Computational Validations of the Asymptotic Matching Conjectures

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July 18, 2005

Abstract

We describe several computational validations of the asymptotic matching conjectures for r-regular bipartite graphs. These validations are based on algorithms for computation of d-dimensional monomer-dimer entropies in statistical mechanics and asymptotic combinatorics. The lower bound conjecture is applied to improve the lower bounds on the monomer dimer entropies in three dimensions.

2000 Mathematics Subject Classification: 05A15, 05A16, 05C70, 05C80, 82B20

Keywords and phrases: Matching and asymptotic growth of average matchings for r-regular bipartite graphs, monomer-dimer partitions and entropies.

1 Introduction

The monomer-dimer covers of infinite graphs G, and in particular of the infinite graph induced by the lattice $\mathbb{Z}^d$, is one of the widely used models in statistical physics. See for example [1, 2, 4, 5, 6, 10, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24].

Let $G = (V, E)$ be an undirected graph with vertices V and edges E. G can be a finite or infinite graph. A *dimer* is a domino occupying an edge $e = (u, v) \in E$. It can be viewed as two neighboring atoms occupying the

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vertices $u, v \in V$ and forging a bond between themselves. A monomer is an atom occupying a vertex $w \in V$, which does not form a bond with any other vertex in V. A *monomer-dimer cover* of G is a subset E' of E such that any two distinct edges $e, f \in E'$ do not have a common vertex. Thus E' describes all dimers in the corresponding monomer-dimer cover of G. All vertices $V' \subset V$, which are not on any edge $e \in E'$, are the monomers of the monomer-dimer cover represented by E'. E' is referred to here as a *matching*. E' is called a *perfect matching* if $V' = \emptyset$, i.e. all the vertices of G are covered by the dimers.

Consider first a finite graph $G = (V, E)$. Then E' is called an *l-matching* if $\#E' = l$. Note that $2l \leq \#V$. Let $\phi(l, G) \geq 0$ be the number of l-matchings in G for any $m \in \mathbb{Z}_+$. (Note that $\phi(0, G) = 1$ and $\phi(l, G) = 0$ if there are no l-matching in G.) Let $\psi(x, G) := \sum_{l=0}^{\infty} \phi(l, G) x^l$ denote the matching generating polynomial of G.

Let $G = (V, E)$ be an infinite graph and $p \in [0, 1]$. One defines $h_G(p)$, the G monomer-dimer entropy of density p as follows. Let $G_n = (V_n, E_n)$, $V_n \subset V, n = 1, 2, \ldots, V_n \nearrow V$ be a sequence of finite graphs where G_n *converges* to G as $n \to \infty$. (For example, each G_n can be an induced subgraph of G on the vertices V_n, i.e. $E_n = E \cap (V_n \times V_n)$. Sometimes it is useful to have different boundary conditions, where $E_n \supset E \cap (V_n \times V_n)$ as discussed below.) Then

$$h_G(p) = \sup : \limsup_{n \to \infty} \frac{\log \phi(l_n, G_n)}{\#V_n}, \quad (1.1)$$

$$\texttt{over all sequences } l_n \in \mathbb{Z}_+ \texttt{ satisfying } \lim_{n \to \infty} \frac{2l_n}{\#V_n} = p \in [0, 1]. \quad (1.2)$$

$h_G(1)$ is called the *dimer entropy* of G, while $h_G := \sup_{p \in [0,1]} h_G(p)$ is called the *monomer-dimer entropy* of G.

We now consider the classical case in statistical physics: the lattice $\mathbb{Z}^d$, consisting of all d-dimensional vectors $\mathbf{i} = (i_1, \ldots, i_d)$ with integer coordinates. (As usual we denote by $\mathbb{Z}, \mathbb{Z}_+, \mathbb{N}$ the set of integer, the set of nonnegative integers and the set of positive integers.) Let $\mathbf{e}_k = (\delta_{k1}, \ldots, \delta_{kd})$ be the unit vector in the direction of the coordinate x_k for $k = 1, \ldots, d$. Then $G = (V = \mathbb{Z}^d, E)$, where $(\mathbf{i}, \mathbf{j}) \in E \iff \mathbf{j} - \mathbf{i} = \pm \mathbf{e}_k$ for some $k \in [1, d]$. Note that G is an infinite $2d$ regular graph.

Let $h_d(p) := h_G(p)$ for any $p \in [0, 1]$ and $h_d := \sup_{p \in [0,1]} h_d(p)$. ($h_d$ and $\tilde{h}_d := h_d(1)$ are called the d-monomer-dimer entropy and the d-dimer entropy respectively [10].) For $d = 1$ it is known that [10, §4]:

$$h_1(p) = \left(1 - \frac{p}{2}\right) \log \left(1 - \frac{p}{2}\right) - \frac{p}{2} \log \frac{p}{2} - (1 - p) \log(1 - p), \quad p \in [0, 1]. \quad (1.3)$$

The value of planar dimer entropy $h_2(1)$ was computed in [5] and [18]

$$h_2(1) = \frac{1}{\pi} \sum_{q=0}^{\infty} \frac{(-1)^q}{(2q+1)^2} = 0.29156090\ldots$$

The exact values of $h_2(p)$ for $p \in (0,1)$ and $h_d(p)$ for $d \geq 3, p \in (0,1]$ are unknown. According to Jerrum [20] the two-dimensional monomer-dimer systems are computationally intractible. In [1] Baxter gave an "intuitive" computation of 19 values of $h_2(p)$ with 10 digits , using sophisticated heuristical arguments. His computations were recently verified by rigorous mathematical methods in [11].

