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Institute of Mathematics

Ph.D. thesis

Algebraic and analytic methods in graph theory

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Chapter 1

Introduction

This thesis revolves around two main topics. In the first part we consider the behaviour of roots of graph polynomials, notably the chromatic polynomial and the matching polynomial, on a sequence of graphs that is convergent in the Benjamini-Schramm sense. In the second part we suggest a possible structural characterization for positive graphs along with some partial results to support our conjecture. The two areas are connected by the use of algebraic and analytic tools in a graph-theoretic setting, especially homomorphisms and measures but also convergence, moments, quantum graphs and some spectral theory.

For a finite graph G, let $\mathrm{ch}_G(q)$ denote the number of proper colorings of G with q colors. Discovered by Birkhoff [9], this is a polynomial in q, called the *chromatic polynomial* of G. While some of its coefficients, roots and substitutions correspond to classical graph-theoretic invariants of G, chromatic roots also play an important role in statistical mechanics, where they control the behaviour of the antiferromagnetic Potts model at zero temperature. In particular, physicists are interested in the so-called thermodynamic limit, where the underlying graph is a lattice with size approaching infinity.

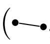
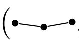
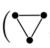
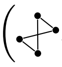
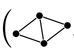
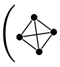
In the last decade, convergence of graph sequences became an important concept in mathematics. Motivated by efforts to better understand the structure of the internet, social networks and other huge networks in biology, physics and industrial processes, several theories appeared. The main idea in each of the theories is that we have a very large graph that is impractical to process or even to know its edges precisely, but we can sample it in some way and then produce smaller graphs that are structurally similar to it in the sense that they give rise to similar samples. If we have a sequence of graphs whose samples approximate those of the original graph arbitrarily closely then we say that this sequence converges to the original graph.

The most prevalent theories are the one about convergence of dense graphs by Lovász and Szegedy [38] and the one about convergence of bounded degree graphs by Benjamini and Schramm [8]. The latter one is also useful as a generalization of the aforementioned thermodynamic limit. Given a sequence of finite graphs G_n with bounded degree, we call it *convergent in the Benjamini-Schramm sense* if for every positive R and finite rooted graph α the probability that the R-ball centered at a uniform random vertex of G_n is isomorphic to α is convergent. In other words, we can not statistically distinguish G_n from $G_{n'}$ for large n and n' by randomly sampling them with a fixed radius of sight. For instance, we can approximate the infinite lattice $\mathbb{Z}^d$ using bricks with side lengths tending to infinity.

In Chapter 2, which is joint work with Miklós Abért, we examine the behaviour of chromatic roots on a Benjamini-Schramm convergent graph sequence. We define the *root measure* as the uniform distribution on the roots. We show that for a convergent sequence of graphs the root measure also converges in a certain sense.

The most natural sense here would be weak convergence, meaning that the integral of any continuous function wrt. the measure is convergent. However, this does not generally hold, as evidenced by the merged sequence of paths and cycles which is still BS convergent but the corresponding measures converge to different limits. Instead we prove *convergence in holomorphic moments*, showing that the integral of any holomorphic function wrt. the measure is convergent. In many cases we can use a separate argument to restrict the chromatic roots to a well-behaved set where convergence in holomorphic moments does imply weak convergence.

Our main vehicle of proof is counting homomorphisms. For two finite graphs F and G let $\hom(F, G)$ denote the number of edge-preserving mappings from $V(F)$ to $V(G)$. Moments of the chromatic root measure can be written as a linear combination of homomorphism numbers from connected graphs. For instance, the third moment equals

$p_3(G) = \frac{1}{8}\hom($  $, G) + \frac{3}{4}\hom($  $, G) + \frac{1}{4}\hom($  $, G) -$
$\frac{3}{8}\hom\Big($  $, G\Big) + \frac{3}{4}\hom($  $, G) - \frac{1}{8}\hom\Big($  $, G\Big)$.

Since these homomorphism numbers converge after normalization, so do the moments themselves, therefore we get the convergence of measures. It also follows that the normalized logarithm of the chromatic polynomial, called the free energy, converges to a real analytic function outside a disc, which answers a question of Borgs [10, Problem 2].

Our results have been recently extended by Csikvári and Frenkel [16] to a much broader class of polynomials, namely multiplicative graph polynomials of bounded exponential type. In addition to the chromatic polynomial this includes the Tutte polynomial, the modified matching polynomial, the adjoint polynomial and the Laplacian characteristic polynomial.

In light of this generalization we also investigate the matching measure in Chapter 3, which is joint work with Miklós Abért and Péter Csikvári. The *matching polynomial* of a finite graph G is defined as

$$\sum_k (-1)^k m_k(G) x^{|V(G)|-2k}$$

where $m_k(G)$ denotes the number of matchings in G with exactly k edges. It also relates to statistical physics, this time to the monomer-dimer model. We can follow our path from Chapter 2 by defining the matching measure as the uniform distribution on the roots of the matching polynomial, and since the Heilmann-Lieb theorem [32] constrains these roots to a compact subset of the real line, we get weak convergence from the Csikvári-Frenkel result, allowing us to automatically extend the definition to infinite vertex transitive lattices.

Alternatively, one can use spectral theory to define the matching measure directly on an infinite vertex transitive lattice L. A walk in L is called self-avoiding if it touches every vertex of L at most once. We can define the *tree of self-avoiding walks* at v by connecting two of them if one is a one step extension of the other. As proved in Chapter 3, the matching measure of L equals the spectral measure of this tree.

We continue by expressing the free energies of monomer-dimer models on Euclidean lattices from their respective matching measures, which allows us to give new, strong estimates. While free energies are traditionally estimated using the Mayer series, the advantage of our approach is that certain natural functions can be integrated along the measure even if the corresponding series do not converge.

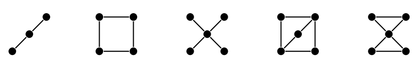
In general, no explicit formulae are known for the matching measures themselves, only in some special cases like the infinite d-regular tree. We can show, however, that the matching measure of a broad class of infinite lattices is atomless.

In Chapter 4 we turn our focus towards positive graphs. This chapter is joint work with Omar Antolín Camarena, Endre Csóka, Gábor Lippner and László Lovász. We already considered homomorphism numbers in Chapter 2, but here we extend the definition to allow weighted target graphs. By adding a real weight w_{ij} to each edge ij of the finite graph G we have

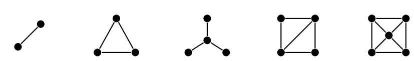
$$\hom(F,G) = \sum_{\varphi:V(F)\to V(G)} \prod_{ij\in E(F)} w_{\varphi(i)\varphi(j)}.$$

Using arbitrary real edge weights means that the homomorphism number can easily become negative. It turns out, however, that there are certain finite graphs F that always exhibit a nonnegative $\hom(F,G)$ regardless of the weighted graph G. We call such an F a *positive graph*.

The following are some examples of positive graphs:



while the ones below are not positive:



For instance, K_3 is not positive, since $\hom(K_3,G) < 0$ if G is a copy of K_3 with all edges having weight -1. This construction shows that no graph having an odd number of edges can be positive.

But why is the cycle of length 4 positive? We can write

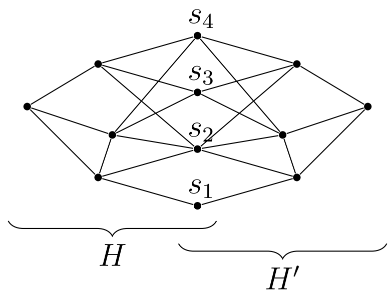
$$\hom(C_4,G) = \sum_{\varphi} w_{\varphi(1)\varphi(2)} w_{\varphi(2)\varphi(3)} w_{\varphi(3)\varphi(4)} w_{\varphi(4)\varphi(1)} =$$

$$= \sum_{\substack{\varphi(1)\\ \varphi(3)}} \Big(\sum_{\varphi(2)} w_{\varphi(1)\varphi(2)} w_{\varphi(2)\varphi(3)} \Big) \Big(\sum_{\varphi(4)} w_{\varphi(3)\varphi(4)} w_{\varphi(4)\varphi(1)} \Big) =$$

$$= \sum_{\substack{\varphi(1)\\ \varphi(3)}} \Big(\sum_{\varphi(2)} w_{\varphi(1)\varphi(2)} w_{\varphi(2)\varphi(3)} \Big)^2$$

Once we fix the images of two opposite vertices, the number of homomorphisms into any target graph G can be written as a square. So the total homomorphism number is a sum of squares and thus nonnegative.

This construction can be generalized. Suppose we have a graph H where the vertices $s_1, s_2, \ldots s_k$ form an independent set. Let H' be a disjoint copy of H and identify each s_i with s_i'. A graph F obtained this way is called *symmetric*.



Once we fix the images of the s_i's, H and H' have the same number of homomorphisms into our target graph G, and these mappings are independent from each other. Therefore the total number of homomorphisms is again a sum of squares, and thus all symmetric graphs are positive.

We conjecture that this implication is in fact an equivalence, i.e. all positive graphs are also symmetric.

To prove some special cases of the conjecture, we introduce a partitioning technique that allows us to disprove the positivity of certain graphs. The idea is to restrict the set of possible images for each vertex. In a simplified explanation, we may color the vertices of both F and G and only consider those homomorphisms that map each vertex into one of the same color. There are colored graphs F that feature a nonnegative $\hom(F, G)$ into any colored and edge-weighted graph G, and these obviously only depend on the partition $\mathcal{N}$ of $V(F)$ corresponding to the coloring. Such an $\mathcal{N}$ is called a *positive partition* of $V(F)$. (For the full analytic definition, see Chapter 4.)

Several operations on positive partitions preserve their positivity, such as merging classes together or restricting the underlying graph F to the union of certain classes. We may also split a class according to the degrees of the vertices, or even the number of edges going from a given vertex into some other specific class.

Starting from the trivial partition on F and successively dividing classes using these operations, we get to the *walk-tree partition* of F where two vertices belong to the same class if and only the universal cover of F as seen from these two vertices are isomorphic. Therefore any union of classes from the walk-tree partition of a positive graph is still positive, which immediately proves the conjecture for trees, and combined with a computer search also proves the conjecture for all graphs on at most 10 vertices, except one.

We end the chapter with some statements about positive graphs, including that they have a homomorphic image with at least half the original number of nodes, in which every edge has an even number of pre-images.

Acknowledgement

I am very grateful to my supervisor, László Lovász, for his guidance, interesting topic suggestions and his two invitations to Princeton. His book [36] also helped me find my way around the vast topic of graph convergence. I would like to express my gratitude towards Miklós Abért for his mission in fostering cooperation between young researchers at the Rényi Institute, and also for his direct guidance.

I would like to thank Péter Csikvári, Endre Csóka and Dávid Kunszenti-Kovács for their valuable discussions. Péter also helped me with correcting some inconsistencies in the thesis.

Several people have suggested ideas or remarks for the individual articles that this thesis consists of. I am thankful to Gábor Halász and Lewis Bowen regarding Chapter 2, Paolo Butera and Paul Federbush respecting Chapter 3 and Sergey Norin and Oleg Pikhurko concerning Chapter 4.

On a more personal note, I owe a lot to my family for the supportive atmosphere, to the various communities I belonged to during my years of being a phd student, and to God for not giving up along the way.

Chapter 2

Chromatic measure and Benjamini-Schramm convergence

This chapter is based on the article [2], which is joint work with Miklós Abért.

2.1 Introduction

Let G be a finite undirected graph without multiple edges and loops. A map $f : V(G) \to \{1, \ldots, q\}$ is a *proper coloring* if for all edges $(x, y) \in E(G)$ we have $f(x) \neq f(y)$. For a positive integer q let $\mathrm{ch}_G(q)$ denote the number of proper colorings of G with q colors. Then ch_G is a polynomial in q, called the *chromatic polynomial* of G. The complex roots of ch_G are called the *chromatic roots* of G.

The study of chromatic polynomials and its roots has been initiated by Birkhoff. Since then, the subject has gotten considerable interest, partially because of its connection to statistical mechanics. In particular, the chromatic roots control the behaviour of the antiferromagnetic Potts model at zero temperature. For a survey on the subject see [47].

For a finite graph G, a finite rooted graph α and a positive integer R, let $\mathbf{P}(G, \alpha, R)$ denote the probability that the R-ball centered at a uniform random vertex of G is isomorphic to α. We say that a graph sequence (G_n) of bounded degree is *Benjamini-Schramm convergent* if for all finite rooted graphs α and $R > 0$, the probabilities $\mathbf{P}(G_n, \alpha, R)$ converge (see [8]). This means that one can not statistically distinguish G_n and $G_{n'}$ for large n and n' by sampling them from a random vertex with a fixed radius of sight. An example (that is regularly used in statistical physics) is to approximate the infinite lattice $\mathbb{Z}^d$ by bricks with all the side lengths tending to infinity. More generally, amenable vertex transitive graphs can be obtained as the Benjamini-Schramm limits of their Følner sequences.

For a simple graph G let μ_G, the *chromatic measure of* G denote the uniform distribution on its chromatic roots. By a theorem of Sokal [46], μ_G is supported on the open disc of radius Cd around 0, denoted by

$$D = B(0, Cd)$$

where d is the maximal degree of G and $C < 8$ is an absolute constant.

Theorem 2.1. *Let (G_n) be a Benjamini-Schramm convergent graph sequence of absolute degree bound d, and $\widetilde{D}$ an open neighborhood of the closed disc $\overline{D}$. Then for every holomorphic function $f : \widetilde{D} \to \mathbb{C}$, the sequence*

$$\int_D f(z) d\mu_{G_n}(z)$$

converges.

Let ln denote the principal branch of the complex logarithm function. For a simple graph G and $z \in \mathbb{C}$ let

$$\mathrm{t}_G(z) = \frac{\ln \mathrm{ch}_G(z)}{|V(G)|}$$

where this is well-defined. In statistical mechanics, $\mathrm{t}_G(z)$ is called the *entropy per vertex* or the *free energy* at z. In their recent paper [11], Borgs, Chayes, Kahn and Lovász proved that if (G_n) is a Benjamini-Schramm convergent graph sequence of absolute degree bound d, then $\mathrm{t}_{G_n}(q)$ converges for every positive integer $q > 2d$. Theorem 2.1 yields the following.

Theorem 2.2. *Let (G_n) be a Benjamini-Schramm convergent graph sequence of absolute degree bound d with $|V(G_n)| \to \infty$. Then $\mathrm{t}_{G_n}(z)$ converges to a real analytic function on $\mathbb{C} \setminus \overline{D}$.*

In particular, $\mathrm{t}_{G_n}(z)$ converges for all $z \in \mathbb{C} \setminus \overline{D}$. Theorem 2.2 answers a question of Borgs [10, Problem 2] who asked under which circumstances the entropy per vertex has a limit and whether this limit is analytic in $1/z$. Note that for an amenable quasi-transitive graph and its Følner sequences, this was shown to hold in [42].

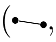
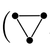
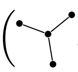
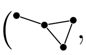
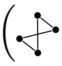
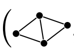
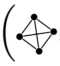
To prove Theorem 2.1 we show that for a finite graph G and for every k, the number

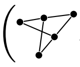
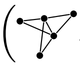
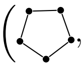
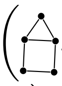
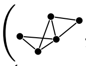
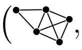
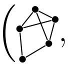
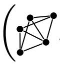
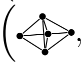
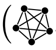
$$p_k(G) = |V(G)| \int_D z^k d\mu_G(z)$$

can be expressed as a fixed linear combination of $\hom(H, G)$ where the H are connected finite graphs and $\hom(H, G)$ denotes the number of graph homomorphisms from H to G. Since a sequence of graphs G_n of bounded degree is Benjamini-Schramm convergent if and only if

$$\frac{\hom(H, G_n)}{|V(G_n)|}$$

converges for all connected graphs H. This gives convergence of all the holomorphic moments of μ_{G_n}, and this is equivalent to Theorem 2.1. For instance, for the fourth moment we get

$p_4(G) = -\frac{1}{3}\hom($$, G) + \frac{4}{3}\hom($$, G) - \frac{1}{2}\hom($$, G) + \frac{1}{3}\hom\Big($$, G\Big) +$
$\hom($$, G) - \frac{1}{2}\hom\Big($$, G\Big) + \hom($$, G) - \frac{1}{3}\hom\Big($$, G\Big) -$

$\frac{1}{3}\,\mathrm{hom}\Big($$, G\Big) + \frac{1}{3}\,\mathrm{hom}\Big($$, G\Big) + \frac{2}{5}\,\mathrm{hom}\Big($$, G\Big) - 2\,\mathrm{hom}\Big($$, G\Big) +$
$2\,\mathrm{hom}\Big($$, G\Big) - \mathrm{hom}\Big($$, G\Big) + \mathrm{hom}\Big($$, G\Big) - \frac{1}{2}\,\mathrm{hom}\Big($$, G\Big) +$
$\frac{1}{3}\,\mathrm{hom}\Big($$, G\Big) - \frac{1}{30}\,\mathrm{hom}\Big($$, G\Big).$

One could speculate that assuming Benjamini-Schramm convergence of G_n, maybe the complex measures μ_{G_n} themselves will weakly converge. That is, Theorem 2.1 would hold for any continuous real function on D or, equivalently, convergence would hold in all the moments

$$\int_D z^k \overline{z}^j \, d\mu_{G_n}(z).$$

However, this is not true in general, as the following easy counterexample shows. Let P_n denote the path of length n and let C_n denote the cycle of length n. Then P_n and C_n converge to the same object, the infinite rooted path, while we have

$$\mathrm{ch}_{P_n}(z) = z(z-1)^{n-1} \text{ and } \mathrm{ch}_{C_n}(z) = (z-1)^n + (-1)^n(z-1).$$

Thus, the weak limit of μ_{P_n} is the Dirac measure on 1 and the weak limit of μ_{C_n} is the normalized Lebesgue measure on the unit circle centered at 1.

Still, using Theorem 2.1, we are able to prove the weak convergence of μ_{G_n} for some natural sequences of graphs. For example, let $T_n = C_4 \times P_n$ denote the $4 \times n$ tube, i.e. the cartesian product of the 4-cycle with a path on n vertices. T_n is a 4-regular graph except at the ends of the tube.

Proposition 2.3. *The chromatic measures μ_{T_n} weakly converge.*

The proof is as follows: as Salas and Sokal [45] showed, the pointwise limit X of supports of μ_{T_n} is part of a particular algebraic curve, so any subsequential weak limit is supported on X. The complement of X is connected, so by Mergelyan's theorem [40], every continuous function on X can be uniformly approximated by polynomials. Using Theorem 2.1 this yields weak convergence of μ_{T_n}. See Section 2.4 for details.

In this case one can use the so-called transfer matrix method to control the support of the chromatic measures (see [45] for various models related to the square lattice). In general, even for models of the square lattice, the complement of the limiting set may not be connected, and hence one can not invoke Mergelyan's theorem. It is expected, however, that for any model where the transfer matrix method can be used, the chromatic measures do converge weakly.

Another naturally interesting case is when the girth of G (the minimal size of a cycle) is large. One can show that

$$\int_D z^k \, d\mu(z) = \frac{|E(G)|}{|V(G)|} \quad (1 \le k \le \mathrm{girth}(G) - 2)$$

that is, the moments are all the same until the girth is reached (see Lemma 2.13). This implies that for a sequence of d-regular graphs G_n with girth tending to infinity, the limit of the free entropy

$$\lim_{n\to\infty} \mathrm{t}_{G_n}(z) = \ln q + \frac{d}{2}\ln(1-\frac{1}{q})$$

for $q > Cd$. This is one of the main results in [6]. Note that their proof works for $q > d+1$, while our approach only works for $q > Cd$. The advantage of our approach is that it gives an explicit estimate on the number of proper colorings of large girth graphs.

Theorem 2.4. *Let G be a finite graph of girth g and maximal degree d. Then for all $q > Cd$ we have*

$$\left|\frac{\ln \mathrm{ch}_G(q)}{|V(G)|} - \left(\ln q + \frac{|E(G)|}{|V(G)|}\ln(1-\frac{1}{q})\right)\right| \leq 2\frac{(Cd/q)^{g-1}}{1-Cd/q}.$$

When G is d-regular with asymptotically maximal girth, i.e. $g = c\ln|V(G)|$, this yields

$$\left|\frac{\ln \mathrm{ch}_G(q)}{|V(G)|} - \left(\ln q + \frac{d}{2}\ln(1-\frac{1}{q})\right)\right| \leq O(|V(G)|^{-c'})$$

for some explicit constant $c' > 0$. Counting the number of proper colorings of random d-regular graphs have been considered in [6]. These graphs do not have logarithmic girth, but they have few shorter cycles, so one can obtain a similar result for them.

Here we wish to raise attention to an interesting phenomenon, of which we only have some computational evidence. We have computed the chromatic measures of several 3-regular large girth graphs and surprisingly, it looks like one may also get weak convergence of chromatic measures.

