Theory of Computation of Multidimensional Entropy with an Application to the Monomer-Dimer Problem

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Abstract

Consider all colorings of a finite box in a multi-dimensional grid with a given number of colors subject to given local constraints. We outline the most recent theory for the computation of the exponential growth rate of the number of such colorings as a function of the dimensions of the box. As an application we compute the monomer-dimer constant for the 2-dimensional grid to 9 decimal digits, agreeing with the heuristic computations of Baxter, and for the 3-dimensional grid with an error smaller than 1.35%.

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1 Introduction

The exponential growth rate h (with respect to the natural logarithm) of the number of configurations on a multi-dimensional grid arises in the study of various statistical physics (or combinatorial) systems [31, 12]. In mathematics h is called the *topological entropy* [14]; in information theory h (with respect to $\log_2$) is called the *multi-dimensional capacity* [35]; and in physics e^h is referred to as the entropy (per atom) of the corresponding "hard model". The 1-dimensional case is easy, namely e^h is equal to the spectral radius $\rho(A)$ of a certain matrix A called the "transfer matrix". There are very few 2-dimensional models where the value of h is known in closed form [10, 23, 26, 27, 2]. In all other cases there are estimates based on: (a) asymptotic expansions, e.g., [29, 1, 17]; (b) Monte-Carlo methods, e.g., [20, 3]; (c) bounds, e.g., [19, 7, 28, 6, 11, 30]. In what follows we give a complete up-to-date theory

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of the computation of h by calculating lower and upper bounds. It refines the techniques described in [15] by using an automorphism subgroup of a given graph. A fundamental problem in lattice statistics is the monomer-dimer problem (see [24]). As a demonstration of our techniques, we compute the topological entropy of the monomer-dimer covers of the 2-dimensional grid $h_2 = .66279897$ (which agrees with the heuristic estimation $e^{h_2} = 1.940215351$ due to Baxter [1]) and of the 3-dimensional grid $.7653 \le h_3 \le .7862$. These numerical results are much better than previously known ones.

Consider the grid $\mathbb{Z}^d$ in d-dimensional space $\mathbb{R}^d$. At each point of the grid we place an element of a set of n kinds of colors (atoms) denoted by $\langle n \rangle := \{1, \ldots, n\}$. Certain restrictions may be imposed on the colorings. For example, the restrictions of the *hard model* are specified by a directed d-graph $\Gamma := (\Gamma_1, \ldots, \Gamma_d)$ called a *nearest neighbor digraph*, with $\Gamma_k \subseteq \langle n \rangle \times \langle n \rangle$, in the sense that two atoms of kinds p and q are allowed to occupy respectively the adjacent grid points $\mathbf{i} = (i_1, \ldots, i_d)$ and $\mathbf{i} + \mathbf{e}_k$ (where $\mathbf{e}_k := (\delta_{1k}, \ldots, \delta_{dk})$) only if $(p, q) \in \Gamma_k$. We call such a placement a Γ-*configuration* or Γ-*cover*. This general model is anisotropic, since the Γ_k can be distinct. A digraph Γ_k is called *symmetric* when $(p, q) \in \Gamma_k \Leftrightarrow (q, p) \in \Gamma_k$. We call Γ a *symmetric isotropic nearest neighbor digraph* when $\Gamma_1 = \cdots = \Gamma_d = \Delta$, and Δ is symmetric. Let $\mathbf{m} = (m_1, \ldots, m_d) \in \mathbb{N}^d$, where $\mathbb{N} := \{1, 2, \ldots\}$, and consider the box $\langle \mathbf{m} \rangle := \langle m_1 \rangle \times \cdots \times \langle m_d \rangle$ of dimensions $m_1, \ldots, m_d$. Let $W(\mathbf{m})$ be the set of all Γ-configurations of $\mathrm{vol}(\mathbf{m}) := m_1 \cdots m_d$ atoms in the box $\langle \mathbf{m} \rangle$. It is easy to show that the multisequence $\log \#W(\mathbf{m})$ for $\mathbf{m} \in \mathbb{N}^d$ is *subadditive* in each coordinate, i.e., $\log \#W(\mathbf{m} + p\mathbf{e}_k) \le \log \#W(\mathbf{m}) + \log \#W(\mathbf{m} + (p - m_k)\mathbf{e}_k)$ for all $\mathbf{m} \in \mathbb{N}^d$, $p \in \mathbb{N}$ and $k \in \langle d \rangle$. From this it can be shown that the following limit exists and is non-negative or equal to $-\infty$ (we use $\mathbf{m} \to \infty$ as an abbreviation of $m_1, \ldots, m_d \to \infty$):

$$h = h(\Gamma) := \lim_{\mathbf{m} \to \infty} \frac{\log \#W(\mathbf{m})}{\mathrm{vol}(\mathbf{m})}, \tag{1.1}$$

and each $\mathbf{m} \in \mathbb{N}^d$ satisfies

$$h \le \frac{\log \#W(\mathbf{m})}{\mathrm{vol}(\mathbf{m})}. \tag{1.2}$$

The limit $h(\Gamma)$ is the exponential growth rate of $\#W(\mathbf{m})$ per atom, also called *entropy* or *Shannon capacity*. It follows from König's Infinity Lemma [9, Section 2.5], [8] that $h = \log 0 = -\infty$ if and only if there are no Γ-covers of $\mathbb{Z}^d$. The case $d = 1$ is well understood: $h = \log \rho(A)$, where A is the incidence matrix for the digraph Γ_1; there exist Γ-covers if and only if Γ_1 has a directed cycle, and in that case h is also the exponential growth rate per atom of the number of periodic Γ-covers of $\mathbb{Z}$ [14]. A periodic Γ-cover of $\mathbb{Z}^d$ with period $\mathbf{m}$ (i.e., a Γ-cover $\phi = (\phi_{\mathbf{i}})_{\mathbf{i} \in \mathbb{Z}^d}$ satisfying $\phi_{\mathbf{i} + m_k \mathbf{e}_k} = \phi_{\mathbf{i}}$ for all $\mathbf{i} \in \mathbb{Z}^d$ and $k \in \langle d \rangle$) is equivalent to a Γ-cover of the torus $T(\mathbf{m}) := (\mathbb{Z}/m_1\mathbb{Z}) \times \cdots \times (\mathbb{Z}/m_d\mathbb{Z})$. For $d \ge 2$, the question whether there exist Γ-covers is undecidable and h is not computable in general [4, 22]. (By saying that a quantity Q is *computable* we mean that given $\epsilon > 0$, we can find in a finite number of steps, depending on ϵ, a rational number r satisfying $|Q - r| < \epsilon$.) Equivalently, there is a d-digraph Γ for which there are Γ-covers of $\mathbb{Z}^d$ but none is periodic. Hence there are no nontrivial lower bounds for h in this case. A fundamental result in [14] asserts that if at least $d - 1$ digraphs out of $\Gamma_1, \ldots, \Gamma_d$ are symmetric, then the exponential growth rate per atom of the number of periodic configurations is equal to h and h is computable, i.e., we have lower bounds for h that converge to h. For $d = 2, 3$ this will also follow from our results in Section 3. These results hold in particular for a symmetric isotropic nearest neighbor digraph.

We mention briefly the topological entropy. Let $W_{\text{top}}(\mathbf{m})$ be the set of all distinct restrictions of Γ-covers of $\mathbb{Z}^d$ to the box $\langle \mathbf{m} \rangle$. The multisequence $\log \# W_{\text{top}}(\mathbf{m})$ witn $\mathbf{m} \in \mathbb{N}^d$ is also subadditive, and the *topological entropy* of Γ is defined by

$$h_{\text{top}}(\Gamma) := \lim_{\mathbf{m} \to \infty} \frac{\log \# W_{\text{top}}(\mathbf{m})}{\text{vol}(\mathbf{m})}.$$

Since $W_{\text{top}}(\mathbf{m}) \subseteq W(\mathbf{m})$, we have $h_{\text{top}}(\Gamma) \leq h(\Gamma)$; a result in [14] asserts that equality holds.

We now elaborate our results. Fix $\mathbf{m}' := (m_1, \ldots, m_{d-1}) \in \mathbb{N}^{d-1}$ and let $\Gamma' := (\Gamma_1, \ldots, \Gamma_{d-1})$. Let $\Omega_d(\mathbf{m}')$ be the transfer digraph between Γ'-covers of $\langle \mathbf{m}' \rangle$ with respect to Γ_d. That is, the vertex set of $\Omega_d(\mathbf{m}')$ is the set of Γ'-covers of $\langle \mathbf{m}' \rangle$, and vertices u, v satisfy $(u, v) \in \Omega_d(\mathbf{m}')$ if and only if $[u, v] \in W(\mathbf{m}', 2)$, where $[u, v]$ is the configuration consisting of u, v occupying the levels $x_d = 1, 2$ of $\langle (\mathbf{m}', 2) \rangle$, respectively. We show that $h \leq \frac{\log \rho(\Omega_d(\mathbf{m}'))}{\text{vol}(\mathbf{m}')}$, where by definition, the spectral radius of a digraph is the spectral radius of its incidence matrix. When $\Gamma_1, \ldots, \Gamma_{d-1}$ are symmetric, this upper bound can be improved as follows. Let $\Theta_d(\mathbf{m}')$ be the induced subdigraph of $\Omega_d(\mathbf{m}')$ whose vertices are the periodic Γ'-covers of $\langle \mathbf{m}' \rangle$ with period $\mathbf{m}'$. Then we show [15]

$$h(\Gamma) \leq \frac{\log \rho(\Theta_d(\mathbf{m}'))}{\text{vol}(\mathbf{m}')}, \quad m_1, \ldots, m_{d-1} \text{ even}, \Gamma_1, \ldots, \Gamma_{d-1} \text{ symmetric}. \tag{1.3}$$

Furthermore, for $\Gamma_1, \ldots, \Gamma_{d-1}$ symmetric, we give various lower bounds for h in terms of $\log \rho(\Theta_d(\mathbf{m}'))$ for various values of $\mathbf{m}'$. For example, for $d = 2$ we show that

$$h(\Gamma_1, \Gamma_2) \geq \frac{\log \rho(\Theta_2(p + 2q)) - \log \rho(\Theta_2(2q))}{p}, \quad p \in \mathbb{N},\ q \in \mathbb{N} \cup \{0\},\ \Gamma_1 \text{ symmetric}. \tag{1.4}$$

See [15] for slightly different lower bounds for h, which do not use periodicity. All of these upper and lower bounds converge to the true entropy when $\mathbf{m}' \to \infty$.

We can enhance the efficiency of computing the spectral radius $\rho(\Lambda)$ of a digraph $\Lambda \subseteq N \times N$ as follows. To compute $\rho(\Lambda)$ one needs to compute the spectral radius of its 0-1 $N \times N$ incidence matrix A. Suppose that $\mathcal{G} \subseteq S_N$ is an automorphism subgroup of Λ. Let $\mathcal{O} = \langle N \rangle / \mathcal{G}$ be the orbit space under the action of $\mathcal{G}$ and set $M = \# \mathcal{O}$. Let $\Lambda' \subseteq \mathcal{O} \times \mathcal{O}$ be the multidigraph induced by Λ and $\mathcal{G}$. That is, for $\mu, \nu \in \mathcal{O}$, the multiplicity of the edge (μ, ν) of Λ' is $\widehat{a}_{\mu,\nu} = \sum_{j \in \nu} a_{i,j}$ for any $i \in \mu$. We show that $\rho(\Lambda)$ is also the spectral radius of the $M \times M$ nonnegative integer matrix $\widehat{A}$. If $M \ll N$, then the computation of $\rho(\widehat{A})$ may be feasible on a desktop computer, whereas the computation of $\rho(A)$ may be infeasible on a supercomputer.

We show that the automorphism group of $\Theta_d(\mathbf{m}')$ contains a subgroup isomorphic to the group of translations of $T(\mathbf{m}')$. If $\Gamma_1 = \cdots = \Gamma_{d-1} = \Delta$ and Δ is symmetric, then the automorphism group of $\Theta_d(\mathbf{m}')$ contains a subgroup isomorphic to the group of rigid motions of $T(\mathbf{m}')$ (motions preserving the distance on $T(\mathbf{m}')$, i.e., translations, reflections and coordinate transpositions for equal dimensions). For example, $T(m)$ has m translations and $2m$ rigid motions if $m > 2$.

We now discuss the monomer-dimer covers of $\mathbb{Z}^d$, see [12]. A *dimer* is a domino consisting of two neighboring atoms occupying the places $\mathbf{i}, \mathbf{i}+\mathbf{e}_k \in \mathbb{Z}^d$. A *monomer* is a single atom occupying the place $\mathbf{i} \in \mathbb{Z}^d$. A *monomer-dimer cover*, respectively *dimer cover*, of $\mathbb{Z}^d$ is a partition of $\mathbb{Z}^d$ into monomers and dimers, respectively dimers. We denote by h_d and $\widetilde{h}_d$ the entropies of the monomer-dimer and dimer covers, respectively. It is fairly easy to compute the values $h_1 = \log \frac{1+\sqrt{5}}{2}$ and $\widetilde{h}_1 = 0$. The big breakthrough in the sixties was a close formula for $\widetilde{h}_2$ in [10, 23]. The exact values of h_d for $d \geq 2$ and $\widetilde{h}_d$ for $d \geq 3$ are unknown.

A seminal contribution to the study of upper and lower bounds and estimates for $\widetilde{h}_d$ and h_d was given in [18, 19, 20, 21]. In particular, it was shown in [18] that for $p \in [0,1]$, there exists the entropy $\lambda_d(p)$ of the monomer-dimer covers of $\mathbb{Z}^d$, where p is the "density" of dimers, i.e., the number of dimers in the cover divided by one half of the volume. The entropy $\lambda_d(p)$ is a continuous concave function of p and $\lambda_d(1) = \widetilde{h}_d$. It is shown here that $h_d = \max_{p\in[0,1]} \lambda_d(p)$. It was pointed out by Kingman, see [19], that the van der Waerden conjecture for permanents of doubly-stochastic matrices gives a lower bound for $\widetilde{h}_d$. The improved lower bound for the permanents of 0-1 matrices [33] gives the currently best lower bound $\widetilde{h}_3 \geq 0.440075$. A recent breakthrough [7] gives the upper bound $\widetilde{h}_3 \leq 0.463107$, improved in [28] to $\widetilde{h}_3 \leq 0.457547$.

It is shown in [15] that the dimer covers can be encoded as $\widetilde{\Lambda}$-covers for an appropriate d-digraph $\widetilde{\Lambda} = (\widetilde{\Lambda}_1, \ldots, \widetilde{\Lambda}_d)$, where all digraphs are on the set of vertices $\langle 2d \rangle$. We show that the monomer-dimer covers can be similarly encoded as Λ-configurations for an appropriate d-digraph $\Lambda = (\Lambda_1, \ldots, \Lambda_d)$, where all digraphs are on the set of vertices $\langle 2d+1 \rangle$. Unfortunately, in these encodings the digraphs Γ_k, $\widetilde{\Gamma}_k$ are not symmetric, so (1.3) and the lower bounds like (1.4) do not apply directly. One of the purposes of this paper is to show that the entropies h_d and $\widetilde{h}_d$ nevertheless obey upper and lower bounds converging to the true entropies, similar to (1.3) and (1.4). The bounds for h_d are stated in terms of the spectral radii of certain multidigraphs $\Theta_d(\mathbf{m}')$. The automorphism group of $\Theta_d(\mathbf{m}')$ has a subgroup isomorphic to the the group of rigid motions of $T(\mathbf{m}')$. This fact enables us to compute the values of h_2 and h_3 with good precision. We also show that $\lambda_d(p)$ can be bounded below by using the generalized van der Waerden conjecture (Tverberg's conjecture), proved by the first author in [13]. For $d = 2, 3$, this lower bound is better than those of [5] and [21] except for very high p. Our lower bound for $\lambda_d(p)$ yields in particular a lower bound for h_d. For $d = 2$ this lower bound is somewhat weaker than the one obtained from the numerical computations of $\rho(\Theta_d(\mathbf{m}'))$, but for $d = 3$ the situation is reversed.

See [16] for a general theory of monomer-dimer covers of an arbitrary graph. Finally it is worth mentioning the theoretical work [25], which shows that the general monomer-dimer problem in arbitrary planar graphs is computationally intractable.

The contents of the paper is as follows. In Section 2 we discuss the the general theory of $\mathbb{Z}^d$ subshifts of finite type (SOFT). In Section 3 we prove the main inequalities of the entropy of $\mathbb{Z}^d$-SOFT with $d-1$ symmetric digraphs $\Gamma_1, \ldots, \Gamma_{d-1}$. In Section 4 we recall the main features of the entropy of the monomer-dimer and dimer covers. In Section 5 we give lower bounds for the entropy of the monomer-dimer covers with a fixed dimer density using the lower bounds for permanents. In Section 6 we show that there exist analogs of the upper and lower bounds discussed in Section 3 that apply to the monomer-dimer and dimer entropy. In Section 7 we discuss using automorphism subgroups to reduce the computations. In Section 8 we give numerical upper and lower bounds for h_2, $\widetilde{h}_2$, h_3, $\widetilde{h}_3$, and compare graphically our lower bounds for $\lambda_2(p)$ and $\lambda_3(p)$ with the known lower bounds and estimates.

2 SOFT and NNSOFT

Let $\langle n\rangle^{\mathbb{Z}^d}$ be the set of all colorings $\phi : \mathbb{Z}^d \to \langle n\rangle$ of $\mathbb{Z}^d$ with colors from $\langle n\rangle = \{1,\dots,n\}$. Given a d-digraph $\Gamma = (\Gamma_1,\dots,\Gamma_d)$ on $\langle n\rangle \times \langle n\rangle$, let $\Gamma^{\mathbb{Z}^d} \subseteq \langle n\rangle^{\mathbb{Z}^d}$ be the set of all Γ-covers, namely colorings $\phi = (\phi_{\mathbf{m}})_{\mathbf{m}\in\mathbb{Z}^d}$ in $\langle n\rangle^{\mathbb{Z}^d}$ such that for each $\mathbf{i} \in \mathbb{Z}^d$ and $k \in \langle d\rangle$, the restriction of ϕ to the line through $\mathbf{i}$ in the direction of $\mathbf{e}_k$, i.e., $(\phi_{\mathbf{i}+j\mathbf{e}_k})_{j\in\mathbb{Z}}$, is a bi-infinite walk on Γ_k. In ergodic theory, $\Gamma^{\mathbb{Z}^d}$ is called a *nearest neighbor subshift of finite type (NNSOFT)*. Note that for an NNSOFT $\Gamma^{\mathbb{Z}^d}$ and for $\mathbf{m} \in \mathbb{N}^d$, $W(\mathbf{m})$ is the set of all configurations $\psi \in \langle n\rangle^{\langle\mathbf{m}\rangle}$ such that $\mathbf{i}, \mathbf{i}+\mathbf{e}_k \in \langle\mathbf{m}\rangle$ imply $(\psi_{\mathbf{i}}, \psi_{\mathbf{i}+\mathbf{e}_k}) \in \Gamma_k$.

A general subshift of finite type can be described as follows. Let $\mathbf{M} \in \mathbb{N}^d$ and a nonempty subset $\mathcal{P} \subseteq \langle n\rangle^{\langle\mathbf{M}\rangle}$ be given. Every element $a \in \mathcal{P}$ is viewed as an allowed coloring (configuration) of the box $\langle\mathbf{M}\rangle$ with n colors. For $\mathbf{i} \in \mathbb{Z}^d$, we define the shifted coloring $\tau_{\mathbf{i}}(a)$ of $a \in \mathcal{P}$ as the coloring of the shifted box $\langle\mathbf{M}\rangle + \mathbf{i}$ that gives to the point $\mathbf{x}+\mathbf{i}$ the same color that a gives to $\mathbf{x} \in \langle\mathbf{M}\rangle$. We denote by $\tau_{\mathbf{i}}(\mathcal{P})$ the set $\{\tau_{\mathbf{i}}(a) : a \in \mathcal{P}\}$, and regard it as the set of allowed colorings of $\langle\mathbf{M}\rangle + \mathbf{i}$. A coloring $\phi \in \langle n\rangle^{\mathbb{Z}^d}$ is called a $\mathcal{P}$*-state* if for each $\mathbf{i} \in \mathbb{Z}^d$ the restriction of ϕ to $\langle\mathbf{M}\rangle+\mathbf{i}$ is in $\tau_{\mathbf{i}}(\mathcal{P})$. We denote by $\langle n\rangle^{\mathbb{Z}^d}(\mathcal{P})$ the set of all $\mathcal{P}$-states. In ergodic theory the set $\langle n\rangle^{\mathbb{Z}^d}(\mathcal{P})$ is called a *subshift of finite type (SOFT)* [32].

