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Matching Measure, Benjamini–Schramm Convergence and the Monomer–Dimer Free Energy

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Abstract We define the *matching measure* of a lattice L as the spectral measure of the tree of self-avoiding walks in L. We connect this invariant to the monomer–dimer partition function of a sequence of finite graphs converging to L. This allows us to express the monomer–dimer free energy of L in terms of the matching measure. Exploiting an analytic advantage of the matching measure over the Mayer series then leads to new, rigorous bounds on the monomer–dimer free energies of various Euclidean lattices. While our estimates use only the computational data given in previous papers, they improve the known bounds significantly.

Keywords Monomer–dimer model · Matching polynomial · Benjamini–Schramm convergence · Self-avoiding walks

1 Introduction

The aim of this paper 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 the first and second authors, Frenkel and Kun [1]. There are essentially two ways to define it: in this paper we take the path of giving a direct, spectral definition for infinite vertex transitive lattices, using self-avoiding walks and

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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 1.1 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 Sect. 2.

To make sense of why we call this the matching measure, we need the notion of Benjamini–Schramm convergence. 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* be

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

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 [16] we show that ρ_L can be obtained as the thermodynamical limit of the ρ_{G_n}.

Theorem 1.2 *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 [12,24,28] 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 [19,20], Hammersley and Menon [21] and Baxter [5] obtained the first (non-rigorous) estimates for the free energy. Then Friedland and Peled [14] 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. [13]) on Friedland's asymptotic matching conjecture which was finally proved by Gurvits [17]. Meanwhile, a non-rigorous estimate $[0.7833, 0.7861]$ was obtained via matrix permanents [23]. Concerning rigorous results, the most significant improvement was obtained recently by Gamarnik and Katz [15] 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 [7]. This paper uses Mayer-series with many coefficients computed in the expansion. The related paper [6] 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 Sect. 3, in particular, in Table 1. 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 1.3 *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 [27] 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 1.2 one can show that the matching measures of hypersimple cubic lattices admit no atoms.

Theorem 1.4 *The matching measures $\rho_{\mathbb{Z}^d}$ have no atoms.*

In Sect. 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 Sect. 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 [4,10,18], under the name *connective constant*.

The paper is organized as follows. In Sect. 2, we define the basic notions and prove Theorem 1.2. In Sect. 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 Sect. 4, we prove Theorem 1.4.

2 Matching Measure

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

Throughout the paper, 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

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

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 $\varphi(u) = v$.

2.2 Matching Measure and Tree of Self-avoiding Walks

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

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

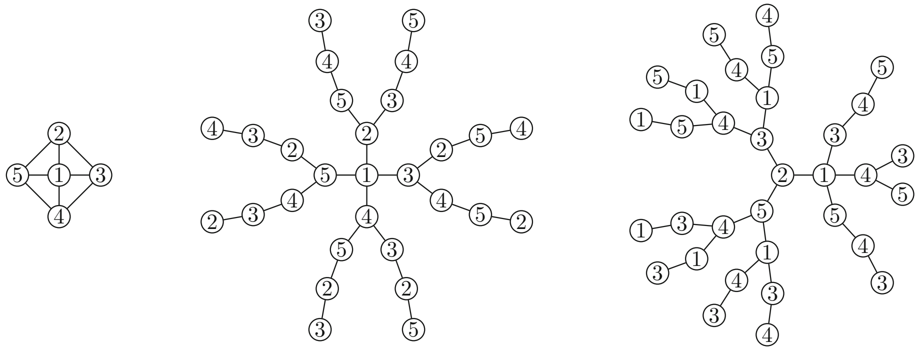

Fig. 1 The pyramid graph and its trees of self-avoiding walks starting from ① and ② respectively

where $m_k(G)$ denotes the number of k-matchings in G.

Definition 2.1 The *matching measure* of a finite graph is defined as

$$\rho_G = \frac{1}{v(G)} \sum_{z_i:\ \mu(G,z_i)=0} \delta(z_i),$$

where $\delta(s)$ is the Dirac-delta measure on s, and we take every z_i into account with its multiplicity.

In other words, it is the probability measure of uniform distribution on the zeros of the matching polynomial of G.

The fundamental theorem for the matching polynomial is the following.

Theorem 2.2 (Heilmann and Lieb [22]) *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 (Fig. 1). The following figure illustrates that in general, $T_v(G)$ very much depends on the choice of v.

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

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

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. The following theorem is just a reformulation of Corollary 2.2 of Chapter 6 in [16].

Theorem 2.3 *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 2.3 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 $2\sqrt{D-1}$, see for instance [22].

To prove Theorem 2.3 we need the following result of Godsil [16] which connects the matching polynomial of the original graph G and the tree of self-avoiding walks:

Theorem 2.4 (Theorem 1.1 of Chapter 6 in [16]) *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 2.5 *(a)* (Exercise 5 of Chapter 2 in [16].) *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) (Theorem 1.1 (d) of Chapter 1 in [16].) For any graph G, we have

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

Proof of Theorem 2.3 First, let us use part (a) of Proposition 2.5 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 2.4 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 2.4. Let us use part (b) of Proposition 2.5:

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

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. □

Now we define Benjamini–Schramm convergence.