Problem 2.5. *Let G_n be a sequence of d-regular graphs with girth tending to infinity. Does μ_{G_n} weakly converge?*

This would be interesting because one could consider the limit as the 'chromatic measure of the d-regular infinite tree'. Observe that any subsequential weak limit μ of μ_{G_n} satisfies

$$\int_D z^k d\mu(z) = \frac{d}{2} \quad (k \geq 1)$$

that is, the holomorphic moments of μ are independent of k. While Figure 2.1 looks very promising, one misleading aspect of it may be that 3-regular graphs having 32 vertices and (maximal possible) girth 7 may exhibit structural restrictions that are much stronger than just large girth.

It would be interesting to generalize our results to the Tutte polynomial $T_G(x,y)$. This two-variable polynomial encodes a lot of interesting invariants of G. For instance, $T_G(z,0) = \mathrm{ch}_G(z)$, $T_G(2,1)$ counts the number of forests, $T_G(1,1)$ is the number of spanning trees

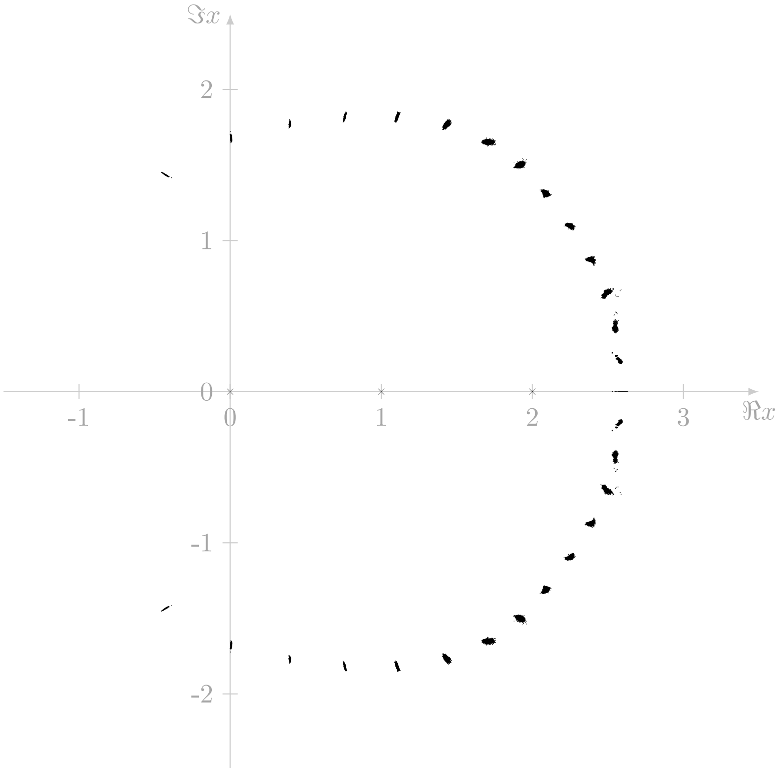


Figure 2.1: Chromatic roots of the 30368 cubic graphs of size 32 and girth 7

and $T_G(1,2)$ is the number of connected spanning subgraphs. By a result of Lyons [39], we know that

$$\frac{\log T_{G_n}(1,1)}{|V(G_n)|}$$

converges for a Benjamini-Schramm convergent sequence of graphs G_n of bounded degree. Also, in [11] it is shown that the same holds at the places (q,y) where $0 \le y < 1$ and q is large enough in terms of the maximal degree. It would be interesting to see whether this also holds at other places. The places $(2,1)$ and $(1,2)$ would be good test points as they have a natural combinatorial meaning. Also, it is not clear whether Theorem 2.1 holds for $p_G(z) = T_G(z, y_0)$ for all fixed y_0. Note that even for the chromatic polynomial, in general, the above log convergence will not hold, for instance at $(2,0)$, because cycles of even and odd length converge to the same limit, but even cycles have a proper 2-coloring, while odd cycles do not. This may not be so surprising, since $T_G(2,0) \le 2^{c(G)}$ where $c(G)$ is the number of components of G. So for a nontrivial graph sequence G_n, $T_{G_n}(2,0)$ is subexponential in $|V(G_n)|$, which points to the proximity of roots of T_{G_n}. To apply Theorem 2.1 in its present form, one needs that some small neighbourhood of the place is sparse in terms of roots.

Remark. Note that recently Csikvári and Frenkel [16] generalized Theorem 2.2 to a large class of graph polynomials, including the Tutte polynomial. In particular, they show that convergence holds for the normalized log of $T(x,y)$ where x, y have large enough absolute value.

2.2 Preliminaries

For a simple graph H on n vertices let the number of legal colorings of H with q colors be denoted by $\mathrm{ch}_H(q)$. Then for any edge e of H the following recursion holds:

$$\mathrm{ch}_H(q) = \mathrm{ch}_{H\setminus e}(q) - \mathrm{ch}_{H/e}(q)$$

where $H \setminus e$ is obtained from H by deleting e and H/e is obtained by gluing the endpoints of e and erasing multiple edges and loops. This implies that ch_H is a polynomial of degree n in q with integer coefficients, called the *chromatic polynomial* of G and that the above recursion holds for the polynomials themselves. It also follows that the constant coefficient of ch_H is zero and its main coefficient is 1. So, we can write

$$\mathrm{ch}_H(z) = z^n - e_1(H)z^{n-1} + \ldots + (-1)^k e_k(H)z^{n-k} + \ldots + (-1)^{n-1}e_{n-1}(H)z =$$
$$= \prod_{i=1}^{n}(z - \lambda_i(H)).$$

The $e_k(H)$ are called the *chromatic coefficients* of H and $\lambda_i(H)$ are its *chromatic roots.* For $k \geq 0$ let

$$p_k(H) = \sum_{i=1}^{n} \lambda_i^k(H).$$

The Newton identities establish connections between the roots and coefficients of a polynomial. In this chapter we will use the following version:

$$p_k = (-1)^{k-1}ke_k + \sum_{i=1}^{k-1}(-1)^{k-i-1}p_i e_{k-i}.$$

Let H, G be simple graphs. A map $f : V(H) \to V(G)$ is a *homomorphism* if for all edges $(x, y) \in E(H)$ we have $(f(x), f(y)) \in E(G)$. We denote the number of homomorphisms from H to G by $\hom(H, G)$. The quantity $\hom(H, G)$ is nice to work with, mainly because of the following property.

Lemma 2.6. *Let H be the disjoint union of H_1 and H_2. Then*

$$\hom(H, G) = \hom(H_1, G)\hom(H_2, G)$$

for all simple graphs G.

We leave the proof to the reader.

For a random rooted graph G, a finite rooted graph α and a positive integer R, let $\mathbf{P}(G, \alpha, R)$ denote the probability that the R-ball centered at the root of G is isomorphic to α. Analogously, for an unrooted finite graph G, let $\mathbf{P}(G, \alpha, R)$ denote the probability that the R-ball centered at a uniform random vertex of G is isomorphic to α. A graph sequence G_n has bounded degree if there is an absolute upper bound on the degrees of vertices of G_n.

A graph sequence (G_n) of bounded degree is *Benjamini-Schramm convergent* if for all finite rooted graphs α and $R > 0$ the probabilities $\mathbf{P}(G_n, \alpha, R)$ converge.

The limit of a Benjamini-Schramm convergent sequence of graphs is the random rooted graph G satisfying

$$\mathbf{P}(G, \alpha, R) = \lim_{n\to\infty} \mathbf{P}(G_n, \alpha, R)$$

for all $R > 0$ and α. It is easy to see that G is well defined. In the most transparent case, G is just one graph, which then has to be vertex transitive. For instance, the d dimensional lattice

$$\mathbb{Z}^d = \lim_{n\to\infty} (\mathbb{Z}/n\mathbb{Z})^d = \lim_{n\to\infty} B_n^d$$

where $(\mathbb{Z}/n\mathbb{Z})^d$ is the d dimensional torus and B_n^d is the box of side length n in $\mathbb{Z}^d$. The same way, one can obtain any connected vertex transitive amenable graph as a limit. Let G be a connected vertex transitive graph of bounded degree. A sequence of connected subgraphs F_n of G is a *Følner sequence*, if

$$\lim_{n\to\infty} \frac{|\partial F_n|}{|V(F_n)|} = 0$$

where ∂F_n denotes the external vertex boundary of F_n. Note that G is amenable if and only if it has a Følner sequence. It is easy to show that any connected vertex transitive amenable graph is the Benjamini-Schramm limit of its Følner sequences.

Let us consider now the d-regular tree T_d, which is in many senses the farthest possible from being amenable. One can obtain T_d as the limit of finite graphs, but it is worth to point out that T_d can *not* be obtained as a limit of finite trees. Indeed, the expected degrees of finite trees are approximately 2 and this passes on to their limits. It is a good exercise to understand what the limit of the balls in T_d is (it is a fixed tree where the root is random). The right way to approximate T_d in Benjamini-Schramm convergence is to take finite d-regular graphs G_n with girth tending to infinity.

Benjamini-Schramm convergence can also be expressed in terms of graph homomorphisms using the following lemma (see [36], Proposition 5.6).

Lemma 2.7. *Let G_n be a graph sequence of bounded degree. Then G_n is Benjamini-Schramm convergent if and only if for every finite connected graph H, the limit*

$$\lim_{n\to\infty} \frac{\hom(H, G_n)}{|V(G_n)|}$$

exists.

Note that one needs connectedness in Lemma 2.7, as $\hom(H, G)$ may be the order of $|V(G)|^c$ where c is the number of components in H.

2.3 Expressing moments from homomorphisms

In this section we give an explicit formula for the holomorpic moments of the chromatic measure in terms of graphs homomorphisms.

For a finite, simple graph G let $\mathcal{P}(G)$ be defined as the set of partitions of $V(G)$ where no edge of G connects two vertices in the same class. A partition $P \in \mathcal{P}(G)$ can be considered as a surjective homomorphism from G to the simple graph G/P obtained by contracting each class of P and erasing multiple edges. For simple graphs G and T let

$$\mathcal{P}(G,T) = \{P \in \mathcal{P}(G) \mid G/P \cong T\}$$

be the collection of partitions of G with quotient isomorphic to T. For $P \in \mathcal{P}(G)$ let

$$\|P\| = \prod_{p \in P} (|p| - 1)!$$

where $p \in P$ runs through the P-classes.

Let $\mathrm{Aut}(G)$ denote the automorphism group of G. Let $\mathcal{G}(k)$ denote the set of graphs without isolated vertices, where the number of vertices minus the number of components equals k and let

$$\mathcal{G}(\leq k) = \cup_{j \leq k} \mathcal{G}(j).$$

Note that $\mathcal{G}(\leq k)$ is a finite set.

Base parameters. Now we introduce a sequence of parameters that will connect moments with chromatic coefficients. For a simple graph T and $k > 0$ let

$$c_k(T) = \sum_{G \in \mathcal{G}(k)} \frac{(-1)^{|E(G)|+|V(G)|+|V(T)|+k}}{|\mathrm{Aut}(G)|} \sum_{P \in \mathcal{P}(G,T)} \|P\|.$$

It turns out that these parameters allow us to express $e_k(H)$ in a nice way.

Lemma 2.8. *Let H be a simple graph. Then we have*

$$e_k(H) = \sum_{T \in \mathcal{G}(\leq k)} c_k(T) \hom(T,H).$$

Proof. We derive the lemma from two easy claims. Let $\mathrm{inj}(G,H)$ denote the number of injective homomorphisms from G to H.

Claim 1. We have

$$e_k(H) = \sum_{G \in \mathcal{G}(k)} \frac{(-1)^{|E(G)|+k}}{|\mathrm{Aut}(G)|} \mathrm{inj}(G,H).$$

To see this, we use the following identity, that is sometimes used as a definition.

$$\mathrm{ch}_H(z) = \sum_{\substack{G \subseteq H \\ \text{spanning}}} (-1)^{|E(G)|} z^{c(G)}$$

where $c(G)$ is the number of connected components in the spanning subgraph G. It is enough to prove this for positive integer values of z. In this case, there are exactly $z^{c(G)}$

colorings that violate the legal coloring constraint for all edges of G, and the equation follows from the inclusion-exclusion principle.

The value of $e_k(H)$ is $(-1)^k$ times the coefficient of z^{n-k}, which contains the terms where $c(G) = n - k$, or equivalently, where the graph G, when erasing its isolated vertices, is in $\mathcal{G}_k$. A graph G is counted as many times as it appears in H as a spanning subgraph, which equals $\mathrm{inj}(G, H)/\left|\mathrm{Aut}(G)\right|$. Claim 1 is proved.

Claim 2. Let $G \in \mathcal{G}(k)$ and let H be a simple graph. Then we have

$$\mathrm{inj}(G, H) = \sum_{T \in \mathcal{G}(\leq k)} \left((-1)^{|V(G)|+|V(T)|} \sum_{P \in \mathcal{P}(G,T)} \|P\| \right) \mathrm{hom}(T, H).$$

To see this, let us consider the partially ordered set $\mathcal{P}(G)$ with respect to refinement. For $P, P' \in \mathcal{P}(G)$ with $P' \leq P$ (i.e. P' refines P), let $p_1, \ldots, p_r$ be a list of the P-classes and let a_i be the number of P'-classes contained in p_i $(1 \leq i \leq r)$. Let $s = \sum_{i=1}^{r} a_i$ be the number of classes in P'. Then the Mobius function is

$$\mu(P', P) = (-1)^{r+s} \prod_{i=1}^{r} (a_i - 1)!$$

(see e.g. [43]). In particular, for the discrete partition P_0 we get

$$\mu(P_0, P) = (-1)^{|V(G)|+|V(G/P)|} \|P\|.$$

On the other hand, we have

$$\mathrm{hom}(G/P', H) = \sum_{P' \leq P \in \mathcal{P}(G)} \mathrm{inj}(G/P, H).$$

Now the Mobius inversion formula yields

$$\mathrm{inj}(G, H) = \sum_{P \in \mathcal{P}(G)} (-1)^{|V(G)|+|V(G/P)|} \|P\| \, \mathrm{hom}(G/P, H)$$

which, when collecting terms by $T = G/P \in \mathcal{G}(\leq k)$ gives the formula in Claim 2.

The lemma follows from substituting the formula in Claim 2 into the formula in Claim 1 and collecting terms. $\square$

Now we show that the base parameters of a disconnected graph can be expressed as a convolution of the base parameters of its connected components, normalized by a constant computed from the multiplicities:

Lemma 2.9. *Let T be the disjoint union of the connected graphs $T_1, T_2, \ldots, T_l$. Let $S = \{j \mid \nexists i < j : T_i \cong T_j\}$ contain the indices of nonisomorphic T_j's and $m_j = |\{i \mid T_i \cong T_j\}|$ denote the multiplicity of T_j. Define $\sigma = \prod_{j \in S} m_j!$. Then for all $k > 0$ we have*

$$c_k(T) = \frac{1}{\sigma} \sum_{\substack{(x_1,\ldots,x_l) \\ x_1+\cdots+x_l=k}} \prod_{j=1}^{l} c_{x_j}(T_j).$$

Proof. Recall that

$$c_k(T) = \sum_{G \in \mathcal{G}(k)} \frac{(-1)^{|E(G)|+|V(G)|+|V(T)|+k}}{|\mathrm{Aut}(G)|} \sum_{P \in \mathcal{P}(G,T)} \|P\| .$$

For a fixed G and P, the connected components of G/P can be identified with $T_1, T_2, \dots, T_l$ in σ possible ways. Each of these matchings gives a subdivision $G = G_1 \cup G_2 \cup \ldots \cup G_l$ by applying the inverse image of the quotient map to the T_i's. The restrictions $P_i = P|_{G_i}$ of the partition P satisfy $P_i \in \mathcal{P}(G_i, T_i)$ and

$$\prod_{j=1}^{l} \|P_j\| = \|P\| .$$

Therefore

$$c_k(T) = \sum_{G \in \mathcal{G}(k)} \frac{(-1)^{|E(G)|+|V(G)|+|V(T)|+k}}{|\mathrm{Aut}(G)|} \sum_{G = G_1 \cup \ldots \cup G_l} \sum_{\substack{P_j \in \mathcal{P}(G_j, T_j) \\ 1 \le j \le l}} \frac{1}{\sigma} \prod_{j=1}^{l} \|P_j\| .$$

If we already know the isomorphism classes of $G_1, G_2, \dots, G_l$, there are still

$$\frac{|\mathrm{Aut}(G)|}{\prod_{j=1}^{l} |\mathrm{Aut}(G_j)|}$$

possibilities to arrange them as a subdivision of G. It follows that $c_k(T)$ equals

$$\sum_{\substack{(x_1,\dots,x_l) \\ x_1+\ldots+x_l=k}} \sum_{\substack{G_j \in \mathcal{G}(x_j) \\ 1 \le j \le l}} \frac{|\mathrm{Aut}(G)|}{\prod_{j=1}^{l} |\mathrm{Aut}(G_j)|} \cdot \frac{(-1)^{|E(G)|+|V(G)|+|V(T)|+k}}{|\mathrm{Aut}(G)|} \sum_{\substack{P_j \in \mathcal{P}(G_j, T_j) \\ 1 \le j \le l}} \frac{1}{\sigma} \prod_{j=1}^{l} \|P_j\| .$$

By using

$$|E(G)| + |V(G)| + |V(T)| + k = \sum_{j=1}^{l} (|E(G_j)| + |V(G_j)| + |V(T_j)| + x_j)$$

and rearranging we get

$$c_k(T) = \frac{1}{\sigma} \sum_{\substack{(x_1,\dots,x_l) \\ x_1+\ldots+x_l=k}} \prod_{j=1}^{l} \sum_{G_j \in \mathcal{G}(x_j)} \frac{(-1)^{|E(G_j)|+|V(G_j)|+|V(T_j)|+x_j}}{|\mathrm{Aut}(G_j)|} \sum_{P_j \in \mathcal{P}(G_j, T_j)} \|P_j\| =$$

$$= \frac{1}{\sigma} \sum_{\substack{(x_1,\dots,x_l) \\ x_1+\ldots+x_l=k}} \prod_{j=1}^{l} c_{x_j}(T_j). \ \square$$

We can use the following variant of Lemma 2.9 when we would like to detach one connected component of T at a time:

Lemma 2.10. *Let T be the disjoint union of the connected graphs $T_1, T_2, \dots, T_l$ where $l \geq 2$. Let $S = \{j \mid \nexists i < j : T_i \cong T_j\}$ contain the indices of nonisomorphic T_j's. Then we have*

$$kc_k(T) - \sum_{i=1}^{k-1} \sum_{j \in S} ic_i(T_j)c_{k-i}(T \setminus T_j) = 0.$$

Proof. Let m_j denote the multiplicity of T_j and $\sigma = \prod_{j \in S} m_j!$ as in Lemma 2.9. Since isomorphic T_j's have identical $c_i(T_j)$ and $c_{k-i}(T \setminus T_j)$, it follows that

$$\sum_{j \in S} ic_i(T_j)c_{k-i}(T \setminus T_j) = \sum_{t=1}^{l} \frac{i}{m_t} c_i(T_t)c_{k-i}(T \setminus T_t).$$

By using Lemma 2.9 for T and σ and also for $T \setminus T_t$ and $\frac{\sigma}{m_t}$ we obtain:

$$kc_k(T) - \sum_{i=1}^{k-1} \sum_{j \in S} ic_i(T_j)c_{k-i}(T \setminus T_j) = kc_k(T) - \sum_{i=1}^{k-1} \sum_{t=1}^{l} \frac{i}{m_t} c_i(T_t)c_{k-i}(T \setminus T_t) =$$

$$= \frac{k}{\sigma} \sum_{\substack{(x_1,\dots,x_l) \\ x_1+\dots+x_l=k}} \prod_{j=1}^{l} c_{x_j}(T_j) - \sum_{i=1}^{k-1} \sum_{t=1}^{l} \frac{i}{m_t} \cdot \frac{m_t}{\sigma} \sum_{\substack{(x_1,\dots,x_l) \\ x_1+\dots+x_l=k \\ x_t=i}} \prod_{j=1}^{l} c_{x_j}(T_j) =$$

$$= \frac{1}{\sigma} \sum_{\substack{(x_1,\dots,x_l) \\ x_1+\dots+x_l=k}} \left(k - \sum_{t=1}^{l} x_t\right) \prod_{j=1}^{l} c_{x_j}(T_j) = 0.$$

The last equation follows from $k - \sum_{t=1}^{l} x_t = 0$. $\square$

Now we show that $p_k(H)$ can be expressed using the number of homomorphisms from *connected* graphs.