Each NNSOFT $\Gamma^{\mathbb{Z}^d}$ is a special kind of SOFT obtained by letting $\mathbf{M} = (2,\dots,2)$ and letting $\mathcal{P}$ be the set of all colorings $\psi \in \langle n\rangle^{\langle\mathbf{M}\rangle}$ such that $\mathbf{i}, \mathbf{i}+\mathbf{e}_k \in \langle\mathbf{M}\rangle$ imply $(\psi_{\mathbf{i}}, \psi_{\mathbf{i}+\mathbf{e}_k}) \in \Gamma_k$. Conversely, each SOFT $\langle n\rangle^{\mathbb{Z}^d}(\mathcal{P})$ can be encoded as an NNSOFT $\Gamma^{\mathbb{Z}^d}$, where $\Gamma = (\Gamma_1,\dots,\Gamma_d)$ are defined as follows. Take $N = \#\mathcal{P}$ and use a bijection between $\mathcal{P}$ and $\langle N\rangle$. The digraph $\Gamma_k \subseteq \langle N\rangle \times \langle N\rangle$ is defined so that for $a, b \in \mathcal{P}$ we have $(a,b) \in \Gamma_k$ if and only if there is a configuration $\phi \in \langle n\rangle^{\langle\mathbf{M}+\mathbf{e}_k\rangle}$ such that the restriction of ϕ to $\langle\mathbf{M}\rangle$ is a and the restriction of ϕ to $\langle\mathbf{M}\rangle + \mathbf{e}_k$ is $\tau_{\mathbf{e}_k}(b)$ [14]. Because of this equivalence, we will be dealing here with NNSOFT only.

In the sequel we shall be taking lim sup and lim inf of real multisequences $(a_{\mathbf{m}})_{\mathbf{m}\in\mathbb{N}^d}$ as $\mathbf{m} \to \infty$. In order to be clear, we define these here and prove that they are limits of subsequences. We also define the limit of real multisequence in terms of lim sup and lim inf, which is equivalent to other definitions in the literature.

Definition 2.1 *Let $(a_{\mathbf{m}})_{\mathbf{m}\in\mathbb{N}^d}$ be a multisequence of real numbers. Then*

(a) $\limsup_{\mathbf{m}\to\infty} a_{\mathbf{m}}$ *is defined as the supremum (possibly $\pm\infty$) of all numbers of the form* $\limsup_{q\to\infty} a_{\mathbf{m}_q}$*, where $(\mathbf{m}_q)_{q\in\mathbb{N}}$ is a sequence in $\mathbb{N}^d$ satisfying* $\lim_{q\to\infty} \mathbf{m}_q = \infty$*, i.e.,* $\lim_{q\to\infty}(\mathbf{m}_q)_i = \infty$ *for each $i \in \langle d\rangle$. We define* $\liminf_{\mathbf{m}\to\infty} a_{\mathbf{m}}$ *similarly.*

(b) $\lim_{\mathbf{m}\to\infty} a_{\mathbf{m}} = \alpha$ *means* $\limsup_{\mathbf{m}\to\infty} a_{\mathbf{m}} = \liminf_{\mathbf{m}\to\infty} a_{\mathbf{m}} = \alpha$.

Proposition 2.2 *If* $\limsup_{\mathbf{m}\to\infty} a_{\mathbf{m}} = \alpha$*, then there exists a sequence $(\mathbf{n}_q)_{q\in\mathbb{N}} \subseteq \mathbb{N}^d$ satisfying* $\lim_{q\to\infty} \mathbf{n}_q = \infty$ *such that the sequence $(a_{\mathbf{n}_q})_{q\in\mathbb{N}}$ has a limit and* $\lim_{q\to\infty} a_{\mathbf{n}_q} = \alpha$*. Similarly for* lim inf.

Proof. Since the lim sup of each real sequence is the limit of a subsequence, we may assume that we have a sequence of convergent subsequences $\{a_{\mathbf{m}_q^j}\}$ satisfying $\lim_{q\to\infty} a_{\mathbf{m}_q^j} = \alpha_j$ and $\lim_{q\to\infty} \mathbf{m}_q^j = \infty$ for each $j \in \mathbb{N}$, and $\lim_{j\to\infty} \alpha_j = \alpha$. Note that $\alpha_j \le \alpha$ for all j by definition of the supremum. If $\alpha_j = \alpha$ for some j, there is nothing to prove. This is true in particular if $\alpha = -\infty$, for then $\alpha_j = -\infty = \alpha$ for each j. Therefore we may assume that $\alpha \in \mathbb{R} \cup \{\infty\}$ and that $\alpha_j < \alpha_{j+1}$ for all j.

Assume first that $\alpha \in \mathbb{R}$. Then for each $j \in \mathbb{N}$ there exists a $q(j) \in \mathbb{N}$ such that $\mathbf{m}_{q(j+1)}^{j+1} > 2\mathbf{m}_{q(j)}^j$ and $|a_{\mathbf{m}_{q(j)}^j} - \alpha_j| < \frac{1}{2^j}$. Then we can take $\mathbf{n}_j = \mathbf{m}_{q(j)}^j$ and the result follows. Similarly, if $\alpha = \infty$, then for each $j \in \mathbb{N}$ there exists a $q(j) \in \mathbb{N}$ such that $\mathbf{m}_{q(j+1)}^{j+1} > 2\mathbf{m}_{q(j)}^j$ and $a_{\mathbf{m}_{q(j)}^j} > \alpha_j - 1$, and again we can take $\mathbf{n}_j = \mathbf{m}_{q(j)}^j$. $\square$

Let $W_{\rm per}(\mathbf{m}) \subseteq \Gamma^{\mathbb{Z}^d}$ be the set of periodic Γ-covers with period $\mathbf{m}$. Then

$$h_{\rm per}(\Gamma) := \limsup_{\mathbf{m}\to\infty} \frac{\log \# W_{\rm per}(\mathbf{m})}{\mathrm{vol}(\mathbf{m})} \tag{2.1}$$

is called the *periodic entropy* of $\Gamma^{\mathbb{Z}^d}$. Clearly $h_{\rm per}(\Gamma) \le h(\Gamma)$.

3 Main Inequalities for Symmetric NNSOFT

For $d \ge 2$, consider $\mathbf{m} = (m_1, \ldots, m_d) \in \mathbb{N}^d$ and $\mathbf{m}^- := (m_2, \ldots, m_d)$. Let $W_{{\rm per},\{1\}}(\mathbf{m})$ be the set of Γ-configurations in the box $\langle \mathbf{m} \rangle$ that correspond to Γ-covers of $T(m_1) \times \langle \mathbf{m}^- \rangle$, i.e., that can be extended periodically in the direction of $\mathbf{e}_1$ with period m_1 into Γ-covers of $\mathbb{Z} \times \langle \mathbf{m}^- \rangle$. We can view these configurations as $\widehat{\Gamma}$-configurations in the box $\langle \mathbf{m}^- \rangle$, where $\widehat{\Gamma} = (\widehat{\Gamma}_2, \ldots, \widehat{\Gamma}_d)$, for each j the vertex set of $\widehat{\Gamma}_j$ is the set $\Gamma_{1,{\rm per}}^{m_1}$ of closed walks $a = (a_1, \ldots, a_{m_1}, a_1)$ of length m_1 on Γ_1, and where $(a, b) \in \widehat{\Gamma}_j$ if and only if $(a_i, b_i) \in \Gamma_j$ for $i = 1, \ldots, m_1$. For this reason, the following limit exists and is equal to the entropy $h(\widehat{\Gamma}_2, \ldots, \widehat{\Gamma}_d)$ of the NNSOFT $\widehat{\Gamma}^{\mathbb{Z}^{d-1}}$:

$$\overline{h}(m_1, \Gamma) := \lim_{\mathbf{m}^-\to\infty} \frac{\log \# W_{{\rm per},\{1\}}(\mathbf{m})}{\mathrm{vol}(\mathbf{m}^-)}, \quad m_1 \in \mathbb{N}. \tag{3.1}$$

We define $W^-(\mathbf{m}^-)$ as the set of $(\Gamma_2, \ldots, \Gamma_d)$-covers of the box $\langle \mathbf{m}^- \rangle$. In the degenerate case $m_1 = 0$, we define $W_{{\rm per},\{1\}}(0, \mathbf{m}^-)$ to be simply $W^-(\mathbf{m}^-)$ and $(\widehat{\Gamma}_2, \ldots, \widehat{\Gamma}_d)$ to be simply $(\Gamma_2, \ldots, \Gamma_d)$. Then (3.1) is also valid for $m_1 = 0$, where we understand $\overline{h}(0, \Gamma)$ to be $h(\Gamma_2, \ldots, \Gamma_d)$.

Theorem 3.1 *Consider the NNSOFT* $\Gamma^{\mathbb{Z}^d}$ *for* $d \ge 2$. *Let* $h(\Gamma)$ *and* $\overline{h}(r, \Gamma)$ *be defined by (1.1) and (3.1), respectively. Assume that* Γ_1 *is symmetric. Then for all* $p, r \in \mathbb{N}$ *and* $q \in \mathbb{N} \cup \{0\}$,

$$\frac{\overline{h}(2r, \Gamma)}{2r} \ge h(\Gamma) \ge \frac{\overline{h}(p + 2q, \Gamma) - \overline{h}(2q, \Gamma)}{p}. \tag{3.2}$$

Proof. Fix $\mathbf{m}^- = (m_2, \ldots, m_d) \in \mathbb{N}^{d-1}$ and let $\Omega_1(\mathbf{m}^-)$ be the following transfer digraph on the vertex set $W^-(\mathbf{m}^-)$, analogous to the transfer digraph $\Omega_d(\mathbf{m}')$ described in Section 1. Vertices u, v satisfy $(u, v) \in \Omega_1(\mathbf{m}^-)$ if and only if $[u, v] \in W(2, \mathbf{m}^-)$, where $[u, v]$ is the configuration consisting of u, v occupying the levels $x_1 = 1, 2$ of $\langle(2, \mathbf{m}^-)\rangle$, respectively. Let $N = \#W^-(\mathbf{m}^-)$ and let $C(\mathbf{m}^-)$ be the $N \times N$ 0-1 incidence matrix of $\Omega_1(\mathbf{m}^-)$, with spectral radius $\rho(C(\mathbf{m}^-)$. As a nonnegative matrix, $C(\mathbf{m}^-)$ satisfies (see e.g., [15])

$$\log \rho(C(\mathbf{m}^-)) = \lim_{k\to\infty} \frac{\log \mathbf{1}^\top C(\mathbf{m}^-)^k \mathbf{1}}{k},$$

where $\mathbf{1} = (1, \dots, 1)^\top$. Since $\mathbf{1}^\top C(\mathbf{m}^-)^k \mathbf{1}$ is the number of walks of length k on $\Omega_1(\mathbf{m}^-)$, which correspond to Γ-covers of $\langle(k, \mathbf{m}^-)\rangle$, we obtain

$$\frac{\log \rho(C(\mathbf{m}^-))}{\mathrm{vol}(\mathbf{m}^-)} = \lim_{k\to\infty} \frac{\log \#W(k, \mathbf{m}^-)}{k\ \mathrm{vol}(\mathbf{m}^-)}. \tag{3.3}$$

Now send $m_2, \dots, m_d$ to ∞, and observe that by (1.1) and (1.2), the right-hand side of (3.3) converges to $h(\Gamma)$ and is an upper bound for it for each $\mathbf{m}^-$. Thus we obtain [14]

$$\frac{\log \rho(C(\mathbf{m}^-))}{\mathrm{vol}(\mathbf{m}^-)} \geq h(\Gamma), \qquad \mathbf{m}^- \in \mathbb{N}^{d-1}, \tag{3.4}$$

and

$$\lim_{\mathbf{m}^-\to\infty} \frac{\log \rho(C(\mathbf{m}^-))}{\mathrm{vol}(\mathbf{m}^-)} = h(\Gamma). \tag{3.5}$$

Next, we observe that

$$\mathrm{tr}\, C(\mathbf{m}^-)^q = \#W_{\mathrm{per},\{1\}}(q, \mathbf{m}^-), \qquad q \in \mathbb{N} \cup \{0\}, \tag{3.6}$$

where $C(\mathbf{m}^-)^0$ is the $N \times N$ identity matrix. Recall that the trace of $C(\mathbf{m}^-)^q$ is given by

$$\mathrm{tr}\, C(\mathbf{m}^-)^q = \sum_{i=1}^{N} \lambda_i^q, \qquad q \in \mathbb{N} \cup \{0\},$$

where $\lambda_1, \dots, \lambda_N$ be the eigenvalues of $C(\mathbf{m}^-)$. By definition of the spectral radius, $\rho(C(\mathbf{m}^-)) = \max_{i\in\langle N\rangle} |\lambda_i|$. Our assumption that Γ_1 is symmetric means that $\Omega_1(\mathbf{m}^-)$ and hence $C(\mathbf{m}^-)$ are symmetric. Therefore $\lambda_1, \dots, \lambda_N$ are real, and hence $\mathrm{tr}\, C(\mathbf{m}^-)^{2r} \geq \rho(C(\mathbf{m}^-))^{2r}$ for each $r \in \mathbb{N}$. Taking logarithms and using (3.6), we obtain

$$\frac{\log \#W_{\mathrm{per},\{1\}}(2r, \mathbf{m}^-)}{2r\, \mathrm{vol}(\mathbf{m}^-)} \geq \frac{\log \rho(C(\mathbf{m}^-))}{\mathrm{vol}(\mathbf{m}^-)}, \qquad r \in \mathbb{N}. \tag{3.7}$$

Sending $m_2, \dots, m_d$ to ∞ in (3.7) and using (3.1) and (3.5), we deduce the upper bound for $h(\Gamma)$ in (3.2).

To prove the lower bound in (3.2), we note that

$$\begin{aligned}\mathrm{tr}\, C(\mathbf{m}^-)^{p+2q} = \sum_i \lambda_i^{p+2q} \leq \sum_i |\lambda_i|^{p+2q} = \sum_i |\lambda_i|^p \lambda_i^{2q} \\ \leq \sum_i \rho(C(\mathbf{m}^-))^p \lambda_i^{2q} = \rho(C(\mathbf{m}^-))^p\, \mathrm{tr}\, C(\mathbf{m}^-)^{2q},\end{aligned}$$

and thus by (3.6)

$$\rho(C(\mathbf{m}^-))^p \geq \frac{\mathrm{tr}\, C(\mathbf{m}^-)^{p+2q}}{\mathrm{tr}\, C(\mathbf{m}^-)^{2q}} = \frac{\#W_{\mathrm{per},\{1\}}(p + 2q, \mathbf{m}^-)}{\#W_{\mathrm{per},\{1\}}(2q, \mathbf{m}^-)}. \tag{3.8}$$

This yields that

$$\frac{\log \rho(C(\mathbf{m}^-))}{\mathrm{vol}(\mathbf{m}^-)} \geq \frac{\log \#W_{\mathrm{per},\{1\}}(p+2q,\mathbf{m}^-) - \log \#W_{\mathrm{per},\{1\}}(2q,\mathbf{m}^-)}{p\,\mathrm{vol}(\mathbf{m}^-)}. \tag{3.9}$$

Sending $\mathbf{m}^-$ to ∞ and using (3.5) and (3.1) (recalling that the latter holds for $m_1 \in \mathbb{N} \cup \{0\}$), we deduce the lower bound in (3.2). □

When $d = 2$, $\overline{h}(m_1, \Gamma)$ is the entropy of the NNSOFT $\widehat{\Gamma}_2^{\mathbb{Z}}$ (recall that $\widehat{\Gamma}_2$ is simply Γ_2 when $m_1 = 0$). Since this is a 1-dimensional NNSOFT, that entropy is equal to $\log \rho(\widehat{\Gamma}_2)$. We denote $\rho(\widehat{\Gamma}_2)$ by $\theta_2(m_1)$, and obtain the following corollary to Theorem 3.1.

Corollary 3.2 *Let $d = 2$ and assume that Γ_1 is symmetric. Then for all $p, r \in \mathbb{N}$ and $q \in \mathbb{N} \cup \{0\}$,*

$$\frac{\log \theta_2(2r)}{2r} \geq h(\Gamma) \geq \frac{\log \theta_2(p+2q) - \log \theta_2(2q)}{p}, \tag{3.10}$$

where θ_2 is defined above.

In (3.10), we take $q = 0$ and $p = 2r$, and send r to ∞. Clearly the upper and lower bounds then converge to $h(\Gamma)$. Hence $h(\Gamma)$ is computable [14]. For completeness of the exposition we reproduce a short proof of (1.3) for any $d \geq 2$ given in [15]. We use the following straightforward lemma.