The properties of the entropy $h_d(p)$ for any $p \in [0,1]$ was studied by Hammersley and his collaborators in the [14, 15, 16, 17]. Let us mention two properties that of interest in this context. For any $m \in \mathbb{N}$ let $\langle m \rangle := \{1, \ldots, m\} = [1, m] \cap \mathbb{Z}$ be the set of integers between 1 and m. For any $\mathbf{m} = (m_1, \ldots, m_d) \in \mathbb{N}^d$ let $\langle \mathbf{m} \rangle := \langle m_1 \rangle \times \ldots \times \langle m_d \rangle \subset \mathbb{N}^d$ is the set of points in the lattice $\mathbb{Z}^d$ located in the box $[1, m_1] \times \ldots \times [1, m_d]$ in $\mathbb{R}^d$. Denote by $\mathrm{vol}(\mathbf{m}) := \prod_{i=1}^d m_i$ the volume of the box $\langle \mathbf{m} \rangle$. Let $G(\mathbf{m}) := (\langle \mathbf{m} \rangle, E(\mathbf{m}))$ be the subgraph of $(\mathbb{Z}^d, E)$ induced by $\langle \mathbf{m} \rangle$, i.e. $(\mathbf{i}, \mathbf{j}) \in E(\mathbf{m}) \iff \mathbf{i}, \mathbf{j} \in \langle \mathbf{m} \rangle$ and $\mathbf{i} - \mathbf{j} = \pm \mathbf{e}_k$ for some $k \in \langle d \rangle$. Let $\mathbf{m}_n := (m_{1,n}, \ldots, m_{d,n}), n \in \mathbb{N}$ be a sequence of lattice points in $\mathbb{N}^d$, such that $\mathbf{m}_n \to \infty \iff m_{k,n} \to \infty$ as $n \to \infty$ for each $k = 1, \ldots, d$. Then for any sequence $l_n \in [0, \frac{\mathrm{vol}(\mathbf{m}_n)}{2}] \cap \mathbb{N}$ the following conditions hold:

$$\lim_{n \to \infty} \frac{\log \phi(l_n, G(\mathbf{m}_n))}{\mathrm{vol}(\mathbf{m}_n)} = h_d(p) \ \texttt{if} \ \mathbf{m}_n \to \infty \ \texttt{and} \ \lim_{n \to \infty} \frac{2l_n}{\mathrm{vol}(\mathbf{m}_n)} = p \in [0,1]. \tag{1.4}$$

The above characterization yields that of $h_d(p)$ is a concave continuous function on $[0,1]$.

Let $T(\mathbf{m}) := (\langle \mathbf{m} \rangle, \tilde{E}(\mathbf{m}))$ be the torus on $\langle \mathbf{m} \rangle$. Thus two vertices $\mathbf{i}, \mathbf{j} \in \langle \mathbf{m} \rangle$ in $T(\mathbf{m})$ are neighbors if $(\mathbf{i}, \mathbf{j}) \in E(\mathbf{m})$, or for any $m_k > 2$ the vertices $(i_1, \ldots, i_{k-1}, 1, i_{k+1}, \ldots, i_d)$ and $(i_1, \ldots, i_{k-1}, m_k, i_{k+1}, \ldots, i_d)$ are adjacent for any $k \in \langle d \rangle$ and $(i_1, \ldots, i_{k-1}, i_{k+1}, \ldots, i_d) \in \mathbb{N}^{d-1}$. Clearly $\phi(l, T(\mathbf{m})) \geq \phi(l, G(\mathbf{m}))$ for any $l \in \mathbb{Z}_+$. It was shown in [10] that the condition (1.4) can be replaced by the corresponding condition on the torus:

$$\lim_{n \to \infty} \frac{\log \phi(l_n, T(\mathbf{m}_n))}{\mathrm{vol}(\mathbf{m}_n)} = h_d(p) \ \texttt{if} \ \mathbf{m}_n \to \infty \ \texttt{and} \ \lim_{n \to \infty} \frac{2l_n}{\mathrm{vol}(\mathbf{m}_n)} = p \in [0,1]. \tag{1.5}$$

(The assumption $l_n \in [0, \frac{\mathrm{vol}(\mathbf{m}_n)}{2}] \cap \mathbb{N}$ is assumed.)

There are several advantages of considering $T(\mathbf{m})$ over $G(\mathbf{m})$. Assume that is that $m_k > 2$ for $k = 1, \ldots, d$. First, the graph $T(\mathbf{m})$ is a $2d$-regular graph. Second, the automorphism group of $T(\mathbf{m})$ is quite big, which can be very well exploited, using the general method of [22], for the computations of $h_d, \tilde{h}_d$ [10] and for the computations of any $h_d(p)$ [11].

The fact that $T(2\mathbf{m})$ is $2d$-regular bipartite graph was exploited in [10] to find a relatively good lower bound

$$fh_d(p) = \tfrac{1}{2}(-p \log p - 2(1-p) \log(1-p) + p \log 2d - p)$$

for $h_d(p)$ for any $p \in [0,1]$. This lower bound is obtained by noting that if $G = (V, E)$ is an r-regular bipartite graph then $\phi(l, G) \geq f_r(l, \#V)$, where the

function $f_r(l,2n) := \binom{n}{l}^2 l! \left(\frac{r}{n}\right)^l$ is determined from the proof of Tverberg's conjecture by the first named author in [7]. (Tverberg's conjecture states that the minimum of the sum of all $l \times l$ permanental minors of $n \times n$ doubly stochastic matrices is achieved only at the flat matrix $J_n = (\frac{1}{n})$.)

