Dimer coverings on random multiple chains of planar honeycomb lattice

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The problem of counting dimer coverings on random graphs has been intensively studied for a long time by mathematicians and computer scientists [1, 2, 3]. In the statistical physics language, the logarithm of the expectation $\mathbb{E}(\mathcal{K}(G))$ on random graph G is also called the annealed entropy of G. In, [1], Zdeborová and Mézard studied the annealed entropy on random regular and Erdös-Rényi random graphs by means of the cavity method, in which an analytic result for the entropy in random regular and Erdös-Rényi random graph had been obtained. But it is clear that most of the samples of these two types of random graph are far away from molecular graph.

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Stimulated by the widely existence of benzenoid hydrocarbons [4] and the produce of two-dimensional material graphene [5]. We consider a particular random planar honeycomb lattice model whose samples existed in the real would. The growth procedure of the model is inspired by the growth of single walledgraphene zigzag nanotubes [5]. In our knowledge this random model is the first one whose sample is existed in the real world.

In statistical physics a dimer represents a diatomic molecule. The dimer model was firstly considered by Roberts in 1935 [6], and by Fowler and Rushbrook [7], which was introduced in order to describe the absorption of diatomic molecules on crystal surface. In graph theoretic terms, a dimer is a molecule which can be placed on a graph G such that it covers an edge and the two incident vertices. A dimer arrangement is a set of dimers placed on G such that no vertex is covered by more than one dimer. A dimer arrangement which covers all vertices in G is called a (pure) dimer covering, or *perfect matching* in terms of graph theory. The dimer model is a classical statistical mechanics model dealing with the set of all dimer coverings of a graph [8].

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Historically the underlying graph for dimer covering problem is taken to be a regular lattice in two dimensions, e.g., the square grid, the honeycomb lattice, or a finite part of such a lattice. The dimer model for planar quadratic lattice were considered by Kasteleyn [9] and by Temperley and Fisher independently in the 1960's who computed the partition function [10, 11] by using different methods and arrived at the same results. Later in [12], Elkies et al. provided a proof for the explicit expression of the number of dimers on Aztec diamond. In [13] Sachs and Zeritz obtained the entropy constant of dimers of another type of finite plane quadratic lattices.

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Based on these results, it could be observed that the shape of the boundary of planar quadratic lattices has a strong effect on its free energy per dimer while the other types of lattices are different. Another similar phenomenon pointed out by Propp [14] and Klein [15] is that the shape of the boundary of a finite sub-region of a quadratic planar lattice has a strong effect on the local entropy and local statistics (frequencies of local patterns) of a random dimer configuration. Many fundamental observations about the dimer and monomer-dimer model in general lattice graphs have been given by Heilmann and Lieb [16, 17].

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As the carbon atom framework of a typical benzenoid hydrocarbon compound, the honeycomb lattice received particular interests from chemists and mathematicians. A large number of works on determining K, i.e., the number of perfect matchings, for various honeycomb lattices were established in literature, e.g., in [4, 18] and the references cited therein. In [19], Klein considered the long-range order for spin pairing in valence bond theory in which three types of dimers are distinguished. Klein et al. also found some further results for the honeycomb lattice strips of arbitrary widths, arbitrary lengths, and arbitrary long-range-order values [20, 21].

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The above results show that the shape of the boundary of a planar honeycomb lattice has a strong effect on its free energy per dimer. For details, we may refer to a survey article of Kenyon [30], in which the boundary effects in, and methods for, planar lattices are summarized.

The *partition function* of the dimer model was introduced as to distinguish various type of dimers, which could be viewed as a density function of energy levels. For the planar honeycomb lattice, Elser studied the partition function by using generating function approach and gave the expression for the hexagon shaped honeycomb lattice [23]. In general, Yan, Yeh and Zhang [18] gave an unified expression of the partition functions for honeycomb lattice, which distinguishes the three types of dimers with different thermodynamic activities. Based on this partition function, they established an algebraic solution to the free energy per dimer for many types of planar honeycomb lattices with fixed shape of boundaries.

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We denote by L_n the straight condensed hexagonal chain of n hexagons and, for convenience, we always place L_n in such a position that its interior edges are vertical. A two-layer multiple chain $H_{2,n}$ is constructed by fusing two copies of L_n . There are two ways of fusing: one is called the α -type fusion, as shown in Figure 1(a) and the other is called the β -type fusion, as shown in Figure 1(b).