Theorem 2.11. *Let H be a simple graph on n vertices and let $k > 0$ be an integer. Then*

$$p_k(H) = \sum_{\substack{T \in \mathcal{G}(\leq k) \\ T \text{ is connected}}} (-1)^{k-1} kc_k(T) \hom(T, H).$$

Proof. The Newton identites tell us that

$$p_k(H) = (-1)^{k-1} ke_k(H) + \sum_{i=1}^{k-1} (-1)^{k-i-1} p_i(H) e_{k-i}(H)$$

for all $k > 0$. Using induction on k, we can assume that the result holds for all $j < k$. Lemma 2.8 gives us a formula for $e_k(H)$ in the parameters $c_k(T)$, namely we have

$$e_k(H) = \sum_{T \in \mathcal{G}(\leq k)} c_k(T) \hom(T, H).$$

Using that hom is multiplicative (stated as Lemma 2.6) we get $p_k(H)$ as a fixed linear combination of the $\hom(T, H)$'s. Let $q_k(T)$ denote the formal coefficient of $\hom(T, H)$ in this sum. So, we have

$$p_k(H) = \sum_{T \in \mathcal{G}(\leq k)} q_k(T) \hom(T, H).$$

This leads to the following equality for all T:

$$q_k(T) = (-1)^{k-1} k c_k(T) + \sum_{i=1}^{k-1} (-1)^{k-i-1} \sum_{\substack{U_1 \in \mathcal{G}(\leq i) \\ U_2 \in \mathcal{G}(\leq k-i) \\ U_1 \cup U_2 = T}} q_i(U_1) c_{k-i}(U_2)$$

where T is isomorphic to the disjoint union of U_1 and U_2.

Let $T \in \mathcal{G}(\leq k)$. We claim that

$$q_k(T) = (-1)^{k-1} k c_k(T)$$

if T is connected and 0 otherwise. If T is connected then it is impossible to choose U_1 and U_2 in the second sum above, so the claim holds. If T is disconnected then as in Lemma 2.10, let T be the disjoint union of the connected graphs $T_1, T_2, \ldots, T_l$ and let S contain the indices of nonisomorphic T_j's. Using induction on k we can assume that $q_i(U_1) = 0$ unless U_1 is isomorphic to one of the T_j's. This gives

$$q_k(T) = (-1)^{k-1} k c_k(T) + \sum_{i=1}^{k-1} (-1)^{k-i-1} \sum_{j \in S} q_i(T_j) c_{k-i}(T \setminus T_j).$$

We know from the induction hypothesis that $q_i(T_j) = (-1)^{i-1} i c_i(T_j)$ and therefore we get

$$q_k(T) = (-1)^{k-1} \left(k c_k(T) - \sum_{i=1}^{k-1} \sum_{j \in S} i c_i(T_j) c_{k-i}(T \setminus T_j) \right)$$

which is 0 according to Lemma 2.10. $\square$

2.4 Convergence of chromatic measures

In this section we prove Theorem 2.1, Theorem 2.2 and Proposition 2.3. For the convenience of the reader, we state the theorems again.

Theorem 2.1. *Let (G_n) be a Benjamini-Schramm convergent graph sequence of absolute degree bound d, and $\widetilde{D}$ an open neighborhood of the closed disc $\overline{D}$. Then for every holomorphic function $f : \widetilde{D} \to \mathbb{C}$, the sequence*

$$\int_D f(z) d\mu_{G_n}(z)$$

converges.

Proof. We have

$$\int_D z^k d\mu_G(z) = \frac{1}{|V(G)|} \sum_{i=1}^{|V(G)|} \lambda_i^k(G) = \frac{p_k(G)}{|V(G)|}$$

for $k \geq 0$.

Since f is holomorphic, it equals its Taylor series

$$f(z) = \sum_{n=0}^{\infty} a_n z^n$$

on an open neighborhood of $\overline{D}$. Let

$$f_k(z) = \sum_{n=0}^{k} a_n z^n$$

denote the partial sums. The f_k's converge uniformly on D, so we also know that

$$F_k(G) = \int_D f_k(z) d\mu_G(z) = \sum_{n=0}^{k} a_n \int_D z^n d\mu_G(z) = \sum_{n=0}^{k} a_n \frac{p_n(G)}{|V(G)|}$$

converges to

$$F(G) = \int_D f(z) d\mu_G(z)$$

uniformly on the set of graphs G with μ_G supported on D. By Theorem 2.11 we have

$$p_n(G) = \sum_{\substack{T \in \mathcal{G}(\leq n) \\ T \text{ is connected}}} (-1)^{n-1} n c_n(T) \hom(T, G).$$

By rearranging, this gives

$$F_k(G) = \sum_T b_{k,T} \frac{\hom(T, G)}{|V(G)|}$$

where T runs through connected graphs on at most $k+1$ vertices. Now let G_n be a Benjamini-Schramm convergent sequence of graphs. By Lemma 2.7, the sequences

$$\frac{\hom(T, G_n)}{|V(G_n)|}$$

converge for every connected T. (Note that for non-connected T this is in general false). This implies that $F_k(G_n)$ is convergent for every k. Since we already know that $F_k(G_n)$ uniformly converges to $F(G_n)$ for every n, we obtain that $F(G_n)$ is also convergent. It also follows that

$$F(G_n, u) = \int_D f(z+u) d\mu_{G_n}(z)$$

uniformly converges to a holomorphic function in a neighborhood of 0. □

We are ready to prove Theorem 2.2.

Theorem 2.2. *Let (G_n) be a Benjamini-Schramm convergent graph sequence of absolute degree bound d with $|V(G_n)| \to \infty$. Then $\mathrm{t}_{G_n}(z)$ converges to a real analytic function on $\mathbb{C} \setminus \overline{D}$.*

Proof. The principal branch of the complex logarithm function only takes values with an imaginary part in $(-\pi, \pi]$. Therefore $\Im \mathrm{t}_{G_n}(z)$ is always in the interval $\left(\frac{-\pi}{|V(G_n)|}, \frac{\pi}{|V(G_n)|}\right]$ and $|V(G_n)| \to \infty$ implies $\Im \mathrm{t}_{G_n}(z) \to 0$.

To prove convergence for the real part $\Re \mathrm{t}_{G_n}(z)$, consider a fixed $z_0 \in \mathbb{C} \setminus \overline{D}$. Since the disc $B(z_0, Cd)$ is bounded away from 0, there exists a branch $\ln^*$ of the complex logarithm function whose branch cut is a half-line emanating from 0 that is disjoint from the disc. It follows that $f(z) = \ln^*(z_0 - z)$ is holomorphic on an open neighborhood of $\overline{D}$. According to Theorem 2.1,

$$\int_D \ln^*(z_0 - z) d\mu_{G_n}(z)$$

converges uniformly in a neighborhood of z_0, which implies that

$$\Re \mathrm{t}_{G_n}(z_0) = \frac{\Re \ln \mathrm{ch}_{G_n}(z_0)}{|V(G_n)|} = \frac{\sum\limits_{\lambda \text{ root}} \Re \ln(z_0 - \lambda)}{|V(G_n)|} = \int_D \Re \ln(z_0 - z) d\mu_{G_n}(z) =$$

$$= \int_D \Re \ln^*(z_0 - z) d\mu_{G_n}(z) = \Re \int_D \ln^*(z_0 - z) d\mu_{G_n}(z)$$

is locally uniformly convergent as a function of z_0. Since $\Re \ln(z_0 - \lambda)$ is a harmonic function for all chromatic roots λ, so is $\Re \mathrm{t}_{G_n}(z_0)$, and the harmonicity of $\lim \mathrm{t}_{G_n}(z_0) = \lim \Re \mathrm{t}_{G_n}(z_0)$ follows from local uniform convergence. The observation that all harmonic functions are real analytic concludes the proof. □

Now we prove Proposition 2.3. Note that already Salas and Sokal [45] showed that the pointwise limit of supports of μ_{T_n} is part of a particular algebraic curve. For convenience, we include some details on that, also adding a picture on the supporting set, but we do not introduce the transfer matrix method here. See [45] for a description of the transfer matrix method.

Proposition 2.3. *The chromatic measures μ_{T_n} weakly converge.*

Proof. We defined T_n as the cartesian product of C_4 and P_n. By the transfer matrix method we obtain

$$\mathrm{ch}_{T_n}(z) = v_1 M^{n-1} \underline{\mathbf{1}}^\mathsf{T}$$

with

$$v_1 = \begin{pmatrix} z^4-6z^3+11z^2-6z & 2z^3-6z^2+4z & z^2-z \end{pmatrix}$$

$$M = \begin{pmatrix} z^4-10z^3+41z^2-84z+73 & 2z^3-14z^2+38z-40 & z^2-5z+8 \\ z^4-10z^3+40z^2-77z+60 & 2z^3-13z^2+32z-29 & z^2-4z+5 \\ z^4-10z^3+39z^2-70z+48 & 2z^3-12z^2+26z-20 & z^2-3z+3 \end{pmatrix}$$

$$\underline{\mathbf{1}}^\mathsf{T} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}.$$

Using the eigenvectors of M as our new basis we can diagonalize M and rewrite the above expression as

$$\mathrm{ch}_{T_n}(z) = u_1 D^{n-1} u_2$$

where

$$u_1 = \begin{pmatrix} \frac{z^7-10z^6+44z^5-105z^4+143z^3-109z^2+36z+z^3r-2z^2r+zr}{2z^3-12z^2+28z-24} \\ \frac{z^7-10z^6+44z^5-105z^4+143z^3-109z^2+36z-z^3r+2z^2r-zr}{2z^3-12z^2+28z-24} \\ 0 \end{pmatrix}^\mathsf{T}$$

$$D = \begin{pmatrix} \frac{z^4-8z^3+29z^2-55z+46+r}{2} & 0 & 0 \\ 0 & \frac{z^4-8z^3+29z^2-55z+46-r}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$u_2 = \begin{pmatrix} \frac{z^4-8z^3+27z^2-47z+36+r}{2r} \\ \frac{-z^4+8z^3-27z^2+47z-36+r}{2r} \\ 0 \end{pmatrix}$$

and

$$r = \sqrt{z^8-16z^7+118z^6-526z^5+1569z^4-3250z^3+4617z^2-4136z+1776}.$$

The matrix D^{n-1} is straightforward to calculate, so we get the following closed formula for the chromatic polynomial:

$$\mathrm{ch}_{T_n}(z) = a_1\lambda_1^{n-1} + a_2\lambda_2^{n-1}$$

where

$$a_i = \frac{z(z-1)(z^4-8z^3+27z^2-47z+36+r_i)(z^5-9z^4+35z^3-70z^2+73z-36+zr_i-r_i)}{4r_i(z-2)(z^2-4z+6)}$$

and

$$\lambda_i = \frac{z^4-8z^3+29z^2-55z+46+r_i}{2}$$

with $r_{1,2} = \pm r$.

We are interested in the complex roots of this expression if n is very large. We don't need to specify them exactly, but we'll prove a necessary condition. If the eigenvalues λ_i differ in their absolute value for some z, there will be an arbitrarily large multiplicative gap between $a_1\lambda_1^{n-1}$ and $a_2\lambda_2^{n-1}$ for any values of a_i unless both $a_1\lambda_1 = 0$ and $a_2\lambda_2 = 0$ holds.

It follows that all roots must have $|\lambda_1| = |\lambda_2|$ with the possible exception of a finite set consisting of the roots and singularities of a_1, a_2, λ_1 and λ_2, or equivalently, the roots of

$$\begin{gathered} z(z-1)(z-2)(2z-5)(z^2-3z+1)(z^2-4z+6)\cdot \\ \cdot(z^6-12z^5+61z^4-169z^3+269z^2-231z+85)\cdot \\ \cdot(z^8-16z^7+118z^6-526z^5+1569z^4-3250z^3+4617z^2-4136z+1776). \end{gathered}$$

Let's ignore this set $\mathcal{S}$ of special roots for now and concentrate on the general case of $|\lambda_1| = |\lambda_2|$:

$$\begin{gathered} \lambda_1\overline{\lambda_1} = \lambda_2\overline{\lambda_2} \\ \frac{z^4-8z^3+29z^2-55z+46+r}{2} \cdot \frac{\overline{z}^4-8\overline{z}^3+29\overline{z}^2-55\overline{z}+46+\overline{r}}{2} = \\ = \frac{z^4-8z^3+29z^2-55z+46-r}{2} \cdot \frac{\overline{z}^4-8\overline{z}^3+29\overline{z}^2-55\overline{z}+46-\overline{r}}{2} \\ (z^4-8z^3+29z^2-55z+46)\overline{r} + (\overline{z}^4-8\overline{z}^3+29\overline{z}^2-55\overline{z}+46)r = 0 \end{gathered}$$

Our last expression means that $(z^4-8z^3+29z^2-55z+46)\overline{r}$ is purely imaginary, which is equivalent to its square being a nonpositive real. When calculated, this gives a degree 14 algebraic curve clipped by a degree 16 algebraic curve, shown as the set $\mathcal{C}$ on the Figure 2.2.

It follows that the curve $\mathcal{C}$ is compact, has an empty interior and its complement is connected. Hence the same holds for $\mathcal{C}' = \mathcal{C} \cup \mathcal{S}$.

Now Mergelyan's theorem [40] says that every continuous function on $\mathcal{C}'$ can be uniformly approximated by polynomials. This implies that if two probability measures μ_1 and μ_2 are supported on $\mathcal{C}'$ and the holomorphic moments satisfy

$$\int_{\mathcal{C}'} z^k d\mu_1(z) = \int_{\mathcal{C}'} z^k d\mu_2(z) \quad (k \geq 1)$$

then

$$\int_{\mathcal{C}'} f(z) d\mu_1(z) = \int_{\mathcal{C}'} f(z) d\mu_2(z)$$

for all continuous functions $f : \mathcal{C}' \to \mathbb{R}$. Hence, we have $\mu_1 = \mu_2$. Since any subsequential weak limit of μ_{T_n} is supported on $\mathcal{C}'$, we get that μ_{T_n} is weakly convergent. $\square$

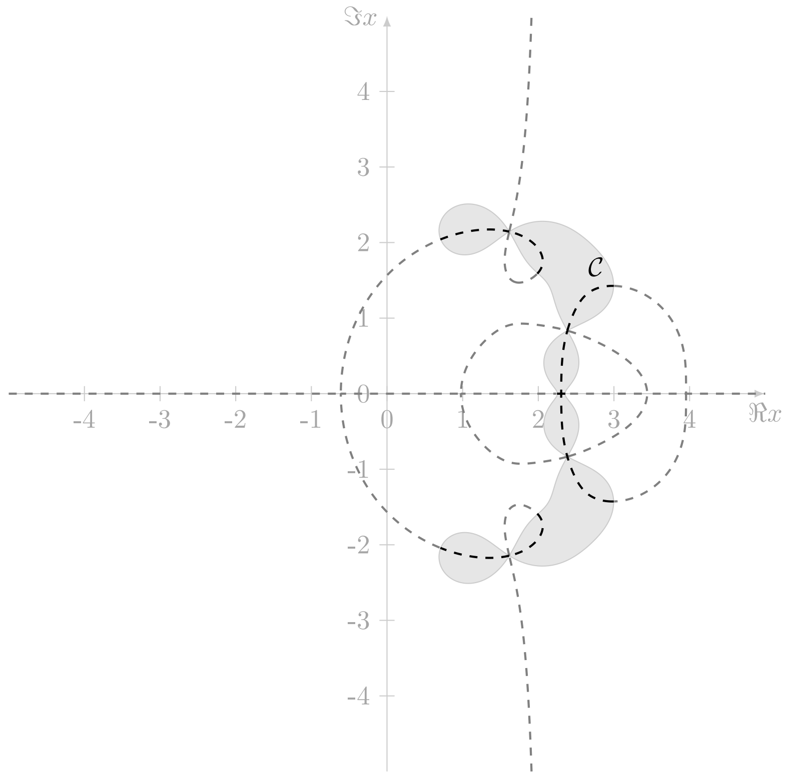


Figure 2.2: Possible limit points of chromatic roots of $T_n = C_4 \times P_n$ as $n \to \infty$

Remark. As we saw in the introduction, weak convergence does not hold in general. The phenomenon where an associated measure blows up by a small change of the graph but keeps its holomorphic moments unchanged also occurs in the spectral theory of *directed* graphs. Namely, the weak limit of the eigenvalue distributions of the directed path of length n is the Dirac measure at 0, while for the directed n-cycle the limit is the uniform measure on the unit circle centered at 0. In both the chromatic and the spectral case, the reason is that the change only affects the coefficients of small index in the corresponding polynomial, and the k-th moment only depends on the k highest index coefficients. It would be interesting to study this blow-up phenomenon using just abstract polynomials.

2.5 Graphs of large girth

In this section we study graphs with large girth and prove Theorem 2.4.

Lemma 2.12. *Suppose that the finite graphs G and H both have girth at least g and $|E(G)| = |E(H)|$. Then $e_i(G) = e_i(H)$ holds for $i = 0, 1, \ldots, g-2$.*

Proof. We use induction on $|E(G)| = |E(H)|$. If the number of edges is zero, the claim is trivial, as is when $g \leq 3$. Otherwise pick $e \in E(G)$ and $f \in E(H)$ arbitrarily and use the deletion-contraction argument:

$$e_i(G) = e_i(G \setminus e) + e_{i-1}(G/e)$$
$$e_i(H) = e_i(H \setminus f) + e_{i-1}(H/f)$$

The claim follows from the observation that $G \setminus e$ and $H \setminus f$ have girth $\geq g$ while G/e and H/f have girth $\geq g-1$. $\square$

Lemma 2.13. *Let G be a finite graph with girth $\geq g$. Then $p_i(G) = |E(G)|$ for $i = 1, 2, \ldots, g-2$.*

Proof. Let H be an arbitrary tree on $|E(G)|+1$ vertices and use the previous lemma. Since the chromatic polynomial of H is $q(q-1)^{|E(G)|}$, we have $e_i(H) = \binom{|E(G)|}{i}$ for $i \leq |E(G)|$, which translates into $e_i(G) = \binom{|E(G)|}{i}$ for $i \leq g-2$. Substituting the e_i's into Newton's identities completes the proof. $\square$

Theorem 2.4. *Let G be a finite graph of girth g and maximal degree d. Then for all $q > Cd$ we have*

$$\left| \frac{\ln \mathrm{ch}_G(q)}{|V(G)|} - \left(\ln q + \frac{|E(G)|}{|V(G)|} \ln(1 - \frac{1}{q}) \right) \right| \leq 2 \frac{(Cd/q)^{g-1}}{1 - Cd/q}.$$

Proof. The normalized log of the chromatic polynomial can be expanded as

$$\frac{\ln \mathrm{ch}_G(q)}{|V(G)|} = \int_D \ln(q-z) d\mu_G(z) = \ln q + \int_D \ln\left(1 - \frac{z}{q}\right) d\mu_G(z) =$$
$$= \ln q - \sum_{n=1}^{\infty} \frac{1}{nq^n} \int_D z^n d\mu_G(z)$$

where the Sokal bound $|z| \leq Cd$ gives the constraint

$$\left| \int_D z^n d\mu_G(z) \right| \leq (Cd)^n$$

for the holomorphic moments, and our last lemma implies

$$\int_D z^n d\mu_G(z) = \frac{p_n(G)}{|V(G)|} = \frac{|E(G)|}{|V(G)|}$$

for $n \leq g-2$. We also know that any real number $x \in [0, 1)$ satisfies

$$\sum_{n=g-1}^{\infty} \frac{x^n}{n} = \int_0^x \sum_{n=g-2}^{\infty} t^n dt = \int_0^x \frac{t^{g-2}}{1-t} dt \leq x \cdot \frac{x^{g-2}}{1-x} = \frac{x^{g-1}}{1-x}.$$

Now we have

$$\left|\frac{\ln \mathrm{ch}_G(q)}{|V(G)|} - \left(\ln q + \frac{|E(G)|}{|V(G)|}\ln(1-\frac{1}{q})\right)\right| =$$

$$= \left|\left(\ln q - \sum_{n=1}^{\infty}\frac{1}{nq^n}\int\limits_D z^n d\mu_G(Z)\right) - \left(\ln q - \sum_{n=1}^{\infty}\frac{1}{nq^n}\cdot\frac{|E(G)|}{|V(G)|}\right)\right| \le$$

$$\le \left|\sum_{n=g-1}^{\infty}\frac{1}{nq^n}\left(\int\limits_D z^n d\mu_G(z) - \frac{|E(G)|}{|V(G)|}\right)\right| \le \sum_{n=g-1}^{\infty}\frac{1}{nq^n}\left(\left|\int\limits_D z^n d\mu_G(z)\right| + \frac{|E(G)|}{|V(G)|}\right) \le$$

$$\le \sum_{n=g-1}^{\infty}\frac{(Cd)^n + |E(G)|/|V(G)|}{nq^n} \le \sum_{n=g-1}^{\infty}\frac{2(Cd)^n}{nq^n} \le 2\frac{(Cd/q)^{g-1}}{1-Cd/q}\ .$$

The theorem holds. □

2.6 Appendix

In the appendix we publish some data that may be useful for further analysis.