In the case of the perfect matching Schrijver improved the lower bound $f_r(n,2n)$ for r-regular bipartite graphs [25]. His improvement translated to the improvement of the lower bound $fh_d(1)$. In [9] the Schrijver lower bound was conjecturally generalized to $\phi(l,G) \geq g_r(l,\#V) \geq f_r(l,\#V)$ for any r-regular bipartite graph. This conjecture implies the following lower bound

$$h_d(p) \geq gh_{2d}(p), \ \texttt{for any} \ p \in (0,1] \ \texttt{and} \ d \geq 2, \tag{1.6}$$

where

$$gh_r(p) := p\log r - p\log p - 2(1-p)\log(1-p) + (r-p)\log(1-\frac{p}{r}), \tag{1.7}$$

for any integer $r \geq 2$. Note that $h_1(p) = gh_2(p)$.

The conjectured lower bound (1.6) also follows from:

Conjecture 1.1 *(**The lower asymptotic matching conjecture**.) Let $G_n = (V_n, E_n), n \in \mathbb{N}$ be a sequence of $r \geq 2$ regular bipartite graphs, where $\#V_n \to \infty$. Assume that the sequence $l_n \in [0, \frac{\#V_n}{2}] \cap \mathbb{N}, n \in \mathbb{N}$ satisfies $lim_{n\to\infty} \frac{2l_n}{\#V_n} = p \in (0,1)$. Then*

$$\liminf_{n\to\infty} \frac{\log \phi(l_n, G_n)}{\#V_n} \geq gh_r(p). \tag{1.8}$$

[25] yields the validity of (1.8) for $p = 1$ under the assumptions of Conjecture 1.1. Hence $h_d(1) \geq gh_{2d}(1)$ for any $d \in \mathbb{N}$. In particular $h_3(1) \geq 0.440075$, which is the best known lower bound. A recent massive computation performed by the third named author in [22] gives the best known upper bound $h_3(1) \leq 0.457547$.

The conjectured lower bound (1.6) yields a lower bound for the d-monomer-dimer entropy h_d. In particular one has $h_3 \geq 0.784992989$, which is the best lower bound known. The numerical computations in [10] yield the best known upper bound $h_3 \leq 0.7862023450$. (The numerical computations in [10] for the lower bound h_3 were not as good as the lower bound $h_3 \geq .7652789557$, which was obtained using the lower bound $fh_d(p)$ for $h_d(p)$ as explained above.)

We also have a corresponding **upper asymptotic matching conjecture** which is slightly more technical to state. (See §4.) For $r = 2$ we proved these conjectures in [9].

The main purpose of this paper is to report on a number of computations to test these two conjectures. All of our computations are inside the interval given by the upper and lower asymptotic conjectures. We believe that the computational and theoretical setting discussed in this paper are of interest by itself and to researchers in asymptotic combinatorics, which is widely used in statistical physics.

We now outline briefly the main setting of our computations for the verification of the two asymptotic conjectures. It is well known that the asymptotic growth of many configurations in statistical physics are given in terms of the spectral radius of the transfer matrix. See for example [10]. In this paper we construct infinite families $G_n = (V_n, E_n), n \in \mathbb{N}$ of r-regular bipartite graphs, which are coded by a specific incidence matrix $A \in \{0,1\}^{N \times N}$. Using programs based on software developed by the third named author one obtains the transfer matrix $B(t) \in \mathbb{R}^{2^N \times 2^N}$, corresponding to the matching generating polynomial with the value $x = e^{2t}$. Using the properties of the *pressure function* $P(t), t \in \mathbb{R}$, studied in detail in [11], we compute the pressure function $P(t)$ in terms of the spectral radius $\rho(B(t))$. Then the left-hand side of (1.8) for the constructed sequence of graphs $G_n = (V_n, E_n), n \in \mathbb{N}$, denoted by $h(A, p)$, is computed by using $\rho(B(t))$ and its derivative. (In this setting $p = p(t)$.) We then compare $h(A, p(t))$ to the upper and lower bound given by the lower and upper asymptotic conjecture.

We now survey briefly the contents of our paper. In §2 we discuss the sequence of tori graphs, which are considered in [10] and [11] to compute h_2, h_3 and $h_2(p)$. In §3 we describe a fairly general construction of sequences of regular graphs, which includes the sequence of tori graphs. In §4 we describe the upper matching conjecture and its asymptotic version, called the upper asymptotic matching conjecture. In §5 we describe our computational results, which support the conjectures stated in this paper. In §6 we identify an infinite graph with the maximal pressure among other infinite graphs in certain families of sequences described in §3.

2 An example of sequence of tori

As a motivation for our construction we consider first the example of a sequence of graphs that give the lower and upper bounds for h_d and $h_d(1)$ for the graph $G = (\mathbb{Z}^d, E)$ considered in [10], and the lower and upper bounds for the pressure $P(t)$ discussed in [11].