Figure 1

We denote by $[L_n]_{\theta}$ the two-layer multiple chain obtained by the θ -type fusion and call the second layer (bottom) the θ -type, where $\theta \in {\alpha, \beta}$. A multiple chain with *m* layers is therefore constructed by successively fusing *m* copies of L_n and is denoted by $H_{m,n} = [\cdots [[[L_n]_{\theta_1}]_{\theta_2}] \cdots]_{\theta_{m-1}}$, or $H_{m,n} = \theta_1 \theta_2 \cdots \theta_{m-1}$ for short, where $\theta_i \in {\alpha, \beta}$ and $i = 1, 2, \cdots, m-1$. Similarly, we call the *i*-th layer in such $H_{m,n}$ the θ_{i-1} -type, $i = 2, 3, \cdots, m$. The multiple chain $\alpha \alpha \beta \beta \alpha$ with n = 6 is depicted in Figure 2.

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Let us consider the vertical edges in each layer. An edge *b* is said to be a dimer edge of a dimer covering *K* if *b* is covered by a dimer in *K*, see Figure 2. It could be observed that there is exactly one dimer edge in each layer for any dimer covering *K*, for details we may refer to [20]. Let the vertical edges in each layer be numbered by $1, 2, 3, \dots, n + 1$, in an order from the left to the right. Let $K(H_{m,n}, i)$ be the number of dimer coverings of $H_{m,n}$ which contain the *i*-th vertical edge in the *m*-th layer.

Since $H_{m,n}$ is a bipartite graph, we may color its vertices using two colors, say the black and the white, such that the adjacent vertices have different colors, as illustrated in Figure 2. Let (i, s)and (i - 1, t) be the unique dimer edges in the *i*-th and (i - 1)-th layer of a dimer covering K, respectively. For convenience, we label the black vertices incident to the vertical edges in the *i*-th layer by $b_1, b_2, \cdots, b_{n+1}$ in an order from the left to the right, respectively. Similarly, we label the white vertices incident to the vertical edges in the (i-1)-th layer by w_1, w_2, \dots, w_{n+1} , as shown in Figure 2.

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Assume that the *i*-th layer is of β -type as illustrated in Figure 2. Since (i, s) is the unique dimer edge in the *i*-th layer, b_{n+1} must match w_{n+1} (i.e., $b_{n+1}w_{n+1}$ must be a dimer edge) and therefore, b_n must match w_n . In this way, b_j must match w_j for each $j \in \{s + 1, s + 2, \cdots, n + 1\}$. This means that the unique dimer edge (i - 1, t) in the (i - 1)-th layer must locate at the left-hand side of the edge (i - 1, s + 1) (also the edge (i, s)), i.e., $t \leq s$. The discussion is similar if the *i*-th layer is of α -type.

Conversely, if we choose one vertical edge from each layer as a dimer edge such that the dimer edge in the (i - 1)-th layer $(i \in \{2, 3, \dots, m\})$ locates at the left-hand (resp., right-hand) side of the dimer edge in the *i*-th layer if the *i*-th layer is of β -type (resp., α -type), then these dimer edges determine an unique dimer covering. Let $H_{m-1,n}$ be obtained from $H_{m,n}$ by removing the last layer. Then the above argument shows that:

If the *m*-th layer of $H_{m,n}$ is of α -type, then

$$K(H_{m,n},i) = \sum_{j=i}^{n+1} K(H_{m-1,n},j)$$

and if the *m*-th layer of $H_{m,n}$ is of β -type, then

$$K(H_{m,n},i) = \sum_{j=1}^{i} K(H_{m-1,n},j).$$

Proposition 2.1. Let

 $V(H_{m,n}) = (K(H_{m,n}, 1), K(H_{m,n}, 2), \cdots, K(H_{m,n}, n+1))$. If the *m*-th layer is of α -type then $V(H_{m,n}) = V(H_{m-1,n})M_{\alpha}$ and if the m-th layer is of β -type then $V(H_{m,n}) = V(H_{m-1,n})M_{\beta}$, where M_{α} and M_{β} are the transfer matrices defined by