For abbreviation, we use the following terminology:

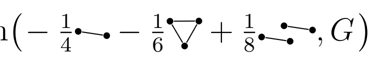
$$\mathrm{hom}\left(\sum_{i=1}^{n} \alpha_i G_i, H\right) = \sum_{i=1}^{n} \alpha_i \,\mathrm{hom}(G_i, H)$$

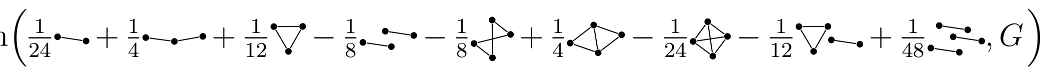
where the G_i and H are finite graphs.

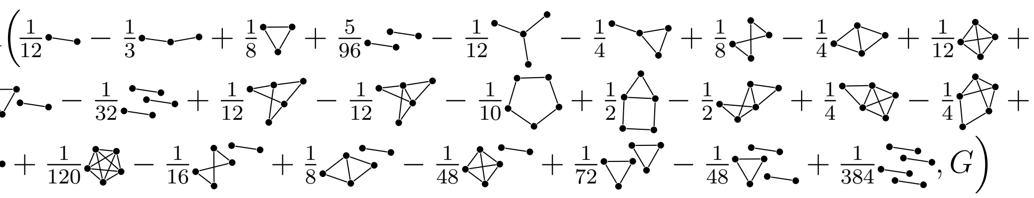
One can express the first 4 chromatic coefficients as a linear combination of homomorphisms as follows:

$e_0(G) = \mathrm{hom}(\bullet, G)$

$e_1(G) = \mathrm{hom}$ 

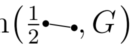
$e_2(G) = \mathrm{hom}$ 

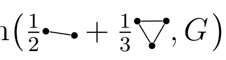
$e_3(G) = \mathrm{hom}$ 

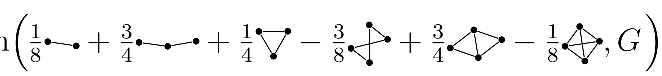
$e_4(G) = \mathrm{hom}$ 

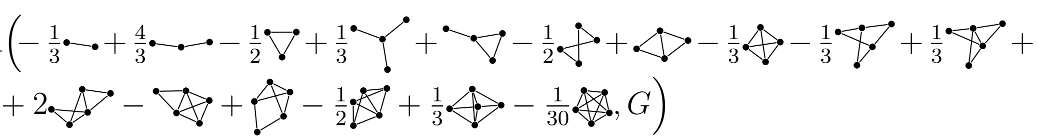
Also, one can express the first 5 chromatic moments as a linear combination of homomorphisms as follows.

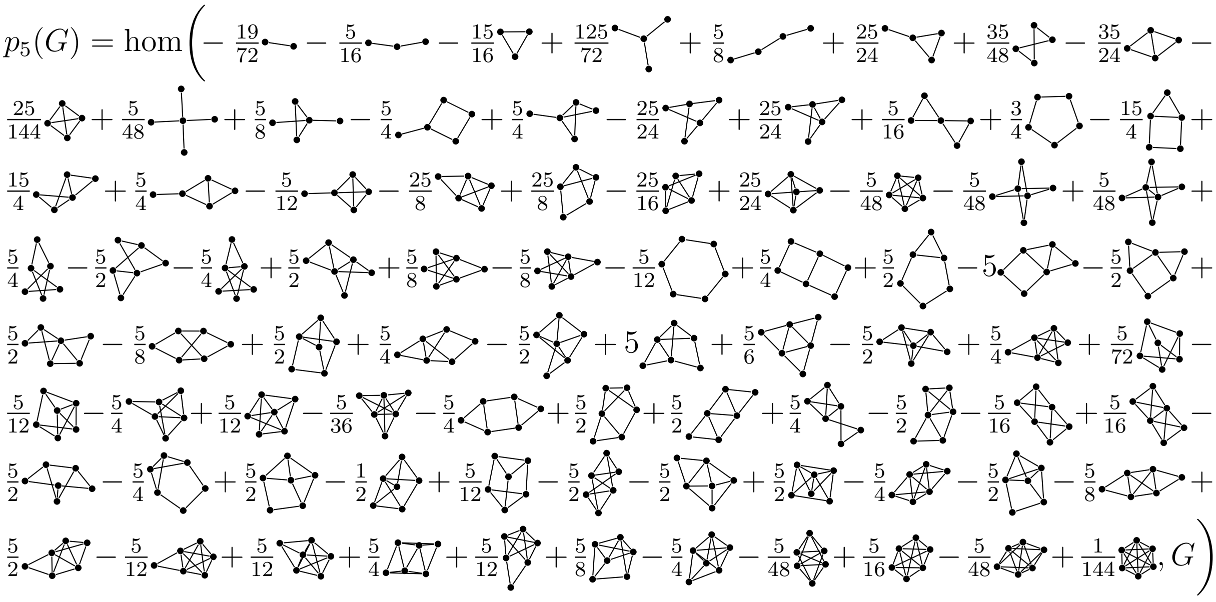
$p_0(G) = \mathrm{hom}(\bullet, G)$

$p_1(G) = \mathrm{hom}$ 

$p_2(G) = \mathrm{hom}$ 

$p_3(G) = \mathrm{hom}$ 

$p_4(G) = \mathrm{hom}$ 


p5(G) = hom(− 19/72 − 5/16 − 15/16 + 125/72 + 5/8 + 25/24 + 35/48 − 35/24 −
25/144 + 5/48 + 5/8 − 5/4 + 5/4 − 25/24 + 25/24 + 5/16 + 3/4 − 15/4 +
15/4 + 5/4 − 5/12 − 25/8 + 25/8 − 25/16 + 25/24 − 5/48 − 5/48 + 5/48 +
5/4 − 5/2 − 5/4 + 5/2 + 5/8 − 5/8 − 5/12 + 5/4 + 5/2 − 5 − 5/2 +
5/2 − 5/8 + 5/2 + 5/4 − 5/2 + 5 + 5/6 − 5/2 + 5/4 + 5/72 −
5/12 − 5/4 + 5/12 − 5/36 − 5/4 + 5/2 + 5/2 + 5/4 − 5/2 − 5/16 + 5/16 −
5/2 − 5/4 + 5/2 − 1/2 + 5/12 − 5/2 − 5/2 + 5/2 − 5/4 − 5/2 − 5/8 +
5/2 − 5/12 + 5/12 + 5/4 + 5/12 + 5/8 − 5/4 − 5/48 + 5/16 − 5/48 + 1/144, G)

Chapter 3

Matching measure and the monomer-dimer free energy

This chapter is based on the article [3], which is joint work with Miklós Abért and Péter Csikvári.

3.1 Introduction

The aim of this chapter is to define the matching measure of an infinite lattice L and show how it can be used to analyze the behaviour of the monomer-dimer model on L. The notion of matching measure has been recently introduced by Abért, Csikvári, Frenkel and Kun in [1]. There are essentially two ways to define it: in this chapter we take the path of giving a direct, spectral definition for infinite vertex transitive lattices, using self-avoiding walks and then connect it to the monomer-dimer model via graph convergence. Recall that a graph L is *vertex transitive* if for any two vertices of L there exists an automorphism of L that brings one vertex to the other.

Let v be a fixed vertex of the graph L. A walk in L is *self-avoiding*, if it touches every vertex at most once. There is a natural graph structure on the set of finite self-avoiding walks starting at v: we connect two walks if one is a one step extension of the other. The resulting graph is an infinite rooted tree, called the *tree of self-avoiding walks of L starting at v*.

Definition 3.1. *Let L be an infinite vertex transitive lattice. The* matching measure ρ_L *is the spectral measure of the tree of self-avoiding walks of L starting at v, where v is a vertex of L.*

By vertex transitivity, the definition is independent of v. For a more general definition, also covering lattices that are not vertex transitive, see Section 3.2.

To make sense of why we call this the matching measure, we need to recall the notion of Benjamini–Schramm convergence from Chapter 2. Let G_n be a sequence of finite graphs. We say that G_n Benjamini–Schramm converges to L, if for every $R > 0$, the probability that the R-ball centered at a uniform random vertex of G_n is isomorphic to the R-ball in L tends to 1 as n tends to infinity. That is, if by randomly sampling G_n and looking at a bounded distance, we can not distinguish it from L in probability.

All Euclidean lattices L can be approximated this way by taking sequences of boxes with side lengths tending to infinity, by bigger and bigger balls in L in its graph metric, or by suitable tori. When L is a Bethe lattice (a d-regular tree), finite subgraphs never converge to L and the usual way is to set G_n to be d-regular finite graphs where the minimal cycle length tends to infinity.

For a finite graph G and $k > 0$ let $m_k(G)$ be the number of monomer-dimer arrangements with k dimers (matchings of G using k edges). Let $m_0(G) = 1$. Let the *matching polynomial*

$$\mu(G, x) = \sum_k (-1)^k m_k(G) x^{|G|-2k}$$

and let ρ_G, the *matching measure of* G be the uniform distribution on the roots of $\mu(G, x)$. Note that $\mu(G, x)$ is just a reparametrization of the monomer-dimer partition function. The matching polynomial has the advantage over the partition function that its roots are bounded in terms of the maximal degree of G.

Using previous work of Godsil [25] we show that ρ_L can be obtained as the thermodynamical limit of the ρ_{G_n}.

Theorem 3.2. *Let L be an infinite vertex transitive lattice and let G_n Benjamini–Schramm converge to L. Then ρ_{G_n} weakly converges to ρ_L and $\lim_{n\to\infty} \rho_{G_n}(\{x\}) = \rho_L(\{x\})$ for all $x \in \mathbb{R}$.*

So in this sense, the matching measure can be thought of as the 'root distribution of the partition function for the infinite monomer-dimer model', transformed by a fixed reparametrization.

It turns out that the matching measure can be effectively used as a substitute for the Mayer series. An important advantage over it is that certain natural functions can be integrated along this measure even in those cases when the corresponding series do not converge. We demonstrate this advantage by giving new, strong estimates on the free energies of monomer-dimer models for Euclidean lattices, by expressing them directly from the matching measures.

The computation of monomer-dimer and dimer free energies has a long history. The precise value is known only in very special cases. Such an exceptional case is the Fisher-Kasteleyn-Temperley formula [21, 34, 44] for the dimer model on $\mathbb{Z}^2$. There is no such exact result for monomer-dimer models. The first approach for getting estimates was the use of the transfer matrix method. Hammersley [28, 29], Hammersley and Menon [30] and Baxter [7] obtained the first (non-rigorous) estimates for the free energy. Then Friedland and Peled [23] proved the rigorous estimates $0.6627989727 \pm 10^{-10}$ for $d = 2$ and the range $[0.7653, 0.7863]$ for $d = 3$. Here the upper bounds were obtained by the transfer matrix method, while the lower bounds relied on the Friedland-Tverberg inequality. The lower bound in the Friedland-Peled paper was subsequently improved by newer and newer results (see e.g. [22]) on Friedland's asymptotic matching conjecture which was finally proved by L. Gurvits [26]. Meanwhile, a non-rigorous estimate $[0.7833, 0.7861]$ was obtained via matrix permanents [33]. Concerning rigorous results, the most significant improvement was obtained recently by D. Gamarnik and D. Katz [24] via their new method which they called sequential cavity method. They obtained the range $[0.78595, 0.78599]$. More precise, but non-rigorous estimates can be found in the paper [14]. This chapter uses Mayer-series with many coefficients computed in the expansion. The related paper [13] may lead to further development through the so-called Positivity conjecture of the authors.

Here we only highlight one computational result. More data can be found in Section 3.3, in particular, in Table 3.2. Let $\tilde{\lambda}(L)$ denote the monomer-dimer free energy of the lattice L, and let $\mathbb{Z}^d$ denote the d-dimensional hyper-simple cubic lattice.

Theorem 3.3. *We have*

$$\tilde{\lambda}(\mathbb{Z}^3) = 0.7859659243 \pm 9.88 \cdot 10^{-7},$$

$$\tilde{\lambda}(\mathbb{Z}^4) = 0.8807178880 \pm 5.92 \cdot 10^{-6}.$$

$$\tilde{\lambda}(\mathbb{Z}^5) = 0.9581235802 \pm 4.02 \cdot 10^{-5}.$$

The bounds on the error terms are rigorous.

Our method allows to get efficient estimates on arbitrary lattices. The computational bottleneck is the tree of self-avoiding walks, which is famous to withstand theoretical interrogation.

It is natural to ask what are the actual matching measures for the various lattices. In the case of a Bethe lattice $\mathbb{T}_d$, the tree of self-avoiding walks again equals $\mathbb{T}_d$, so the matching measure of $\mathbb{T}_d$ coincides with its spectral measure. This explicit measure, called Kesten-McKay measure has density

$$\frac{d}{2\pi} \frac{\sqrt{4(d-1) - t^2}}{d^2 - t^2} \chi_{\{|t| \leq 2\sqrt{d-1}\}}.$$

We were not able to find such explicit formulae for any of the Euclidean lattices. However, using Theorem 3.2 one can show that the matching measures of hypersimple cubic lattices admit no atoms.

Theorem 3.4. *The matching measures $\rho_{\mathbb{Z}^d}$ have no atoms.*

In Section 3.4 we prove a more general result which also shows that for instance, the matching measure of the hexagonal lattice has no atoms. For some images on the matching measures of $\mathbb{Z}^2$ and $\mathbb{Z}^3$ see Section 3.4. We expect that the matching measures of all hypersimple cubic lattices are absolutely continuous with respect to the Lebesque measure. We also expect that the radius of support of the matching measure (that is, the spectral radius of the tree of self-avoiding walks) carries further interesting information about the lattice. Note that the *growth* of this tree for $\mathbb{Z}^d$ and other lattices has been under intense investigation [5, 19, 27], under the name *connective constant*.

The chapter is organized as follows. In Section 3.2, we define the basic notions and prove Theorem 3.2. In Section 3.3 we introduce the entropy function $\lambda_G(p)$ for finite graphs G and related functions, and we gather their most important properties. We also extend this concept to lattices. In this section we provide the computational data too. In Section 3.4, we prove Theorem 3.4.

3.2 Matching measure

3.2.1 Notations

This section is about the basic notions and lemmas needed later. Since the same objects have different names in graph theory and statistical mechanics, for the convenience of the reader, we start with a short dictionary.

Graph theory	Statistical mechanics
vertex	site
edge	bond
k-matching	monomer-dimer arrangement with k dimers
perfect matching	dimer arrangement
degree	coordination number
d-dimensional grid ($\mathbb{Z}^d$)	hyper-simple cubic lattice
infinite d-regular tree ($\mathbb{T}_d$)	Bethe lattice
path	self-avoiding walk

Table 3.1: A dictionary between graph theory and statistical mechanics

Throughout the chapter, G denotes a finite graph with vertex set $V(G)$ and edge set $E(G)$. The number of vertices is denoted by $|G|$. For an infinite graph L, we will use the word *lattice*. The *degree* of a vertex is the number of its neighbors. A graph is called *d-regular* if every vertex has degree exactly d. The graph $G - v$ denotes the graph obtained from G by erasing the vertex v together with all edges incident to v.

For a finite or infinite graph T, let $l^2(T)$ denote the Hilbert space of square summable real functions on $V(T)$. The *adjacency operator* $A_T : l^2(T) \to l^2(T)$ is defined by

$$(A_T f)(x) = \sum_{(x,y)\in E(T)} f(y) \qquad (f \in l^2(T)).$$

When T is finite, in the standard base of vertices, A_T is a square matrix, where $a_{u,v} = 1$ if the vertices u and v are adjacent, otherwise $a_{u,v} = 0$. For a finite graph T, the characteristic polynomial of A_T is denoted by $\phi(T, x) = \det(xI - A_T)$.

A *matching* is set of edges having pairwise distinct endpoints. A *k-matching* is a matching consisting of k edges. A graph is called *vertex-transitive* if for every vertex pair u and v, there exists an automorphism φ of the graph for which $\varphi(u) = v$.

3.2.2 Matching measure and tree of self-avoiding walks

The *matching polynomial* of a finite graph G is defined as

$$\mu(G,x) = \sum_k (-1)^k m_k(G) x^{|G|-2k},$$

where $m_k(G)$ denotes the number of k-matchings in G. Let ρ_G, the *matching measure* of G be the uniform distribution on the zeros of the matching polynomial of G.

The fundamental theorem for the matching polynomial is the following.

Theorem 3.5 (Heilmann and Lieb [32]). *The roots of the matching polynomial $\mu(G,x)$ are real, and if the largest degree D is greater than 1, then all roots lie in the interval $[-2\sqrt{D-1}, 2\sqrt{D-1}]$.*

A walk in a graph is *self-avoiding* if it touches every vertex at most once. For a finite graph G and a root vertex v, one can construct $T_v(G)$, the *tree of self-avoiding walks at v* as follows: its vertices correspond to the finite self-avoiding walks in G starting at v, and we connect two walks if one of them is a one-step extension of the other. The following figure illustrates that in general, $T_v(G)$ very much depends on the choice of v.

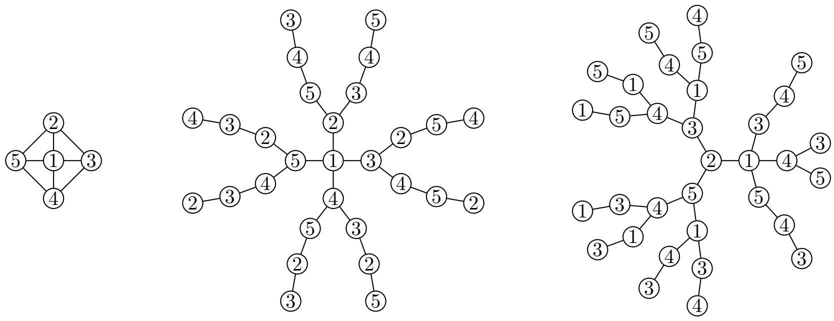


Figure 3.1: The pyramid graph and its trees of self-avoiding walks starting from ① and ② respectively.

Recall that the spectral measure of a (possibly infinite) rooted graph (T,v) is defined as follows. Assume that T has bounded degree. Then the adjacency operator $A_T : l^2(T) \to l^2(T)$ is bounded and self-adjoint, hence it admits a spectral measure $P_T(X)$ ($X \subseteq \mathbb{R}$ Borel). This is a projection-valued measure on $\mathbb{R}$ such that for any polynomial $F(x)$ we have

$$F(A) = \int F(x) dP_x \tag{Sp}$$

where $P_x = P((-\infty, x))$. We define $\delta_{(T,v)}$, the *spectral measure of T at v* by

$$\delta_{(T,v)}(X) = \langle P_T(X)\chi_v, P_T(X)\chi_v\rangle = \langle P_T(X)\chi_v, \chi_v\rangle \quad (X \subseteq \mathbb{R} \text{ Borel})$$

where χ_v is the characteristic vector of v. It is easy to check that $\delta_{(T,v)}$ is a probability measure supported on the spectrum of the operator A_T. Also, by (Sp), for all $k \geq 0$, the k-th moment of $\delta_{(T,v)}$ equals

$$\int x^k d\delta_{(T,v)} = \left\langle A^k \chi_v, \chi_v \right\rangle = a_k(T,v)$$

where $a_k(T, v)$ is the number of returning walks of length k starting at v.

It turns out that the matching measure of a finite graph equals the average spectral measure over its trees of self-avoiding walks.

Theorem 3.6. *Let G be a finite graph and let v be a vertex of G chosen uniformly at random. Then*

$$\rho_G = \mathbb{E}_v \delta_{(T_v(G),v)}.$$

Equivalently, for all $k \geq 0$, the k-th moment of ρ_G equals the expected number of returning walks of length k in $T_v(G)$ starting at v.

In particular, Theorem 3.6 gives one of the several known proofs for the Heilmann-Lieb theorem. Indeed, spectral measures are real and the spectral radius of a tree with degree bound D is at most $2\sqrt{D-1}$.

To prove Theorem 3.6 we need the following result of Godsil [25] which connects the matching polynomial of the original graph G and the tree of self-avoiding walks:

Theorem 3.7. *[25] Let G be a finite graph and v be an arbitrary vertex of G. Then*

$$\frac{\mu(G - v, x)}{\mu(G, x)} = \frac{\mu(T_v(G) - v, x)}{\mu(T_v(G), x)}.$$

We will also use two well-known facts which we gather in the following proposition:

Proposition 3.8. *[25] (a) For any tree or forest T, the matching polynomial $\mu(T, x)$ coincides with the characteristic polynomial $\phi(T, x)$ of the adjacency matrix of the tree T:*

$$\mu(T, x) = \phi(T, x).$$

(b) For any graph G, we have

$$\mu'(G, x) = \sum_{v \in V} \mu(G - v, x).$$

Proof of Theorem 3.6. First, let us use part (a) of Proposition 3.8 for the tree $T_v(G)$ and the forest $T_v(G) - v$:

$$\frac{\mu(T_v(G) - v, x)}{\mu(T_v(G), x)} = \frac{\phi(T_v(G) - v, x)}{\phi(T_v(G), x)}.$$

On the other hand, for any graph H and vertex u, we have

$$\frac{\phi(H - u, x)}{\phi(H, x)} = x^{-1} \sum_{k=0}^{\infty} c_k(u) x^{-k},$$

where $c_k(u)$ counts the number of walks of length k starting and ending at u. So this is exactly the moment generating function of the spectral measure with respect to the vertex u. Putting together these with Theorem 3.7 we see that

$$\frac{\mu(G - v, x)}{\mu(G, x)} = \frac{\mu(T_v(G) - v, x)}{\mu(T_v(G), x)} = x^{-1} \sum_{k=0}^{\infty} a_k(v) x^{-k}$$

is the moment generating function of the spectral measure of the tree of self-avoiding walks with respect to the vertex v.