Assume that the dimension $d > 1$. Let $\mathbf{m}' := (m_1, \ldots, m_{d-1}) \in \mathbb{N}^{d-1}$ be fixed and assume that $m_i > 3$ for $i = 1, \ldots, d-1$. Consider the sequence of d-dimensional torii $T((\mathbf{m}', n)) = (V_n, E_n), n = 3, 4, \ldots$. Each torus is a $2d$-regular graph. If $m_1, \ldots, m_{d-1}$ and n are even then $T((\mathbf{m}', n))$ is bipartite. The vertex set of $T((\mathbf{m}', n)$ is the set $V_n := \langle(\mathbf{m}', n)\rangle$. V_n can be viewed as composed of n layers of vertices $\langle \mathbf{m}' \rangle$. The edges between all vertices $\langle \mathbf{m}' \rangle$ in each level k are given as in the $d-1$ dimensional torus $T(\mathbf{m}')$. The other edges of $T((\mathbf{m}', n))$ are going from level k to level $k+1$ for $k = 1, \ldots, n$, where the level $n+1$ is identified with the level 1. (We also identify level 0 with the level n.) The rule for the edges between the level k and the level $k+1$ is independent of k. Thus the vertices $(\mathbf{i}', k)$ and $(\mathbf{j}', k+1)$ in V_n are adjacent if and only if $\mathbf{i}' = \mathbf{j}'$. The adjacency matrix between the two vertices $\mathbf{i}'$ in the level k and $\mathbf{j}'$ in the level $k+1$ is given by the $0-1$ matrix $A(\mathbf{m}') := (a_{\mathbf{i}'\mathbf{j}'})_{\mathbf{i}', \mathbf{j}' \in \langle \mathbf{m}' \rangle}$, which is

an identity matrix of order $N = \mathrm{vol}(\mathbf{m}')$.

Let us recall first the computation of the monomer-dimer entropy h_d given in [10]. The entries transfer matrix $B(\mathbf{m}') = (b_{ST})_{S,T\subset\langle\mathbf{m}'\rangle}$ are indexed by two subsets of S, T of $\langle\mathbf{m}'\rangle$. (These subsets may be empty.) First $b_{ST} = 0$ if $S \cap T \neq \emptyset$. Second assume that $S \cap T = \emptyset$ then b_{ST} counts the number of the monomer-dimer covers of the subgraph of $T(\mathbf{m}')$ induced by the set vertices $\langle\mathbf{m}'\rangle\backslash(S \cup T)$. Note that any subgraph of $T(\mathbf{m}')$ induced by a set $U \subset \langle\mathbf{m}'\rangle$ can be covered by monomers. Hence $b_{ST} \geq 1$. (If $S \cup T = \langle\mathbf{m}\rangle$ then $b_{ST} = 1$.) It is not hard to see that the product of n terms $b_{S_1S_2}b_{S_2S_3}\dots b_{S_{n-1}S_n}b_{S_nS_1}$ corresponds to all monomer-dimer covers of $G_n = T((\mathbf{m}', n))$ with the following conditions. For each level $k = 1, \dots, n$ the dimers going from the level k to $k-1$ are located at the set S_k and the dimers going from the level k to the level $k+1$ are located at the set S_{k+1}. Let $\Phi(G_n) := \sum_{l=0}^{\infty}\phi(l, G_n)$ number of all possible monomer-dimer covering $T((\mathbf{m}', n))$. Then the trace of $B(\mathbf{m}')^n$, denoted by $\mathrm{tr}\, B(\mathbf{m}')^n$, is equal to $\Phi(G_n)$. It is shown in [10]

$$\lim_{n\to\infty}\frac{\log\Phi(G_n)}{\#V_n} = \frac{\log\rho(B(\mathbf{m}'))}{\mathrm{vol}(\mathbf{m}')},\ h_d = \lim_{\mathbf{m}'\to\infty}\frac{\log\rho(B(\mathbf{m}'))}{\mathrm{vol}(\mathbf{m}')}, \quad (2.1)$$
$$\texttt{and}\ \ h_d \leq \frac{\log\rho(B(2\mathbf{m}'))}{\mathrm{vol}(2\mathbf{m}')}\ \ \texttt{for any}\ \ \mathbf{m}' \in \mathbb{N}^{d-1}.$$

(Here $2\mathbf{m}' := (2m_1, \dots, 2m_{d-1})$.) The lower bounds for h_d are also expressed in terms of linear combinations of certain $\log\rho(B)$ corresponding to different values of $\mathbf{m}'$.

Let $T((\mathbf{m}', \mathbb{Z}))$ be an infinite graph given by the set of vertices $\langle\mathbf{m}'\rangle\times\mathbb{Z}$ and the following set of edges $\tilde{E}(\mathbf{m}', \mathbb{Z})$. $((\mathbf{i}', p), (\mathbf{j}', q)) \in \tilde{E}(\mathbf{m}', \mathbb{Z})$ if either $p = q$ and $(\mathbf{i}', \mathbf{j}') \in \tilde{E}(\mathbf{m}')$ or $|p - q| = 1$ and $\mathbf{i}' = \mathbf{j}'$. Thus the sequence of graphs $G_n := T((\mathbf{m}', n)), n = 3, 4, \dots$ converges to $G := T((\mathbf{m}', \mathbb{Z}))$. Let $h_G(p)$ be defined by (1.1-1.2). We now show how to compute $h_G(p)$ using the pressure function.

