Combinatorial and Computational Aspects of the Monomer-Dimer Problem: Extended abstract

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The exponential growth rate h (with respect to the natural logarithm) of the number of configurations on a multi-dimensional grid arises in the theory of various phenomena [3]. In physics e^h is viewed as the entropy (per atom) of the corresponding "hard model"; in mathematics h is called the *topological entropy* [5]; and in information theory h (with respect to $\log_2$) is called the *multi-dimensional capacity* [12]. In the 1-dimensional case e^h is equal to the spectral radius $\rho(\Gamma)$ of certain digraph Γ. There are very few 2-dimensional model where the value of h is known in closed form. In [7] we give a complete up-to-date theory of the computation of h by using lower and upper bounds that converge to h. It refines the techniques described in [6] by using an automorphism subgroup of a certain graph. As a demonstration of these techniques, we compute the topological entropy of the monomer-dimer covers of the 2-dimensional grid to 8 decimal digits and of the 3-dimensional grid with an error smaller than 1.35%.

Let $\mathbb{Z}^d$ be the grid of integer points in d-dimensional space $\mathbb{R}^d$. 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. In other words, h_d is the limit of the logarithm of the number of monomer-dimer covers of a box in $\mathbb{Z}^d$ divided by the volume of the box, as the dimensions of the box grow to infinity; and similarly for $\widetilde{h}_d$. It is straightforward 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 [2]. The exact values of h_d for $d \geq 2$ and $\widetilde{h}_d$ for $d \geq 3$ are unknown.

It was shown in [8] 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 $\lambda_d(1) = \widetilde{h}_d$. We show that $h_d = \max_{p\in[0,1]} \lambda_d(p)$. The van der Waerden conjecture for permanents of doubly-stochastic matrices gives a lower bound on $\widetilde{h}_d$. The improved lower bound for the permanents of 0-1 matrices [11] gives the currently best lower bound $\widetilde{h}_3 \geq 0.440075$. A recent breakthrough [1] gives the upper bound $0.463107 \geq \widetilde{h}_3$, improved to $0.457547 \geq \widetilde{h}_3$ by Lundow [10].

In [7] it is to shown that the entropies h_d and $\widetilde{h}_d$ obey upper and lower bounds similar to the upper and the lower for the entropy of configurations with the symmetric isotropic nearest neighbor graph. The bounds for h_d are stated in terms of the spectral radii of certain multigraphs whose automorphism group has a subgroup isomorphic to the the group of rigid motions of the $(d-1)$-dimensional torus $(\mathbb{Z}/m_1\mathbb{Z}) \times \cdots \times (\mathbb{Z}/m_{d-1}\mathbb{Z})$. 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 [4]. In particular, these lower bounds yield a lower bound for h_d. For $d = 2$ this lower bound is somewhat weaker than the one obtained from the numerical computations, but for $d = 3$ the situation is reversed.

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