Now let us consider the left hand side of Theorem 3.7. Let us use part (b) of Proposition 3.8:

$$\mu'(G,x) = \sum_{u \in V} \mu(G-u,x).$$

This implies that

$$\mathbb{E}_v \frac{\mu(G-v,x)}{\mu(G,x)} = \frac{1}{|G|}\frac{\mu'(G,x)}{\mu(G,x)} = x^{-1}\sum_{k=0}^{\infty} \mu_k x^{-k},$$

where

$$\mu_k = \frac{1}{|G|}\sum \lambda^k,$$

where the summation goes through the zeros of the matching polynomial. In other words, μ_k is k-th moment of the matching measure defined by the uniform distribution on the zeros of the matching polynomial. Putting everything together we see that

$$\mu_k = \mathbb{E}_v a_k(v).$$

Since both ρ_G and $\mathbb{E}_v \rho(v)$ are supported on $\{|x| \le \|A_G\|\}$, we get that the two measures are equal. $\square$

We already defined Benjamini–Schramm convergence in Chapter 2, but we give an extended definition here that also includes a notion of the limit, at least in the special case when it is a vertex transitive lattice.

Definition 3.9. *For a finite graph G, a finite rooted graph α and a positive integer r, let $\mathbb{P}(G,\alpha,r)$ be the probability that the r-ball centered at a uniform random vertex of G is isomorphic to α. We say that a graph sequence (G_n) of bounded degree is* Benjamini–Schramm convergent *if for all finite rooted graphs α and $r > 0$, the probabilities $\mathbb{P}(G_n,\alpha,r)$ converge. Let L be a vertex transitive lattice. We say that (G_n)* Benjamini–Schramm converges to *L, if for all positive integers r, $\mathbb{P}(G_n,\alpha_r,r) \to 1$ where α_r is the r-ball in L.*

Example 3.10. *Let us consider a sequence of boxes in $\mathbb{Z}^d$ where all sides converge to infinity. This will be Benjamini–Schramm convergent graph sequence since for every fixed r, we will pick a vertex which at least r-far from the boundary with probability converging to* 1*. For all these vertices we will see the same neighborhood. This also shows that we can impose arbitrary boundary condition, for instance periodic boundary condition means that we consider the sequence of toroidal boxes. Boxes and toroidal boxes will be Benjamini–Schramm convergent even together.*

We prove the following generalization of Theorem 3.2.

Theorem 3.11. *Let (G_n) be a Benjamini–Schramm convergent bounded degree graph sequence. Then the sequence of matching measures ρ_{G_n} is weakly convergent. If (G_n) Benjamini–Schramm converges to the vertex transitive lattice L, then ρ_{G_n} weakly converges to ρ_L and $\lim_{n\to\infty} \rho_{G_n}(\{x\}) = \rho_L(\{x\})$ for all $x \in \mathbb{R}$.*

Remark 3.12. The first part of the theorem was first proved in [1]. The proof given there relied on a general result on graph polynomials given in [16]. For completeness, we give an alternate self-contained proof here.

We will use the following theorem of Thom [48]. See also [4] where this is used for Benjamini–Schramm convergent graph sequences.

Theorem 3.13 (Thom)**.** *Let $(q_n(z))$ be a sequence of monic polynomials with integer coefficients. Assume that all zeros of all $q_n(z)$ are at most R in absolute value. Let ρ_n be the probability measure of uniform distribution on the roots of $q_n(z)$. Assume that ρ_n weakly converges to some measure ρ. Then for all $\theta \in \mathbb{C}$ we have*

$$\lim_{n\to\infty} \rho_n(\{\theta\}) = \rho(\{\theta\}).$$

Proof of Theorem 3.2 and 3.11. For $k \geq 0$ let

$$\mu_k(G) = \int z^k \, d\rho_G(z)$$

be the k-th moment of ρ_G. By Theorem 3.6 we have

$$\mu_k(G) = \mathbb{E}_v a_k(G, v)$$

where $a_k(G, v)$ denotes the number of closed walks of length k of the tree $T_v(G)$ starting and ending at the vertex v.

Clearly, the value of $a_k(G, v)$ only depends on the k-ball centered at the vertex v. Let $TW(\alpha) = a_k(G, v)$ where the k-ball centered at v is isomorphic to α. Note that the value of $TW(\alpha)$ depends only on the rooted graph α and does not depend on G.

Let $\mathcal{N}_k$ denote the set of possible k-balls in G. The size of $\mathcal{N}_k$ and $TW(\alpha)$ are bounded by a function of k and the largest degree of G. By the above, we have

$$\mu_k(G) = \mathbb{E}_v a_k(G, v) = \sum_{\alpha \in \mathcal{N}_k} \mathbb{P}(G, \alpha, k) \cdot TW(\alpha).$$

Since (G_n) is Benjamini–Schramm convergent, we get that for every fixed k, the sequence of k-th moments $\mu_k(G_n)$ converges. The same holds for $\int q(z)\, d\rho_{G_n}(z)$ where q is any polynomial. By the Heilmann–Lieb theorem, ρ_{G_n} is supported on $[-2\sqrt{D-1}, 2\sqrt{D-1}]$ where D is the absolute degree bound for G_n. Since every continuous function can be uniformly approximated by a polynomial on $[-2\sqrt{D-1}, 2\sqrt{D-1}]$, we get that the sequence (ρ_{G_n}) is weakly convergent.

Assume that (G_n) Benjamini–Schramm converges to L. Then for all $k \geq 0$ we have $\mathbb{P}(G_n, \alpha_k, k) \to 1$ where α_k is the k-ball in L, which implies

$$\lim_{n\to\infty} \mu_k(G_n) = \lim_{n\to\infty} \sum_{\alpha \in \mathcal{N}_k} \mathbb{P}(G_n, \alpha, k) \cdot TW(\alpha) = TW(\alpha_k) = a_k(L, v)$$

where v is any vertex in L. This means that all the moments of ρ_L and $\lim \rho_{G_n}$ are equal, so $\lim \rho_{G_n} = \rho_L$.

Since the matching polynomial is monic with integer coefficients, Theorem 3.13 gives $\lim_{n\to\infty} \rho_{G_n}(\{x\}) = \rho_L(\{x\})$ for all $x \in \mathbb{R}$. □

3.3 The function $\lambda_G(p)$

Let G be a finite graph, and recall that $|G|$ denotes the number of vertices of G, and $m_k(G)$ denotes the number of k-matchings ($m_0(G) = 1$). Let t be the activity, a non-negative real number, and

$$M(G,t) = \sum_{k=0}^{\lfloor |G|/2 \rfloor} m_k(G) t^k,$$

We call $M(G,t)$ the matching generating function or the partition function of the monomer-dimer model. Clearly, it encodes the same information as the matching polynomial. Let

$$p(G,t) = \frac{2t \cdot M'(G,t)}{|G| \cdot M(G,t)},$$

and

$$F(G,t) = \frac{\ln M(G,t)}{|G|} - \frac{1}{2} p(G,t) \ln(t).$$

Note that

$$\tilde{\lambda}(G) = F(G,1)$$

is called the monomer-dimer free energy.

The function $p = p(G,t)$ is a strictly monotone increasing function which maps $[0,\infty)$ to $[0,p^*)$, where $p^* = \frac{2\nu(G)}{|G|}$, where $\nu(G)$ denotes the number of edges in the largest matching. If G contains a perfect matching, then $p^* = 1$. Therefore, its inverse function $t = t(G,p)$ maps $[0,p^*)$ to $[0,\infty)$. (If G is clear from the context, then we will simply write $t(p)$ instead of $t(G,p)$.) Let

$$\lambda_G(p) = F(G, t(p))$$

if $p < p^*$, and $\lambda_G(p) = 0$ if $p > p^*$. Note that we have not defined $\lambda_G(p^*)$ yet. We simply define it as a limit:

$$\lambda_G(p^*) = \lim_{p \nearrow p^*} \lambda_G(p).$$

We will show that this limit exists, see part (d) of Proposition 3.15. Later we will extend the definition of $p(G,t), F(G,t)$ and $\lambda_G(p)$ to infinite lattices L.

The intuitive meaning of $\lambda_G(p)$ is the following. Assume that we want to count the number of matchings covering p fraction of the vertices. Let us assume that it makes sense: $p = \frac{2k}{|G|}$, and so we wish to count $m_k(G)$. Then

$$\lambda_G(p) \approx \frac{\ln m_k(G)}{|G|}.$$

The more precise formulation of this statement will be given in Proposition 3.15. To prove this proposition we need some preparation.

We will use the following theorem of Darroch.

Lemma 3.14 (Darroch's rule [17]). *Let $P(x) = \sum_{k=0}^{n} a_k x^k$ be a polynomial with only positive coefficients and real zeros. If*

$$k - \frac{1}{n-k+2} < \frac{P'(1)}{P(1)} < k + \frac{1}{k+2},$$

then k is the unique number for which $a_k = \max(a_1, a_2, \dots, a_n)$. If, on the other hand,

$$k + \frac{1}{k+2} < \frac{P'(1)}{P(1)} < k + 1 - \frac{1}{n-k+1},$$

then either a_k or a_{k+1} is the maximal element of $a_1, a_2, \dots, a_n$.

Proposition 3.15. *Let G be a finite graph.*
(a) Let nG be n disjoint copies of G. Then

$$\lambda_G(p) = \lambda_{nG}(p).$$

(b) If $p < p^*$, then

$$\frac{d}{dp}\lambda_G(p) = -\frac{1}{2}\ln t(p).$$

(c) The limit

$$\lambda_G(p^*) = \lim_{p \nearrow p^*} \lambda_G(p)$$

exists.
(d) Let $k \leq \nu(G)$ and $p = \frac{2k}{|G|}$. Then

$$\left| \lambda_G(p) - \frac{\ln m_k(G)}{|G|} \right| \leq \frac{\ln |G|}{|G|}.$$

(e) Let $k = \nu(G)$, then for $p^* = \frac{2k}{|G|}$ we have

$$\lambda_G(p^*) = \frac{\ln m_k(G)}{|G|}.$$

(f) If for some function $f(p)$ we have

$$\lambda_G(p) \geq f(p) + o_{|G|}(1)$$

then

$$\lambda_G(p) \geq f(p).$$

Proof. (a) Let nG be the disjoint union of n copies of G. Note that

$$M(nG, t) = M(G, t)^n$$

implying that $p(nG, t) = p(G, t)$ and $\lambda_{nG}(p) = \lambda_G(p)$.

(b) Since

$$\lambda_G(p) = \frac{\ln M(G, t)}{|G|} - \frac{1}{2} p(G, t) \ln(t)$$

we have

$$\frac{d\lambda_G(p)}{dp} = \left(\frac{1}{|G|} \cdot \frac{M'(G,t)}{M(G,t)} \cdot \frac{dt}{dp} - \frac{1}{2}\left(\ln(t) + p \cdot \frac{1}{t} \cdot \frac{dt}{dp}\right)\right) = -\frac{1}{2}\ln(t),$$

since

$$\frac{1}{|G|} \cdot \frac{M'(G,t)}{M(G,t)} = \frac{p}{2t}$$

by definition.

(c) From $\frac{d}{dp}\lambda_G(p) = -\frac{1}{2}\ln t(p)$ we see that if $p > p(G,1)$, the function $\lambda_G(p)$ is monotone decreasing. (Note that we also see that $\lambda_G(p)$ is a concave-down function.) Hence

$$\lim_{p \nearrow p^*} \lambda_G(p) = \inf_{p > p(G,1)} \lambda_G(p).$$

(d) First, let us assume that $k < \nu(G)$. In case of $k = \nu(G)$, we will slightly modify our argument. Let $t = t(p)$ be the value for which $p = p(G,t)$. The polynomial

$$P(G,x) = M(G,tx) = \sum_{j=0}^{n} m_j(G) t^j x^j$$

considered as a polynomial in variable x, has only real zeros by Theorem 3.5. Note that

$$k = \frac{p|G|}{2} = \frac{P'(G,1)}{P(G,1)}.$$

Darroch's rule says that in this case $m_k(G)t^k$ is the unique maximal element of the coefficient sequence of $P(G,x)$. In particular

$$\frac{M(G,t)}{|G|} \leq m_k(G)t^k \leq M(G,t).$$

Hence

$$\lambda_G(p) - \frac{\ln|G|}{|G|} \leq \frac{\ln m_k(G)}{|G|} \leq \lambda_G(p).$$

Hence in case of $k < \nu(G)$, we are done.

If $k = \nu(G)$, then let p be arbitrary such that

$$k - \frac{1}{2} < \frac{p|G|}{2} < k.$$

Again we can argue by Darroch's rule as before that

$$\lambda_G(p) - \frac{\ln|G|}{|G|} \leq \frac{\ln m_k(G)}{|G|} \leq \lambda_G(p).$$

Since this is true for all p sufficiently close to $p^* = \frac{2\nu(G)}{|G|}$ and

$$\lambda_G(p^*) = \lim_{p \nearrow p^*} \lambda_G(p),$$

we have

$$\left| \frac{\ln m_k(G)}{|G|} - \lambda_G(p^*) \right| \leq \frac{\ln |G|}{|G|}$$

in this case too.

(e) By part (a) we have $\lambda_{nG}(p) = \lambda_G(p)$. Note also that if $k = \nu(G)$, then $m_{nk}(nG) = m_k(G)^n$. Applying the bound from part (d) to the graph nG, we obtain that

$$\left| \frac{\ln m_k(G)}{|G|} - \lambda_G(p^*) \right| \leq \frac{\ln |nG|}{|nG|}.$$

Since

$$\frac{\ln |nG|}{|nG|} \to 0$$

as $n \to \infty$, we get that

$$\lambda_G(p^*) = \frac{\ln m_k(G)}{|G|}.$$

(f) This is again a trivial consequence of $\lambda_{nG}(p) = \lambda_G(p)$. $\square$

Our next aim is to extend the definition of the function $\lambda_G(p)$ for infinite lattices L. We also show an efficient way of computing its values if p is sufficiently separated from p^*.

The following theorem was known in many cases for thermodynamic limit.

Theorem 3.16. *Let (G_n) be a Benjamini–Schramm convergent sequence of bounded degree graphs. Then the sequences of functions*
(a)

$$p(G_n, t),$$

(b)

$$\frac{\ln M(G_n, t)}{|G_n|}$$

converge to strictly monotone increasing continuous functions on the interval $[0, \infty)$. If, in addition, every G_n has a perfect matching then the sequences of functions
(c)

$$t(G_n, p),$$

(d)

$$\lambda_{G_n}(p)$$

are convergent for all $0 \leq p < 1$.

Remark 3.17. In part (c), we used the extra condition to ensure that $p^* = 1$ for all these graphs. We mention that H. Nguyen and K. Onak [41], and independently G. Elek and G. Lippner [20] proved that for a Benjamini–Schramm convergent graph sequence (G_n), the following limit exits:

$$\lim_{n\to\infty} \frac{2\nu(G_n)}{|G_n|} = \lim_{n\to\infty} p^*(G_n).$$

In particular, one can extend part (c) to graph sequences without perfect matchings. Since we are primarily interested in lattices with perfect matchings, we leave it to the Reader.

To prove Theorem 3.16, we essentially repeat an argument of the paper [1].

Proof of Theorem 3.16. First we prove part (a) and (b). For a graph G let $S(G)$ denote the set of zeros of the matching polynomial $\mu(G,x)$, then

$$M(G,t) = \prod_{\substack{\lambda\in S(G)\\ \lambda>0}} (1+\lambda^2 t) = \prod_{\lambda\in S(G)} (1+\lambda^2 t)^{1/2}.$$

Then

$$\ln M(G,t) = \sum_{\lambda\in S(G)} \frac{1}{2}\ln\left(1+\lambda^2 t\right).$$

By differentiating both sides we get that

$$\frac{M'(G,t)}{M(G,t)} = \sum_{\lambda\in S(G)} \frac{1}{2}\frac{\lambda^2}{1+\lambda^2 t}.$$

Hence

$$p(G,t) = \frac{2t\cdot M'(G,t)}{|G|\cdot M(G,t)} = \frac{1}{|G|}\sum_{\lambda\in S(G)} \frac{\lambda^2 t}{1+\lambda^2 t} = \int \frac{tz^2}{1+tz^2}\, d\rho_G(z).$$

Similarly,

$$\frac{\ln M(G,t)}{|G|} = \frac{1}{|G|}\sum_{\lambda\in S(G)} \frac{1}{2}\ln\left(1+\lambda^2 t\right) = \int \frac{1}{2}\ln\left(1+tz^2\right)\, d\rho_G(z).$$

Since (G_n) is a Benjamini–Schramm convergent sequence of bounded degree graphs, the sequence (ρ_{G_n}) weakly converges to some ρ^* by Theorem 3.11. Since both functions

$$\frac{tz^2}{1+tz^2} \quad \text{and} \quad \frac{1}{2}\ln\left(1+tz^2\right)$$

are continuous, we immediately obtain that

$$\lim_{n\to\infty} p(G_n,t) = \int \frac{tz^2}{1+tz^2}\, d\rho^*(z),$$

and

$$\lim_{n\to\infty} \frac{\ln M(G_n,t)}{|G_n|} = \int \frac{1}{2}\ln\left(1+tz^2\right)\, d\rho^*(z).$$

Note that both functions

$$\frac{tz^2}{1+tz^2} \quad \text{and} \quad \frac{1}{2}\ln\left(1+tz^2\right)$$

are strictly monotone increasing continuous functions in the variable t. Thus their integrals are also strictly monotone increasing continuous functions.

To prove part (c), let us introduce the function

$$p(L,t) = \int \frac{tz^2}{1+tz^2}\, d\rho^*(z).$$

We have seen that $p(L,t)$ is a strictly monotone increasing continuous function, and equals $\lim_{n\to\infty} p(G_n,t)$. Since for all G_n, $p^*(G_n)=1$, we have $\lim_{t\to\infty} p(G_n,t)=1$ for all n. This means that $\lim_{t\to\infty} p(L,t)=1$. Hence we can consider inverse function $t(L,p)$ which maps $[0,1)$ to $[0,\infty)$. We show that

$$\lim_{n\to\infty} t(G_n,p) = t(L,p)$$

pointwise. Assume by contradiction that this is not the case. This means that for some p_1, there exists an ε and an infinite sequence n_i for which

$$|t(L,p_1) - t(G_{n_i},p_1)| \geq \varepsilon.$$

We distinguish two cases according to
(i) there exists an infinite sequence (n_i) for which

$$t(G_{n_i},p_1) \geq t(L,p_1)+\varepsilon,$$

or (ii) there exists an infinite sequence (n_i) for which

$$t(G_{n_i},p_1) \leq t(L,p_1)-\varepsilon.$$

In the first case, let $t_1 = t(L,p_1)$, $t_2 = t_1+\varepsilon$ and $p_2 = p(L,t_2)$. Clearly, $p_2 > p_1$. Note that

$$t(G_{n_i},p_1) \geq t(L,p_1)+\varepsilon = t_2$$

and $p(G_{n_i},t)$ are monotone increasing functions, thus

$$p(G_{n_i},t_2) \leq p(G_{n_i},t(G_{n_i},p_1)) = p_1 = p_2-(p_2-p_1) = p(L,t_2)-(p_2-p_1).$$

This contradicts the fact that

$$\lim_{n\to\infty} p(G_{n_i},t_2) = p(L,t_2).$$

In the second case, let $t_1 = t(L,p_1)$, $t_2 = t_1-\varepsilon$ and $p_2 = p(L,t_2)$. Clearly, $p_2 < p_1$. Note that

$$t(G_{n_i},p_1) \leq t(L,p_1)-\varepsilon = t_2$$

and $p(G_{n_i}, t)$ are monotone increasing functions, thus

$$p(G_{n_i}, t_2) \geq p(G_{n_i}, t(G_{n_i}, p_1)) = p_1 = p_2 + (p_1 - p_2) = p(L, t_2) + (p_1 - p_2).$$

This again contradicts the fact that

$$\lim_{n\to\infty} p(G_{n_i}, t_2) = p(L, t_2).$$

Hence $\lim_{n\to\infty} t(G_n, p) = t(L, p)$.