Lemma 3.3 *Let $\Gamma = (\Gamma_1, \ldots, \Gamma_d)$ and $\mathbf{m} \in \mathbb{N}^d$, put $\Gamma' = (\Gamma_1, \ldots, \Gamma_{d-1})$ and $\mathbf{m}' = (m_1, \ldots, m_{d-1})$, and let $\Theta_d(\mathbf{m}')$ be the transfer digraph between Γ'-covers of $T(\mathbf{m}')$ with respect to Γ_d. Let $\widehat{\Gamma}_2, \ldots, \widehat{\Gamma}_d$ be defined as in the beginning of this section, put $\widehat{\Gamma}' = (\widehat{\Gamma}_2, \ldots, \widehat{\Gamma}_{d-1})$ and $\widetilde{\mathbf{m}} = (m_2, \ldots, m_{d-1})$, and let $\widehat{\Theta}_d(\widetilde{\mathbf{m}})$ be the transfer digraph between $\widehat{\Gamma}'$-covers of $T(\widetilde{\mathbf{m}})$ with respect to $\widehat{\Gamma}_d$. Then $\Theta_d(\mathbf{m}')$ and $\widehat{\Theta}_d(\widetilde{\mathbf{m}})$ are isomorphic, and in particular $\rho(\Theta_d(\mathbf{m}')) = \rho(\widehat{\Theta}_d(\widetilde{\mathbf{m}}))$.*

Proof. We use the following bijection between the vertices u of $\Theta_d(\mathbf{m}')$ and the vertices $\widehat{u}$ of $\widehat{\Theta}_d(\widetilde{\mathbf{m}})$. Given $u = (\phi_{\mathbf{i}})_{\mathbf{i} \in \langle \mathbf{m}' \rangle}$, we have

$$(\phi_{\mathbf{i}}, \phi_{\mathbf{i}+\mathbf{e}_k}) \in \Gamma_k, \quad k = 1, \ldots, d-1, \tag{3.11}$$

where the addition $\mathbf{i} + \mathbf{e}_k$ is understood modulo m_k, i.e., $m_k + 1$ is 1. Then the corresponding $\widehat{u}$ is defined to be $\widehat{u} = (\widehat{\phi}_{\mathbf{j}})_{\mathbf{j} \in \langle \widetilde{\mathbf{m}} \rangle}$, where $\widehat{\phi}_{\mathbf{j}} = (\phi_{(q,\mathbf{j})})_{q=1}^{m_1}$. We note that $\widehat{\phi}_{\mathbf{j}}$ is indeed a Γ_1-cover of $T(m_1)$ and thus a vertex of $\widehat{\Gamma}_2, \ldots, \widehat{\Gamma}_{d-1}$ by (3.11) with $\mathbf{i} = (q, \mathbf{j})$ and $k = 1$. In order to show that $\widehat{u}$ is a $\widehat{\Gamma}'$-cover of $T(\widetilde{\mathbf{m}})$ and thus a vertex of $\widehat{\Theta}_d(\widetilde{\mathbf{m}})$, we need to show that $(\widehat{\phi}_{\mathbf{j}}, \widehat{\phi}_{\mathbf{j}+\mathbf{e}'_k}) \in \widehat{\Gamma}_k$ for $k = 2, \ldots, d-1$. This means showing that $(\phi_{(q,\mathbf{j})}, \phi_{(q,\mathbf{j}+\mathbf{e}'_k)}) \in \Gamma_k$ for $k = 2, \ldots, d-1$ and $q = 1, \ldots, m_1$, which follows in turn from (3.11) with $\mathbf{i} = (q, \mathbf{j})$. It is easy to see that the correspondence $u \mapsto \widehat{u}$ can be inverted. It remains to show that $(u, v) \in \Theta_d(\mathbf{m}') \Leftrightarrow (\widehat{u}, \widehat{v}) \in \widehat{\Theta}_d(\widetilde{\mathbf{m}})$. We prove only the $\Rightarrow$ part. Let $u = (\phi_{\mathbf{i}})_{\mathbf{i} \in \langle \mathbf{m}' \rangle}$ and $v = (\psi_{\mathbf{i}})_{\mathbf{i} \in \langle \mathbf{m}' \rangle}$ be Γ'-covers of $T(\mathbf{m}')$. The assumption $(u, v) \in \Theta_d(\mathbf{m}')$ means that $(\phi_{\mathbf{i}}, \psi_{\mathbf{i}}) \in \Gamma_d$ for all $\mathbf{i} \in \langle \mathbf{m}' \rangle$. Applying this with $\mathbf{i} = (q, \mathbf{j})$, $q = 1, \ldots, m_1$ and $\mathbf{j} \in \langle \widetilde{\mathbf{m}} \rangle$ shows that $(\widehat{\phi}_{\mathbf{j}}, \widehat{\psi}_{\mathbf{j}}) \in \widehat{\Gamma}_d$ for all $\mathbf{j} \in \langle \widetilde{\mathbf{m}} \rangle$, which means in turn that $(\widehat{u}, \widehat{v}) \in \widehat{\Theta}_d(\widetilde{\mathbf{m}})$. □

Theorem 3.4 *Let $d \geq 2$ and consider the NNSOFT $\Gamma^{\mathbb{Z}^d}$, where $\Gamma = (\Gamma_1, \dots, \Gamma_d)$. For $\mathbf{m}' = (m_1, \dots, m_{d-1}) \in \mathbb{N}^{d-1}$ and $\Gamma' = (\Gamma_1, \dots, \Gamma_{d-1})$, let $\Theta_d(\mathbf{m}')$ be the transfer digraph between Γ'-covers of $T(\mathbf{m}')$ with respect to Γ_d. Assume that $\Gamma_1, \dots, \Gamma_{d-1}$ are symmetric and $m_1, \dots, m_{d-1}$ are even. Then*

$$h(\Gamma) \leq \frac{\log \rho(\Theta_d(\mathbf{m}'))}{\operatorname{vol}(\mathbf{m}')}.$$

Proof. The proof is by induction on d. For $d = 2$ the result is equivalent to the upper bound in (3.10). For the inductive step, observe that the upper bound of (3.2) with $r = m_1/2$ yields $h(\Gamma) \leq \overline{h}(m_1, \Gamma)/m_1$. Recall that $\overline{h}(m_1, \Gamma)$ is the entropy of the NNSOFT $\widehat{\Gamma}^{\mathbb{Z}^{d-1}}$, where $\widehat{\Gamma} = (\widehat{\Gamma}_2, \dots, \widehat{\Gamma}_d)$ is as in Lemma 3.3. Since $\Gamma_2, \dots, \Gamma_{d-1}$ are symmetric, so are $\widehat{\Gamma}_2, \dots, \widehat{\Gamma}_{d-1}$, and therefore the induction hypothesis applied to $\widehat{\Gamma}^{\mathbb{Z}^{d-1}}$ gives $\overline{h}(m_1, \Gamma) \leq \log \rho(\widehat{\Theta}_d(\widetilde{\mathbf{m}}))/\operatorname{vol}(\widetilde{\mathbf{m}})$, where $\widetilde{\mathbf{m}}$ and $\widehat{\Theta}_d$ are also as in the lemma. Applying this lemma completes the proof. $\square$

Corollary 3.5 *Let $\Gamma = (\Gamma_1, \Gamma_2, \Gamma_3)$ and assume that Γ_1 and Γ_2 are symmetric. For $(m_1, m_2) \in \mathbb{N}^2$, let $\Theta_3(m_1, m_2)$ be the transfer digraph between (Γ_1, Γ_2)-covers of $T(m_1, m_2)$ with respect to Γ_3, and let $\theta_3(m_1, m_2)$ be its spectral radius. Let $\theta_3(0, m_2)$ be the spectral radius of the transfer digraph between Γ_2-covers of $T(m_2)$ with respect to Γ_3. Let $\theta_3(m_1, 0)$ be the spectral radius of the transfer digraph between Γ_1-covers of $T(m_1)$ with respect to Γ_3. Then for all $r, t, p, u, v \in \mathbb{N}$ and $q, s \in \mathbb{N} \cup \{0\}$ we have*

$$\begin{aligned} \frac{\log \theta_3(2r, 2t)}{4rt} &\geq h(\Gamma) \\ &\geq \frac{\log \theta_3(p + 2q, u + 2s) - \log \theta_3(p + 2q, 2s)}{up} - \frac{\log \theta_3(2q, 2v)}{2vp}. \end{aligned} \tag{3.12}$$

Proof. The upper bound in (3.12) follows directly from Theorem 3.4 for $d = 3$. To show the lower bound we use the lower bound in (3.2), which is valid since Γ_1 is symmetric. This gives

$$h(\Gamma_1, \Gamma_2, \Gamma_3) \geq \frac{\overline{h}(p + 2q, (\Gamma_1, \Gamma_2, \Gamma_3)) - \overline{h}(2q, (\Gamma_1, \Gamma_2, \Gamma_3))}{p}. \tag{3.13}$$

For each $a \in \mathbb{N}$ we have $\overline{h}(a, (\Gamma_1, \Gamma_2, \Gamma_3)) = h(\widehat{\Gamma}_2, \widehat{\Gamma}_3)$, where $\widehat{\Gamma}_2, \widehat{\Gamma}_3$ are digraphs on the vertex set $\Gamma^a_{1,\mathrm{per}}$ as in the beginning of this section. Since Γ_2 is symmetric, so is $\widehat{\Gamma}_2$, and we can apply the lower bound of Corollary 3.2 to $(\widehat{\Gamma}_2, \widehat{\Gamma}_3)$ to obtain

$$h(\widehat{\Gamma}_2, \widehat{\Gamma}_3) \geq \frac{\log \theta_3(a, u + 2s) - \log \theta_3(a, 2s)}{u}, \tag{3.14}$$

where $\theta_3(a, b) = \rho(\widehat{\Theta}_3(b)) = \rho(\Theta_3(a, b))$ by Lemma 3.3. Inequality (3.14) is also valid for $s = 0$, since we defined $\theta_3(a, 0)$ to be the spectral radius of $\widehat{\Gamma}_3$, exactly as in Corollary 3.2 for the degenerate case. Using (3.14) for $a = p + 2q$ gives

$$\overline{h}(p + 2q, (\Gamma_1, \Gamma_2, \Gamma_3)) \geq \frac{\log \theta_3(p + 2q, u + 2s) - \log \theta_3(p + 2q, 2s)}{u}. \tag{3.15}$$

Applying the upper bound of Corollary 3.2 to $(\widehat{\Gamma}_2, \widehat{\Gamma}_3)$, we obtain

$$h(\widehat{\Gamma}_2, \widehat{\Gamma}_3) \leq \frac{\log \theta_3(a, 2v)}{2v}. \tag{3.16}$$

Inequality (3.16) is also valid for $a = 0$, since in that case $(\widehat{\Gamma}_2, \widehat{\Gamma}_3) = (\Gamma_2, \Gamma_3)$; this follows from applying Theorem 3.4 to (Γ_2, Γ_3) and the definition of $\theta_3(0, 2v)$. Using (3.16) for $a = 2q$ gives

$$\overline{h}(2q, (\Gamma_1, \Gamma_2, \Gamma_3)) \leq \frac{\log \theta_3(2q, 2v)}{2v}. \tag{3.17}$$

Finally, substitution of (3.15) and (3.17) in (3.13) yields the lower bound of (3.12). □

4 Dimer and Monomer-Dimer Covers of $\mathbb{Z}^d$

As in [15], the set of monomer-dimer covers, respectively dimer covers, of $\mathbb{Z}^d$ is an NNSOFT $\Gamma^{\mathbb{Z}^d}$, respectively $\widetilde{\Gamma}^{\mathbb{Z}^d}$, where Γ and $\widetilde{\Gamma}$ are defined as follows. We encode a monomer-dimer cover of $\mathbb{Z}^d$ as a coloring of $\mathbb{Z}^d$ with the $2d+1$ colors $1, \ldots, 2d+1$: a dimer in the direction of $\mathbf{e}_k$ occupying the adjacent points $\mathbf{i}, \mathbf{i}+\mathbf{e}_k$ is encoded by the color k at $\mathbf{i}$ and the color $k+d$ at $\mathbf{i}+\mathbf{e}_k$; a monomer at $\mathbf{i}$ is encoded by the color $2d+1$ at $\mathbf{i}$. This imposes restrictions on the coloring, which are expressed by the d-digraph $\Gamma = (\Gamma_1, \ldots, \Gamma_k)$ on the set of vertices $\langle 2d+1 \rangle$, where

- $(k, q) \in \Gamma_k \Leftrightarrow q = k + d$;
- for $j \neq k$, $(j, q) \in \Gamma_k \Leftrightarrow q \neq k + d$.

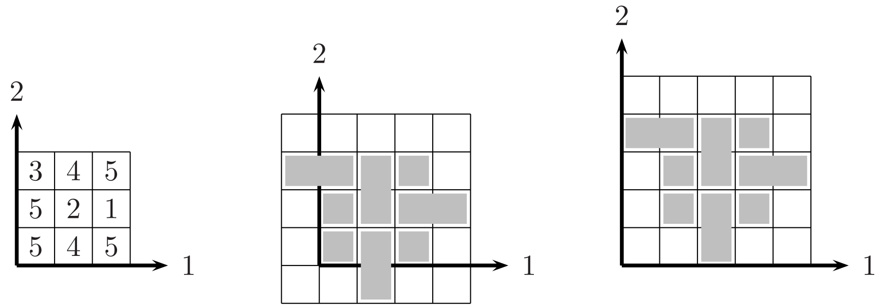
It is easy to check that this gives a bijection between the monomer-dimer covers of $\mathbb{Z}^d$ and $\Gamma^{\mathbb{Z}^d}$. Similarly, if $\widetilde{\Gamma} = (\widetilde{\Gamma}_1, \ldots, \widetilde{\Gamma}_d)$ is obtained from Γ by removing the vertex $2d+1$, then there is a bijection between the dimer covers of $\mathbb{Z}^d$ and $\widetilde{\Gamma}^{\mathbb{Z}^d}$.

The disadvantage of these encodings is that Γ_k and $\widetilde{\Gamma}_k$ are not symmetric, so we cannot apply the results of Section 3 directly. However, as pointed out in [7] for the dimer problem, there is a hidden symmetry, which enables us to obtain results analogous to those of Section 3.

Recall that $W(\mathbf{m})$ denotes the set of Γ-colorings of $\langle \mathbf{m} \rangle \subseteq \mathbb{N}^d$. Consider a Γ-coloring $\phi \in W(\mathbf{m})$ with the Γ defined above. Certain points $\mathbf{i}$ on the boundary of $\langle \mathbf{m} \rangle$ can receive colors indicating that $\mathbf{i}$ is one half of a dimer whose other half is outside $\langle \mathbf{m} \rangle$. Therefore ϕ corresponds to a monomer-dimer cover of a "box with protrusions" T satisfying $\langle \mathbf{m} \rangle \subseteq T \subseteq \langle \mathbf{m} + 2\mathbf{1} \rangle - \mathbf{1}$, where $\mathbf{1} := (1, \ldots, 1) \in \mathbb{N}^d$, such that each monomer in the cover is contained in $\langle \mathbf{m} \rangle$ and each dimer in the cover has a nonempty intersection with $\langle \mathbf{m} \rangle$. We translate T by $\mathbf{1}$ to move it into $\mathbb{N}^d$, and thus ϕ corresponds to a monomer-dimer cover of a set S satisfying $\langle \mathbf{m} \rangle + \mathbf{1} \subseteq S \subseteq \langle \mathbf{m} + 2\mathbf{1} \rangle$ such that each monomer in the cover is contained in $\langle \mathbf{m} \rangle + \mathbf{1}$ and each dimer in the cover has a nonempty intersection with $\langle \mathbf{m} \rangle + \mathbf{1}$. Conversely, each monomer-dimer cover of such a set S satisfying these conditions corresponds to a Γ-coloring of $\langle \mathbf{m} \rangle$. This is illustrated in Figure 1.

Similarly, $\widetilde{W}(\mathbf{m})$ denotes the set of $\widetilde{\Gamma}$-colorings of $\langle \mathbf{m} \rangle$, and there is a bijection between $\widetilde{W}(\mathbf{m})$ and the set of dimer covers of a set S satisfying $\langle \mathbf{m} \rangle + \mathbf{1} \subseteq S \subseteq \langle \mathbf{m} + 2\mathbf{1} \rangle$ such that each dimer in the cover has a nonempty intersection with $\langle \mathbf{m} \rangle + \mathbf{1}$.

Let $W_{\mathrm{per}}(\mathbf{m})$, respectively $\widetilde{W}_{\mathrm{per}}(\mathbf{m})$, denote the set of Γ-colorings, respectively $\widetilde{\Gamma}$-colorings, of $\langle \mathbf{m} \rangle$ that can be extended periodically to Γ-colorings, respectively $\widetilde{\Gamma}$-colorings, of $\mathbb{Z}^d$ with period $\mathbf{m}$. It corresponds to the set of monomer-dimer covers,



(a) (b) (c)

Figure 1: (a) Γ-coloring of $\langle \mathbf{m} \rangle = \langle (3,3) \rangle$; (b) The corresponding monomer-dimer cover of T; (c) The corresponding monomer-dimer cover of S.

respectively dimer covers, of $T(\mathbf{m})$ and satisfies $W_{\mathrm{per}}(\mathbf{m}) \subseteq W(\mathbf{m})$, $\widetilde{W}_{\mathrm{per}}(\mathbf{m}) \subseteq \widetilde{W}(\mathbf{m})$.

Finally, let $W_0(\mathbf{m})$, respectively $\widetilde{W}_0(\mathbf{m})$, be the set of Γ-colorings of $\langle \mathbf{m} \rangle$ for which S defined above is equal to $\langle \mathbf{m} \rangle + \mathbf{1}$, i.e., each dimer in the corresponding cover of S is contained in $\langle \mathbf{m} \rangle$. To emphasize the fact that the dimers do not protrude out of $\langle \mathbf{m} \rangle$, we refer to these covers as *tilings*. We have $W_0(\mathbf{m}) \subseteq W_{\mathrm{per}}(\mathbf{m})$, $\widetilde{W}_0(\mathbf{m}) \subseteq \widetilde{W}_{\mathrm{per}}(\mathbf{m})$. We can see that $\#W(\mathbf{m}) \leq \#W_0(\mathbf{m} + 2\mathbf{1})$, because we can extend the monomer-dimer cover of S into a member of $W_0(\langle \mathbf{m} + 2\mathbf{1} \rangle)$ by tiling $\langle \mathbf{m} + 2\mathbf{1} \rangle \setminus S$ with monomers.

From the discussion above, we have

$$\#W_0(\mathbf{m}) \leq \#W_{\mathrm{per}}(\mathbf{m}) \leq \#W(\mathbf{m}) \leq \#W_0(\mathbf{m} + 2\mathbf{1}), \tag{4.1}$$

$$\#\widetilde{W}_0(\mathbf{m}) \leq \#\widetilde{W}_{\mathrm{per}}(\mathbf{m}) \leq \#\widetilde{W}(\mathbf{m}), \tag{4.2}$$

$$\#\widetilde{W}_0(\mathbf{m}) \leq \#W_0(\mathbf{m}), \tag{4.3}$$

$$\#\widetilde{W}_{\mathrm{per}}(\mathbf{m}) \leq \#W_{\mathrm{per}}(\mathbf{m}), \tag{4.4}$$

$$\#\widetilde{W}(\mathbf{m}) \leq \#W(\mathbf{m}). \tag{4.5}$$

Recall that the d-dimensional monomer-dimer entropy h_d is defined by

$$h_d := \lim_{\mathbf{m} \to \infty} \frac{\log \#W(\mathbf{m})}{\mathrm{vol}(\mathbf{m})}.$$

From (4.1), we obtain

$$\begin{aligned} \liminf_{\mathbf{m} \to \infty} \frac{\log \#W_0(\mathbf{m})}{\mathrm{vol}(\mathbf{m})} &= \liminf_{\mathbf{m} \to \infty} \frac{\log \#W_0(\mathbf{m} + 2\mathbf{1})}{\mathrm{vol}(\mathbf{m} + 2\mathbf{1})} \\ &= \liminf_{\mathbf{m} \to \infty} \frac{\log \#W_0(\mathbf{m} + 2\mathbf{1})}{\mathrm{vol}(\mathbf{m})} \geq h_d \geq \limsup_{\mathbf{m} \to \infty} \frac{\log \#W_0(\mathbf{m})}{\mathrm{vol}(\mathbf{m})}. \end{aligned}$$

This and one more application of (4.1) give

$$h_d := \lim_{\mathbf{m} \to \infty} \frac{\log \#W(\mathbf{m})}{\mathrm{vol}(\mathbf{m})} = \lim_{\mathbf{m} \to \infty} \frac{\log \#W_{\mathrm{per}}(\mathbf{m})}{\mathrm{vol}(\mathbf{m})} = \lim_{\mathbf{m} \to \infty} \frac{\log \#W_0(\mathbf{m})}{\mathrm{vol}(\mathbf{m})}. \tag{4.6}$$

Similarly, the d-dimensional dimer entropy $\widetilde{h}_d$ is defined by

$$\widetilde{h}_d := \lim_{\mathbf{m}\to\infty} \frac{\log \#\widetilde{W}(\mathbf{m})}{\mathrm{vol}(\mathbf{m})}.$$

This expression is known to satisfy

$$\widetilde{h}_d = \lim_{\mathbf{m}\to\infty, \frac{\mathrm{vol}(\mathbf{m})}{2}\in\mathbb{N}} \frac{\log \#\widetilde{W}_{\mathrm{per}}(\mathbf{m})}{\mathrm{vol}(\mathbf{m})} = \lim_{\mathbf{m}\to\infty, \frac{\mathrm{vol}(\mathbf{m})}{2}\in\mathbb{N}} \frac{\log \#\widetilde{W}_0(\mathbf{m})}{\mathrm{vol}(\mathbf{m})}. \tag{4.7}$$

The proof of (4.7) is more involved, and follows from the results proved in [18], as we show now. For $\mathbf{m} \in \mathbb{N}^d$ and $s \in \left[0, \frac{\mathrm{vol}(\mathbf{m})}{2}\right] \cap \mathbb{Z}$, let $W_0(\mathbf{m}, s)$ be the subset of $W_0(\mathbf{m})$ consisting of the monomer-dimer tilings of $\langle \mathbf{m} \rangle$ that have exactly s dimers. As pointed out in [18], $W_0(\mathbf{m}, s) \neq \emptyset$ by induction on d. It is shown in [18] that there exists a function $\lambda_d(\cdot) : [0,1] \to \mathbb{R}_+$ such that for all sequences $(\mathbf{m}_q)_{q\in\mathbb{N}}$ and $(s_q)_{q\in\mathbb{N}}$ satisfying

$$s_q \in \left[0, \frac{\mathrm{vol}(\mathbf{m}_q)}{2}\right] \cap \mathbb{Z}, \quad \lim_{q\to\infty} \mathbf{m}_q = \infty, \quad \lim_{q\to\infty} \frac{2s_q}{\mathrm{vol}(\mathbf{m}_q)} = p \in [0,1], \tag{4.8}$$

the following equality holds

$$\lim_{q\to\infty} \frac{\log \#W_0(\mathbf{m}_q, s_q)}{\mathrm{vol}(\mathbf{m}_q)} = \lambda_d(p). \tag{4.9}$$

Furthermore, the function $\lambda_d(p)$ is a continuous concave function of p on $[0,1]$. We call $\lambda_d(p)$ the *monomer-dimer entropy with dimer density* p.