Let S, T be two disjoint subsets of $\langle\mathbf{m}'\rangle$. Let $E' \subset \tilde{E}(\mathbf{m}')$ be an l-matching of $T(\mathbf{m}')$ so that each edge $(u, v) \in E'$ represents a dimer occupying two adjacent vertices in $T(\mathbf{m}')$ located in $\langle\mathbf{m}'\rangle\backslash(S \cup T)$. To this matching we correspond a monomial x^l. Let $c_{ST}(x)$ be the sum of all such monomials. $c_{ST}(x)$ is the matching generating polynomial for the graph $T(\mathbf{m}', S, T)$, the subgraph of $T(\mathbf{m}')$ induced by the subset of vertices $\langle\mathbf{m}'\rangle\backslash(S \cup T)$. We let $c_{ST}(x) = 0$ if $S, T \subset \langle\mathbf{m}'\rangle$ and $S \cap T \neq \emptyset$. Then $b_{ST} = c_{ST}(1)$. Let $b_{ST}(t) := c_{ST}(e^{2t})e^{(\#S+\#T)t}$ and $B(\mathbf{m}, t) := (b_{ST}(t))_{S,T\subset\langle\mathbf{m}'\rangle}$. Then the pressure $P(t)$, for $T((\mathbf{m}', \mathbb{Z}))$, on is defined as

$$P(t) = \frac{\log\rho(B(\mathbf{m}, t))}{\mathrm{vol}(\mathbf{m}')}, \quad t \in \mathbb{R}. \quad (2.2)$$

(We suppressed the dependence of $P(t)$ on $\mathbf{m}'$.) $P(t)$ is a smooth convex function of $t \in \mathbb{R}$. Then

$$h_G(p(t)) = P(t) - tP'(t)\ \ \texttt{and}\ \ p(t) = P'(t)\ \ \texttt{for any}\ \ t \in \mathbb{R}. \quad (2.3)$$

Furthermore $h_G(p)$ is a concave function. See [11] or [9].

3 A construction of sequences of graphs

We now generalize the construction in the previous section to a general construction of a sequence of regular graphs. Let $F = (U, D)$ be an undirected graph with the set of vertices U and the set of edges D. For $n \geq 2$ let $G_n := (V_n, E_n)$ be the following graph. $V_n = U \times \langle n \rangle$, i.e. we can view V_n consisting of n copies of U arranged in the n layers $(U,1), (U,2), \ldots, (U,n)$. We let $(U,0) := (U,n), (U,n+1) := (U,1)$. Then

1. For any $u, v \in U$ and $k \in \langle n \rangle$ $((u,k),(v,k)) \in E_n \iff (u,v) \in D$.

2. Any other edges of E_n are between the vertices (U,k) and $(U,k+1)$ for $k = 1, \ldots, n$.

3. Let $A = (a_{uv})_{u,v \in U}$ be a given nonzero $0-1$ matrix. Then for each $k \in \langle n \rangle$ $((u,k),(v,k+1)) \in E_n \iff a_{uv} = 1$. We call A the *connection* matrix.

4. For any two subsets $S, T \subset U$, (S, T may be empty), let $\tilde{a}_{ST} \in \mathbb{Z}_+$ be defined as follows. If $\#S \neq \#T$ then $\tilde{a}_{ST} = 0$. Assume that $\#S = \#T$. Let $\mathcal{B}(S,T)$ be the set of all bijections $\beta : S \to T$. Then $\tilde{a}_{\emptyset\emptyset} = 1$ and $\tilde{a}_{ST} = \sum_{\beta \in \mathcal{B}(S,T)} \prod_{s \in S} a_{s\beta(s)}$ for $\#S = \#T \geq 1$.

   Thus $\tilde{a}_{ST}$ is the number of perfect matchings in the subgraph of the bipartite graph on the set of vertices $(U,1) \cup (U,2)$, and the set edges $E \subset (U,1) \times (U,2)$ given by A, and induced by the subset of vertices $(S,1) \cup (T,2)$. Let $\tilde{A} := (\tilde{a}_{ST})_{S,T \subset U}$ be a $2^{\#U} \times 2^{\#U}$ matrix with nonnegative integer entries.

5. For any two disjoint subsets $S, T \subset U$, let $c_{ST}(x)$ be the matching generating polynomial of the subgraph of F induced by the set of vertices $U \backslash (S \cup T)$. For non-disjoint subset $S, T \subset U$ let $c_{ST}(x) = 0$. Let $M(t) := (c_{ST}(e^{2t}) e^{(\#S + \#T)t})_{S,T \subset U}$ and $B(t) := M(t)\tilde{A}$ be $2^{\#U} \times 2^{\#U}$ nonnegative matrices for any $t \in \mathbb{R}$. Then $\log \rho(B(t))$ is a continuous convex function on $\mathbb{R}$. If $B(1)$ is an irreducible matrix then $\log \rho(B(t))$ is a C^∞ function.

Then the sequence $G_n, n = 2, \ldots$ has the following properties:

- If F is connected then each G_n is connected.

- Assume that F is bipartite, where $U = U_1 \cup U_2, D \subset U_1 \times U_2$. Suppose that the edges between the two consecutive levels of vertices (U,k) and $(U,k+1)$ are either between (U_i,k) and $(U_i,k+1)$ for $i = 1,2$ or between (U_i,k) and $(U_{i+1},k+1)$ for $i = 1,2$. ($U_3 := U_1$.) If n is even then G_n is bipartite.