In the following, we will consider to generate $H_{m,n}$ randomly subject to the Bernoulli distribution on the two types of fusing. That is, the probability that the α -type fusing occurs in each layer is equal to a constant, say $p \in [0, 1]$, which is independent to the parameter m. Correspondingly, the probability that the β -type fusing occurs in each layer is equal to the constant 1 - p. In this way, we get the ensemble of random multiple chains $H_{m,n}$ and denote it by $\mathcal{H}(m, n, p)$. Let $\mathbb{E}(K(H_{m,n}))$ (or \mathbb{E}_m for simplicity) and $\mathbb{E}(K(H_{m,n},i))$ (or $\mathbb{E}_m(i)$ for simplicity) be the expected values of $K(H_{m,n})$ and $K(H_{m,n},i)$, respectively, where $i = 1, 2, \cdots, n+1$. Let $M_p = pM_\beta + (1-p)M_\alpha$.

Theorem 2.1. Let $H_{m,n} \in \mathcal{H}(m, n, p)$. Then

$$\mathbb{E}(K(H_{m,n})) = UM_p^{m-1}U^T,$$

where $U = (1, 1, \dots, 1)$ and U^T is the transpose of U.

By the linear algebra theory, the power of M_p could be represented in terms of the eigenvalues of M_p . To this end, we have the following proposition.

Proposition 2.2. The characteristic polynomial of the transfer matrix M_p is

$$P(\lambda) = \det(\lambda I - M_p)$$

= $(\lambda - 1)(\lambda - 1 + p)^n - p \sum_{i=1}^n (\lambda - p)^i (\lambda - 1 + p)^{n-i}$

and the largest (in modulus) eigenvalue of M_p is

$$\lambda_{\max} = \begin{cases} 1, & \text{if } p = 0, 1, \\ 1 + \frac{1}{2}n, & \text{if } p = \frac{1}{2}, \\ \frac{pq - q + p}{1 - q}, & \text{otherwise,} \end{cases}$$
(1)

where $q = (\frac{1}{p} - 1)^{\frac{1}{n+1}}$. 张 福 基(合作者: 任海珍,钱建国) Dimer covering

Dimer coverings on random multiple chains of planar honeycon

Applying Cayley-Hamilton Theorem to M_p , we have

$$M_P^{n+1} + c_1 M_P^n + c_2 M_P^{n-1} + \dots + c_n M_P + c_{n+1} I = O,$$

where *I* is the $(n + 1) \times (n + 1)$ identity matrix, *O* is the $(n + 1) \times (n + 1)$ matrix of all 0's and c_i is the coefficient of λ^i in (2), $i = 1, 2, \dots, n + 1$. Then by Theorem 2.1, we get the recurrence relation of the form

$$\mathbb{E}_{m} + c_{1}\mathbb{E}_{m-1} + c_{2}\mathbb{E}_{m-2} + \dots + c_{n}\mathbb{E}_{m-n} + c_{n+1}\mathbb{E}_{m-n-1} = 0.$$
(2)

By Proposition 2.2 and the theory of linear difference equation with constant coefficients, the homogeneous solution of (2) is given by:

Case 1. If p = 0 or 1 then is

$$\mathbb{E}(\mathcal{K}(\mathcal{H}_{m,n})) = \sum_{k=1}^{n+1} a_k m^{n+1-k} 1^m,$$

where a_k are the constant coefficients, $k = 1, 2, \dots, n+1$. Case 2. If $p = \frac{1}{2}$ then

$$\mathbb{E}(\mathcal{K}(\mathcal{H}_{m,n})) = b_{n+1}\left(\frac{1}{2}\right)^m + \sum_{k=1}^n b_k m^{n-k} \left(1+\frac{n}{2}\right)^m,$$

where b_k are the constant coefficients, $k = 1, 2, \dots, n + 1$.

Case 3. If $p \neq 0, 1, \frac{1}{2}$, then

$$\mathbb{E}(K(H_{m,n})) = \sum_{t=1}^{\frac{n}{2}} (a_t(b_t - il_t)^m + a'_t(b_t + il_t)^m) + a_0 \left(\frac{pq - q + p}{1 - q}\right)^m$$

if n is even and

$$\mathbb{E}(K(H_{m,n})) = \sum_{t=1}^{\frac{n+1}{2}-1} (a_t(b_t - il_t)^m + a_t'(b_t + il_t)^m) + a_0 \left(\frac{pq - q + p}{1 - q}\right)^m + a_{n+1} \left(\frac{-pq + q + p}{1 + q}\right)^m$$

if *n* is odd, where a_0 , a_{n+1} , a_t , a'_t , b_t and l_t , $t = 1, 2, \dots, \frac{n}{2}$ are the constant coefficients, $q = (\frac{1}{p} - 1)^{\frac{1}{n+1}}$ and $b_t \pm i l_t$ are conjugate complex roots.