Theorem 4.1 *Let $\widetilde{W}(\mathbf{m})$, $\widetilde{W}_{\mathrm{per}}(\mathbf{m})$, $\widetilde{W}_0(\mathbf{m})$ be defined as above. Then (4.7) and the following equalities hold*

$$\lambda_d(0) = 0, \tag{4.10}$$

$$\lambda_d(1) = \widetilde{h}_d, \tag{4.11}$$

$$\max_{p\in[0,1]} \lambda_d(p) = h_d. \tag{4.12}$$

Proof. The proof of (4.10) is easy: pick any sequence $\mathbf{m}_q$ satisfying $\lim_{q\to\infty} \mathbf{m}_q = \infty$, and take $s_q = 0$ for all q. Then conditions (4.8) hold for $p = 0$, and consequently (4.9) holds. But $\#W_0(\mathbf{m}_q, 0) = 1$, since there is only one way to cover a box with monomers, and (4.10) follows.

We prove (4.7) and (4.11) together. Pick a sequence $(\mathbf{m}_q)_{q\in\mathbb{N}} \subseteq \mathbb{N}^d$ such that the $\mathrm{vol}(\mathbf{m}_q)$ are even and $\lim_{q\to\infty} \mathbf{m}_q = \infty$, and take $s_q = \frac{\mathrm{vol}(\mathbf{m}_q)}{2}$. Then the conditions given in (4.8) hold for $p = 1$, and consequently (4.9) holds. But $W_0(\mathbf{m}_q, s_q) = \widetilde{W}_0(\mathbf{m}_q)$, and therefore

$$\lim_{\mathbf{m}\to\infty, \frac{\mathrm{vol}(\mathbf{m})}{2}\in\mathbb{N}} \frac{\log \#\widetilde{W}_0(\mathbf{m})}{\mathrm{vol}(\mathbf{m})} = \lambda_d(1). \tag{4.13}$$

In view of (4.2) and (4.13), we obtain

$$\lim_{\mathbf{m}\to\infty} \frac{\log \#\widetilde{W}(\mathbf{m})}{\mathrm{vol}(\mathbf{m})} \ge \limsup_{\mathbf{m}\to\infty, \frac{\mathrm{vol}(\mathbf{m})}{2}\in\mathbb{N}} \frac{\log \#\widetilde{W}_{\mathrm{per}}(\mathbf{m})}{\mathrm{vol}(\mathbf{m})}$$
$$\ge \liminf_{\mathbf{m}\to\infty, \frac{\mathrm{vol}(\mathbf{m})}{2}\in\mathbb{N}} \frac{\log \#\widetilde{W}_{\mathrm{per}}(\mathbf{m})}{\mathrm{vol}(\mathbf{m})} \ge \liminf_{\mathbf{m}\to\infty, \frac{\mathrm{vol}(\mathbf{m})}{2}\in\mathbb{N}} \frac{\log \#\widetilde{W}_0(\mathbf{m})}{\mathrm{vol}(\mathbf{m})} = \lambda_d(1). \quad (4.14)$$

For $\mathbf{m} \ge (2,\dots,2) \in \mathbb{N}^d$, let $a(\mathbf{m}) := 2\,\mathrm{vol}(\mathbf{m}) \sum_{i=1}^d \frac{1}{m_i}$ be the surface area of $\langle \mathbf{m} \rangle$ and let

$$w(\mathbf{m}) := \sum_{s\in[\frac{\mathrm{vol}(\mathbf{m})-a(\mathbf{m})}{2}, \frac{\mathrm{vol}(\mathbf{m})}{2}]\cap\mathbb{Z}} \#W_0(\mathbf{m}, s),$$
$$\widetilde{\omega}(\mathbf{m}) := \max_{s\in[\frac{\mathrm{vol}(\mathbf{m})-a(\mathbf{m})}{2}, \frac{\mathrm{vol}(\mathbf{m})}{2}]\cap\mathbb{Z}} \#W_0(\mathbf{m}, s),$$
$$\widetilde{s}(\mathbf{m}) := \arg\max_{s\in[\frac{\mathrm{vol}(\mathbf{m})-a(\mathbf{m})}{2}, \frac{\mathrm{vol}(\mathbf{m})}{2}]\cap\mathbb{Z}} \#W_0(\mathbf{m}, s).$$

In words, $w(\mathbf{m})$ is the sum of $\#W_0(\mathbf{m}, s)$ where s ranges over those numbers of dimers that are sufficient to cover the interior of $\langle \mathbf{m} \rangle$, i.e., the elements of $\langle \mathbf{m} \rangle$ not on its boundary; $\widetilde{\omega}(\mathbf{m})$ is the largest summand in that sum; and $\widetilde{s}(\mathbf{m})$ is a number of dimers achieving the maximum.

Clearly $\widetilde{\omega}(\mathbf{m}) \le w(\mathbf{m}) \le \frac{a(\mathbf{m})+2}{2}\widetilde{\omega}(\mathbf{m})$, and therefore

$$\limsup_{\mathbf{m}\to\infty} \frac{\log \widetilde{\omega}(\mathbf{m})}{\mathrm{vol}(\mathbf{m})} = \limsup_{\mathbf{m}\to\infty} \frac{\log w(\mathbf{m})}{\mathrm{vol}(\mathbf{m})}. \quad (4.15)$$

By Proposition 2.2, there exists a sequence $(\mathbf{n}_q)_{q\in\mathbb{N}} \subseteq \mathbb{N}^d$ satisfying

$$\lim_{q\to\infty} \mathbf{n}_q = \infty, \quad \lim_{q\to\infty} \frac{\log \widetilde{\omega}(\mathbf{n}_q)}{\mathrm{vol}(\mathbf{n}_q)} = \limsup_{\mathbf{m}\to\infty} \frac{\log \widetilde{\omega}(\mathbf{m})}{\mathrm{vol}(\mathbf{m})}. \quad (4.16)$$

Let $t_q := \widetilde{s}(\mathbf{n}_q)$ for each $q \in \mathbb{N}$, and so $\#W_0(\mathbf{n}_q, t_q) = \widetilde{\omega}(\mathbf{n}_q)$. Clearly $\lim_{q\to\infty} \frac{2t_q}{\mathrm{vol}(\mathbf{n}_q)} = 1$, and so conditions (4.8) hold for $\mathbf{n}_q, t_q$ with $p = 1$, and consequently (4.9) holds for them. Hence by (4.16)

$$\limsup_{\mathbf{m}\to\infty} \frac{\log \widetilde{\omega}(\mathbf{m})}{\mathrm{vol}(\mathbf{m})} = \lambda_d(1). \quad (4.17)$$

Next we assert that $\#\widetilde{W}(\mathbf{m}) \le w(\mathbf{m} + 2\mathbf{1})$. Indeed, each cover in $\widetilde{W}(\mathbf{m})$ can be shifted by $\mathbf{1}$ and extended by monomers to a tiling in $W_0(\mathbf{m} + 2\mathbf{1}, s)$ for one of the s appearing in the sum $w(\mathbf{m} + 2\mathbf{1})$. Therefore by (4.15) and (4.17)

$$\lim_{\mathbf{m}\to\infty} \frac{\log \#\widetilde{W}(\mathbf{m})}{\mathrm{vol}(\mathbf{m})} \le \limsup_{\mathbf{m}\to\infty} \frac{\log w(\mathbf{m} + 2\mathbf{1})}{\mathrm{vol}(\mathbf{m})}$$
$$= \limsup_{\mathbf{m}\to\infty} \frac{\log w(\mathbf{m})}{\mathrm{vol}(\mathbf{m})} = \limsup_{\mathbf{m}\to\infty} \frac{\log \widetilde{\omega}(\mathbf{m})}{\mathrm{vol}(\mathbf{m})} = \lambda_d(1). \quad (4.18)$$

Inequalities (4.14) and (4.18) combined, along with (4.2), complete the proof of (4.7) and (4.11).

We now prove (4.12). As $W_0(\mathbf{m}, s) \subseteq W_0(\mathbf{m})$, it follows that $\lambda_d(p) \le h_d$ for all $p \in [0,1]$. To complete the proof, we exhibit a $p^* \in [0,1]$ satisfying the reverse inequality. For each $\mathbf{m} \in \mathbb{N}^d$, let

$$\omega(\mathbf{m}) := \max_{s \in [0, \frac{\mathrm{vol}(\mathbf{m})}{2}] \cap \mathbb{Z}} \#W_0(\mathbf{m}, s),$$
$$s(\mathbf{m}) := \arg\max_{s \in [0, \frac{\mathrm{vol}(\mathbf{m})}{2}] \cap \mathbb{Z}} \#W_0(\mathbf{m}, s),$$
$$p(\mathbf{m}) := \frac{2s(\mathbf{m})}{\mathrm{vol}(\mathbf{m})} \in [0,1],$$

so that $\omega(\mathbf{m}) = \#W_0(\mathbf{m}, s(\mathbf{m}))$.

Observe that $\#W_0(\mathbf{m}) = \sum_{s \in [0, \frac{\mathrm{vol}(\mathbf{m})}{2}] \cap \mathbb{Z}} \#W_0(\mathbf{m}, s) \le \frac{\mathrm{vol}(\mathbf{m})+2}{2} \omega(\mathbf{m})$, and therefore, by (4.6),

$$h_d \le \liminf_{\mathbf{m} \to \infty} \frac{\log \omega(\mathbf{m})}{\mathrm{vol}(\mathbf{m})}. \tag{4.19}$$

From the bounded sequence $(p(q\mathbf{1}))_{q \in \mathbb{N}}$ choose a convergent subsequence $(p(q_k\mathbf{1}))_{k \in \mathbb{N}}$ and set $p^* := \lim_{k \to \infty} p(q_k\mathbf{1}) \in [0,1]$. Then conditions (4.8) hold for the sequences $q_k\mathbf{1}$ and $s(q_k\mathbf{1})$ with p^*, and therefore (4.9) yields

$$\lim_{k \to \infty} \frac{\log \omega(q_k\mathbf{1})}{q_k^d} = \lambda_d(p^*). \tag{4.20}$$

By the definition of lim inf we have $\liminf_{\mathbf{m} \to \infty} \frac{\log \omega(\mathbf{m})}{\mathrm{vol}(\mathbf{m})} \le \lim_{k \to \infty} \frac{\log \omega(q_k\mathbf{1})}{q_k^d}$. Hence by (4.19) and (4.20), we obtain $h_d \le \lambda_d(p^*)$. □

Proposition 4.2 *Let $d \in \mathbb{N}$. Then for each $\mathbf{m} \in \mathbb{N}^d$*

$$\frac{\log \#W(\mathbf{m})}{\mathrm{vol}(\mathbf{m})} \ge h_d \ge \frac{\log \#W_0(\mathbf{m})}{\mathrm{vol}(\mathbf{m})}, \tag{4.21}$$
$$\frac{\log \#\widetilde{W}(\mathbf{m})}{\mathrm{vol}(\mathbf{m})} \ge \widetilde{h}_d \ge \frac{\log \#\widetilde{W}_0(\mathbf{m})}{\mathrm{vol}(\mathbf{m})}. \tag{4.22}$$

These upper and lower bounds converge to h_d and $\widetilde{h}_d$, respectively, hence the latter are computable.

Proof. The upper bounds follow from the general theory of NNSOFT (1.2), and their convergence from (1.1). For the lower bounds, let $k \in \mathbb{N}$ and consider the box $\langle k\mathbf{m} \rangle$. It can be decomposed into k^d shifted copies of $\langle \mathbf{m} \rangle$. Hence

$$\#W_0(k\mathbf{m}) \ge \#W_0(\mathbf{m})^{k^d}, \quad \#\widetilde{W}_0(k\mathbf{m}) \ge \#\widetilde{W}_0(\mathbf{m})^{k^d}.$$

Sending k to ∞ and using (4.6) and (4.7), we deduce the lower bounds as well as their convergence. □

We conclude this section by computing the various quantities in question for $d = 1$ and illustrating Theorem 4.1 for that case, where everything can be found explicitly. $\#W_0(m)$ is the number of monomer-dimer tilings of $\langle m \rangle$. Clearly it satisfies $\#W_0(1) = 1$, $\#W_0(2) = 2$ and $\#W_0(m) = \#W_0(m-1) + \#W_0(m-2)$ for $m \geq 3$. It follows that $\#W_0(m) = F_{m+1}$, where $F_m = \frac{1}{\sqrt{5}}\left(\frac{1+\sqrt{5}}{2}\right)^m - \frac{1}{\sqrt{5}}\left(\frac{1-\sqrt{5}}{2}\right)^m$ are the Fibonacci numbers. $\#W_{\rm per}(m)$ is the number of monomer-dimer tilings of $T(m)$, and it satisfies $\#W_{\rm per}(1) = 1$, $\#W_{\rm per}(2) = 3$ (one monomer tiling and two dimer tilings), and $\#W_{\rm per}(m) = \#W_0(m) + \#W_0(m-2)$ for $m \geq 3$ (the second term counting the tilings with a dimer occupying 1 and m). It follows that $\#W_{\rm per}(m) = F_{m+1} + F_{m-1} = L_m$, where $L_m = \left(\frac{1+\sqrt{5}}{2}\right)^m + \left(\frac{1-\sqrt{5}}{2}\right)^m$ are the Lucas numbers. $\#W(m)$ is the number of monomer-dimer covers of $\langle m\rangle$, where a dimer may protrude from 1 to 0 , or from m to $m+1$. It satisfies $\#W(1) = 3$, $\#W(2) = 5$ and $\#W(m) = \#W_0(m) + 2\#W_0(m-1) + \#W_0(m-2)$ for $m \geq 3$ (the three terms representing covers with zero, one, or two protruding dimers, respectively). It follows that $\#W(m) = L_m + 2F_m = \left(1 + \frac{2}{\sqrt{5}}\right)\left(\frac{1+\sqrt{5}}{2}\right)^m + \left(1 - \frac{2}{\sqrt{5}}\right)\left(\frac{1-\sqrt{5}}{2}\right)^m$. From these values we see that $\frac{\log \#W(m)}{m}$, $\frac{\log \#W_{\rm per}(m)}{m}$ and $\frac{\log \#W_0(m)}{m}$ converge to $h_1 = \log \frac{1+\sqrt{5}}{2}$, in accordance with (4.6).

To determine $\lambda_1(p)$, it is enough to consider rational $p \in [0,1]$ by continuity, and then only $n \in \mathbb{N}$ such that $s = \frac{pn}{2} \in \mathbb{N}$, and send such n to ∞, by(4.8)–(4.9). Then $\#W_0(s,n)$ is the number of linear arrangements of s dimers and $n-2s$ monomers, which is equal to $\binom{n-s}{s}$. An application of Stirling's approximation then gives [18]

$$\begin{aligned}\lambda_1(p) = \lim_{n\to\infty} \frac{1}{n} \log \binom{\left(1-\frac{p}{2}\right)n}{\frac{pn}{2}} \\ = \left(1-\frac{p}{2}\right)\log\left(1-\frac{p}{2}\right) - \frac{p}{2}\log\frac{p}{2} - (1-p)\log(1-p).\end{aligned}$$

We see that $\lambda_1(0) = 0$ and $\lambda_1(1) = 0 = \widetilde{h}_1$ in accordance with (4.10) and (4.11). It is straightforward to verify that

$$\max_{p\in[0,1]} \lambda_1(p) = \lambda_1\left(1 - \frac{1}{\sqrt{5}}\right) = \log\frac{1+\sqrt{5}}{2} = h_1,$$

in accordance with (4.12).

5 Lower Bounds for Monomer-Dimer Entropy with Dimer Density p

For an $m \times n$ matrix A, denote by $\operatorname{perm}_s A$ the sum of the permanents of all $s \times s$ submatrices of A. For a graph G, a *matching* is a set of vertex-disjoint edges, and $W(G,s)$ denotes the set of all matchings of size s in G, which can be regarded as covers of the vertex set $V(G)$ of G by s dimers (edges) and $|V(G)| - 2s$ monomers (isolated vertices). If G is a bipartite graph with color classes $\langle m\rangle$ and $\langle n\rangle$, its *incidence matrix* is the $m \times n$ 0-1 matrix $A = A(G)$ such that $a_{ij} = 1$ if and only if $\{i,j\}$ is an edge of G. In that case it is immediate that $\#W(G,s) = \operatorname{perm}_s A(G)$. A bipartite graph G is said to be *r-regular* if each vertex of G has degree r, or equivalently $A(G)$ has all row sums and column sums equal to r, so that $\frac{1}{r}A(G)$ is *doubly-stochastic* (a nonnegative matrix with all row sums and column sums equal to 1, necessarily a square matrix).

Theorem 5.1 *Let G be an r-regular bipartite graph with n vertices in each color class. Then*

$$\#W(G,s) \geq \binom{n}{s}^2 s! \left(\frac{r}{n}\right)^s. \tag{5.1}$$

Proof. A result of the first author [13] states that if B is a doubly-stochastic $n \times n$ matrix, then $\mathrm{perm}_s B \geq \mathrm{perm}_s J_n$, where J_n is the $n \times n$ matrix with all entries equal to $\frac{1}{n}$. Since $\frac{1}{r}A(G)$ is doubly-stochastic, $\mathrm{perm}_s \frac{1}{r}A(G) = \frac{1}{r^s}\mathrm{perm}_s A(G)$ and $\mathrm{perm}_s J_n = \binom{n}{s}^2 \frac{s!}{n^s}$, the result follows. □

The recent result of Schrijver [33] improves this lower bound for the case $s = n$ if r is constant and n tends to infinity: under the assumptions of Theorem 5.1

$$\#W(G,n) \geq \left(\frac{(r-1)^{r-1}}{r^{r-2}}\right)^n. \tag{5.2}$$

It would be of interest to similarly improve the lower bound of Theorem 5.1 in the interesting range n large and $s/n \geq r > 0$ (see below).

In a recent paper [34], Wanless gives an alternative lower bound to (5.1), namely $\#W(G,s) \geq \binom{n}{s}\left(\frac{(r-1)^{r-1}}{r^{r-2}}\right)^s$. It turns out that except for $\frac{s}{n}$ close to 1, the bound (5.1) is better.

