i) \quad (3.10)$$

for $u_1, v_1, \ldots, u_l, v_l \in V$.

Let $H = ([n], E)$ be a graph. Let for $i \in [n]$, $h_i \in V^\otimes d(i)$. (Recall that $d(i)$ denotes the degree of vertex $i$.) Assume that we have some specific ordering of $\delta(i)$ for each $i \in [n]$. Then $(H, h_1, \ldots, h_n)$ is called a tensor network. To a tensor network we can associate an element of $\mathbb{F}$ by contracting the network, as we will now describe.

For $1 \leq i < j \leq l \in \mathbb{N}$ the contraction $C_{i,j}^l : \forall \in \mathbb{N}$ the contraction $C_{i,j}^l$ is the unique linear map

$$C_{i,j}^l : V^\otimes l \to V^\otimes l-2 \quad (3.11)$$

satisfying

$$v_1 \otimes \cdots \otimes v_l \mapsto (v_i, v_j) v_1 \otimes \cdots \otimes v_{i-1} \otimes v_{i+1} \cdots \otimes v_{j-1} \otimes v_{j+1} \otimes \cdots \otimes v_l.$$

Let $h = h_1 \otimes \cdots \otimes h_n \in V^\otimes 2m$, where $m$ denotes the cardinality of $E$. An edge $e \in E$ gives rise to a unique contraction $C_{i,j}^{2m}$ for some $i, j \in [2m]$. Then the contraction of $(H, h)$ along $e$ is the pair $(H', h')$ where $H'$ is the graph obtained from $H$ by removing $e$ and identifying the endpoints of $e$ (an edge parallel to...
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$e$ becomes a loop in this way) and $h' := C_{ij}^{2m}(h)$. Note that $h'$ is again of the form $h' = h_1' \otimes \cdots \otimes h_m'$, with $n' = n$ if $e$ is a loop and $n' = n - 1$ otherwise. If $m = 1$, this contraction just gives an element of $\mathbb{F}$. The contraction of the tensor network $(H, h_1, \ldots, h_n)$ is the element of $\mathbb{F}$ obtained by recursively contracting $(H, h)$ along any sequence of edges $e_1, \ldots, e_m$. (This does not depend on the chosen sequence as the form is symmetric and bilinear.)

Suppose that $V$ has an orthonormal basis $e_1, \ldots, e_k$ with respect to $(\cdot, \cdot)$. (If $\mathbb{F}$ is algebraically closed, an orthonormal basis always exists, but for example for $\mathbb{F} = \mathbb{R}$ such a basis need not exist.) Define for $\phi : [d] \to [k]$, $e_\phi := e_{\phi(1)} \otimes \cdots \otimes e_{\phi(d)}$ and note that the $e_\phi$ form an orthonormal basis for $V^\otimes d$. Let $x_1, \ldots, x_k$ be the associated dual basis for $V^*$ and let $h \in \mathbb{F}[x_1, \ldots, x_k]^*$. Let $H([n], E)$ be a graph and let for $v \in [n], h_v$ be the restriction of $h$ to the space of homogeneous polynomials of degree $d(v)$. We can view $h_v$ as a symmetric tensor in $V^\otimes d(v)$. That is, for each $\phi : [d(v)] \to [k]$,

$$(h_v, e_\phi) = h(x_{\phi(1)} \cdots x_{\phi(d(v))}).$$

(3.12)

Then it is easy to see that $p_H(H)$ is equal to the contraction of the tensor network $(H, h_1, \ldots, h_n)$ (taking any ordering of $\delta(i)$ for $i \in [n]$, as the $h_i$ are symmetric). This will be spelled out in Section 6.2. For completeness, we will now sketch a proof of this fact here. Using (3.12) we find that

$$p_H(H) = \sum_{\phi : E \to [k]} \prod_{i=1}^{n} h(\prod_{e \in \delta(i)} x_{\phi(e)}) = \sum_{\phi : E \to [k]} \prod_{i=1}^{n} (h_i, \bigotimes_{e \in \delta(i)} e_{\phi(i)})$$

(3.13)

$$= \sum_{\phi : E \to [k]} (h_1 \otimes \cdots \otimes h_n, \bigotimes_{e \in E} e_{\phi(e)}).$$

The last line of (3.13) is equal to the contraction of $(H, h_1, \ldots, h_n)$, as for any $v \in V^\otimes 2$, $C_{12}^2(v) = \sum_{i=1}^{k} (v, e_i \otimes e_i)$.

Remark. Using tensor networks, we obtain a coordinate-free definition of partition function of edge-coloring models. Many results in this thesis have analogues that are coordinate-free, but for the sake of concreteness, we will mostly work with a fixed orthonormal basis and formulas such as (3.7).