Definition 2.6 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 2.7 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 1.2.

Theorem 2.8 *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 2.9 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 [8]. For completeness, we give an alternate self-contained proof here.

We will use the following theorem of Thom [29]. See also [3] where this is used for Benjamini–Schramm convergent graph sequences.

Theorem 2.10 (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 1.2 and 2.8 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 2.3 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 2.10 gives $\lim_{n\to\infty} \rho_{G_n}(\{x\}) = \rho_L(\{x\})$ for all $x \in \mathbb{R}$. □

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 3.2. 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 3.2. To prove this proposition we need some preparation.

We will use the following theorem of Darroch.

Lemma 3.1 (Darroch's rule [9]) *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 3.2 *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 $k \le \nu(G)$ and $p = \frac{2k}{|G|}$. Then

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

(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

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

then

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

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

□

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 3.3 *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 $0 \le p < 1$.

Remark 3.4 In part (c), we used the extra condition to ensure that $p^* = 1$ for all these graphs. We mention that Nguyen and Onak [26], and independently Elek and Lippner [11] 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 3.3, we essentially repeat an argument of the paper [1].

Proof of Theorem 1.2 and 2.8 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 2.8. 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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Definition 3.5 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

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

and

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

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 3.6 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

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

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'.

3.1 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 $k \le N$. 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

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

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

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

and

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

Hence

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

How can we compute the moment sequence (μ_k)? One way is to use its connection with the Mayer series (see Remark 3.6). A good source of Mayer series coefficients is the paper of Butera and Pernici [7], where they computed b_n for $1 \le n \le 24$ for various lattices. (More precisely, they computed $d_n = b_n/2$ with the notation of the paper [7] since they expanded the function $\rho(t) = p(t)/2$.) This means that we know μ_k for $k \le 49$ for these lattices. For instance, for the square lattice $\mathbb{Z}^2$, the sequence $\mu_0, \mu_1, \mu_2, \ldots$ starts as $1, 0, 4, 0, 28, 0, 232, 0, 2084, \ldots$ (see Table 1 of [7].)

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:

$$1, 0, 3, 0, 15, 0, 87, 0, 543, 0, 3543, 0, 23817, 0, 163551, 0, 1141119, 0, 8060343, 0,$$

Table 1 Monomer-dimer free energy estimates for hyper-simple cubic lattices and the honeycomb lattice

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

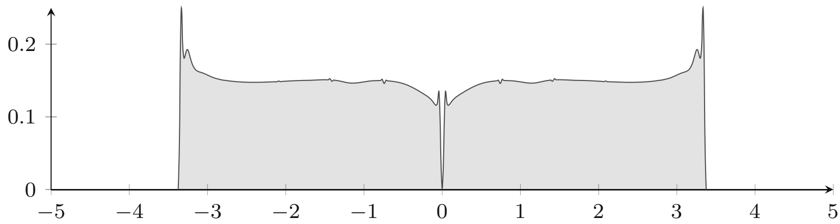

Fig. 2 An approximation for the matching measure of $\mathbb{Z}^2$, obtained by smoothing the matching measure of the finite grid $C_{10} \times P_{100}$ by convolution with a triweight kernel.

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

The following table contains some numerical results. The bound on the error terms are rigorous. The paper [7] contains very similar non-rigorous results.

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 1, the measure ρ_L is atomless. We use the following lemmas (Fig. 2).

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

Lemma 4.1 [16,22]

(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 Ku and Chen [25].

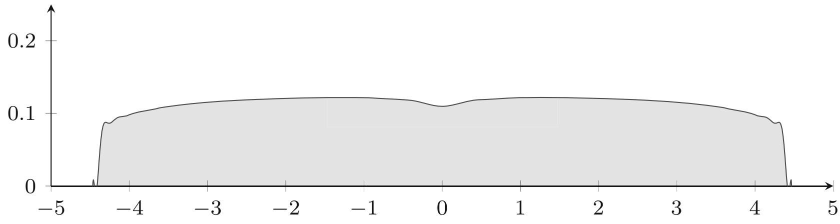

Fig. 3 An approximation for the matching measure of $\mathbb{Z}^3$. Working with reasonably sized finite grids would have been computationally too expensive, so this time we took the L_2 projection of the infinite measure to the space of degree 48 polynomials which can be calculated from the sequence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

Lemma 4.2 [25] *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 1.4.

Theorem 4.3 *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 of Theorem 3.3 We prove the two statements together. Let $\text{mult}(G_n, \theta)$ denote the multiplicity of θ as a zero of $\mu(G_n, x)$. Then by Theorem 2.10 we have

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

Note that by Lemma 4.1 we have $\text{mult}(G_n, \theta)$ 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 $\text{mult}(G_n, \theta) = 1$ by Lemma 4.2. This means that in both cases $\rho_L(\{\theta\}) = 0$. □

Proof of Theorem 1.4 (Proof of Theorem 1.4) Note that $\mathbb{Z}^d$ satisfies both conditions of Theorem 4.3 by taking boxes or using part (b), taking toroidal boxes (Fig. 3).

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