Theorem 5.2 *Let $d \in \mathbb{N}$, $p \in [0,1]$ and recall the definition of $\lambda_d(p)$, the monomer-dimer entropy with dimer density p, given by (4.8)–(4.9). Then*

$$\lambda_d(p) \geq \tfrac{1}{2}(-p\log p - 2(1-p)\log(1-p) + p\log 2d - p). \tag{5.3}$$

Furthermore, the dimer entropy $\widetilde{h}_d$ and monomer-dimer entropy h_d satisfy

$$\widetilde{h}_d = \lambda_d(1) \geq \tfrac{1}{2}((2d-1)\log(2d-1) - (2d-2)\log 2d), \tag{5.4}$$

and

$$h_d \geq \tfrac{1}{2}(-p(d)\log p(d) - 2(1-p(d))\log(1-p(d)) + p(d)\log 2d - p(d)), \tag{5.5}$$

where

$$p(d) = \frac{4d+1-\sqrt{8d+1}}{4d}. \tag{5.6}$$

Proof. Let $\mathbf{m} = (m_1,\ldots,m_d) \in \mathbb{N}^d$ and assume that $m_1,\ldots,m_d$ are all even. Let G be the adjacency graph of $T(\mathbf{m})$. That is, the color classes of G are the sets $\{\mathbf{i} \in T(\mathbf{m}) : i_1+\cdots+i_d \text{ even}\}$ and $\{\mathbf{j} \in T(\mathbf{m}) : j_1+\cdots+j_d \text{ odd}\}$, and $\{\mathbf{i},\mathbf{j}\}$ is an edge of G if and only if $\mathbf{i}$ and $\mathbf{j}$ are neighbors on $T(\mathbf{m})$, i.e., $\mathbf{j} = \mathbf{i} \pm \mathbf{e}_k$ for some $k \in \langle d \rangle$, where the addition is the standard addition in the group $(\mathbb{Z}/m_1\mathbb{Z}) \times \cdots \times (\mathbb{Z}/m_d\mathbb{Z})$. Then G is a $2d$-regular bipartite graph on $2n = \mathrm{vol}(\mathbf{m})$ vertices, and $W(G,s)$ is the set $W_{\mathrm{per}}(\mathbf{m},s)$ of monomer-dimer covers of $T(\mathbf{m})$ having exactly s dimers. Theorem 5.1 yields that $\#W_{\mathrm{per}}(\mathbf{m},s) \geq \binom{n}{s}^2 s!\left(\frac{2d}{n}\right)^s$. There is an injection f from $W_{\mathrm{per}}(\mathbf{m},s)$ to $W_0(\mathbf{m}+\mathbf{1},s)$, the set of monomer-dimer tilings of $\langle \mathbf{m}+\mathbf{1} \rangle$ having exactly s dimers: if $c \in W_{\mathrm{per}}(\mathbf{m},s)$, then $f(c)$ is obtained from c by replacing each dimer in c occupying the points $\mathbf{i} = (i_1,\ldots,i_d)$ and $\mathbf{j} = \mathbf{i} + \mathbf{e}_k$ such that $i_k = m_k$ and

$j_k = 0$ by a dimer occupying the points $\mathbf{i}$ and $(i_1, \dots, i_{k-1}, m_k + 1, i_{k+1}, \dots, i_d)$. Therefore $\#W_0(\mathbf{m} + \mathbf{1}, s) \geq \binom{n}{s}^2 s! \left(\frac{2d}{n}\right)^s$. Let $(\mathbf{m}_q)_{q \in \mathbb{N}} \subseteq \mathbb{N}^d$ and $(s_q)_{q \in \mathbb{N}} \subseteq \mathbb{N}$ be sequences such that all the coordinates of each $\mathbf{m}_q$ are even, $\lim_{q \to \infty} \mathbf{m}_q = \infty$ and $\lim_{q \to \infty} \frac{2s_q}{\mathrm{vol}(\mathbf{m}_q)} = p$. Set $n_q = \frac{\mathrm{vol}(\mathbf{m}_q)}{2}$. Then conditions (4.8) hold, and consequently (4.9) does. Therefore

$$\lambda_d(p) = \lim_{q \to \infty} \frac{\log \#W_0(\mathbf{m}_q, s_q)}{|\mathbf{m}_q|} = \lim_{q \to \infty} \frac{\log \#W_0(\mathbf{m}_q + \mathbf{1}, s_q)}{|\mathbf{m}_q|}$$
$$\geq \lim_{q \to \infty} \frac{\log \binom{n_q}{s_q}^2 s_q! \left(\frac{2d}{n_q}\right)^{s_q}}{2n_q} = \lim_{n \to \infty} \frac{1}{2n} \log \binom{n}{pn}^2 (pn)! \left(\frac{2d}{n}\right)^{pn}.$$

Manipulating the limit in the right-hand side of the inequality above and using the equality $\lim_{r \to \infty} \frac{1}{r}(\log r! - \log r^r) = -1$, we deduce the inequality (5.3).

Let $(\mathbf{m}_q)_{q \in \mathbb{N}}$ again satisfy the assumptions that all the coordinates of each $\mathbf{m}_q$ are even and $\lim_{q \to \infty} \mathbf{m}_q = \infty$, but this time set $s_q = n_q = \frac{\mathrm{vol}(\mathbf{m}_q)}{2}$. Using the inequality (5.2) for $\#W_{\mathrm{per}}(\mathbf{m}_q, n_q)$ and (4.11), we deduce the inequality (5.4).

To prove (5.5), we use (4.12). We easily verify that the right-hand side of (5.3) is a strictly concave function of p in $[0, 1]$, and $p(d)$ given in (5.6) is its unique critical point in that interval, hence its maximizing point there. □

For $d = 2, 3$, inequality (5.5) yields

$$h_2 \geq 0.6358077435 \tag{5.7}$$
$$h_3 \geq 0.7652789557. \tag{5.8}$$

For $d = 3$, inequality (5.4) yields $\widetilde{h}_3 \geq 0.440075842$, which is the best known lower bound.

6 Upper and Lower Bounds for h_d and $\widetilde{h}_d$ Using Spectral Radii

For $d \in \mathbb{N}$, $K \subseteq \langle d \rangle$ and $\mathbf{m} \in \mathbb{N}^d$, we denote by $\langle \mathbf{m}_K \rangle$ the projection of $\langle \mathbf{m} \rangle$ on the coordinates with indices in K. Let $W_{\mathrm{per},K}(\mathbf{m})$, respectively $\widetilde{W}_{\mathrm{per},K}(\mathbf{m})$, be the set of monomer-dimer covers, respectively dimer covers, of $T(\mathbf{m}_K) \times \langle \mathbf{m}_{\langle d \rangle \setminus K} \rangle$. Thus $W_{\mathrm{per},\langle d \rangle}(\mathbf{m}) = W_{\mathrm{per}}(\mathbf{m})$ and $\widetilde{W}_{\mathrm{per},\langle d \rangle}(\mathbf{m}) = \widetilde{W}_{\mathrm{per}}(\mathbf{m})$. Note that by the isotropy of our Γ, $\#W_{\mathrm{per},K}(\mathbf{m})$ and $\#\widetilde{W}_{\mathrm{per},K}(\mathbf{m})$ are invariant under permutations of the components of $\mathbf{m}$ if K undergoes a corresponding change.

In order to analyze $W_{\mathrm{per},\{d\}}(\mathbf{m})$, we focus on the dimers in the cover lying along the direction $\mathbf{e}_d$. More precisely, with $\mathbf{m}' = (m_1, \dots, m_{d-1})$, we consider $\langle \mathbf{m}' \rangle \times T(m_d)$ as consisting of m_d levels isomorphic to $\langle \mathbf{m}' \rangle$. A subset S of the points in level q is covered by dimers joining levels $q-1$ and q (with level 0 understood as level m_d); a subset T disjoint from S is covered by dimers joining levels q and $q+1$ (with level $m_d + 1$ understood as level 1); and the remainder U of level q is covered by monomers and dimers lying entirely within level q. We are interested in counting the coverings of U subject to various restrictions. With that in mind, for $\mathbf{m}' \in \mathbb{N}^{d-1}$ we define an undirected graph $G(\mathbf{m}')$ whose vertices are the subsets of $\langle \mathbf{m}' \rangle$ in which subsets S and T are adjacent if and only if $S \cap T = \emptyset$. When $S \cap T = \emptyset$ we also define the following, using $U = \langle \mathbf{m}' \rangle \setminus (S \cup T)$:

$a_{ST} =$ number of monomer-dimer tilings of U.

$b_{ST} =$ number of monomer-dimer tilings of U viewed as a subset of $T(\mathbf{m}')$.

$p_{ST} =$ number of monomer-dimer covers of U, viewed as a subset of $T(m_1) \times \langle (m_2, \ldots, m_{d-1}) \rangle$, each monomer within U, and each dimer meeting U but not $S \cup T$.

$c_{ST} =$ number of monomer-dimer covers of U, each monomer within U, and each dimer meeting U but not $S \cup T$.

Thus in the tilings/covers counted by a_{ST}, b_{ST}, p_{ST}, c_{ST}, each monomer lies within U and each dimer meets U but not $S \cup T$. In a_{ST}, each dimer occupies two points of U that are adjacent in $\langle \mathbf{m}' \rangle$. In b_{ST}, each dimer occupies two points of U that are adjacent in $T(\mathbf{m}')$, so is allowed to "wrap around". In p_{ST}, the dimers in the direction of $\mathbf{e}_1$ are allowed to "wrap around" and the other dimers are allowed to "protrude out" of $\langle (m_2, \ldots, m_{d-1}) \rangle$. In c_{ST}, the dimers may "protrude" out of $\langle \mathbf{m}' \rangle$. Therefore $a_{ST} \le b_{ST} \le p_{ST} \le c_{ST}$. By definition, if $U = \emptyset$, then $a_{ST} = b_{ST} = p_{ST} = c_{ST} = 1$. Notice that when $d = 2$, there is no distinction between b_{ST} and p_{ST}.

We define the matrices $A(\mathbf{m}')$, $B(\mathbf{m}')$, $P(\mathbf{m}')$, $C(\mathbf{m}')$ with rows and columns indexed by subsets of $\langle \mathbf{m}' \rangle$ as follows:

$$A(\mathbf{m}')_{ST} = \begin{cases} a_{ST} & \text{if } S \cap T = \emptyset \\ 0 & \text{if } S \cap T \neq \emptyset, \end{cases}$$

$$B(\mathbf{m}')_{ST} = \begin{cases} b_{ST} & \text{if } S \cap T = \emptyset \\ 0 & \text{if } S \cap T \neq \emptyset, \end{cases}$$

$$P(\mathbf{m}')_{ST} = \begin{cases} p_{ST} & \text{if } S \cap T = \emptyset \\ 0 & \text{if } S \cap T \neq \emptyset, \end{cases}$$

$$C(\mathbf{m}')_{ST} = \begin{cases} c_{ST} & \text{if } S \cap T = \emptyset \\ 0 & \text{if } S \cap T \neq \emptyset. \end{cases}$$

Thus $A(\mathbf{m}')$, $B(\mathbf{m}')$, $P(\mathbf{m}')$, $C(\mathbf{m}')$ are symmetric matrices—here is the "hidden symmetry" referred to in Section 4—of integers satisfying $0 \le A(\mathbf{m}') \le B(\mathbf{m}') \le P(\mathbf{m}') \le C(\mathbf{m}')$ (where the inequalities indicate componentwise comparisons). We denote by $\alpha(\mathbf{m}'), \beta(\mathbf{m}'), \pi(\mathbf{m}'), \gamma(\mathbf{m}')$ their spectral radii, respectively, and consequently $\alpha(\mathbf{m}') \le \beta(\mathbf{m}') \le \pi(\mathbf{m}') \le \gamma(\mathbf{m}')$.

In an analogous way, we define $\widetilde{a}_{ST}$, $\widetilde{b}_{ST}$, $\widetilde{p}_{ST}$, $\widetilde{c}_{ST}$, where there are no monomers in the tilings and covers, the matrices $\widetilde{A}(\mathbf{m}')$, $\widetilde{B}(\mathbf{m}')$, $\widetilde{P}(\mathbf{m}')$, $\widetilde{C}(\mathbf{m}')$, and their spectral radii $\widetilde{\alpha}(\mathbf{m}'), \widetilde{\beta}(\mathbf{m}'), \widetilde{\pi}(\mathbf{m}'), \widetilde{\gamma}(\mathbf{m}')$.

Each of these eight symmetric matrices can be considered as the adjacency matrix of an undirected multigraph, where the multiplicity of an edge is the corresponding matrix entry. This multigraph is a weighted version of $G(\mathbf{m}')$. If the multigraph is bipartite, we say that the matrix is *bipartite*; if the multigraph is connected, we say that the matrix is *irreducible*; if the multigraph is disconnected, we say that the matrix is a *direct sum*; if the multigraph is connected and the greatest common divisor of the lengths of all its closed walks is 1, or equivalently if for sufficiently high powers of the matrix all entries are strictly positive, we say that the matrix is *primitive*.

Proposition 6.1 *Let* $2 \le d \in \mathbb{N}$ *and* $\mathbf{m} = (\mathbf{m}', m_d) \in \mathbb{N}^d$. *Then*

(a) $\operatorname{tr} A(\mathbf{m}')^{m_d}$ *is the number of monomer-dimer tilings of* $\langle \mathbf{m}' \rangle \times T(m_d)$ *and* $\operatorname{tr} \widetilde{A}(\mathbf{m}')^{m_d}$ *is the number of dimer tilings of* $\langle \mathbf{m}' \rangle \times T(m_d)$;

(b) $\operatorname{tr} B(\mathbf{m}')^{m_d} = \#W_{\mathrm{per}}(\mathbf{m})$ *and* $\operatorname{tr} \widetilde{B}(\mathbf{m}')^{m_d} = \#\widetilde{W}_{\mathrm{per}}(\mathbf{m})$;

(c) $\operatorname{tr} P(\mathbf{m}')^{m_d} = \#W_{\mathrm{per},\{1,d\}}(\mathbf{m})$ *and* $\operatorname{tr} \widetilde{P}(\mathbf{m}')^{m_d} = \#\widetilde{W}_{\mathrm{per},\{1,d\}}(\mathbf{m})$;

(d) $\operatorname{tr} C(\mathbf{m}')^{m_d} = \#W_{\mathrm{per},\{d\}}(\mathbf{m})$ *and* $\operatorname{tr} \widetilde{C}(\mathbf{m}')^{m_d} = \#\widetilde{W}_{\mathrm{per},\{d\}}(\mathbf{m})$;

(e) for $m_d \ge 2$, *if column vector* $\mathbf{x} = (x_S)_{S \subseteq \langle \mathbf{m}' \rangle}$ *is given by* $x_S = b_{S\emptyset}$, *then* $\mathbf{x}^\top B(\mathbf{m}')^{m_d-2}\mathbf{x} = \#W_{\mathrm{per},\langle d-1 \rangle}(\mathbf{m})$,
if vector $\mathbf{y}$ *is given by* $y_S = c_{S\emptyset}$, *then* $\mathbf{y}^\top C(\mathbf{m}')^{m_d-2}\mathbf{y} = \#W(\mathbf{m})$,
if $\mathbf{z} = (z_S)_{S \subseteq \langle \mathbf{m}' \rangle}$ *is given by* $z_S = p_{S\emptyset}$, *then* $\mathbf{z}^\top P(\mathbf{m}')^{m_d-2}\mathbf{z} = \#W_{\mathrm{per},\{1\}}(\mathbf{m})$;
if column vector $\widetilde{\mathbf{x}} = (\widetilde{x}_S)_{S \subseteq \langle \mathbf{m}' \rangle}$ *is given by* $\widetilde{x}_S = \widetilde{b}_{S\emptyset}$, *then* $\widetilde{\mathbf{x}}^\top \widetilde{B}(\mathbf{m}')^{m_d-2}\widetilde{\mathbf{x}} = \#\widetilde{W}_{\mathrm{per},\langle d-1 \rangle}(\mathbf{m})$,
if $\widetilde{\mathbf{y}}$ *is given by* $\widetilde{y}_S = \widetilde{c}_{S\emptyset}$, *then* $\widetilde{\mathbf{y}}^\top \widetilde{C}(\mathbf{m}')^{m_d-2}\widetilde{\mathbf{y}} = \#\widetilde{W}(\mathbf{m})$,
if vector $\widetilde{\mathbf{z}}$ *is given by* $\widetilde{z}_S = \widetilde{p}_{S\emptyset}$, *then* $\widetilde{\mathbf{z}}^\top \widetilde{P}(\mathbf{m}')^{m_d-2}\widetilde{\mathbf{z}} = \#\widetilde{W}_{\mathrm{per},\{1\}}(\mathbf{m})$;

(f) the matrices $A(\mathbf{m}')$, $B(\mathbf{m}')$, $P(\mathbf{m}')$, $C(\mathbf{m}')$ *are primitive;*

(g) if $\operatorname{vol}(\mathbf{m}')$ *is odd, then* $\widetilde{A}(\mathbf{m}')$, $\widetilde{B}(\mathbf{m}')$ *are bipartite, otherwise they are direct sums.*

Proof. We begin with proving the first part of (b), its second part and (a), (c), (d) and (e) being similar. Assume first that $m_d = 1$, and let $\phi \in W_{\mathrm{per}}(\mathbf{m})$. Since ϕ can be extended periodically in the direction of $\mathbf{e}_d$ with period 1, it can be viewed as an element of $W_{\mathrm{per}}(\mathbf{m}')$. Therefore $\#W_{\mathrm{per}}(\mathbf{m}) = \#W_{\mathrm{per}}(\mathbf{m}')$. We have $\operatorname{tr} B(\mathbf{m}') = \sum_{S \subseteq \langle \mathbf{m}' \rangle} b_{SS}$. Only the term $S = \emptyset$ contributes to the sum, and for this term we have $U = \langle \mathbf{m}' \rangle$ and $b_{\emptyset\emptyset} = \#W_{\mathrm{per}}(\mathbf{m}')$. Hence $\operatorname{tr} B(\mathbf{m}') = \#W_{\mathrm{per}}(\mathbf{m}')$. Now assume that $m_d > 1$, and consider any closed path $S_1, S_2, \ldots, S_{m_d}, S_1$ of length m_d in $G(\mathbf{m}')$. For each $\mathbf{p}' \in S_q$ place a dimer occupying the points $(\mathbf{p}', q)$ and $(\mathbf{p}', q+1)$ (with m_d+1 wrapping around to 1). We want to extend these dimers to a monomer-dimer tiling of $T(\mathbf{m}') \times T(m_d) = T(\mathbf{m})$, i.e., to a member of $W_{\mathrm{per}}(\mathbf{m})$, by monomers and by dimers not in the direction of $\mathbf{e}_d$, i.e., lying within the levels $1, \ldots, m_d$. The number of choices of such monomers and dimers to fill the remainder of level q is given by $b_{S_{q-1}S_q}$, and so the number of extensions to a member of $W_{\mathrm{per}}(\mathbf{m})$ is $b_{S_1S_2} b_{S_2S_3} \cdots b_{S_{m_d-1}S_{m_d}} b_{S_{m_d}S_1}$. Conversely, each member of $W_{\mathrm{per}}(\mathbf{m})$ is obtained in this way. Hence $\#W_{\mathrm{per}}(\mathbf{m})$ is the sum of all the products of the above form, namely $\operatorname{tr} B(\mathbf{m}')^{m_d}$.

To prove (f), we note that $A(\mathbf{m}')$ is irreducible, since whenever $S \cap T = \emptyset$, U can be tiled by monomers and therefore each subset of $\langle \mathbf{m}' \rangle$ is adjacent to $\emptyset$ in the graph of $A(\mathbf{m}')$. Furthermore, $A(\mathbf{m}')$ is primitive since the graph has a cycle of length 1 from $\emptyset$ to $\emptyset$. Since $A(\mathbf{m}') \le B(\mathbf{m}') \le P(\mathbf{m}') \le C(\mathbf{m}')$, $B(\mathbf{m}')$, $P(\mathbf{m}')$, and $C(\mathbf{m}')$ are also primitive.