3.5 The orthogonal group

As in the previous section, let $V$ be a $k$-dimensional vector space over $\mathbb{F}$ that is equipped with a nondegenerate symmetric bilinear form $(\cdot, \cdot)$. The orthogonal group $O_k(\mathbb{F})$ is the group of invertible linear maps $g : V \to V$ such that
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\((gu, gv) = (u, v)\) for all \(u, v \in V\). We do not indicate the dependency on the bilinear form. Moreover, we will usually write \(O_k\) instead of \(O_k(\mathbb{F})\).

If \(V\) admits an orthonormal basis \(e_1, \ldots, e_k\) with respect to \((\cdot, \cdot)\), then, with respect to this basis, \(O_k\) is the set of \(\mathbb{F}\)-valued \(k \times k\) matrices \(g\) such that \(g^T g = I\), where \(I\) denotes the \(k \times k\) identity matrix.

By \(O(V)\) we denote the algebra generated by the linear maps on \(V\). If we choose a basis \(x_1, \ldots, x_k\) for \(V^*\), this is just the polynomial ring \(R\). The group \(O_k\) acts on \(O(V)\) as follows:

\[
\text{for } p \in O(V), \ g \in O_k \text{ and } v \in V, \ (gp)(v) := p(g^{-1}v). \quad (3.14)
\]

This action induces an action on \(O(V)^*\) (and hence on edge-coloring models) as follows:

\[
\text{for } h \in O(V)^*, \ p \in O(V) \text{ and } g \in O_k, \ (gh)(p) = h(g^{-1}p). \quad (3.15)
\]

The orthogonal group acts linearly on \(V^\otimes l\):

\[
\text{for } v = v_1 \otimes \cdots \otimes v_l \in V^\otimes l \text{ and } g \in O_k, \ gv := gv_1 \otimes \cdots \otimes gv_l. \quad (3.16)
\]

It is a well-known fact that \(V\) and \(V^*\) are isomorphic as \(O_k\)-modules. Indeed, define the map \(\tau : V \to V^*\) by \(\tau(v)(u) = (v, u)\) for \(v, u \in V\). Then for \(g \in O_k\)

\[
\tau(gv)(u) = (gv, u) = (v, g^{-1}u) = (g\tau(v))(u). \quad (3.17)
\]

So for the \(O_k\)-action it does not matter whether we think of a \(k\)-color edge-coloring model \(h\) as a linear function on the polynomial ring or as a collection of symmetric tensors. Sometimes it will be more convenient to think of \(h\) as an element of \(O(V)^*\) (or \(R^*\)) and sometimes it is more convenient to think of \(h\) as a collection of symmetric tensors.

As contractions are by definition \(O_k\)-invariant, the tensor network interpretation of the partition function function of \(h\) immediately implies that it is invariant under the action of \(O_k\):

\[
\text{for each } g \in O_k \text{ and any graph } H, \ p_{gh}(H) = p_h(H). \quad (3.18)
\]

### 3.6 Computational complexity

It is by all means not a surprise that computing the partition functions of edge- or vertex-coloring models is generally hard, as already deciding whether a
3.6. Computational complexity

A graph can be properly colored with $k$ colors is NP-complete for $k \geq 3$. In fact, computing the number of $k$-colorings of a graph is known to be #P-complete for $k \geq 3$.

There are so-called dichotomy results about the complexity of evaluating $p_{a,B}$ for certain classes of vertex-coloring models $(a, B)$. This roughly means that $p_{a,B}$ can be computed in polynomial time if $(a, B)$ has a special structure and that it is #P-complete otherwise. We refer to [21, 10, 11] for more details.

Lovász [38] (see also [40]) showed that if for some $l \in \mathbb{N}$, the vertex-connection matrix $N_{f,l}$ has finite rank, then there exists a polynomial time algorithm that computes $f$ on graphs of treewidth bounded by $l$. This implies that for graphs of bounded treewidth, $p_{a,B}(H)$ can be computed in polynomial time.

Partition functions of edge-coloring models can be seen as a special case of a so-called Holant problems (cf. [12, 13]). In [12, 13] Cai, Lu and Xia prove a dichotomy result for a particular class of Holant problems. As far as we know no complete classification for the complexity of computing partition functions of edge-coloring models has been obtained. But the main message is that these are generally hard problems, unless the edge-coloring model has some special structure.

We should remark however, that using the interpretation of partition functions of edge-coloring models as contractions of tensor networks, we can conclude by a result of Markov and Shi [48], who used tensor networks in the field of quantum computing to simulate quantum computation, that for graphs of bounded degree and bounded treewidth the partition function of a $k$-color edge-coloring model can be computed in polynomial time. Using the fact that for a $k$-color edge-coloring model $h$ such that $h(x^a) = 0$ if $|a| > d$, the rank of its $l$-th vertex-connection matrix is bounded by $(kd)^l$ (as follows from Proposition 5.5), this also follows from the result of Lovász.