Finally, we show that $\lambda_{G_n}(p)$ converges for all p. Let $t = t(L, p)$, and

$$\lambda_L(p) = \lim_{n\to\infty} \frac{\ln M(G_n, t)}{|G_n|} - \frac{1}{2} p \ln(t).$$

Note that

$$\lambda_{G_n}(p) = \frac{\ln M(G_n, t_n)}{|G_n|} - \frac{1}{2} p \ln(t_n),$$

where $t_n = t(G_n, p)$. We have seen that $\lim_{n\to\infty} t_n = t$. Hence it is enough to prove that the functions

$$\frac{\ln M(G_n, u)}{|G_n|}$$

are equicontinuous. Let us fix some u_0 and let

$$H(u_0, u) = \max_{z\in[-2\sqrt{D-1}, 2\sqrt{D-1}]} \left| \frac{1}{2} \ln\left(1 + u_0 z^2\right) - \frac{1}{2} \ln\left(1 + u z^2\right) \right|.$$

Clearly, if $|u - u_0| \leq \delta$ for some sufficiently small δ, then $H(u_0, u) \leq \varepsilon$, and

$$\left| \frac{\ln M(G_n, u)}{|G_n|} - \frac{\ln M(G_n, u_0)}{v(G_n)} \right| = \left| \int \frac{1}{2} \ln\left(1 + u_0 z^2\right)\, d\rho_{G_n}(z) - \int \frac{1}{2} \ln\left(1 + u z^2\right)\, d\rho_{G_n}(z) \right| \leq$$

$$\leq \int \left| \frac{1}{2} \ln\left(1 + u_0 z^2\right) - \frac{1}{2} \ln\left(1 + u z^2\right) \right| d\rho_{G_n}(z) \leq \int H(u, u_0)\, d\rho_{G_n}(z) \leq \varepsilon.$$

This completes the proof of the convergence of $\lambda_{G_n}(p)$. □

Definition 3.18. *Let L be an infinite lattice and (G_n) be a sequence of finite graphs which is Benjamini–Schramm convergent to L. For instance, G_n can be chosen to be an exhaustion of L. Then the sequence of measures (ρ_{G_n}) weakly converges to some measure which we will call ρ_L, the matching measure of the lattice L. For $t > 0$, we can introduce*

$$p(L, t) = \int \frac{tz^2}{1 + tz^2}\, d\rho_L(z)$$

and

$$F(L, t) = \int \frac{1}{2} \ln\left(1 + tz^2\right)\, d\rho_L(z) - \frac{1}{2} p(L, t) \ln(t).$$

If the lattice L contains a perfect matching, then we can choose G_n such that all G_n contain a perfect matching. Then $p(L,t)$ maps $[0,\infty)$ to $[0,1)$ in a monotone increasing way, and we can consider its inverse function $t(L,p)$. Finally, we can introduce

$$\lambda_L(p) = F(L, t(L,p))$$

for all $p \in [0,1)$. We will define $\lambda_L(1)$ as

$$\lambda_L(1) = \lim_{p \nearrow 1} \lambda_L(p).$$

Remark 3.19. In the literature, the so-called Mayer series are computed for various lattices L:

$$p(L,t) = \sum_{n=1}^{\infty} b_n t^n$$

for small enough t. Let us compare it with

$$p(L,t) = \int \frac{tz^2}{1+tz^2}\, d\rho_L(z) = \int \left(\sum_{n=1}^{\infty} (-1)^{n+1} z^{2n} t^n \right) d\rho_L(z) = \sum_{n=1}^{\infty} (-1)^{n+1} \left(\int z^{2n} d\rho_L(z) \right) t^n.$$

Hence if we introduce the moment sequence

$$\mu_k = \int z^k d\rho_L(z),$$

we see that

$$\mu_{2n} = \int z^{2n} d\rho_L(z) = (-1)^{n+1} b_n.$$

Note that $\mu_0 = 1$ and $\mu_{2n-1} = 0$ since the matching measures are symmetric to 0. Since the support of the measure ρ_L lie in the interval $[-2\sqrt{D-1}, 2\sqrt{D-1}]$, we see that the Mayer series converges whenever $|t| < \frac{1}{4(D-1)}$. We also would like to point out that the integral is valid for all $t > 0$, while the Mayer series does not converge if t is 'large'.

3.3.1 Computation of the monomer-dimer free energy

The monomer-dimer free energy of a lattice L is $\tilde{\lambda}(L) = F(L,1)$. Its computation can be carried out exactly the same way as we proved its existence: we use that

$$\tilde{\lambda}(L) = F(L,1) = \int \frac{1}{2} \ln\left(1+z^2\right)\, d\rho_L(z).$$

Assume that we know the moment sequence (μ_k) for $k \leq N$. Then let us choose a polynomial of degree at most N, which uniformly approximates the function

$$\frac{1}{2} \ln\left(1+z^2\right)$$

on the interval $[-2\sqrt{D-1}, 2\sqrt{D-1}]$, where D is the coordination number of L. A good polynomial approximation can be found by Remez's algorithm. Assume that we have a polynomial

$$q(z) = \sum_{k=0}^{N} c_k z^k$$

for which

$$\left| \frac{1}{2} \ln\left(1+z^2\right) - q(z) \right| \leq \varepsilon$$

for all $z \in [-2\sqrt{D-1}, 2\sqrt{D-1}]$. Then

$$\left| \tilde{\lambda}(L) - \int q(z)\, d\rho_L(z) \right| \leq \int \left| \frac{1}{2} \ln\left(1+z^2\right) - q(z) \right| d\rho_L(z) \leq \varepsilon,$$

and

$$\int q(z)\, d\rho_L(z) = \sum_{k=0}^{N} c_k \mu_k.$$

Hence

$$\left| \tilde{\lambda}(L) - \sum_{k=0}^{N} c_k \mu_k \right| \leq \varepsilon.$$

How can we compute the moment sequence (μ_k)? One way is to use its connection with the Mayer series (see Remark 3.19). A good source of Mayer series coefficients is the paper of P. Butera and M. Pernici [14], where they computed b_n for $1 \leq n \leq 24$ for various lattices. (More precisely, they computed $d_n = b_n/2$ with the notation of the paper [14] since they expanded the function $\rho(t) = p(t)/2$.) This means that we know μ_k for $k \leq 49$ for these lattices. For instance, for the square lattice $\mathbb{Z}^2$, the sequence $\mu_0, \mu_1, \mu_2, \dots$ starts as $1, 0, 4, 0, 28, 0, 232, 0, 2084, \dots$ (See Table 1 of [14].)

The other strategy to compute the moment sequence is to use its connection with the number of closed walks in the self-avoiding walk tree.

Since the moment sequence is missing for the honeycomb lattice (hexagonal lattice), we computed the first few elements of the moment sequence for this lattice:

$$\begin{gathered}
1, 0, 3, 0, 15, 0, 87, 0, 543, 0, 3543, 0, 23817, 0, 163551, 0, 1141119, 0, 8060343, 0, \\
57494385, 0, 413383875, 0, 2991896721, 0, 21774730539, 0, 159227948055, 0, \\
1169137211487, 0, 8615182401087, 0, 63683991513351, 0, 472072258519041, 0, \\
3508080146139867, 0, 26127841824131313, 0, 194991952493587371, 0, \\
1457901080870060919, 0, 10918612274039599755, 0, 81898043907874542705
\end{gathered}$$

The following table contains some numerical results. The bound on the error terms are rigorous. The paper [14] contains very similar non-rigorous results.

Lattice	$\tilde{\lambda}(L)$	Bound on error	$p(L,1)$	Bound on error
2d	0.6627989725	$3.72 \cdot 10^{-8}$	0.638123105	$5.34 \cdot 10^{-7}$
3d	0.7859659243	$9.89 \cdot 10^{-7}$	0.684380278	$1.14 \cdot 10^{-5}$
4d	0.8807178880	$5.92 \cdot 10^{-6}$	0.715846906	$5.86 \cdot 10^{-5}$
5d	0.9581235802	$4.02 \cdot 10^{-5}$	0.739160383	$3.29 \cdot 10^{-4}$
6d	1.0237319240	$1.24 \cdot 10^{-4}$	0.757362382	$8.91 \cdot 10^{-4}$
7d	1.0807591953	$3.04 \cdot 10^{-4}$	0.772099489	$1.95 \cdot 10^{-3}$
hex	0.58170036638	$1.56 \cdot 10^{-9}$	0.600508638	$2.65 \cdot 10^{-8}$

Table 3.2: Numerical estimates of $\tilde{\lambda}(L)$ and $p(L,1)$ with error bounds

3.4 Density function of matching measures.

It is natural problem to investigate the matching measure. One particular question is whether it is atomless or not. In general, ρ_L can contain atoms. For instance, if G is a finite graph then clearly ρ_G consists of atoms. On the other hand, it can be shown that for all lattices in Table 3.2, the measure ρ_L is atomless. We use the following lemmas.

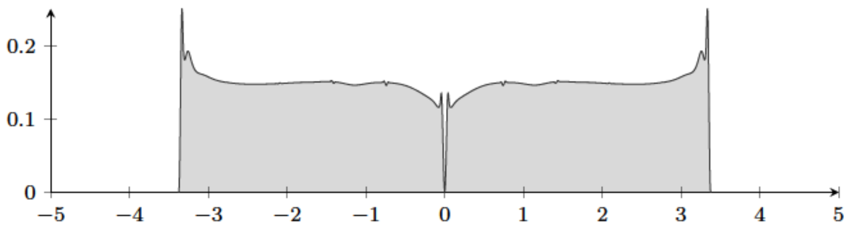


Figure 3.2: An approximation for the matching measure of $\mathbb{Z}^2$, obtained by smoothing the matching measure of the finite grid $C_{10} \times P_{100}$ by convolution with a triweight kernel.

We will only need part (a) of the following lemma, we only give part (b) for the sake of completeness.

Lemma 3.20. *[25, 32] (a) The maximum multiplicity of a zero of $\mu(G,x)$ is at most the number of vertex-disjoint paths required to cover G.*

(b) The number of distinct zeros of $\mu(G,x)$ is at least the length of the longest path in G.

The following lemma is a deep result of C. Y. Ku and W. Chen [35].

Lemma 3.21. *[35] If G is a finite connected vertex transitive graph, then all zeros of the matching polynomial are distinct.*

Now we are ready to give a generalization of Theorem 3.4.

Theorem 3.22. *Let L be a lattice satisfying one of the following conditions.*

(a) The lattice L can be obtained as a Benjamini–Schramm limit of a finite graph sequence G_n such that G_n can be covered by $o(|G_n|)$ disjoint paths.

(b) The lattice L can be obtained as a Benjamini–Schramm limit of connected vertex transitive finite graphs.

Then the matching measure ρ_L is atomless.

Proof. We prove the two statements together. Let $\mathrm{mult}(G_n, \theta)$ denote the multiplicity of θ as a zero of $\mu(G_n, x)$. Then by Theorem 3.13 we have

$$\rho_L(\{\theta\}) = \lim_{n \to \infty} \frac{\mathrm{mult}(G_n, \theta)}{|G_n|}.$$

Note that by Lemma 3.20 we have $\mathrm{mult}(G_n, \theta)$ is at most the number of paths required to cover the graph G_n. In case of connected vertex transitive graphs G_n, we have $\mathrm{mult}(G_n, \theta) = 1$ by Lemma 3.21. This means that in both cases $\rho_L(\{\theta\}) = 0$. □

Proof of Theorem 3.4. Note that $\mathbb{Z}^d$ satisfies both conditions of Theorem 3.22 by taking boxes or using part (b), taking toroidal boxes. □

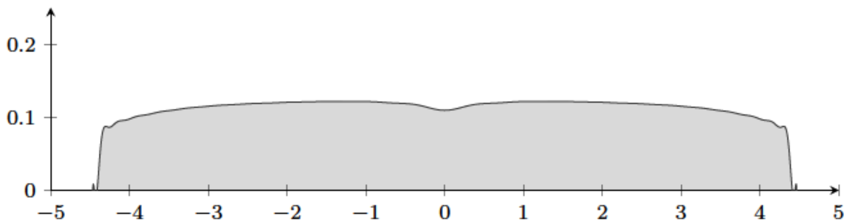


Figure 3.3: An approximation for the matching measure of $\mathbb{Z}^3$. Working with reasonably sized finite grids would have been computationally too expensive, so this time we took the L_2 projection of the infinite measure to the space of degree 48 polynomials which can be calculated from the sequence of moments.

Chapter 4

Positive graphs

This chapter is based on the article [15], which is joint work with Omar Antolín Camarena, Endre Csóka, Gábor Lippner and László Lovász.

4.1 Problem description

For a graph G we are going to denote the set of its vertices by $V(G)$ and the set of its edges by $E(G)$, but may simply write V and E when the it is clear from the context which graph we are talking about.

Let G and H be two simple graphs. A *homomorphism* $G \to H$ is a map $V(G) \to V(H)$ that preserves adjacency. We denote by $\hom(G,H)$ the number of homomorphisms $G \to H$. We extend this definition to graphs H whose edges are weighted by real numbers $\beta_{ij} = \beta_{ji}$ $(i, j \in V(H))$:

$$\hom(G,H) = \sum_{f\colon\, V(G)\to V(H)} \prod_{ij\in E(G)} \beta_{f(i)f(j)}.$$

(One could extend it further by allowing nodeweights, and also by allowing weights in G. Positive nodeweights in H would not give anything new; whether we get anything interesting through weighting G is not investigated here.)

We call the graph G *positive* if $\hom(G,H) \geq 0$ for every edge-weighted graph H (where the edgeweights may be negative). It would be interesting to characterize these graphs; in this chapter we offer a conjecture and line up supporting evidence.

We call a graph *symmetric*, if its vertices can be partitioned into three sets (S, A, B) so that S is an independent set, there is no edge between A and B, and there exists an isomorphism between the subgraphs spanned by $S \cup A$ and $S \cup B$ which fixes S.

Conjecture 4.1. *A graph G is positive if and only if it is symmetric.*

There is an analytic definition for graph positivity which is sometimes more convenient to work with. A *kernel* is a symmetric bounded measurable function $W : [0,1]^2 \to \mathbb{R}$. A map $p: V(G) \to [0,1]$ can be thought of as a homomorphism into W. It also naturally induces a map $p: E(G) \to [0,1]^2$. The *weight* of $p \in [0,1]^{V(G)}$ is then defined as

$$\hom(G, W, p) = \prod_{e \in E} W\big(p(e)\big) = \prod_{(a,b) \in E} W\big(p(a), p(b)\big).$$

The *homomorphism density* of a graph $G = (V, E)$ in a kernel W is defined as the expected weight of a random map:

$$t(G, W) = \int_{[0,1]^V} \hom(G, W, p)\, \mathrm{d}p = \int_{[0,1]^V} \prod_{e \in E} W\big(p(e)\big)\, \mathrm{d}p. \tag{4.1}$$

Graphs with real edge weights can be considered as kernels in a natural way: Let H be a looped-simple graph with edge weights β_{ij}; assume that $V(H) = [n] = \{1, \ldots, n\}$. Split the interval $[0,1]$ into n intervals $J_1, \ldots, J_n$ of equal length, and define

$$W_H(x, y) = \beta_{ij} \quad \text{for} \quad x \in J_i,\ y \in J_j.$$

Then it is easy to check that for every simple graph G and edge-weighted graph H, we have $t(G, W_H) = t(G, H)$, where $t(G, H)$ is a normalized version of homomorphism numbers between finite graphs:

$$t(G, H) = \frac{\hom(G, H)}{|V(H)|^{|V(G)|}}.$$

(For two simple graph G and H, $t(G, H)$ is the probability that a random map $V(G) \to V(H)$ is a homomorphism.)

It follows from the theory of graph limits [12, 38] that positive graphs can be equivalently be defined by the property that $t(G, W) \geq 0$ for every kernel W.

Hatami [31] studied "norming" graphs G, for which the functional $W \mapsto t(G, W)^{|E(G)|}$ is a norm on the space of kernels. Positivity is clearly a necessary condition for this (it is far from being sufficient, however). We don't know whether our Conjecture can be proved for norming graphs.

4.2 Results

In this section, we state our results (and prove those with simpler proofs). First, let us note that the "if" part of the conjecture is easy.

Lemma 4.2. *If a graph G is symmetric, then it is positive.*

Proof. For any map $p: V \to [0,1]$ and any subset $M \subset V$ let p_M denote the restriction of p to M. Let further $G[M]$ denote the subgraph of G spanned by M.

$$\begin{aligned}
t(G,W) &\overset{(4.1)}{=} \int_{[0,1]^V} \prod_{e\in E} W\big(p(e)\big)\ \mathrm{d}p \\
&= \int_{[0,1]^V} \Big(\prod_{e\in G[S\cup A]} W\big(p(e)\big)\Big) \Big(\prod_{e\in G[S\cup B]} W\big(p(e)\big)\Big)\ \mathrm{d}p \\
&= \int_{[0,1]^S} \Big(\int_{[0,1]^A} \prod_{e\in G[S\cup A]} W\big(p(e)\big)\,\mathrm{d}p_A\Big) \Big(\int_{[0,1]^B} \prod_{e\in G[S\cup B]} W\big(p(e)\big)\,\mathrm{d}p_B\Big)\,\mathrm{d}p_S \\
&= \int_{[0,1]^S} \Big(\int_{[0,1]^A} \prod_{e\in G[S\cup A]} W\big(p(e)\big)\,\mathrm{d}p_A\Big)^2 \mathrm{d}p_S \geq 0. \qquad \square
\end{aligned}$$

In the reverse direction, we only have partial results. We are going to prove that the conjecture is true for trees (Corollary 4.20) and for all graphs up to 9 nodes (see Section 4.5).

We state and prove a number of properties of positive graphs. Each of these is of course satisfied by symmetric graphs.

Lemma 4.3. *If G is positive, then G has an even number of edges.*

Proof. Otherwise, choosing W to be the constant -1 kernel we get $t(G,W) = (-1)^{|E(G)|} = -1$. $\square$

We call a homomorphism *even* if the preimage of each edge is has even cardinality.

Lemma 4.4. *If G is positive, then there exists an even homomorphism of G into itself.*

Proof. Let H be obtained from G by assigning random ± 1 weights to its edges, and let f be a random map $V(G) \to V(H)$. Then $\mathsf{E}_f(\hom(G,H,f)) = t(G,H) \geq 0$, and $t(G,H) > 0$ if all weights are 1, so $\mathsf{E}_H\mathsf{E}_f(\hom(G,H,f)) > 0$. Hence there is a f for which $\mathsf{E}_H(\hom(G,H,f)) > 0$. But clearly $\mathsf{E}_H(\hom(G,H,f)) = 0$ unless f is an even homomorphism of G into itself. $\square$

For two looped-simple graphs G_1 and G_2, we denote by $G_1 \times G_2$ their *categorical product*, defined by

$$\begin{aligned}
&V(G_1 \times G_2) = V(G_1) \times V(G_2), \\
&E(G_1 \times G_2) = \big\{\big((i_1,i_2),(j_1,j_2)\big) :\ (i_1,j_1) \in E(G_1), (i_2,j_2) \in E(G_2)\big\}.
\end{aligned}$$

Let K_n^+ denote the complete graph on the vertex set $[n]$ with loops at all vertices, where $n \geq |V(G)|$.

Theorem 4.5. *If a graph G is positive, then there exists an even homomorphism $f:\ G \to K_n^+ \times G$ so that $\big|f(V(G))\big| \geq \frac{1}{2}\big|V(G)\big|$.*

We will prove this theorem in Section 4.4.

There are certain operations on graphs that preserve symmetry. Every such operation should also preserve positiveness. We are going to prove three results of this kind; such results are also useful in proving the conjecture for small graphs.

We need some basic properties of the homomorphism density function: Let G_1 and G_2 be two simple graphs, and let G_1G_2 denote their disjoint union. Then for every kernel W

$$t(G_1G_2, W) = t(G_1, W)t(G_2, W). \tag{4.2}$$

We note that if at least one of G_1 and G_2 is simple (has no loops) then so is the product. The quantity $t(G_1 \times G_2, W)$ cannot be expressed as simply as (4.2), but the following formula will be good enough for us. For a kernel W and looped-simple graph H, let us define the function $W^H : ([0,1]^V)^2 \to \mathcal{R}$ by

$$W^H\big((x_1, \dots, x_k), (y_1, \dots, y_k)\big) = \prod_{(i,j)\in E(H)} W(x_i, y_j) \tag{4.3}$$

(every non-loop edge of H contributes two factors in this product). Then we have

$$t(G \times H, W) = t(G, W^H). \tag{4.4}$$

The following lemma implies that it is enough to prove the conjecture for connected graphs.

Lemma 4.6. *A graph G is positive if and only if every connected graph that occurs among the connected components of G an odd number of times is positive.*

Proof. The "if" part is obvious by (4.2). To prove the converse, let $G_1, \dots, G_m$ be the connected components of a positive graph G. We may assume that these connected components are different and non-positive, since omitting a positive component or two isomorphic components does not change the positivity of G. We want to show that $m = 0$. Suppose that $m \geq 1$.