To prove (g), let $\mathcal{E}, \mathcal{O}$ denote the subsets of $\langle \mathbf{m}' \rangle$ with even and odd cardinality, respectively. If $\widetilde{b}_{ST} > 0$, then U can be tiled by dimers and so $\#U$ must be even. Therefore if $\mathrm{vol}(\mathbf{m}')$ is odd, members of $\mathcal{E}$ are adjacent only to members of $\mathcal{O}$ and vice versa in the graph of $\widetilde{B}(\mathbf{m}')$, and so that graph is bipartite; if $\mathrm{vol}(\mathbf{m}')$ is even, then members of $\mathcal{E}$ are adjacent only to themselves, and the graph is disconnected. The same conclusions hold for $\widetilde{A}(\mathbf{m}')$ since $\widetilde{A}(\mathbf{m}') \le \widetilde{B}(\mathbf{m}')$. $\square$

Lemma 6.2 *Let $2 \le d \in \mathbb{N}$ and $\mathbf{m}' \in \mathbb{N}^{d-1}$. Then*

$$\lim_{m_d\to\infty} \frac{\log \# W_0(\mathbf{m}', m_d)}{m_d} = \log \alpha(\mathbf{m}'), \tag{6.1}$$

$$\lim_{m_d\to\infty} \frac{\log \# W_{\mathrm{per},\langle d-1\rangle}(\mathbf{m}', m_d)}{m_d} = \log \beta(\mathbf{m}'), \tag{6.2}$$

$$\lim_{m_d\to\infty} \frac{\log \# W_{\mathrm{per},\{1\}}(\mathbf{m}', m_d)}{m_d} = \log \pi(\mathbf{m}'), \tag{6.3}$$

$$\lim_{m_d\to\infty} \frac{\log \# W(\mathbf{m}', m_d)}{m_d} = \log \gamma(\mathbf{m}'), \tag{6.4}$$

$$\lim_{m_d\to\infty} \frac{\log \# \widetilde{W}_0(\mathbf{m}', m_d)}{m_d} \le \log \widetilde{\alpha}(\mathbf{m}'), \tag{6.5}$$

$$\lim_{m_d\to\infty} \frac{\log \# \widetilde{W}_{\mathrm{per},\langle d-1\rangle}(\mathbf{m}', m_d)}{m_d} = \log \widetilde{\beta}(\mathbf{m}'), \tag{6.6}$$

$$\lim_{m_d\to\infty} \frac{\log \# \widetilde{W}_{\mathrm{per},\{1\}}(\mathbf{m}', m_d)}{m_d} = \log \widetilde{\pi}(\mathbf{m}'), \tag{6.7}$$

$$\lim_{m_d\to\infty} \frac{\log \# \widetilde{W}(\mathbf{m}', m_d)}{m_d} = \log \widetilde{\gamma}(\mathbf{m}'). \tag{6.8}$$

Proof. From part (a) of Proposition 6.1 we obtain $\#\widetilde{W}_0(\mathbf{m}', m_d) \le \operatorname{tr} \widetilde{A}(\mathbf{m}')^{m_d}$, and therefore

$$\limsup_{m_d\to\infty} \frac{\log \# \widetilde{W}_0(\mathbf{m}', m_d)}{m_d} \le \limsup_{m_d\to\infty} \frac{\log \operatorname{tr} \widetilde{A}(\mathbf{m}')^{m_d}}{m_d} = \log \widetilde{\alpha}(\mathbf{m}'). \tag{6.9}$$

The equality in (6.9) follows from a characterization of $\rho(M)$ for a square matrix $M \ge 0$, namely $\rho(M) = \limsup_{n\to\infty} (\operatorname{tr} M^n)^{\frac{1}{n}}$ (see for example Proposition 10.3 of [15]). Since $-\log \#\widetilde{W}_0(\mathbf{m}', m_d)$ is subadditive in m_d, the first lim sup in (6.9) can be replaced by a lim, which proves (6.5). Similar considerations prove $\lim_{m_d\to\infty} \frac{\log \# W_0(\mathbf{m}', m_d)}{m_d} \le \log \alpha(\mathbf{m}')$. In order to prove the reverse inequality and thus (6.1), observe that each monomer-dimer tiling of $\langle \mathbf{m}' \rangle \times T(m_d)$ extends to a monomer-dimer tiling in $W_0(\mathbf{m}', m_d + 1)$ (as can be seen by replacing each dimer occupying $(\mathbf{m}', 1)$ and $(\mathbf{m}', m_d)$ by a monomer occupying $(\mathbf{m}', 1)$ and a dimer occupying $(\mathbf{m}', m_d)$ and $(\mathbf{m}', m_d + 1)$, and tiling the rest with monomers). Hence $\#W_0(\mathbf{m}', m_d + 1) \ge \operatorname{tr} A(\mathbf{m}')^{m_d}$ by part (a) of Proposition 6.1. Therefore, since

$-\log \#W_0(\mathbf{m}', m_d)$ is subadditive in m_d and thus the limits below exist, we obtain

$$\lim_{m_d\to\infty} \frac{\log \#W_0(\mathbf{m}', m_d)}{m_d} = \lim_{m_d\to\infty} \frac{\log \#W_0(\mathbf{m}', m_d+1)}{m_d}$$
$$\geq \limsup_{m_d\to\infty} \frac{\log \operatorname{tr} A(\mathbf{m}')^{m_d}}{m_d} = \log \alpha(\mathbf{m}').$$

To prove (6.2), (6.3), and (6.4), we use another characterization of the spectral radius. A *vector norm* is a mapping $\|\cdot\| : M_n(\mathbb{C}) \to \mathbb{R}_+$ taking complex matrices of order n to nonnegative reals such that $\|M\| = 0$ only if $M = 0$, $\|zM\| = |z|\|M\|$ for all $z \in \mathbb{C}$, and $\|M + N\| \leq \|M\| + \|N\|$. If $c_{ij} > 0$ for all $i, j \in \langle n\rangle$, then $\|M\| = \sum_{ij} c_{ij}|m_{ij}|$ is a vector norm. Proposition 10.1 of [15] states that if $\|\cdot\|$ is a vector norm, then $\rho(M) = \lim_{k\to\infty} \|M^k\|^{\frac{1}{k}}$. In particular, if $M \geq 0$ and $\mathbf{v}$ is a column vector with positive entries, then $\rho(M) = \lim_{k\to\infty}(\mathbf{v}^\top M^k \mathbf{v})^{\frac{1}{k}}$. Applying this to $M = B(\mathbf{m}'), P(\mathbf{m}'), C(\mathbf{m}')$ and using part (e) of Proposition 6.1 with $\mathbf{v} = \mathbf{x}, \mathbf{z}, \mathbf{y}$ defined there proves (6.2), 6.3), (6.4).

The proof of (6.6) is a little more complicated because the vector $\widetilde{\mathbf{x}}$ in part (e) of Proposition 6.1 is not strictly positive. Therefore we introduce the vector $\widetilde{\mathbf{w}}$ with entries $\widetilde{w}_S = \max(1, \widetilde{x}_S)$. Then, by part (e) of Proposition 6.1, we have $\#\widetilde{W}_{\mathrm{per},\langle d-1\rangle}(\mathbf{m}) = \widetilde{\mathbf{x}}^\top \widetilde{B}(\mathbf{m}')^{m_d-2}\widetilde{\mathbf{x}} \leq \widetilde{\mathbf{w}}^\top \widetilde{B}(\mathbf{m}')^{m_d-2}\widetilde{\mathbf{w}}$. Therefore we obtain

$$\lim_{m_d\to\infty} \frac{\log \#\widetilde{W}_{\mathrm{per},\langle d-1\rangle}(\mathbf{m})}{m_d} \leq \lim_{m_d\to\infty} \frac{\log \widetilde{\mathbf{w}}^\top \widetilde{B}(\mathbf{m}')^{m_d-2}\widetilde{\mathbf{w}}}{m_d} = \log \widetilde{\beta}(\mathbf{m}')$$

(the first lim above existing since $\log \#\widetilde{W}_{\mathrm{per},\langle d-1\rangle}(\mathbf{m})$ is subadditive in m_d). On the other hand $\#\widetilde{W}_{\mathrm{per},\langle d-1\rangle}(\mathbf{m}) \geq \#\widetilde{W}_{\mathrm{per}}(\mathbf{m}) = \operatorname{tr} \widetilde{B}(\mathbf{m}')^{m_d}$ by part (b) of Proposition 6.1. Therefore

$$\lim_{m_d\to\infty} \frac{\log \#\widetilde{W}_{\mathrm{per},\langle d-1\rangle}(\mathbf{m})}{m_d} \geq \limsup_{m_d\to\infty} \frac{\log \operatorname{tr} \widetilde{B}(\mathbf{m}')^{m_d}}{m_d} = \log \widetilde{\beta}(\mathbf{m}').$$

This proves (6.6). To prove (6.8), we show analogously that

$$\lim_{m_d\to\infty} \frac{\log \#\widetilde{W}(\mathbf{m})}{m_d} \leq \log \widetilde{\gamma}(\mathbf{m}'),$$

and on the other hand, by part (d) of Proposition 6.1,

$$\lim_{m_d\to\infty} \frac{\log \#\widetilde{W}(\mathbf{m})}{m_d} \geq \limsup_{m_d\to\infty} \frac{\log \#\widetilde{W}_{\mathrm{per},\{d\}}(\mathbf{m})}{m_d}$$
$$= \limsup_{m_d\to\infty} \frac{\log \operatorname{tr} \widetilde{C}(\mathbf{m}')^{m_d}}{m_d} = \log \widetilde{\gamma}(\mathbf{m}').$$

The proof of (6.7) is similar. □

Proposition 6.3 *Let* $2 \leq d \in \mathbb{N}$ *and* $\mathbf{m}' \in \mathbb{N}^{d-1}$. *Then*

$$\frac{\log \gamma(\mathbf{m}')}{|\mathbf{m}'|_{pr}} \geq h_d \geq \frac{\log \alpha(\mathbf{m}')}{|\mathbf{m}'|_{pr}}, \tag{6.10}$$
$$\frac{\log \widetilde{\gamma}(\mathbf{m}')}{|\mathbf{m}'|_{pr}} \geq \widetilde{h}_d \geq \frac{\log \widetilde{\alpha}(\mathbf{m}')}{|\mathbf{m}'|_{pr}}. \tag{6.11}$$

Proof. The upper bounds follow from the general upper bounds in Proposition 4.2 along with (6.4) and (6.8). The lower bound in (6.10) follows similarly from the general lower bound in Proposition 4.2 along with (6.1). However, since (6.5) only gives a lower bound for $\log\alpha(\mathbf{m}')$, we use a separate argument for the lower bound in (6.11) as follows. For $q \in \mathbb{N}$, $\#\widetilde{W}(q\mathbf{m}', m_d)$ is not smaller than the the number of dimer tilings of $\langle q\mathbf{m}'\rangle \times T(m_d)$, which in turn is not smaller than the number of dimer tilings of $\langle \mathbf{m}'\rangle \times T(m_d)$ raised to the q^{d-1} power. Hence by part (a) of Proposition 6.1 we have

$$\#\widetilde{W}(q\mathbf{m}', m_d) \geq \left(\operatorname{tr} \widetilde{A}^{m_d}\right)^{q^{d-1}},$$

and so

$$\frac{\log \#\widetilde{W}(q\mathbf{m}', m_d)}{\operatorname{vol}(q\mathbf{m}', m_d)} \geq \frac{\log \operatorname{tr} \widetilde{A}^{m_d}}{\operatorname{vol}(\mathbf{m}')m_d}.$$

Therefore

$$\widetilde{h}_d = \lim_{q,m_d\to\infty} \frac{\log \#\widetilde{W}(q\mathbf{m}', m_d)}{\operatorname{vol}(q\mathbf{m}', m_d)} \geq \frac{1}{\operatorname{vol}(\mathbf{m}')} \limsup_{q,m_d\to\infty} \frac{\log \operatorname{tr} \widetilde{A}^{m_d}}{m_d} = \frac{\log \widetilde{\alpha}(\mathbf{m}')}{|\mathbf{m}'|_{pr}}.$$

□

Now we introduce the following notation. For $\mathbf{m} \in \mathbb{N}^d$ and $k \in \langle d\rangle$, $\mathbf{m}^{\sim k} := (m_1, \ldots, m_{k-1}, m_{k+1}, \ldots, m_d) \in \mathbb{N}^{d-1}$. As special cases, we have the previous notation $\mathbf{m}' = \mathbf{m}^{\sim d}$ and $\mathbf{m}^- = \mathbf{m}^{\sim 1}$.

Proposition 6.4 *Let $\mathbf{m} \in \mathbb{N}^d$, and assume that m_d is even. Then each $k \in \langle d-1\rangle$ satisfies*

$$\frac{\log \beta(\mathbf{m}^{\sim d})}{\operatorname{vol}(\mathbf{m})} \leq \frac{\log 2}{m_k} + \frac{\log \beta(\mathbf{m}^{\sim k})}{|\mathbf{m}^{\sim k}|_{pr}}, \tag{6.12}$$

$$\frac{\log \widetilde{\beta}(\mathbf{m}^{\sim d})}{\operatorname{vol}(\mathbf{m})} \leq \frac{\log 2}{m_k} + \frac{\log \widetilde{\beta}(\mathbf{m}^{\sim k})}{|\mathbf{m}^{\sim k}|_{pr}}. \tag{6.13}$$

Proof. We have

$$\begin{aligned}\beta(\mathbf{m}^{\sim d})^{m_d} \leq \operatorname{tr} B(\mathbf{m}^{\sim d})^{m_d} = \#W_{\text{per}}(\mathbf{m}) &= \operatorname{tr} B(\mathbf{m}^{\sim k})^{m_k} \\ &\leq 2^{\operatorname{vol}(\mathbf{m}^{\sim k})}\beta(\mathbf{m}^{\sim k})^{m_k},\end{aligned}$$

where the first inequality follows since $\beta(\mathbf{m}^{\sim d})$ is one of the eigenvalues of $B(\mathbf{m}^{\sim d})$, which are all real, and m_d is even, the next equality from part (b) of Proposition 6.1, the next equality from the same and the fact that $\#W_{\text{per}}(\mathbf{m})$ is invariant under coordinate permutations in $\mathbf{m}$, and the last inequality from the fact that $B(\mathbf{m}^{\sim k})$ has $2^{\operatorname{vol}(\mathbf{m}^{\sim k})}$ eigenvalues, all real, whose absolute values are at most $\beta(\mathbf{m}^{\sim k})$. Taking logarithms and dividing by $|\mathbf{m}|_{pr}$, we deduce (6.12). The inequality (6.13) is obtained in a similar way. □

We define

$$\overline{h}_{d-1}(m_1) := \lim_{\mathbf{m}^-\to\infty} \frac{\log \#W_{\text{per},\{1\}}(m_1, \mathbf{m}^-)}{\operatorname{vol}(\mathbf{m}^-)}, \ m_1 \in \mathbb{N}; \quad \overline{h}_{d-1}(0) := \log 2,$$

$$\breve{h}_{d-1}(m_1) := \lim_{\mathbf{m}^-\to\infty} \frac{\log \#\widetilde{W}_{\text{per},\{1\}}(m_1, \mathbf{m}^-)}{\operatorname{vol}(\mathbf{m}^-)}, \ m_1 \in \mathbb{N}; \quad \breve{h}_{d-1}(0) := \log 2.$$

Notice that for $m_1 \in \mathbb{N}$, $\overline{h}_{d-1}(m_1)$ is the same as $\overline{h}(m_1, \Gamma)$ defined in (3.1) when Γ is the d-digraph encoding the monomer-dimer covers. For this reason, the limit $\overline{h}_{d-1}(m_1)$ exists, and similarly for $\breve{h}_{d-1}(m_1)$. The following theorem is an analog of Theorem 3.1 and Theorem 3.4.

Theorem 6.5 *Let $2 \le d \in \mathbb{N}$, $p, r \in \mathbb{N}$, $q \in \mathbb{N} \cup \{0\}$. Then*

$$\frac{\overline{h}_{d-1}(2r)}{2r} \ge h_d \ge \frac{\overline{h}_{d-1}(p+2q) - \overline{h}_{d-1}(2q)}{p}, \tag{6.14}$$

$$\frac{\breve{h}_{d-1}(2r)}{2r} \ge \widetilde{h}_d \ge \frac{\breve{h}_{d-1}(p+2q) - \breve{h}_{d-1}(2q)}{p}. \tag{6.15}$$

Let $\mathbf{m}' = (m_1, \dots, m_{d-1}) \in \mathbb{N}^{d-1}$ and assume that $m_1, \dots, m_{d-1}$ are even. Then

$$h_d \le \frac{\beta(\mathbf{m}')}{|\mathbf{m}'|_{pr}}, \tag{6.16}$$

$$\widetilde{h}_d \le \frac{\widetilde{\beta}(\mathbf{m}')}{|\mathbf{m}'|_{pr}}. \tag{6.17}$$

Proof. We have

$$\widetilde{h}_d = \lim_{\substack{\mathbf{m}', m_d \to \infty \\ \frac{m_d}{2} \in \mathbb{N}}} \frac{\log \#\widetilde{W}_0(\mathbf{m}', m_d)}{\mathrm{vol}(\mathbf{m}') m_d} \le \liminf_{\mathbf{m}' \to \infty} \frac{\log \widetilde{\alpha}(\mathbf{m}')}{\mathrm{vol}(\mathbf{m}')} \le \limsup_{\mathbf{m}' \to \infty} \frac{\log \widetilde{\gamma}(\mathbf{m}')}{\mathrm{vol}(\mathbf{m}')}$$

$$= \limsup_{\mathbf{m}', m_d \to \infty} \frac{\log \#W(\mathbf{m}', m_d)}{\mathrm{vol}(\mathbf{m}') m_d} = \widetilde{h}_d,$$

where the first equality follows from (4.7), the next inequality from (6.5), the next one from $\widetilde{\alpha}(\mathbf{m}') \le \widetilde{\gamma}(\mathbf{m}')$, the next equality from (6.8), and the last equality again from (4.7). From this and $\widetilde{\alpha}(\mathbf{m}') \le \widetilde{\beta}(\mathbf{m}') \le \widetilde{\gamma}(\mathbf{m}')$, we obtain

$$\widetilde{h}_d = \lim_{\mathbf{m}' \to \infty} \frac{\log \widetilde{\alpha}(\mathbf{m}')}{\mathrm{vol}(\mathbf{m}')} = \lim_{\mathbf{m}' \to \infty} \frac{\log \widetilde{\beta}(\mathbf{m}')}{\mathrm{vol}(\mathbf{m}')} = \lim_{\mathbf{m}' \to \infty} \frac{\log \widetilde{\gamma}(\mathbf{m}')}{\mathrm{vol}(\mathbf{m}')}. \tag{6.18}$$

Similarly (and more simply)

$$h_d = \lim_{\mathbf{m}' \to \infty} \frac{\log \alpha(\mathbf{m}')}{\mathrm{vol}(\mathbf{m}')} = \lim_{\mathbf{m}' \to \infty} \frac{\log \beta(\mathbf{m}')}{\mathrm{vol}(\mathbf{m}')} = \lim_{\mathbf{m}' \to \infty} \frac{\log \gamma(\mathbf{m}')}{\mathrm{vol}(\mathbf{m}')}. \tag{6.19}$$

First we prove (6.16). Let $\mathbf{m}' = (m_1, \dots, m_{d-1}) \in \mathbb{N}$, $m_1, \dots, m_{d-1}$ even, and let $\mathbf{p} = (p_1, \dots, p_{d-1}) \in \mathbb{N}^{d-1}$ be arbitrary. Set

$$\mathbf{m}_1 = (p_1, \dots, p_{d-1}, m_1), \quad \mathbf{m}_2 = (p_2, \dots, p_d, m_1, m_2), \quad \dots,$$
$$\mathbf{m}_{d-1} = (p_d, m_1, \dots, m_{d-1}).$$

Then, using (6.12) with $k = 1$ $d-1$ times, we obtain

$$\frac{\log \beta(\mathbf{p})}{|\mathbf{p}|_{pr}} \le \frac{\log 2}{p_1} + \frac{\log \beta(\mathbf{m}_1^-)}{|\mathbf{m}_1^-|_{pr}} \le \frac{\log 2}{p_1} + \frac{\log 2}{p_2} + \frac{\log \beta(\mathbf{m}_2^-)}{|\mathbf{m}_2^-|_{pr}} \le \cdots$$
$$\le \sum_{j=1}^{d-1} \frac{\log 2}{p_j} + \frac{\log \beta(\mathbf{m}')}{|\mathbf{m}'|_{pr}}.$$

Letting $\mathbf{p} \to \infty$ and using (6.19) for the left-hand side, we deduce (6.16). Similar arguments apply to deduce (6.17).

We now demonstrate the lower bound in (6.14). Let $\mathbf{m}^- \in \mathbb{N}^{d-1}$, $p \in \mathbb{N}$, $q \in \mathbb{N} \cup \{0\}$. Assume first that $q \in \mathbb{N}$. Since $\gamma(\mathbf{m}^-) = \rho(C(\mathbf{m}^-))$ and $C(\mathbf{m}^-)$ is symmetric, it follows as in the arguments for (3.8) that

$$\gamma(\mathbf{m}^-)^p \geq \frac{\operatorname{tr} C(\mathbf{m}^-)^{p+2q}}{\operatorname{tr} C(\mathbf{m}^-)^{2q}} = \frac{\# W_{\mathrm{per},\{1\}}(p+2q, \mathbf{m}^-)}{\# W_{\mathrm{per},\{1\}}(2q, \mathbf{m}^-)}. \tag{6.20}$$

Taking logarithms, dividing by $|\mathbf{m}^-|_{pr}$, letting $\mathbf{m}^- \to \infty$, and using (6.19) and the definition of $\overline{h}_{d-1}(m_1)$, we deduce the lower bound in (6.14) for the case $q \in \mathbb{N}$. If $q = 0$, we have to replace the denominators in (6.20) by $\operatorname{tr} I = 2^{\mathrm{vol}(\mathbf{m}^-)}$, and the lower bound in (6.14) is verified because $h_{d-1}(0)$ was defined to be $\log 2$. The lower bound in (6.15) is proved similarly.