- Assume that F is p-regular. Assume that the matrix A has q 1's in each row and column. Then G_n is $p+2q$-regular graph.

- Assume that F is p-regular bipartite. Let $U = U_1 \cup U_2, D \subset U_1 \times U_2$ and n is even. Assume that the matrix A has the following properties. Each row indexed by $u \in U_1$ and each column indexed by $v \in U_2$ has q 1's, and each row indexed by $v \in U_2$ and each column indexed by $u \in U_1$ has $q-1$ 1's. ($q \in \mathbb{N}$.) Then G_n is $p+2q-1$ regular.

- Then sequence of graphs $G_n, n = 2, 3, \ldots$ converges to the infinite graph $G = (V, E)$, where $V = F \times \mathbb{Z}$. The edges E are either between the two vertices on the same level $(U, k), k \in \mathbb{Z}$, determined by D, or between the vertices of two consecutive levels (U, k) and $(U, k+1)$, given by the incidence matrix A in the way described above.

- $P(t) := \frac{\log \rho(B(t))}{\#U}$ is the pressure of G. Assume that $B(1)$ is an irreducible matrix. Let $h_G(p)$ be defined by (1.1-1.2). Then (2.3) holds.

In the example of $G_n = T((\mathbf{m}', n)), n = 3, 4, \ldots$, discussed in the previous section, we have that $U = T(\mathbf{m}')$ and A is the identity matrix I. Hence $\tilde{A}$ is also the identity matrix.

4 The upper matching conjecture

For $r \geq 2$ let $K_{r,r}$ be a complete bipartite graph on $2r$ vertices, where each vertex has degree r. Then

$$\phi(l, K_{r,r}) = \binom{r}{l}^2 l!, \ l \in \mathbb{Z}_+, \ \texttt{and} \ \psi(x, K_{r,r}) = \sum_{l=0}^{r} \binom{r}{l}^2 l! x^l. \tag{4.1}$$

Conjecture 4.1 *(**The upper matching conjecture**.) Let $G = (V, E)$ be a finite bipartite regular r-regular graph on $2qr$ vertices where $2 \leq q, r \in \mathbb{N}$. Let $qK_{r,r}$ be the graph consisting of q copies of $K_{r,r}$. Then $\phi(l, G) \leq \phi(l, qK_{r,r})$ for $l = 0, \ldots, qr$.*

In [9] we proved the above conjecture for $r = 2$. We also showed that for $r = 2$ $\phi(l, G) \leq \phi(l, qK_{2,2})$ for any 2 regular graph G on $4q$ vertices. (G does not have to be bipartite.) It is plausible that in the above conjecture one can drop the assumption that G is bipartite.

For $l = 0, 1$ the above conjecture is trivial. For $l = qr$ the above conjecture follows from the Minc conjecture proved by Bregman [3].

Let $G_n = (V_n, E_n), n \in \mathbb{N}$ be a sequence of r regular bipartite graphs, where $\#V_n \to \infty$. Let $h_G(p)$ be defined as in (1.1-1.2). Let K be an infinite countable union of $K_{r,r}$. Let $h_K(p)$ be defined as in (1.1-1.2) where $G_n = nK_{r,r}, n \in \mathbb{N}$. Assume for simplicity of the exposition that $\#V_n = 2q_n r$. Then Conjecture

4.1 yields $\phi(l, G_n) \leq \phi(l, q_n K_{r,r})$ for $n \in \mathbb{N}$. Hence $h_G(p) \leq h_K(p)$ for any $p \in [0, 1]$.

We use the pressure $P(t)$ for K to compute $h_K(p)$. Clearly the matching generating polynomial of $qK_{r,r}$ is $\psi(x, K_{r,r})^q$. Hence

$$P_K(t) = \frac{\log \sum_{l=0}^{r} \binom{r}{l}^2 l! e^{2lt}}{2r}, \quad t \in \mathbb{R}. \tag{4.2}$$

This formula follows also from the results of the previous section, where $F = K_{r,r}$ and the incidence matrix A between two levels $(U, 1)$ and $(U, 2)$ is the zero matrix. Then $\rho(B(t)\tilde{A}) = \psi(e^{2t}, K_{r,r})$. The thermodynamics formalism [11] and [9] given by (2.3) yields

$$h_K(p(t)) = \frac{\log \sum_{l=0}^{r} \binom{r}{l}^2 l! e^{2lt}}{2r} - \frac{t \sum_{l=0}^{r} \binom{r}{l}^2 l!(2l) e^{2lt}}{2r \sum_{l=0}^{r} \binom{r}{l}^2 l! e^{2lt}}, \tag{4.3}$$

$$\texttt{where } p(t) = \frac{\sum_{l=0}^{r} \binom{r}{l}^2 l!(2l) e^{2lt}}{2r \sum_{l=0}^{r} \binom{r}{l}^2 l! e^{2lt}} \texttt{ and } t \in \mathbb{R}.$$

Note that

$$p(t) \texttt{ increases on } \mathbb{R}, \lim_{t \to -\infty} p(t) = 0, \texttt{ and } \lim_{t \to \infty} p(t) = 1.$$

Conjecture 4.2 *(**The upper asymptotic matching conjecture**.) Let $G_n = (V_n, E_n), n \in \mathbb{N}$ be a sequence of r regular bipartite graphs, where $\#V_n \to \infty$. Let $h_G(p)$ be defined as in (1.1-1.2). Let $h_K(p)$ be defined by (4.3). Then $h_G(p) \leq h_K(p)$ for any $p \in [0, 1]$.*

It is plausible to assume that Conjecture 4.2 holds under the assumption that each G_n is an r-regular graph.