Claim 4.7. *We can choose kernels $W_1, \dots, W_m$ so that $t(G_i, W_i) < 0$ and $t(G_i, W_j) \neq t(G_j, W_j)$ for $i \neq j$.*

For every i there is a kernel W_i such that $t(G_i, W_i) < 0$, since G_i is not positive. Next we show that for every $i \neq j$ there is a kernel W_{ij} such that $t(G_i, W_{ij}) \neq t(G_j, W_{ij})$. If $|V(G_i)| \neq |V(G_j)|$ then the kernel $W_{ij} = \mathbb{1}(x, y \leq 1/2)$ does the job, as in this case, due to the connectivity of the graphs, $t(G_i, W_{ij}) = (1/2)^{|V(G_i)|}$. So we may suppose that $|V(G_i)| = |V(G_j)|$. Then by [36, p475, Theorem 5.29] there is a simple graph H such that $\hom(G_i, H) \neq \hom(G_j, H)$, and hence we can choose $W_{ij} = W_H$.

Let us denote $\underline{x} = (x_1, \dots, x_m)$ and define $W_j'(\underline{x}) = W_j + \sum_{i\neq j} x_i W_{ij}$. Expanding the product in the definition of $t(-,-)$ one easily sees that $Q_j(\underline{x}) = t(G_i, W_j'(\underline{x}))$ $(i = 1, \dots, m)$ are all different polynomials in the variables $\underline{x}$, and hence their values are all different for a generic choice of $\underline{x}$. If $\underline{x}$ is chosen close to $\underline{0}$, then $t(G_j, W_j'(\underline{x})) < 0$, and hence we can replace W_j by $W_j'(\underline{x})$. This proves the Claim.

Let $W_0 = 1$ denote the identically 1 kernel. For nonnegative integers $k_0, \dots, k_m$, construct a kernel $W_{k_0,\dots,k_m}$ by arranging k_i rescaled copies of W_i for each i on the "diagonal". Then

$$t(G_1 \dots G_m, W_{k_0,\dots,k_m}) \overset{(4.2)}{=} \Big(\sum k_i\Big)^{-\sum|V(G_j)|} \prod_{j=1}^{m}\Big(\sum_{i=0}^{m} k_i t(G_j, W_i)\Big).$$

We know that this expression is nonnegative for every choice of the k_i. Since the right hand side is homogeneous in $k_0, \dots, k_m$, it follows that

$$\prod_{j=1}^{m}\Big(1 + \sum_{i=1}^{m} x_i t(G_j, W_i)\Big) \geq 0 \tag{4.5}$$

for every $x_1, \dots, x_m \geq 0$. But the m linear forms $\ell_j(x) = 1 + \sum_{i=1}^{m} x_i t(G_j, W_i)$ are different by the choice of the W_i, and each of them vanishes on some point of the positive orthant since $t(G_j, W_j) < 0$. Hence there is a point $x \in \mathbb{R}_+^m$ where the first linear form vanishes but the other forms do not. In a small neighborhood of this point the product (4.5) changes sign, which is a contradiction. □

Proposition 4.8. *If G is a positive simple graph and H is any looped-simple graph, then $G \times H$ is positive.*

Proof. Immediate from (4.4). □

Let $G(r)$ be the graph obtained from G by replacing each node with r twins of it. Then $G(r) \cong G \times K_r^\circ$, where K_r° is the complete r-graph with a loop added at every node. Hence we get:

Corollary 4.9. *If G is a positive simple graph, then so is $G(r)$ for every positive integer r.*

As a third result of this kind, we will show that the subgraph of a positive graph spanned by nodes with a given degree is also positive (Corollary 4.18). This proof, however, is more technical and is given in the next section. Unfortunately, these tools do not help us much for regular graphs G.

4.3 Subgraphs of positive graphs

In this section we develop a technique to show that one can partition the vertices of a positive graph in a certain way so that subgraphs spanned by each part are also positive. The main idea is to limit, over what maps $p : V \to [0,1]$ one has to average to check positivity. Using this idea recursively we can finally reduce to maps that take each partition to disjoint subsets of $[0,1]$. This in turn allows us to conclude positivity of the spanned subgraphs.

To this end, first we have to introduce the notion of $\mathcal{F}$-positivity. Let $G = (V, E)$ be a simple graph. For a measurable subset $\mathcal{F} \subseteq [0,1]^V$ and a bounded measurable weight function $\omega : [0,1] \to (0, \infty)$, we define

$$t(G, W, \omega, \mathcal{F}) = \int\limits_{p \in \mathcal{F}} \hom(G, W, \omega, p)\,\mathrm{d}p, \tag{4.6}$$

where the *weight* of a $p : V \to [0,1]$ is

$$\hom(G, W, \omega, p) = \prod_{v \in V} \omega\big(p(v)\big) \prod_{e \in E} W\big(p(e)\big) \tag{4.7}$$

With the measure μ with density function ω (i.e., $\mu(X) = \int_X \omega$), we can write this as

$$t(G, W, \omega, \mathcal{F}) = \int\limits_{\mathcal{F}} \prod_{e \in E} W\big(p(e)\big)\,\mathrm{d}\mu^V(p). \tag{4.8}$$

We say that G is *$\mathcal{F}$-positive* if for every kernel W and function ω as above, we have $t(G, W, \omega, \mathcal{F}) \geq 0$. It is easy to see that G is $[0,1]^V$-positive if and only if it is positive.

We say that $\mathcal{F}_1, \mathcal{F}_2 \subseteq [0,1]^V$ are *equivalent* if there exists a bijection $\varphi : [0,1] \to [0,1]$ such that both φ and φ^{-1} are measurable, and $p \in \mathcal{F}_1 \Leftrightarrow \varphi(p) \in \mathcal{F}_2$, where $\varphi(p)(v) = \varphi\big(p(v)\big)$.

Lemma 4.10. *If $\mathcal{F}_1$ and $\mathcal{F}_2$ are equivalent, then G is $\mathcal{F}_1$-positive if and only if it is $\mathcal{F}_2$-positive.*

Proof. Let φ denote the bijection in the definition of the equivalence. For a kernel W and weight function ω, define the kernel $W^\varphi(x,y) = W\big(\varphi(x), \varphi(y)\big)$, and weight function $\omega^\varphi(x) = \omega\big(\varphi(x)\big)$, and let μ and μ_φ denote the measures defined by ω and ω^φ, respectively. With this notation,

$$\begin{aligned} t(G, W^\varphi, \omega^\varphi, \mathcal{F}_2) &= \int\limits_{\mathcal{F}_2} \prod_{e \in E} W^\varphi\big(p(e)\big)\,\mathrm{d}\mu_\varphi^V(p) \\ &= \int\limits_{\mathcal{F}_1} \prod_{e \in E} W\big(p(e)\big)\,\mathrm{d}\mu^V(p) = t(G, W, \omega, \mathcal{F}_1). \end{aligned}$$

This shows that if G is $\mathcal{F}_2$-positive if and only if it is $\mathcal{F}_1$-positive. □

For a nonnegative kernel $W : [0,1]^2 \to [0,1]$ (these are also called *graphons*), function $\omega : [0,1] \to [0, \infty)$, and $\mathcal{F} \subseteq [0,1]^V$, define

$$s = s(G, W, \omega, \mathcal{F}) = \sup_{p \in \mathcal{F}} \Big(\prod_{v \in V} \omega\big(p(v)\big) \cdot \prod_{e \in E} W\big(p(e)\big) \Big), \tag{4.9}$$

and

$$\mathcal{F}_{max} = \Big\{ p \in \mathcal{F} : \prod_{v \in V} \omega\big(p(v)\big) \cdot \prod_{e \in E} W\big(p(e)\big) = s \Big\}.$$

If the Lebesgue measure $\lambda(\mathcal{F}_{max}) > 0$, then we say that $\mathcal{F}_{max}$ is *emphasizable* from $\mathcal{F}$, and (W, ω) *emphasizes* it.

Lemma 4.11. *If G is $\mathcal{F}_1$-positive and $\mathcal{F}_2$ is emphasizable from $\mathcal{F}_1$, then G is $\mathcal{F}_2$-positive.*

Proof. Suppose that (U, τ) emphasizes $\mathcal{F}_2$ from $\mathcal{F}_1$, and let $s = s(G, U, \tau, \mathcal{F}_1)$. Assume that G is not $\mathcal{F}_2$-positive, then there exists a kernel W and a weight function ω with $t(G, W, \omega, \mathcal{F}_2) < 0$. Consider the kernel $W_n = U^n W$ and weight function $\omega_n = s^{-n/|V|}\tau^n\omega$. Then

$$\prod_{v\in V}\omega_n\big(p(v)\big)\cdot\prod_{e\in E}W_n\big(p(e)\big) = \Big(\prod_{v\in V}\omega\big(p(v)\big)\cdot\prod_{e\in E}W\big(p(e)\big)\Big)\cdot a(p)^n,$$

where

$$a(p) = \frac{1}{s}\prod_{v\in V}\tau\big(p(v)\big)\cdot\prod_{e\in E}U\big(p(e)\big)\begin{cases}= 1 & \text{if } p\in\mathcal{F}_2,\\ < 1 & \text{otherwise.}\end{cases}$$

Thus (by the dominated convergence theorem)

$$\begin{aligned} t(G, W_n, \omega_n, \mathcal{F}_1) &= \int_{\mathcal{F}_1}\prod_{v\in V}\omega_n\big(p(v)\big)\cdot\prod_{e\in E}W_n\big(p(e)\big)\,\mathrm{d}p\\ &\to \int_{\mathcal{F}_2}\prod_{v\in V}\omega\big(p(v)\big)\cdot\prod_{e\in E}W\big(p(e)\big)\,\mathrm{d}p = t(G, W, \omega, \mathcal{F}_2) < 0,\end{aligned}$$

which implies that G is not $\mathcal{F}_1$-positive. $\square$

For a partition $\mathcal{P}$ of $[0,1]$ into a finite number of sets with positive measure and a function $\pi :\ V \to \mathcal{P}$, we call the box $\mathcal{F}(\pi) = \{p \in [0,1]^V :\ p(v) \in \pi(v)\ \forall v \in V\}$ a *partition-box.* Equivalently, a partition-box is a product set $\prod_{v\in V} S_v$, where the sets $S_v \subseteq [0,1]$ are measurable, and either $S_u \cap S_v = \emptyset$ or $S_u = S_v$ for all $u, v \in V$.

A partition $\mathcal{N}$ of V is *positive* if for any partition $\mathcal{P}$ as above, and any $\pi : V \to \mathcal{P}$ such that $\pi^{-1}(\mathcal{P}) = \mathcal{N}$, G is $\mathcal{F}(\pi)$-positive.

Lemma 4.12. *If $\mathcal{F}_1 \supseteq \mathcal{F}_2$ are partition-boxes, and G is $\mathcal{F}_2$-positive, then it is $\mathcal{F}_1$-positive.*

Proof. Let $\mathcal{F}_i$ be a product of classes of partition $\mathcal{P}_i$; we may assume that $\mathcal{P}_2$ refines $\mathcal{P}_1$. For $P \in \mathcal{P}_2$, let $\overline{P}$ denote the class of $\mathcal{P}_1$ containing P. Since every definition is invariant under measure preserving automorphisms of $[0,1]$, we may assume that every partition class of $\mathcal{P}_1$ and $\mathcal{P}_2$ is an interval.

Consider any kernel W and any weight function ω. Let $\varphi :\ [0,1] \to [0,1]$ be the function that maps each $P \in \mathcal{P}_2$ onto $\overline{P}$ in a monotone increasing and affine way. The map φ is measure-preserving, because for each $A \subseteq Q \in \mathcal{P}_1$,

$$\lambda\big(\varphi^{-1}(A)\big) = \sum_{\substack{P\in\mathcal{P}_2\\ P\subseteq Q}}\lambda\big(\varphi^{-1}(A)\cap P\big) = \sum_{\substack{P\in\mathcal{P}_2\\ P\subseteq Q}}\lambda(A)\frac{\lambda(P)}{\lambda(Q)} = \lambda(A). \tag{4.10}$$

Applying φ coordinate-by-coordinate we get a measure preserving map $\psi :\ [0,1]^V \to [0,1]^V$. Then $\psi' = \psi|_{\mathcal{F}_2}$ is an affine bijection from $\mathcal{F}_2$ onto $\mathcal{F}_1$, and clearly $\det(\psi') > 0$.

Hence

$$
\begin{aligned}
t(G, W^\varphi, \omega^\varphi, \mathcal{F}_2) &\overset{(4.6)}{=} \int\limits_{\mathcal{F}_2} \prod_{v\in V} \omega^\varphi\big(p(v)\big) \cdot \prod_{e\in E} W^\varphi\big(p(e)\big)\,\mathrm{d}p \\
&= \int\limits_{\mathcal{F}_2} \prod_{v\in V} \omega\big((\psi'(p))(v)\big) \cdot \prod_{e\in E} W\big((\psi'(p))(e)\big)\,\mathrm{d}p \\
&= \det(\psi')^{-1} \cdot \int\limits_{\mathcal{F}_1} \prod_{v\in V} \omega\big(p(v)\big) \cdot \prod_{e\in E} W\big(p(e)\big)\,\mathrm{d}p \\
&\overset{(4.6)}{=} \det(\psi')^{-1} \cdot t(G, W, \omega, \mathcal{F}_1).
\end{aligned}
$$

Since G is $\mathcal{F}_2$-positive, the left hand side is positive, and hence $t(G, W, \omega, \mathcal{F}_1) \geq 0$, proving that G is $\mathcal{F}_1$-positive. □

Corollary 4.13. *If $\mathcal{N}_2$ refines $\mathcal{N}_1$ and $\mathcal{N}_2$ is positive, then $\mathcal{N}_1$ is positive as well.*

Lemma 4.14. *Suppose that $\mathcal{F}_1$ is a partition-box defined by a partition $\mathcal{P}$ and function π_1. Let $Q \in \mathcal{P}$ and let U be the union of an arbitrary set of classes of $\mathcal{P}$. Let θ be a positive number but not an integer. Split Q into two parts with positive measure, Q^+ and Q^-. Let $\deg(v, U)$ denote the number of neighbors u of v with $\pi_1(u) \subseteq U$. Define*

$$
\pi_2(v) = \begin{cases} \pi_1(v) & \text{if } \pi_1(v) \neq Q, \\ Q^+ & \text{if } \pi_1(v) = Q \text{ and } \deg(v, U) > \theta, \\ Q^- & \text{if } \pi_1(v) = Q \text{ and } \deg(v, U) < \theta, \end{cases}
$$

and let $\mathcal{F}_2$ be the corresponding partition-box. Then there exists a pair (W, ω) emphasizing $\mathcal{F}_2$ from $\mathcal{F}_1$.

Proof. Clearly, $\lambda(\mathcal{F}_2) > 0$. First, suppose that $Q \not\subseteq U$. Let W be 2 in $Q^+ \times U$ and in $U \times Q^+$, and 1 everywhere else. Let $\omega(x)$ be $2^{-\theta}$ if $x \in Q^+$ and 1 otherwise. It is easy to see that the weight of a $p \in \mathcal{F}_1$ is 2^a, where $a = \sum_{v\in p^{-1}(Q^+)} \big(\deg(v, U) - \theta\big)$. This expression is maximal if and only if $p \in \mathcal{F}_2$.

In the case when $Q \subset U$ the only difference is that one has to let $W = 4$ in the intersection $Q^+ \times U \cap U \times Q^+$. □

Corollary 4.15. *If $\mathcal{N}_1$ is a positive partition of the vertex set, U is an arbitrary union of classes, Q is a single class, $\theta > 0$ is not an integer, and $\mathcal{N}_2$ is obtained from $\mathcal{N}_1$ by splitting Q according to whether (by abuse of notation) $\deg(v, U) > \theta$ or not for each vertex $v \in Q$, then $\mathcal{N}_2$ is also positive.*

We can use Corollary 4.15 iteratively: we start with the trivial partition, and refine it so that it remains positive. This is essentially the 1-dimensional Weisfeiler–Lehman algorithm, which classifies vertices recursively ([49], see e. g. [18]). It starts splitting vertices into classes according to their degree. Then in each step it refines the existing classes according to the number of neighbors in each of the current classes. The analogy will be clear from the proofs below. There is a non-iterative description of the resulting partition, and this is what we are going to describe next.

The *walk-tree* of a rooted graph (G, v) is the following infinite rooted tree $R(G, v)$: its nodes are all finite walks starting from v, its root is the 0-length walk, and the parent of any other walk is obtained by deleting its last node. The *walk-tree partition* $\mathcal{R}$ is the partition of V in which two nodes $u, v \in V$ belong to the same class if and only if $R(G, u) \cong R(G, v)$.

Proposition 4.16. *If a graph G is positive, then its walk-tree partition is also positive.*

Proof. Let the k-neighborhood of r in $R(G, r)$ be denoted by $R_k(G, r)$. The *k-walk-tree partition* $\mathcal{R}_k$ is the partition of V in which two nodes $u, v \in V$ belong to the same class if and only if $R_k(G, u) \cong R_k(G, v)$. Clearly, if for two vertices $R(G, u) \neq R(G, v)$ then there is a $k = k(u, v)$ such that $R_k(G, u) \neq R_k(G, v)$. Since V is finite, choosing $k_0 = \max_{u,v \in V} k(u, v)$ we see that $\mathcal{R}_{k_0} = \mathcal{R}$. Thus we are done if we show that $\mathcal{R}_k$ is positive for every k.

We prove this by induction. If $k = 0$ then $\mathcal{R}_0$ is the trivial partition, hence the assertion follows from the positivity of G. Now let us assume that the statement is true for k. Clearly, $R_{k+1}(G, v)$ is determined by the *neighborhood profile*, the multi-set $\{R_k(G, u) : u \sim v\}$. Using Corollary 4.15, we separate each class Q into subclasses so that $u, v \in Q$ end up in the same class if and only if their neighborhood profiles are the same. The new partition is exactly $\mathcal{R}_{k+1}$. □

Corollary 4.17. *Let $G(V, E)$ be a positive graph, and let $S \subset V$ be the union of some classes of the walk-tree partition. Then $G[S]$ is also positive.*

Proof. By Corollary 4.13 the partition $\mathcal{N} = \{S, V \backslash S\}$ is positive. Let $\mathcal{P} = \{[0, 1/2], (1/2, 1]\}$ and define $\pi : V \to \mathcal{P}$ by $\pi(v) = [0, 1/2]$ if and only if $v \in S$. Suppose that $G[S]$ is negative as demonstrated by some W. Let us define

$$W'(x, y) = \begin{cases} W(2x, 2y) & : x, y \in [0, 1/2] \\ 1 & : \text{otherwise} \end{cases}$$

Then $t(G, W', 1, \mathcal{F}(\pi)) < 0$ contradicting the positivity of the partition $\mathcal{N}$. □

Corollary 4.18. *If G is positive, then for each k the subgraph of G spanned by all nodes with degree k is positive as well.* □

Corollary 4.19. *For each odd k the number of nodes of G with degree k must be even.*

Proof. Otherwise, consider the partition-box $\mathcal{F}$ that separates the vertices of G with degree d to class $A = [0, 1/2]$ and the other vertices to $\bar{A} = (1/2, 1]$. Consider the kernel W which is -1 between A and $\bar{A}$ and 1 in the other two cells. Then for each map $p \in [0, 1]^V$, the total degree of the nodes mapped into class A is odd, so there is an odd number of edges between A and $\bar{A}$. So the weight of p is -1, therefore $t(G, W, 1, \mathcal{F}) = -\lambda(\mathcal{F}) < 0$. □

Corollary 4.20. *Conjecture 4.1 is true for trees.*

Proof. From the walk-tree of a vertex v of the tree G, we can easily decode the rooted tree (G, v). We call a vertex *central* if it cuts G into components with at most $|V|/2$ nodes. There can be either one central node or two neighboring central nodes of G. If there are two of them, then their walk-trees are different from the walk-trees of every other node. But these two points span a graph with a single edge, which is not positive, therefore Corollary 4.17 implies that neither is G. If there is only one central node, then consider the walk-trees of its neighbors. If there is an even number of each kind, then G is symmetric (and is thus positive by Lemma 4.2). Otherwise we can find two classes (one consist of the central node, the other consists of an odd number of its neighbors) whose union spans a graph with an odd number of edges, hence it is negative by Lemma 4.3. $\square$

4.4 Homomorphic images of positive graphs

The main goal of this section is to prove Theorem 4.5. In what follows, let n be an integer. Let us fix a graph G. Let $G_{\times n} = K_n^+ \times G$. For a homomorphism $f:\ F \to G_{\times n}$, we call an edge $e \in E(G_{\times n})$ *f-odd* if $\left|f^{-1}(e)\right|$ is odd. We call a vertex $v \in V(G_{\times n})$ *f-odd* if there exists an f-odd edge incident with v. Let $E_{\text{odd}}(f)$ and $V_{\text{odd}}(f)$ denote the set of f-odd edges and nodes of $G_{\times n}$, respectively, and define

$$r(f) = \left|V(F)\right| - \left|f\big(V(F)\big)\right| + \frac{1}{2}\left|V_{\text{odd}}(f)\right|. \tag{4.11}$$