We now prove the upper bound of (6.14). For each $\mathbf{m}' \in \mathbb{N}^{d-1}$ we have

$$\gamma(\mathbf{m}')^{2r} \leq \operatorname{tr} C(\mathbf{m}')^{2r} = \# W_{\mathrm{per},\{d\}}(\mathbf{m}', 2r) = \# W_{\mathrm{per},\{1\}}(2r, \mathbf{m}'),$$

where the inequality above is true because the eigenvalues of the symmetric matrix $C(\mathbf{m}')$ are real and $\gamma(\mathbf{m}')$ is one of them, the first equality follows from part (d) of Proposition 6.1, and the last equality from the invariance under coordinate permutations. Therefore

$$\frac{\log \gamma(\mathbf{m}')}{|\mathbf{m}'|_{pr}} \leq \frac{\log \# W_{\mathrm{per},\{1\}}(2r, \mathbf{m}')}{2r|\mathbf{m}'|_{pr}},$$

and letting $\mathbf{m}' \to \infty$, we deduce the upper bound of (6.14) by (6.19) and the definition of $\overline{h}_{d-1}(m_1)$. Similarly we deduce the upper bound of (6.15). □

The following theorem supplies practical upper and lower bounds for 2- and 3-dimensional monomer-dimer and dimer entropies.

Theorem 6.6 *Let $p, r, t, u, v \in \mathbb{N}$ and $q, s \in \mathbb{N} \cup \{0\}$. Then*

$$\frac{\log \beta(2r)}{2r} \geq h_2 \geq \frac{\log \beta(p+2q) - \log \beta(2q)}{p}, \quad \beta(0) = 2,$$
$$\frac{\log \widetilde{\beta}(2r)}{2r} \geq \widetilde{h}_2 \geq \frac{\log \widetilde{\beta}(p+2q) - \log \widetilde{\beta}(2q)}{p}, \quad \widetilde{\beta}(0) = 2,$$
$$\frac{\log \beta(2r, 2t)}{4rt} \geq h_3 \geq \frac{\log \beta(p+2q, u+2s) - \log \beta(p+2q, 2s)}{up} - \frac{\log \beta(2q, 2v)}{2vp},$$
$$\frac{\log \widetilde{\beta}(2r, 2t)}{4rt} \geq \widetilde{h}_3 \geq \frac{\log \widetilde{\beta}(p+2q, u+2s) - \log \widetilde{\beta}(p+2q, 2s)}{up} - \frac{\log \widetilde{\beta}(2q, 2v)}{2vp},$$
$$\beta(n, 0) = \beta(0, n) = \widetilde{\beta}(n, 0) = \widetilde{\beta}(0, n) = 2^n, \quad n \in \mathbb{N}.$$

Proof. The upper bounds in the above inequalities are the inequalities (6.16) and (6.17). We now show the lower bounds. Equations (6.2) and (6.6) for $d = 2$ yield

$$\overline{h}_1(m_1) = \log \beta(m_1), \quad \breve{h}_1(m_1) = \log \widetilde{\beta}(m_1), \quad m_1 \in \mathbb{N}. \tag{6.21}$$

Hence the lower bounds for $h_2, \widetilde{h}_2$ follow immediately from the lower bounds in (6.14), (6.15), equation (6.21) and the equalities $\overline{h}_1(0) = \breve{h}_1(0) = \log 2$.

In order to establish the lower bounds for h_3 and $\widetilde{h}_3$, we first establish lower and upper bounds for $\overline{h}_2(m_1)$ and $\breve{h}_2(m_1)$ in terms of $\beta(\cdot,\cdot)$ and $\widetilde{\beta}(\cdot,\cdot)$. The definition of $\overline{h}_2(m_1)$ and $\breve{h}_2(m_1)$ and equations (6.3) and (6.7) for $d = 3$ yield

$$\overline{h}_2(m_1) = \lim_{m_2\to\infty} \frac{\log \pi(\mathbf{m}')}{m_2}, \quad \breve{h}_2(m_1) = \lim_{m_2\to\infty} \frac{\log \widetilde{\pi}(\mathbf{m}')}{m_2}, \quad m_1 \in \mathbb{N}, \tag{6.22}$$

where $\mathbf{m}' = (m_1, m_2)$. Since $P(\mathbf{m}')$ is a nonnegative symmetric matrix with spectral radius $\pi(\mathbf{m}')$, it follows as in (3.8) and using part (c) of Proposition 6.1 that

$$\pi(\mathbf{m}')^u \geq \frac{\operatorname{tr} P(\mathbf{m}')^{u+2s}}{\operatorname{tr} P(\mathbf{m}')^{2s}} = \frac{\#W_{\mathrm{per},\{1,3\}}(\mathbf{m}', u+2s)}{\#W_{\mathrm{per},\{1,3\}}(\mathbf{m}', 2s)}.$$

Here $u \in \mathbb{N}$ and $s \in \mathbb{N} \cup \{0\}$. When $s = 0$, $\operatorname{tr} P(\mathbf{m}')^{2s} = 2^{\mathrm{vol}(\mathbf{m}')}$, and so this is the value we use for $\#W_{per,\{1,3\}}(\mathbf{m}', 0)$. Take logarithms of this inequality, divide by m_2 and send m_2 to ∞. Using (6.22) and (6.2) for $d = 3$, we deduce that

$$\overline{h}_2(m_1) \geq \frac{\log \beta(m_1, u+2s) - \log \beta(m_1, 2s)}{u}, \quad m_1 \in \mathbb{N}, \tag{6.23}$$

where $\beta(m_1, 0) := 2^{m_1}$. Similarly

$$\breve{h}_2(m_1) \geq \frac{\log \widetilde{\beta}(m_1, u+2s) - \log \widetilde{\beta}(m_1, 2s)}{u}, \quad m_1 \in \mathbb{N}, \tag{6.24}$$

where $\widetilde{\beta}(m_1, 0) := 2^{m_1}$. For $v \in \mathbb{N}$ we have the inequality $\pi(\mathbf{m}')^{2v} \leq \operatorname{tr} P(\mathbf{m}')^{2v} = \#W_{\mathrm{per},\{1,3\}}(\mathbf{m}', 2v)$. Take logarithms of this inequality, divide by $2vm_2$ and send m_2 to ∞. Using (6.22) and (6.2) for $d = 3$, we deduce that for $m_1 \in \mathbb{N}$

$$\overline{h}_2(m_1) \leq \frac{\log \beta(m_1, 2v)}{2v}. \tag{6.25}$$

Inequality (6.25) also holds for $m_1 = 0$ since by definition $\overline{h}(0) = \log 2$ and $\beta(0, 2v) = 2^{2v}$. Similarly, for $m_1 \in \mathbb{N} \cup \{0\}$

$$\breve{h}_2(m_1) \leq \frac{\log \widetilde{\beta}(m_1, 2v)}{2v}. \tag{6.26}$$

Now we can substitute the bounds (6.23) and (6.25) in the lower bound of (6.14) as appropriate from the signs in the numerator, and obtain the lower bound for h_3 as stated in the theorem, and similarly for $\widetilde{h}_3$. □

7 Using Automorphism Subgroups to Reduce Computations

The nonnegative matrix $B(\mathbf{m}')$ has order 2^n, where $n = \mathrm{vol}(\mathbf{m}')$, and so has 4^n entries. Since its (S, T) entries are positive precisely when $S \cap T = \emptyset$, the number of positive entries is $\sum \binom{n}{i} 2^{n-i} = 3^n$. Hence $B(\mathbf{m}')$ is sparse. However, already for

$\mathbf{m}' = (4,4)$, it has $4.3 \cdot 10^7$ nonzero entries, and the computation of its spectral radius is infeasible for a standard PC. Nevertheless, this computation can be reduced to computing the spectral radii of a suitable nonnegative matrix whose order is the number of orbits of the action of an automorphism subgroup of $B(\mathbf{m}')$. This usage of automorphisms is also used in [7] and [28].

Recall that given an $N \times N$ complex-valued matrix $A = (a_{ij})_1^N$, its automorphism group is the subgroup of the symmetric group S_N on $\langle N \rangle$ defined by

$$\mathrm{Aut}(A) := \{\pi \in S_N \ : \ a_{\pi(i)\pi(j)} = a_{ij} \text{ for all } i,j \in \langle N \rangle\}. \tag{7.1}$$

Let $\mathcal{G}$ be a subgroup of $\mathrm{Aut}(A)$. The action of $\mathcal{G}$ partitions $\langle N \rangle$ into minimal invariant subsets called *orbits*. We denote by $\mathcal{O} := \langle N \rangle / \mathcal{G}$ the orbit space (set of orbits), and by Greek letters $\mu, \nu, \ldots$ its members. We have

$$\sum_{j \in \nu} a_{ij} = \sum_{j \in \nu} a_{\pi(i)\pi(j)} = \sum_{k \in \nu} a_{\pi(i)k}, \qquad \mu, \nu \in \mathcal{O}, \ \ i \in \mu, \ \ \pi \in S_N, \tag{7.2}$$

which means that for given $\mu, \nu \in \mathcal{O}$, the sum $\Sigma_{j \in \nu} a_{ij}$ is the same for all $i \in \mu$. Let $M = \#\mathcal{O}$, and define the $M \times M$ matrix $\widehat{A} = (\widehat{a}_{\mu\nu})_{\mu,\nu \in \mathcal{O}}$ by

$$\widehat{a}_{\mu\nu} = \sum_{j \in \nu} a_{ij}, \quad i \in \mu. \tag{7.3}$$

This is a valid definition by (7.2).

Proposition 7.1 *Let $A = (a_{ij})_1^N$ be a complex-valued matrix. Let $\mathcal{G}$ be a subgroup of* $\mathrm{Aut}\, A$, *$\mathcal{O}$ its orbit space, and $M = \#\mathcal{O}$. Let $\widehat{A}$ be the induced $M \times M$ complex-valued matrix given by (7.3). Then the spectrum (set of eigenvalues) of $\widehat{A}$,* $\mathrm{spec}(\widehat{A})$, *is a subset of* $\mathrm{spec}(A)$, *and in particular $\rho(\widehat{A}) \le \rho(A)$. If A is a real-valued nonnegative matrix, then $\rho(\widehat{A}) = \rho(A)$. If A is real and symmetric, then $\widehat{A}$ is symmetric with respect to an appropriate inner product on $\mathbb{R}^M$, and in particular* $\mathrm{spec}(\widehat{A})$ *is real and $\widehat{A}$ is diagonalizable.*

Proof. Let Π_N be the group of $N \times N$ permutation matrices. Let $\iota : S_N \to \Pi_N$ be the standard representation of S_N. That is $\iota(\pi)(x_i)_{i \in \langle N \rangle} = (x_{\pi(i)})_{i \in \langle N \rangle}$. Let

$$\begin{aligned}\mathcal{X} &:= \{\mathbf{x} \in \mathbb{C}^N : \iota(\pi)(\mathbf{x}) = \mathbf{x} \text{ for all } \pi \in \mathcal{G}\} \\ &= \{(x_i)_{i \in \langle N \rangle} \in \mathbb{C}^N : x_{\pi(i)} = x_i \text{ for all } i \in \langle N \rangle, \pi \in \mathcal{G}\}\end{aligned}$$

be the subspace of vectors that are constant on each orbit of $\mathcal{G}$. Then $\mathcal{X} \subseteq \mathbb{C}^N$ is the largest subspace of $\mathbb{C}^N$ on which $\iota(\mathcal{G})$ acts trivially (as the identity operator). Clearly, $\mathcal{X}$ is isomorphic to $\mathbb{C}^M$. Indeed, each $\mathbf{x} = (x_i) \in \mathcal{X}$ induces a unique vector $\widehat{\mathbf{x}} := (\widehat{x}_\mu)_{\mu \in \mathcal{O}} \in \mathbb{C}^M$, where $\widehat{x}_\mu = x_i$ for any $i \in \mu$. Conversely, each $\mathbf{y} \in \mathbb{C}^M$ induces a unique $\mathbf{x} \in \mathcal{X}$ such that $\mathbf{y} = \widehat{\mathbf{x}}$. Next, we observe that $\mathcal{X}$ is an invariant subspace of A. Indeed, for each $\mathbf{x} = (x_i) \in \mathcal{X}$ and $\pi \in \mathcal{G}$ we have for all $i \in \langle N \rangle$

$$(A\mathbf{x})_i = \sum_{j=1}^N a_{ij} x_j = \sum_{j=1}^N a_{\pi(i)\pi(j)} x_{\pi(j)} = \sum_{k=1}^N a_{\pi(i)k} x_k = (A\mathbf{x})_{\pi(i)},$$

which means that $A\mathbf{x} \in \mathcal{X}$. Moreover, if $\mathbf{x} \in \mathcal{X}$ and $\widehat{\mathbf{x}} = (\widehat{x}_\mu) \in \mathbb{C}^M$ is defined as above, then for any $i \in \mu$ we have $(A\mathbf{x})_i = \sum_{\nu \in \mathcal{O}} \widehat{a}_{\mu\nu} \widehat{x}_\nu$, and consequently

$\widehat{A\mathbf{x}} = \widehat{A}\widehat{\mathbf{x}}$. This means that the action of $A|_{\mathcal{X}}$ is isomorphic the the action of $\widehat{A}$ on $\mathbb{C}^M$. In particular,

$$\operatorname{spec}(\widehat{A}) = \operatorname{spec}(A|_{\mathcal{X}}) \subseteq \operatorname{spec}(A),$$

and therefore

$$\rho(\widehat{A}) \le \rho(A).$$

Assume now that A is nonnegative. Then by the Perron-Frobenius Theorem, $\rho(A) \in \operatorname{spec}(A)$, and A has an eigenvector $\mathbf{x}$ belonging to $\rho(A)$. Since each $\pi \in \operatorname{Aut}(A)$ satisfies $A\iota(\pi) = \iota(\pi)A$, it follows that $\iota(\pi)\mathbf{x}$ is also an eigenvector of A belonging to $\rho(A)$. Hence $\sum_{\pi\in\operatorname{Aut}(A)} \iota(\pi)\mathbf{x} \in \mathcal{X}$ is an eigenvector of A belonging to $\rho(A)$. Therefore $\rho(A) \in \operatorname{spec}(A|_{\mathcal{X}}) = \operatorname{spec}(\widehat{A})$. It follows that $\rho(\widehat{A}) = \rho(A)$.

Finally, assume that A is a real symmetric matrix. That is $(A\mathbf{x}, \mathbf{y}) = (\mathbf{x}, A\mathbf{y})$, where $(\mathbf{x}, \mathbf{y}) = \mathbf{y}^\top \mathbf{x}$ is the standard inner product in $\mathbb{R}^N$. For each $\mu \in \mathcal{O}$, let w_μ be the cardinality of the orbit μ. In $\mathbb{R}^M$ we define the inner product

$$\langle \widehat{\mathbf{x}}, \widehat{\mathbf{y}} \rangle := \sum_{\mu\in\mathcal{O}} w_\mu \widehat{x}_\mu \widehat{y}_\mu. \tag{7.4}$$

Then all $\mathbf{x}, \mathbf{y} \in \mathcal{X}$ satisfy $(\mathbf{x}, \mathbf{y}) = \langle \widehat{\mathbf{x}}, \widehat{\mathbf{y}} \rangle$. Hence $\langle \widehat{A}\widehat{\mathbf{x}}, \widehat{\mathbf{y}} \rangle = \langle \widehat{\mathbf{x}}, \widehat{A}\widehat{\mathbf{y}} \rangle$, i.e., $\widehat{A}$ is symmetric (self adjoint) with respect to the inner product $\langle \cdot, \cdot \rangle$ in $\mathbb{R}^M$. In particular, $\widehat{A}$ has real eigenvalues and is similar to a diagonal matrix. □

We shall now briefly mention the power method for computing $\rho(A)$ where A is a nonnegative symmetric matrix of order N, and a variant of it that works on $\widehat{A}$ of order M, which we used in our computations.

Proposition 7.2 *Let A be a nonnegative symmetric matrix of order N. Choose a scalar $r > 0$ and a positive vector $\mathbf{x}_0 = (x_{0,1}, \dots, x_{0,N})^\top$. For each $m \in \mathbb{N}$, let*

$$\begin{aligned}
\mathbf{x}_m = (x_{m,1}, \dots, x_{m,N})^\top &:= (A + rI)\mathbf{x}_{m-1}, \\
l_m &:= \min_i \frac{x_{m,i}}{x_{m-1,i}}, \\
u_m &:= \max_i \frac{x_{m,i}}{x_{m-1,i}}, \\
r_m &:= \frac{(\mathbf{x}_m, \mathbf{x}_{m-1})}{(\mathbf{x}_{m-1}, \mathbf{x}_{m-1})}.
\end{aligned}$$

Then l_m is nondecreasing and u_m is nonincreasing in m,

$$\begin{gathered}
l_m \le r_m \le \rho(A) + r \le u_m, \qquad m \in \mathbb{N} \\
\lim_{m\to\infty} l_m = \lim_{m\to\infty} u_m = \rho(A) + r,
\end{gathered}$$

and $\mathbf{x}_m/\sqrt{(\mathbf{x}_m, \mathbf{x}_m)}$ converges to an eigenvector of A belonging to $\rho(A)$.

Furthermore, with the notation of Proposition 7.1, if we choose the vector $\mathbf{x}_0$ to be in $\mathcal{X}$, i.e., if $\mathbf{x}_0$ is constant on each orbit of $\mathcal{G}$, then for each $m \in \mathbb{N}$ the vector

$\mathbf{x}_m$ *is also in* $\mathcal{X}$ *(so* $\widehat{\mathbf{x}}_m$ *is defined),*

$$\begin{aligned}
\widehat{\mathbf{x}}_m &= (\widehat{A} + r\widehat{I})\widehat{\mathbf{x}}_{m-1}, \\
l_m &= \min_{\alpha \in \mathcal{O}} \frac{\widehat{x}_{m,\alpha}}{\widehat{x}_{m-1,\alpha}}, \\
u_m &= \max_{\alpha \in \mathcal{O}} \frac{\widehat{x}_{m,\alpha}}{\widehat{x}_{m-1,\alpha}}, \\
r_m &= \frac{\langle \widehat{\mathbf{x}}_m, \widehat{\mathbf{x}}_{m-1} \rangle}{\langle \widehat{\mathbf{x}}_{m-1}, \widehat{\mathbf{x}}_{m-1} \rangle},
\end{aligned}$$

and $\widehat{\mathbf{x}}_m / \sqrt{\langle \widehat{\mathbf{x}}_m, \widehat{\mathbf{x}}_m \rangle}$ *converges to an eigenvector of* $\widehat{A}$ *belonging to* $\rho(\widehat{A}) = \rho(A)$.

For $\mathbf{m}' \in \mathbb{N}^{d-1}$, let $G_T(\mathbf{m}')$ be the adjacency graph of the elements of the torus $T(\mathbf{m}')$. The automorphisms of $G_T(\mathbf{m}')$ act as automorphisms of the symmetric non-negative matrices $B(\mathbf{m}')$ and $\widetilde{B}(\mathbf{m}')$. In view of Proposition 7.2, in order to compute the spectral radii $\beta(\mathbf{m}')$ and $\widetilde{\beta}(\mathbf{m}')$, it is advantageous to use large automorphism subgroups of $G_T(\mathbf{m}')$. The rigid motions of the box $\langle \mathbf{m}' \rangle$ and of the torus $T(\mathbf{m}')$ are automorphisms of $G_T(\mathbf{m}')$.

The rigid motions of $\langle \mathbf{m}' \rangle$ contain: (a) the reflections across the hyperplanes $x_k = \frac{m_k+1}{2}$, $k \in \langle d-1 \rangle$, which commute with each other, and (b) the allowable transpositions, namely those that exchange x_i and x_j in case $m_i = m_j$. Thus if $\mathbf{m}' = m\mathbf{1}$, $m \geq 2$, then the group of rigid motions of the cube $\langle \mathbf{m}' \rangle$ contains a subgroup of order $2^{d-1}(d-1)!$. For $d = 2, 3$, which is our main focus in this paper, the reflections and allowable transpositions generate all the rigid motions of $\langle \mathbf{m}' \rangle$.