5 Computational results

5.1 The Upper Matching Conjecture for Cubic graphs

We have checked the upper matching conjecture for $r = 3$ and n up to 24 by computing the matching generating polynomials for all connected bipartite cubic graphs, up to an isomorphism, in this range. For $n = 6$ and $n = 8$ there is only one cubic bipartite graph of the given size: $K_{3,3}$ and the 3-dimensional hypercube Q_3 respectively. For $n = 10$ there are two graphs to consider and they turn out to have incomparable matching generating functions. The first graph G_1 is shown in Figure 1 and the second graph is the 10 vertex Möbius ladder M_{10}. (M_{10} consists of two copies of path of length 5: $1-2-3-4-5$, denoted by $(P_5, 1)$ and $(P_5, 2)$, where first one connects $(i, 1)$ and $(i, 2)$ by an edge for $i = 1, \ldots, 5$, and then one connects $(1, 1)$ with $(5, 2)$ and $(1, 2)$ with $(5, 1)$.)

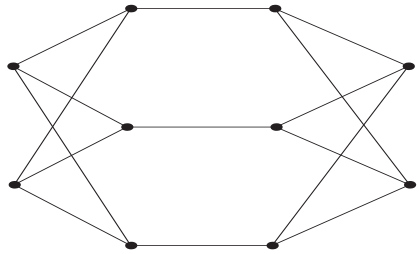


Figure 1: G_1

Their matching generating polynomials are:

$$\psi(x, G_1) := 1 + 15x + 75x^2 + 145x^3 + 96x^4 + 12x^5,$$
$$\psi(x, M_{10}) := 1 + 15x + 75x^2 + 145x^3 + 95x^4 + 13x^5.$$

For n from 12 to 24 the extremal graphs, with the maximal $\phi(l, G)$, are for the form

$$\begin{array}{ll} \frac{n}{6}K_{3,3} & \text{if } 6|n \\ \frac{n-8}{6}K_{3,3} \bigcup Q_3 & \text{if } 6|(n-2) \\ \frac{n-10}{6}K_{3,3} \bigcup (G_1 \text{ or } M_{10}) & \text{if } 6|(n-4) \end{array} \tag{5.1}$$

So for $n = 10, 22$ we do not have a unique extremal graph, which maximizes all $\phi(l, G)$. It seems natural to conjecture that the three graph families given here together make up all the extremal graphs for all n.

5.2 The asymptotic matching conjectures

We have checked the asymptotic matching conjectures for several families like those described in Section 3. In each case we choose U to be a cycle C_l of length l for several values of l and then varied the connection matrix A. In each case we used the described transfer matrix method to compute the entropy for several values of p and then compared with the conjectured bound. In all cases the conjecture was found to hold.

In order to test the conjectured lower bound for a given choice of U and A we first constructed the transfer matrix $B(t)$ for the given graph. Given $B(t)$ we can directly compute $P(t)$ from the maximum eigenvalue as in (2.2). Next we computed $P'(t)$, using the equality

$$\rho'(t) = \eta_1^T \left(\frac{d}{dt} B(t) \right) \eta_2,$$

where η_1^T and η_2 are the left and right eigenvectors of $B(t)$, normalized by the condition $\eta_1^T \eta_2 = 1$. From these values we now compute $h_G(p(t))$ using (2.3). So for each value of t we get a pair $(p(t), h_G(p(t)))$ telling us the asymptotic

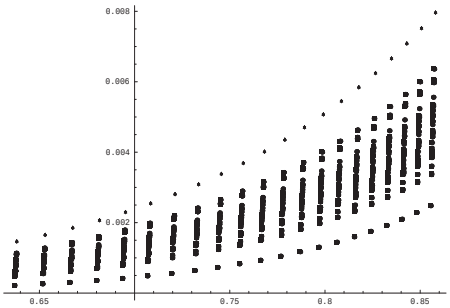


Figure 2: Difference between actual entropy and the lower asymptotic matching conjecture for 4-regular graphs with $U = C_8$

pressure $h_G(p(t))$ at the density $p(t) = P'(t)$. To make all computations exact we chose e^t to be rational numbers, which yielded rational values for all matrix entries.

Example 5.1 (r=4) *In our first family we let l, the length of the cycle $U = C_l$, vary from 4 to 8. We tested all permutation matrices A, which give every vertex (u, k) in G_n one neighbor in the level $k-1$ and one in the level $k+1$, and give rise to a bipartite G_n. We thus have a family of bipartite 4-regular graphs which includes the standard square lattice tori.*

In Figure 2 we plot the difference between the actual values of the entropies $h_G(p)$, for all choices of A, and the lower asymptotic matching conjecture for a given range of densities p. The highest curve correspond to the normal torus graph, i.e it is the graph with the maximum number of matching of a given size in this family.