Lemma 4.21. *Let $G_i = (V_i, E_i)$ $(i = 1, 2)$ be two graphs, let $f:\ G_1G_2 \to G_{\times n}$, and let $f_i:\ G_i \to G_{\times n}$ denote the restriction of f to V_i. Then $r(f) \ge r(f_1) + r(f_2)$.*

Proof. Clearly $|V(G_1G_2)| = |V_1| + |V_2|$ and $|V(f(G_1G_2))| = |f(V_1)| + |f(V_2)| - |f(V_1) \cap f(V_2)|$. Furthermore, $E_{\text{odd}}(f) = E_{\text{odd}}(f_1) \triangle E_{\text{odd}}(f_2)$, which implies that $V_{\text{odd}}(f) \supseteq V_{\text{odd}}(f_1) \triangle V_{\text{odd}}(f_2)$. Hence

$$\begin{aligned} |V_{\text{odd}}(f)| &\ge |V_{\text{odd}}(f_1)| + |V_{\text{odd}}(f_2)| - 2|V_{\text{odd}}(f_1) \cap V_{\text{odd}}(f_2)| \\ &\ge |V_{\text{odd}}(f_1)| + |V_{\text{odd}}(f_2)| - 2|f(V_1) \cap f(V_2)|. \end{aligned}$$

Substituting these expressions in (4.11), the lemma follows. $\square$

Let F^k denote the disjoint union of k copies of a graph F. This lemma implies that if $f:\ F^k \to G_{\times n}$ is any homomorphism and $f_i:\ F \to G_{\times n}$ denotes the restriction of f to the i-th copy of G, then

$$r(f) \ge \sum_{i=1}^{k} r(f_i). \tag{4.12}$$

Let us define

$$\bar{r}(F) = \min\left\{r(f) \middle| n \in \mathbb{N}, f:\ F \to G_{\times n}\right\} \tag{4.13}$$

and

$$q(F) = \min\left\{\left|V(F)\right| - \left|f\big(V(G)\big)\right| \,\middle|\, n \in \mathbb{N}, f:\ G \to G_{\times n} \text{ is even}\right\} \tag{4.14}$$

Since $q(H) = \min\big\{r(f)\big|n \in \mathbb{N}, f:\ G \to G_{\times n} \text{ is even}\big\}$, it follows that

$$q(F) \geq \bar{r}(F). \tag{4.15}$$

Furthermore, if there exists any injective $f:\ G \to G_{\times n}$, then

$$\bar{r}(F) \leq r(f) = \big|V(F)\big| - \big|f\big(V(F)\big)\big| + \frac{1}{2}\big|f\big(V(F)\big)\big| = \frac{1}{2}\big|V(F)\big|. \tag{4.16}$$

Lemma 4.22.

$$\bar{r}(G^k) = k\bar{r}(G). \tag{4.17}$$

Proof. For one direction, take an $f:\ G^k \to G_{\times n}$ with $r(f) = \bar{r}(G^k)$. Then

$$\bar{r}(G^k) = r(f) \overset{(4.12)}{\geq} \sum_{i=1}^{k} r(f_i) \overset{(4.13)}{\geq} \sum_{i=1}^{k} \bar{r}(G) = k \cdot \bar{r}(G).$$

For the other direction, let us choose each f_i so that $r(f_i) = \bar{r}(G)$ and the images $f_i(G)$ are pairwise disjoint. Then

$$\bar{r}(G^k) \overset{(4.13)}{\leq} r(f) = \sum_{i=1}^{k} r(f_i) = \sum_{i=1}^{k} \bar{r}(G) = k \cdot \bar{r}(G). \qquad \square$$

Lemma 4.23.

$$q(G^2) = \bar{r}(G^2). \tag{4.18}$$

Proof. We already know by (4.15) that $q(G^2) \geq \bar{r}(G^2)$. For the other direction, we define $f:\ G^2 \to G_{\times n}$ as follows. We choose f_1 so that $r(f_1) = \bar{r}(G)$. Consider all points $v_1, v_2, ..., v_l$ in $f_1\big(V(G)\big)$ which are not f_1-odd. Let us choose pairwise different nodes $v_1', v_2', ..., v_l'$ disjointly from $f_1\big(V(G)\big)$ so that v_i and v_i' have the same second coordinate in $V(G_{\times n}) \cong V(K_n^+) \times V(G)$. Now we choose f_2 so that for each $x \in V(G)$, if $f_1(x)$ is an f_1-odd point, then $f_2(x) = f_1(x)$, and if $f_1(x) = v_i$, then $f_2(i) = v_i'$.

If an edge $e \in E(G_{\times n})$ is incident to a v_i, then $\big|f_1^{-1}(e)\big|$ is even and $f_2^{-1}(e) = \emptyset$. If e is incident to a v_i', then $\big|f_2^{-1}(e)\big|$ is even and $f_1^{-1}(e) = \emptyset$. If e is not incident to any v_i or v_i', then $\big|f_1^{-1}(e)\big| = \big|f_2^{-1}(e)\big|$. Therefore f is even. Thus,

$$q(G^2) \overset{(4.14)}{\leq} r(f) \overset{(4.11)}{=} \big|V(G^2)\big| - \big|f(V(G^2))\big|$$

$$= 2\big|V(G)\big| - \Big|f_1\big(V(G)\big)\Big| - \Big|f_2\big(V(G)\big)\Big| + \Big|f_1\big(V(G)\big) \cap f_2\big(V(G)\big)\Big|$$

$$= 2\big|V(G)\big| - 2\Big|f_1\big(V(G)\big)\Big| + |V_{\text{odd}}(f_1)| \overset{(4.11)}{=} 2r(f_1) = 2\bar{r}(G) \overset{(4.17)}{=} \bar{r}(G^2). \qquad \square$$

Let $G_{\times n}^w$ denote $K_{|V(G_{\times n})|}$ equipped with an edge-weighting $w:\ E(K_{|V(G_{\times n})|}) \to \{-1, 0, 1\}$, where $w(e) = 0$ if and only if e is a non-edge in $G_{\times n}$. Let the stochastic variable $G_{\times n}^{\pm 1}$ denote $G_{\times n}^w$ with a uniform random w.

Lemma 4.24. *For a fixed graph G, and $n \to \infty$,*

$$\mathsf{E}\big(t(G, G^{\pm 1}_{\times n})\big) = \begin{cases} \Theta\big(n^{-q(G)}\big) & \text{if } q(G) < \infty \\ 0 & \text{otherwise.} \end{cases} \tag{4.19}$$

Proof. If f is not a homomorphism to $G_{\times n}$, then there exists an edge $e \in E(G)$ that $w\big(f(e)\big) = 0$, therefore, $\hom(G, G^w_{\times n}, f) = 0$. If an edge e is f-odd, then changing the weight on e changes the sign of the homomorphism, therefore $\mathsf{E}_w\big(\hom(G, G^w_{\times n}, f)\big) = 0$. On the other hand, if f is an even homomorphism to $G_{\times n}$, then for all w, $\hom(G, G^w_{\times n}, f) = 1$. Therefore, taking a uniformly random homomorphism $f : G \to G_{\times n}$,

$$\mathsf{E}\big(t(G, G^{\pm 1}_{\times n})\big) = \mathsf{E}_w\big(t(G, G^w_{\times n})\big) = \mathsf{E}_w\Big(\mathsf{E}_f\big(\hom(G, G^w_{\times n}, f)\big)\Big)$$

$$= \mathsf{E}_f\Big(\mathsf{E}_w\big(\hom(G, G^w_{\times n}, f)\big)\Big) = \mathsf{P}\big(f \text{ is an even homomorphism } G \to G_{\times n}\big). \tag{4.20}$$

If $q(G) = \infty$ we are done. Otherwise we have

$$(4.20) \le \mathsf{P}\Big(\big|V(G)\big| - \big|f(V(G))\big| \ge q(G)\Big) = O(|G_{\times n}|^{-q(G)}) = O(n^{-q(G)}).$$

On the other hand, consider an even homomorphism $g : G \to G_{\times n}$ with $r(g) = q(G)$. Consider now an arbitrary function $\sigma : V\big(g(G)\big) \to V\big(G_{\times n}\big)$ which does not change the second coordinate of $V(G_{\times n}) \cong V(K_n^+) \times V(G)$. Then $\sigma \circ g$ is also an even homomorphism. These homomorphisms are pairwise different, and the number of such functions σ is $n^{|V(g(G))|}$. Therefore,

$$(4.20) \ge \frac{n^{|V(g(G))|}}{|V(G_{\times n})|^{|V(G)|}} = \Omega(n^{|g(V(G))| - |V(G)|}) \overset{(4.11)}{=} \Omega(n^{-r(g)}) = \Omega(n^{-q(G)}). \qquad \square$$

Now let us turn to the proof of Theorem 4.5. Assume that G is positive, then the random variable $X = t(G, G^{\pm 1}_{\times n})$ is nonnegative. Applying the Cauchy-Schwarz inequality to $X^{1/2}$ and $X^{3/2}$ we get that

$$\mathsf{E}(X) \cdot \mathsf{E}(X^3) \ge \mathsf{E}(X^2)^2. \tag{4.21}$$

Here

$$\mathsf{E}(X^k) = \mathsf{E}\big(t(G, G^{\pm 1}_{\times n})^k\big) \overset{(4.2)}{=} \mathsf{E}\big(t(G^k, G^{\pm 1}_{\times n})\big) \overset{(4.19)}{=} \Theta\big(n^{-q(G^k)}\big),$$

so (4.21) shows that $n^{-q(G)} \cdot n^{-q(G^3)} = \Omega\big(n^{-2q(G^2)}\big)$, thus $q(G) + q(G^3) \le 2q(G^2)$. Hence

$$4\bar{r}(G) \overset{(4.17)}{=} \bar{r}(G) + \bar{r}(G^3) \overset{(4.15)}{\le} q(G) + q(G^3) \le 2q(G^2) \overset{(4.18)}{=} 2\bar{r}(G^2) \overset{(4.17)}{=} 4\bar{r}(G). \tag{4.22}$$

All expressions in (4.22) must be equal, therefore $\bar{r}(G) = q(G)$.

Finally, for an even $f : G \to G_{\times n}$ with $\big|V(G)\big| - \big|f(V(G))\big| = q(G)$, we have

$$\frac{1}{2}\big|V(G)\big| \overset{(4.16)}{\ge} \bar{r}(G) = q(G) = \big|V(G)\big| - \big|f(V(G))\big|,$$

therefore $\big|f\big(V(G)\big)\big| \ge \frac{1}{2}\big|V(G)\big|$. $\square$

4.5 Computational results

We checked Conjecture 4.1 for all graphs on at most 10 vertices using the previous results and a computer program. Starting from the list of nonisomorphic graphs, we filtered out those who violated one of our conditions for being a minimal counterexample. In particular we performed the following tests:

1. Check whether the graph is symmetric, by exhaustive search enumerating all possible involutions of the vertices. If the graph is symmetric, it is not a counterexample.

2. Calculate the number of homomorphisms into graphs represented by 1×1, 2×2 or 3×3 matrices of small integers. (Checking 1×1 matrices is just the same as checking whether or not the number of edges is even.) If we get a negative homomorphism count, the graph is negative and therefore it is not a counterexample.

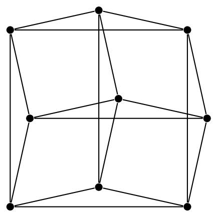
3. Calculate the number of homomorphisms into graphs represented by symbolic 3×3 and 4×4 matrices and perform local minimization on the resulting polynomial from randomly chosen points. Once we reach a negative value, we can conclude that the graph is negative.

4. Partition the vertices of the graph in such a way that two vertices belong to the same class if and only if they produce the same walk-tree (1-dimensional Weisfeiler–Lehman algorithm). Check for all proper subsets of the set of classes whether their union spans an asymmetric subgraph. If we find such a subgraph, the graph is not a minimal counterexample: either the subgraph is not positive and by Corollary 4.17 the original graph is not positive either, or the subgraph is positive, and therefore we have a smaller counterexample.

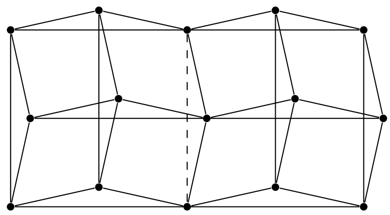
5. Consider only those homomorphisms which map all vertices in the ith class of the partition into vertices $3i + 1$, $3i + 2$ and $3i + 3$ of the target graph represented by a symbolic matrix. If we get a negative homomorphism count, the graph is negative by Proposition 4.16. (In this case we work with a $3k \times 3k$ matrix where k denotes the number of classes of the walk-tree partition, but the resulting polynomial still has a manageable size because we only count a small subset of homomorphisms. Note that if one of the classes consists of a single vertex, we only need one corresponding vertex in the target graph.)

The tests were performed in such an order that the more efficient ones were run first, restricting the later ones to the set of remaining graphs. For example, in step 4, we start with checking whether any of the classes spans an odd number of edges, or whether the number of edges between any two classes is odd. We used the `SAGE` computer-algebra system for our calculations and rewritten the speed-critical parts in `C` using `nauty` for isomorphism checking, `mpfi` for interval arithmetics and Jean-Sébastien Roy's `tnc` package for nonlinear optimization.

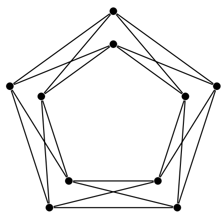
Our automated tests left only 4 graphs as possible counterexamples, out of the 12,293,435 graphs on at most 10 vertices. Of those, the non-positivity of G_1 and G_2 was proved manually by counting the number of homomorphisms into H_1 and H_2, respectively. The dashed edges have weight -1 and all other edges have weight 1.



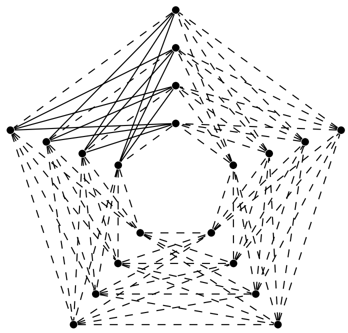
G_1



H_1



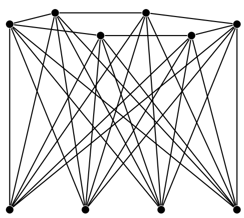
G_2



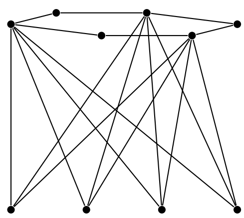
H_2

($H_2 \cong K_2^+ \times G_2 \cong K_4^+ \times C_5$. The edges with weight -1 form two vertex-disjoint cycles of length 5 and 15. The latter one goes three times around.)

The graph G_3 can be shown to be non-positive from the counterexample for G_3^-. We emphasized a tripartition of G_3 by iteratively emphasizing the maximum cut, then we used a generalized version of Corollary 4.17.

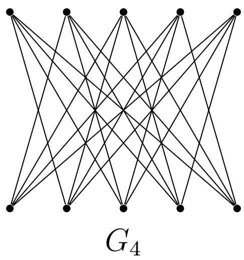


G_3



G_3^-

This leaves only G_4, which is not symmetric, but we could not decide whether it is positive. There was no graph traced back to G_4, therefore, the conjecture is proved to be true for all graphs up to 10 nodes except G_4.



G_4

Notice that all four graphs are regular, as is the case for all remaining graphs on 11 vertices. We have found step 5 of the algorithm quite effective at excluding graphs with nontrivial walk-tree partitions.

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Abstract

A sequence of graphs is convergent in the Benjamini–Schramm sense if the local features of the graphs, i.e. those observable by local sampling, are getting arbitrarily close to being indistinguishable. Formally, G_n is convergent if for every positive R and finite rooted graph α the probability that the R-ball centered at a uniform random vertex of G_n is isomorphic to α is convergent.

The chromatic polynomial of G is defined as the number of proper colorings of G with q colors, which gives a polynomial in q. In Chapter 2 we observe the behaviour of the roots of the chromatic polynomial on a convergent sequence of graphs. To make sense of a limit, we define the root measure as the uniform distribution on the roots. While this measure is not necessarily weakly convergent, we can show that the integral of any holomorphic function according to the measure converges. The proof goes by writing the moments of the root measure as a linear combination of homomorphism numbers into connected graphs, which already satisfy this requirement.

Our results have been generalized by Csikvári and Frenkel to a broader class of graph polynomials, and we build on their work in Chapter 3 where we consider the roots of the matching polynomial. The matching polynomial is defined as $\sum_k (-1)^k m_k(G) x^{|V(G)|-2k}$ with $m_k(G)$ denoting the number of matchings with exactly k edges.

We can define the matching measure of G in analogy with the chromatic measure, as the root measure of the matching polynomial. This time a convergent graph sequence does imply weak convergence of the matching measure, extending its definition to infinite lattices. We prove that the matching measure of an infinite lattice is equivalent to the spectral measure of its tree of self-avoiding walks. Matching measures also allow us to express the free energies of monomer-dimer models in statistical physics, giving us new and strong estimates.

Chapter 4 concerns the other main topic of this thesis, positive graphs. By extending the definition of homomorphism count to weighted target graphs we realize that for some graphs F $\hom(F, G)$ is always nonnegative even if G contains edges with negative weights. Such an F is called a positive graph. We suggest a possible structural characterization stating that a graph is positive if and only if it exhibits a certain kind of symmetry. Then we prove this conjecture for trees and – with the help of a computer program – for all but one graphs on at most 10 vertices.

Chapter 2 is joint work with Miklós Abért. Chapter 3 is joint work with Miklós Abért and Péter Csikvári. Chapter 4 is joint work with Omar Antolín Camarena, Endre Csóka, Gábor Lippner and László Lovász.

Összefoglalás

Egy gráfsorozatot Benjamini–Schramm konvergensnek nevezünk, ha a gráfok lokális jellemzői, vagyis azok, amiket lokális mintavételezéssel megfigyelhetünk, egy idő után megkülönböztethetetlenné válnak, bármilyen kis hibával is nézzük. Formálisan G_n akkor konvergens, ha bármely pozitív R és bármely α véges gyökeres gráf esetén annak a valószínűsége, hogy G_n egy egyenletes véletlen csúcsának R sugarú környezete α-val izomorf, konvergens.

Egy G gráf kromatikus polinomja azt adja meg, hogy hányféleképpen színezhető ki q színnel, ami q-ban egy polinom. A 2. fejezetben a kromatikus polinom gyökeinek viselkedését vizsgáljuk konvergens gráfsorozatokon. Azért, hogy legyen értelme a határértékről beszélni, bevezetjük a gyökmértéket, vagyis a gyökökön vett egyenletes eloszlást. Bár ez a mérték nem feltétlenül gyengén konvergens, belátjuk, hogy bármilyen holomorf függvény integrálja a mérték szerint már konvergens lesz. A bizonyítás azon alapul, hogy a mérték momentumait felírjuk összefüggő gráfokba menő homomorfizmusszámok lineáris kombinációjaként, amik már teljesítik ezt a követelményt.

Ezeket az eredményeket Csikvári Péter és Frenkel Péter általánosították gráfpolinomok egy tágabb osztályára. A 3. fejezetben az ő munkájukra építve vizsgáljuk a párosításpolinom gyökmértékét. A párosítás-polinomot a $\sum_k (-1)^k m_k(G) x^{|V(G)|-2k}$ képlet definiálja, ahol $m_k(G)$ a pontosan k éllel rendelkező párosítások száma.

Egy G gráf párosítás-mértékét a kromatikus mértékhez hasonlóan definiálhatjuk a párosításpolinom gyökmértékeként. Itt már teljesül, hogy konvergens gráfsorozatokra a párosításmérték gyengén konvergens, ezáltal értelmezhetjük végtelen rácsok párosítás-mértékét is. Megmutatjuk, hogy az így nyert mérték megegyezik a rács sétafájának spektrálmértékével. A párosítás-mérték segítségével ki tudjuk fejezni a statisztikus fizikában használt monomerdimer modellek szabadenergiáját is, ami új, a korábban ismerteknél erősebb becsléseket is ad.

A 4 fejezetben rátérünk az értekezés másik fő témájára, a pozitív gráfokra. A homomorfizmusszámokat súlyozott célgráfokra kiterjesztve azt tapasztaljuk, hogy néhány F gráfra a $\hom(F, G)$ homomorfizmusszámok mindig nemnegatívak, akkor is, ha G negatív éleket is tartalmazhat. Az ilyen F-eket pozitív gráfoknak nevezzük. Megfogalmazunk egy sejtést a pozitív gráfok strukturális leírásáról, miszerint egy gráf akkor és csak akkor pozitív, ha egy bizonyos szimmetria-feltételt teljesít. Utána bebizonyítjuk ezt a sejtést fákra és egy számítógépes program segítségével egy kivétellel minden legfeljebb 10 csúcsú gráfra.

A 2. fejezet Abért Miklóssal közös munka, a 3. fejezet Abért Miklóssal és Csikvári Péterrel, míg a 4. fejezet Omar Antolín Camarenával, Csóka Endrével, Lippner Gáborral és Lovász Lászlóval közös kutatáson alapul.