The rigid motions of $T(\mathbf{m}')$ contain, in addition to the rigid motions of $\langle \mathbf{m}' \rangle$, the unit translations $\mathbf{x} \mapsto \mathbf{x} + \mathbf{e}_k$, $k \in \langle d-1 \rangle$. The unit translations generate the group of translations, an Abelian group isomorphic to $(\mathbb{Z}/m_1\mathbb{Z}) \times \cdots \times (\mathbb{Z}/m_{d-1}\mathbb{Z})$ of order $\mathrm{vol}(\mathbf{m}')$. We call the group generated by the reflections, the allowable transpositions and the unit translations *the group of rigid motions of* $T(\mathbf{m}')$. Note that for $T(2)$ the reflection coincides with the unit translation, and similarly for $T(\mathbf{m}')$, if $m_k = 2$ then the reflection across $x_k = \frac{3}{2}$ coincides with the unit translation $\mathbf{x} \mapsto \mathbf{x} + \mathbf{e}_k$. We are aware of additional automorphisms of $G_T(\mathbf{m}')$ if at least two components of $\mathbf{m}'$ are equal to 4: observe that $G_T(4)$ is isomorphic to $G_T(2,2)$, since both are 4-cycles. Therefore $G_T(4,4)$ is isomorphic to $G_T(2,2,2,2)$, and its automorphism group has order at least $2^4 \cdot 4! = 384$, whereas the group of rigid motions of $T(4,4)$ has order $2^2 \cdot 2 \cdot 4^2 = 128$. Similar results hold for $d > 3$.

The following proposition is straightforward:

Proposition 7.3 *Let* $\Gamma_1, \ldots, \Gamma_d \subseteq \langle n \rangle \times \langle n \rangle$ *and* $\Gamma = (\Gamma_1, \ldots, \Gamma_d)$. *Let* $\mathbf{m} = (m_1, \ldots, m_d) \in \mathbb{N}^d$ *and* $\mathbf{m}' = (m_1, \ldots, m_{d-1})$, *and consider the transfer digraph* $\Theta_d(\mathbf{m}')$ *between members of* $W_{\mathrm{per}}(\mathbf{m}')$ *with respect to* Γ_d. *Then the group of translations of* $T(\mathbf{m}')$ *acts a subgroup of automorphisms of* $\Theta_d(\mathbf{m}')$. *If for some* $k \in \langle d-1 \rangle$ Γ_k *is symmetric, then the reflection across the hyperplane* $x_k = \frac{m_k+1}{2}$ *acts as an automorphism of* $\Theta_d(\mathbf{m}')$. *If for some* $p, q \in \langle d-1 \rangle$ $m_p = m_q$ *and* $\Gamma_p = \Gamma_q$, *then the transposition exchanging* x_p *and* x_q *acts as an automorphism of* $\Theta_d(\mathbf{m}')$.

Corollary 7.4 *Let* $\Gamma_1, \ldots, \Gamma_d \subseteq \langle n \rangle \times \langle n \rangle$, $\Gamma = (\Gamma_1, \ldots, \Gamma_d)$, *and assume that* $\Gamma_1, \ldots, \Gamma_{d-1}$ *are symmetric. Let* $\mathbf{m} = (m_1, \ldots, m_d) \in \mathbb{N}^d$ *and* $\mathbf{m}' = (m_1, \ldots, m_{d-1})$,

m_1	$\#\mathcal{O}(m_1)$	$\log\beta(m_1)$	$\frac{\log\beta(m_1)}{m_1}$
4	6	2.6532941163	.66332352908
5	8	3.3135066910	.66270133821
6	13	3.9769139475	.66281899125
7	18	4.6395628723	.66279469604
8	30	5.3023993987	.66279992338
9	46	5.9651887945	.66279875494
10	78	6.6279902386	.66279902386
11	126	7.2907885674	.66279896067
12	224	7.9535877093	.66279897578
13	380	8.6163866375	.66279897212
14	687	9.2791856222	.66279897301
15	1224	9.9419845918	.66279897279
16	2250	10.60478356551861	.662798972844913
17	4112	11.267582538126	.66279897283094

Table 1: Spectral radii for h_2

and assume that for all $p, q \in \langle d-1\rangle$, $\Gamma_p = \Gamma_q$ if $m_p = m_q$. Then the automorphism subgroup of $G_T(\mathbf{m}')$ described above acts as an automorphism subgroup of the transfer digraph $\Theta_d(\mathbf{m}')$.

As an example, consider the upper and lower bounds given by (3.10). The parameter $\theta_2(m)$ appearing there is the spectral radius of the matrix $B(m)$ defined in Section 6, which has an automorphism subgroup of order $2m$, isomorphic to the group of rigid motions of $T(m)$, if $m > 2$. $B(15)$ is $2^{15} \times 2^{15}$, but as we shall see, $\widehat{B}(15)$ is 1224×1224, which makes the computation of its spectral radius feasible on a regular desktop computer.

These observations are our main keys in finding good upper and lower bounds for h_2 and h_3. We point out that [7] was the first work that used these automorphisms of $\widetilde{B}(\mathbf{m}')$ to help obtain a good upper bound for $\widetilde{h}_3$, which was later improved in [28] by similar methods.

8 Numerical Results for Monomer-Dimer Entropy in Two and Three Dimensions

Our results are based on Theorem 6.6, and we compute the spectral radii appearing there using Propositions 7.1 and 7.2, and the automorphism subgroups described in Section 7. We first consider the two-dimensional monomer-dimer entropy. Recall that $\beta(m_1)$ is the spectral radius of $B(m_1)$. Table 1 lists $\log\beta(m_1)$, $\frac{\log\beta(m_1)}{m_1}$, and the number $\#\mathcal{O}(m_1)$ of orbits of the torus $T(m_1)$ under the action of the group of rigid motions of $T(m_1)$. We notice that the sequence $\frac{\log\beta(2r)}{2r}$ is decreasing for $r = 2, \ldots, 8$. Hence $h_2 \le \frac{\log\beta(16)}{16} = .662798972844913$ is the best upper bound for h_2 from our data. The best lower bound for h_2 from our data is $h_2 \ge \frac{\log\beta(17) - \log\beta(16)}{1} = .662798972607$. This improves the lower bound (5.7) from permanents by more than

m_1	$\#\mathcal{O}(m_1)$	$\log\widetilde{\beta}(m_1)$	$\frac{\log\widetilde{\beta}(m_1)}{m_1}$
4	6	1.316957897	.3292
5	8	1.404661127	.2809
6	13	1.843797237	.3073
7	18	2.003260294	.2862
8	30	2.400842203	.3001
9	46	2.594837310	.2883
10	78	2.969359257	.2969
11	126	3.183303939	.2894
12	224	3.543130579	.2953
13	380	3.770113562	.2900
14	687	4.119721251	.2943
15	1224	4.355934472	.2904

Table 2: Spectral radii for $\widetilde{h}_2$

4%. Hence we obtain the value

$$h_2 = .6627989727 \pm .0000000001, \tag{8.1}$$

with 9 correct digits. We also notice that the sequence $\frac{\log\beta(2j+1)}{2j+1}$ is increasing for $j = 2, \ldots, 8$. Suppose that this sequence were increasing for all values of j. Since $\lim_{j\to\infty} \frac{\log\beta(2j+1)}{2j+1} = h_2$ by (6.19), it would follow that $h_2 \geq \frac{\log\beta(17)}{17} = .66279897283094$, so the above hypothesis would give the value $h_2 = .6627989728$ with 10 correct digits, consistent with the value found by Baxter [1]. (Baxter's value of h_2 is accurate to 8 digits, as can be seen by evaluating $\log\frac{\kappa}{s}$ for $s = 1$ in his Table II and varying the last digit of the tabulated $\frac{\kappa}{s}$.) Since the lower bound (5.7) for h_2 is quite close to the correct value of h_2, it is reasonable to assume that the value p^*, for which $\lambda_2(p^*) = h_2$, is fairly close to $p(2) = \frac{9-\sqrt{17}}{8} \sim 0.6096118$. (According to [1], $p^* = 0.63812311$.)

As a check, Table 2 gives $\widetilde{\beta}(m_1)$, the spectral radius of $\widetilde{B}(m_1)$, yielding lower and upper bounds for the known entropy $\widetilde{h}_2 = 0.29156090\ldots$. Again, the sequence $\frac{\log\widetilde{\beta}(2r)}{2r}$ decreases for $r = 2, \ldots, 7$ and the sequence $\frac{\log\widetilde{\beta}(2j+1)}{2j+1}$ increases for $j = 2, \ldots, 7$. Thus the best upper bound for $\widetilde{h}_2$ from our data is $\frac{\log\widetilde{\beta}(14)}{14} = .2943$, which is larger by 0.9% than the true value. The best lower bound is $\frac{\log\widetilde{\beta}(14)-\log\widetilde{\beta}(12)}{2} = 0.2883$, which is smaller by 1.1% than the true value. We notice that $\frac{\log\widetilde{\beta}(15)}{15} = .2905 < \widetilde{h}_2$, consistent with the assumed fact that $\frac{\log\widetilde{\beta}(2j+1)}{2j+1}$ increases for all j.

We now consider the three-dimensional monomer-dimer entropy h_3. Recall that $\beta(m_1, m_2) = \beta(m_2, m_1)$ is the spectral radius of $B(m_1, m_2)$. Table 3 gives $\log\beta(m_1, m_2)$, $\frac{\log\beta(m_1,m_2)}{m_1 m_2}$, and the number $\#\mathcal{O}(m_1, m_2)$ of orbits of the torus $T(m_1, m_2)$ under the action of the group of rigid motions of $T(m_1, m_2)$. (In the case $(m_1, m_2) = (4, 4)$, we recall that the group of rigid motions of $T(2, 2)$ has order 128, and it turns out to have 805 orbits. We also did the computations with the larger automorphism subgroup of $G_T(4, 4)$ of order 384 discussed in Section 7, which turns out to have 402 orbits. Both computations gave the same value of $\beta(4, 4)$.)

(m_1, m_2)	$\#\mathcal{O}(m_1, m_2)$	$\log\beta(m_1, m_2)$	$\frac{\log\beta(m_1,m_2)}{m_1 m_2}$
$(2,2)$	6	3.224405658	.8061014145
$(3,2)$	13	4.768958913	.7948264855
$(4,2)$	34	6.367778959	.7959723699
$(5,2)$	78	7.958105292	.7958105292
$(6,2)$	237	9.550024542	.7958353785
$(7,2)$	687	11.14163679	.7958311993
$(8,2)$	2299	12.73331093	.7958319331
$(3,3)$	25	7.057039652	.7841155169
$(4,3)$	158	9.421594940	.7851329117
$(5,3)$	708	11.77517604	.7850117360
$(4,4)$	805	12.57923752	.7862023450

Table 3: Spectral radii for h_3

(m_1, m_2)	$\#\mathcal{O}(m_1, m_2)$	$\log\widetilde{\beta}(m_1, m_2)$	$\frac{\log\widetilde{\beta}(m_1,m_2)}{m_1 m_2}$
$(2,2)$	6	2.292431670	.5731079175
$(3,2)$	13	3.068671222	.5114452037
$(4,2)$	34	4.151763891	.5189704864
$(5,2)$	78	5.119835223	.5119835223
$(6,2)$	237	6.161467494	.5134556245
$(7,2)$	687	7.168058989	.5120042135
$(3,3)$	25	3.938705096	.4376338996
$(4,3)$	158	5.365527945	.4471273287
$(5,3)$	708	6.635849120	.4423899413
$(4,4)$	805	7.409698288	.4631061430
$(6,3)$	4236	7.97716207	.443175671
$(6,4)$	184854	10.98112634	.4575469308

Table 4: Spectral radii for $\widetilde{h}_3$

Recall that $h_3 \leq \frac{\log\beta(2r,2t)}{4rt}$, and hence the best upper bound for h_3 from our data is $\frac{\log\beta(4,4)}{16} = 0.7862023450$. The best lower bound is $\frac{\log\beta(3,5)-\log\beta(3,4)}{1\cdot 1} - \frac{\log\beta(2,8)}{8\cdot 1} = .761917234$. It turns out that the lower bound (5.8) is better: $h_3 \geq .7652789557$. Of course, had we computed $\beta(m_1, m_2)$ for larger m_1 and m_2, we would eventually improve (5.8). Thus, the best estimates we have are

$$.7652789557 \leq h_3 \leq .7862023450. \tag{8.2}$$

Table 4 lists $\widetilde{\beta}(m_1, m_2)$, the spectral radius of $\widetilde{B}(m_1, m_2)$, which give bounds for $\widetilde{h}_3$. The entry $(m_1, m_2) = (6, 4)$ is taken from [28], which took advantage of the fact that the matrix of order 184854 is a direct sum of 3 matrices. The best upper bound for $\widetilde{h}_3$ is $\frac{\log\widetilde{\beta}(6,4)}{6\cdot 4} = 0.4575469308$, which was reported in [28]. The best lower bound from the data is given by $\frac{\log\widetilde{\beta}(4,6)-\log\widetilde{\beta}(4,4)}{2\cdot 2} - \frac{\log\widetilde{\beta}(2,6)}{6\cdot 2} = .3794013885$, which is a weak lower bound. The best lower bound for $\widetilde{h}_3$ is given by (5.4): $\widetilde{h}_3 \geq 0.4400758$.

We now compare our results for h_2 with the results of [21]. On page 342, Hammersley and Menon tabulate estimates of $\lambda_2(p)$ computed by the Monte Carlo method in increments of 0.05 for $0 \le p \le 1$. The maximal value in their table is .6676 for $p = 0.65$. Hammersley and Menon state, "There are reasons for believing that this Monte Carlo estimate has a small negative bias, probably 1% or 2% too low.". However, since $\lambda_2(p) \le h_2 = .66279897$, the Monte Carlo estimate for $\lambda_2(0.65)$ is at least 0.7% higher than the true value.

We conclude with a comparison of several lower bounds for the monomer-dimer entropy with dimer density p, $\lambda_d(p)$, for $d = 2, 3$. Hammersley and Menon [21] give a lower bound for $\lambda_d(p)$, graphed and tabulated in increments of 0.05, for $0 \le p \le 1$. Bondy and Welsh [5] give another lower bound for $\lambda_d(p)$ that depends on the dimer entropy $\lambda_d(1)$ and increases with it. Since $\lambda_3(1)$ is known only through upper and lower bounds, the bound of [5] improves each time a better lower bound for $\lambda_d(1)$ is found. We computed the lower bound of [5] for $\lambda_3(p)$ using the best available lower bound $\lambda_3(1) = \widetilde{h}_3 \ge 0.4400758$. Hammersley and Menon too tabulated and graphed the bound of [5] for $\lambda_3(p)$, but at the time the available lower bound for $\lambda_3(1)$ was weaker. Figures 2 and 3 illustrate the lower bounds for $\lambda_d(p)$, $d = 2, 3$, due to [21], [5], and Theorem 5.2. Figure 2 also illustrates the Monte Carlo estimates of [21]. It is seen that except for very high p, the best lower bound is given by Theorem 5.2. (As pointed out above, (8.1) implies that the Monte Carlo estimates above the line $y = h_2$ are over estimates.) We also include in the figure estimates of $\lambda_2(p)$ obtained from the heuristic computations of Baxter [1]. One can obtain from the lower bound of [34] a corresponding lower bound for $\lambda_d(p)$. It turns out that for $d = 2, 3$, this bound is dominated by the maximum of the lower bound given by Theorem 5.2 and the lower bound of [5].

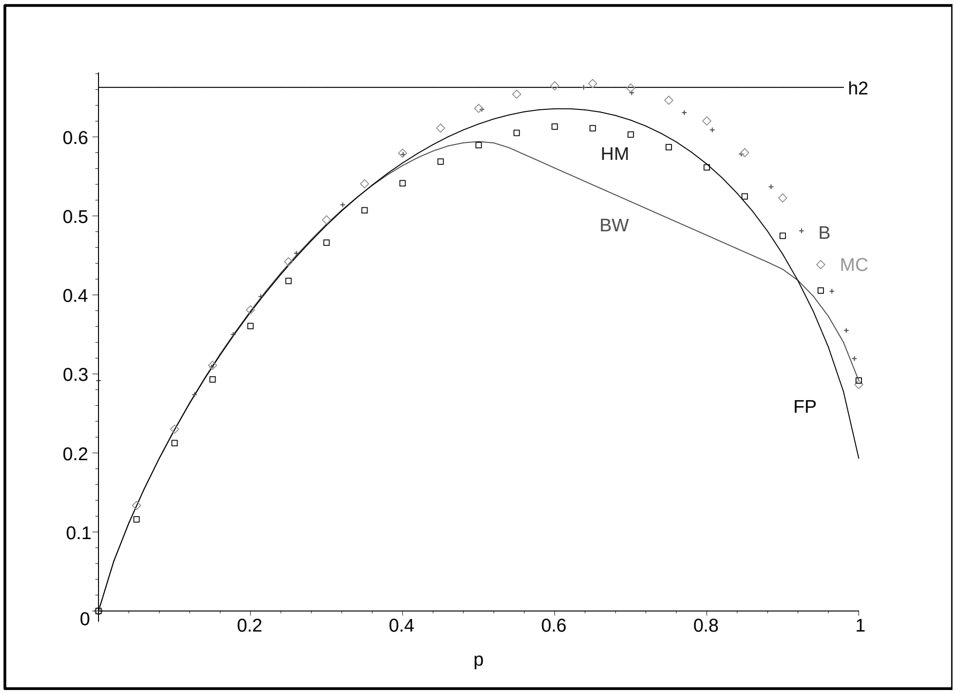


Figure 2: Lower bounds and estimates for $\lambda_2(p)$. HM is the lower bound of [21], BW is the lower bound of [5], FP is the lower bound of Theorem 5.2, MC is the Monte Carlo estimate of [21], B is the estimate from [1], and h2 is the true value of $h_2 = \max \lambda_2(p)$.

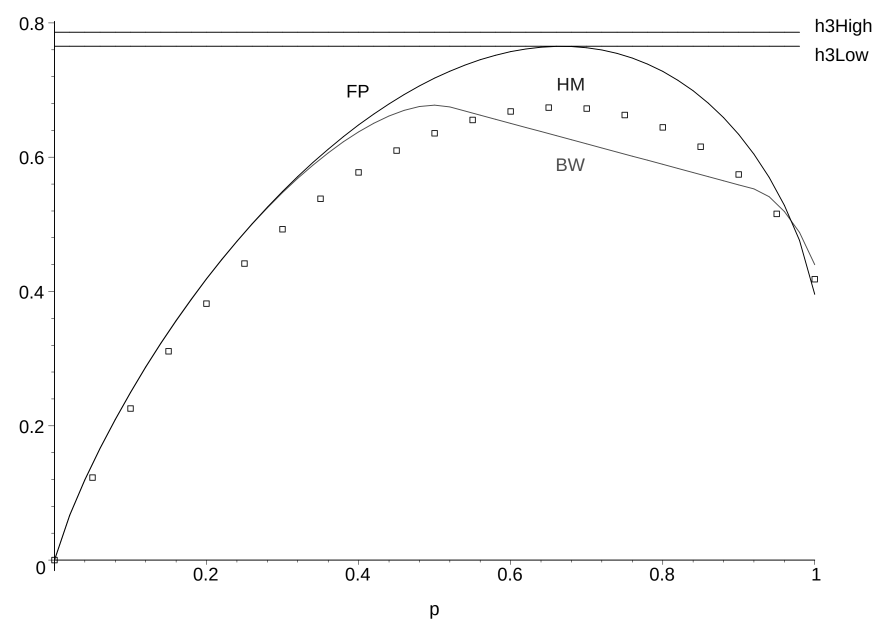


Figure 3: Lower bounds for $\lambda_3(p)$. HM is the lower bound of [21], BW is the lower bound of [5], FP is the lower bound of Theorem 5.2, h3Low and h3High are the best lower and upper bounds for $h_3 = \max \lambda_3(p)$.

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