Example 5.2 (r=3) *For our second example we again chose $U = C_l$ to be a cycle of length l. Here we chose A so that if we number the vertices on the cycle $1, \ldots, l$ the even vertices in the level k have an an odd vertex as a neighbor in the level $k+1$ for $k = 1, \ldots, n$. G_n is cubic, and for l and n even G_n is bipartite. This family includes the torus graphs obtained from the hexagonal lattice which all have girth at least 6. In this case we let the length of the cycle vary from 4 to 10 and again the conjecture was found to hold. In Figure 3 we display the difference between the actual values of the entropies $h_G(p)$, for all choices of A, and the lower asymptotic matching conjecture for a given range of densities p. Here the values typically stayed closer to the conjecture than for the 4-regular case, which is to be expected since this graph family has higher girth.*

Apart from the above tests, we also tested some more arbitrarily chosen connection matrices giving graphs of degree 6. This was done by U as a cycle and choosing the connection matrix A, having two 1's in each row and column. Again the conjecture was found to hold but here the deviation up from the conjectured lower bound was even smaller. This is again expected since the conjecture should become more accurate for graphs of higher degree.

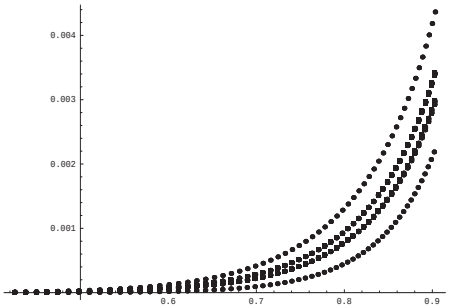


Figure 3: Difference between actual entropy and the lower asymptotic matching conjecture for 3-regular graphs with $U = C_{10}$

6 Infinite graphs with the maximal pressure

In this section we give a partial justification for the computational result in Example 5.1 that the highest curve correspond to the normal torus graph.

Theorem 6.1 *Let $F = (U, D)$ be an undirected graph and consider an infinite graph $G = (V, E)$ defined as follows. $V = U \times \mathbb{Z}$, i.e. the vertices of G consists layers $(U, k), k \in \mathbb{Z}$. The edges E of G connect two vertices on the level $k, j \in \mathbb{Z}$ only if $|k - j| \leq 1$. The edges between any two vertices on level k are given by D. The edges between the level k and the level $k + 1$ are given by $\#U \times \#U$ permutation matrix $A_k = (a_{uv,k})_{u,v \in U}$ for each $k \in \mathbb{Z}$. Thus $((u, k), (v, k + 1)) \in E \iff a_{uv,k} = 1$. Let $M(t), t \in \mathbb{R}$ and $\tilde{A}_k$ be the $2^{\#U} \times 2^{\#U}$ nonnegative matrices defined as in §3. Then the pressure $P_G(t)$ of G is given as*

$$P_G(t) = \limsup_{i,j \to \infty} \frac{\log \operatorname{tr} M(t)\tilde{A}_{-j}M(t)\tilde{A}_{-j+1} \dots M(t)\tilde{A}_i}{(i + j + 1)\#U}. \tag{6.1}$$

Let G_0 be the infinite graph obtained by letting A_k to be the identity matrix for each $k \in \mathbb{Z}$. Then

$$P_{G_0}(t) = \frac{\log \rho(M(t))}{\#U} \geq P_G(t) \tag{6.2}$$

for any $t \in \mathbb{R}$ and any G of the above form. In particular the monomer-dimer entropy h_G of G, which is equal to $P_G(0)$, does not exceed $h_{G_0} = P_{G_0}(0)$.

Proof. Fix $i, j \in \mathbb{N}$ and let $n = i + j + 1$. Define $G_n = (V_n, E_n)$ to be the following graph. V_n consists of n copies of U, labelled as (U, k) for $k = -j, \dots, i$. The edges of E_n are induced by the edges of G, except that the edges from the level i are connected to the edges of the level $-j$, which is identified with the level $i + 1$, by the connection matrix A_i. The arguments of §2 yield that $\psi(e^{2t}, G_n) = \operatorname{tr} M(t)\tilde{A}_{-j}M(t)\tilde{A}_{-j+1} \dots M(t)\tilde{A}_i$. Hence P_G is given by (6.1) [11].

Consider now the case of G_0 where $A_k = I$. Then (6.1) yields $P_{G_0}(t) = \frac{\log \rho(M(t))}{\#U}$. (See for example [8, §10] for the self-contained details of the arguments on matrices used here.) From the definition of $M(t)$ it follows that

$M(t)$ is a nonnegative and symmetric matrix. Hence $\rho(M(t)) = ||M(t)||$, where $||M(t)||$ is the l_2 operator norm of $M(t)$. Since A_k is a permutation it follows that $\tilde{A}_k$ is also a permutation matrix. Hence $||\tilde{A}_k|| = 1$. Thus

$$||M(t)\tilde{A}_{-j}M(t)\tilde{A}_{-j+1}\dots M(t)\tilde{A}_i|| \le ||M(t)||^{i+j+1} = \rho(M(t))^{i+j+1} \Rightarrow$$
$$\operatorname{tr} M(t)\tilde{A}_{-j}M(t)\tilde{A}_{-j+1}\dots M(t)\tilde{A}_i \le 2^{\#U}\rho(M(t))^{i+j+1} \Rightarrow$$
$$P_G(t) \le \frac{\log \rho(M(t))}{\#U}.$$

This proves (6.2).

From the definition of monomer-dimer entropy of G [10] it follows that $h_G = P_G(0)$. Hence $h_G \le h_{G_0}$. □

Conjecture 6.2 *Let the assumptions of Theorem 6.1 hold. Then for any* $p \in [0,1]$ $h_G(p) \le h_{G_0}(p)$.

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