From the above discussion, we can now give the asymptotic property of the annealed entropy:

$$\lim_{m,n\to\infty}\frac{2}{M}\log(\mathbb{E}(\mathcal{K}(H_{m,n})))=0.$$

2. If *m* is fixed,

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$$\lim_{n\to\infty}\frac{2}{M}\log(\mathbb{E}(K(H_{m,n}))) = \lim_{n\to\infty}\frac{m}{mn+m+n}\log(n+1) = 0.$$

3. If *n* is fixed, then

$$\lim_{m \to \infty} \frac{2}{M} \log(\mathbb{E}(K(H_{m,n}))) = \begin{cases} 0, & \text{if } p = 0, 1, \\ \frac{1}{(1+n)} \log(1 + \frac{1}{2}n), & \text{if } p = \frac{1}{2}, \\ \frac{1}{(1+n)} \log \frac{pq - q + p}{1 - q}, & \text{otherwise,} \end{cases}$$

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where
$$q = \left(\frac{1}{p} - 1\right)^{\frac{1}{n+1}}$$
.

We now present some numerical results of $K(H_{m,n})$ for the multiple chains $H_{m,n}$ and $\mathbb{E}(K(H_{m,n}))$ for random multiple chain $H_{m,n} \in \mathcal{H}(m, n, p)$. Note that

$$K(H_{m,n}) = K(H_{m,n}, 1) + K(H_{m,n}, 2) + \cdots + K(H_{m,n}, n+1).$$

Then $K(H_{m,n})$ can be calculated by applying Proposition 2.1 and the numerical result for n = 3 and $m \le 7$ is presented in Table 1. The expected value $\mathbb{E}(K(H_{m,n}))$ for random multiple chain $H_{m,n} \in \mathcal{H}(m, n, p)$ is calculated by applying Theorem 2.1 and the numerical result for n = 3 and $m \le 7$ is presented in Table 2, in which we choose the probability $p = 0.1 \times i, i = 0, 1, 2, \cdots, 10$. The asymptotic behavior is illustrated in Figure 3.

Numerical results

т	H _{m,3}	$K(H_{m,3})$	H _{m,3}	$K(H_{m,3})$	H _{m,3}	$K(H_{m,3})$	H _{m,3}	$K(H_{m,3})$
1	L ₃	4						
2	α	10						
3	$\alpha \alpha$	20	$\alpha\beta$	30				
4	ααα	35	$\alpha\beta\alpha$	85	$\alpha \alpha \beta$	65	$\alpha\beta\beta$	65
5	αααα	56	$\alpha\beta\alpha\alpha$	179	$\alpha \alpha \beta \alpha$	179	$\alpha\beta\beta\alpha$	206
	$\alpha \alpha \alpha \beta$	119	$\alpha\beta\alpha\beta$	246	$\alpha \alpha \beta \beta$	146	lphaetaetaeta	119
6	ααααα	84	$\alpha\beta\alpha\alpha\alpha$	322	$\alpha \alpha \beta \alpha \alpha$	372	$\alpha\beta\beta\alpha\alpha$	457
	$\alpha \alpha \alpha \beta \alpha$	322	$\alpha\beta\alpha\beta\alpha$	707	$\alpha \alpha \beta \beta \alpha$	457	$\alpha\beta\beta\beta\alpha$	399
	$\alpha \alpha \alpha \alpha \alpha \beta$	196	$\alpha\beta\alpha\alpha\beta$	573	$\alpha \alpha \beta \alpha \beta$	523	$\alpha\beta\beta\alpha\beta$	573
	$\alpha \alpha \alpha \beta \beta$	273	$\alpha\beta\alpha\beta\beta$	523	$\alpha \alpha \beta \beta \beta$	273	$\alpha\beta\beta\beta\beta\beta$	196
7	αααααα	120	$\alpha\beta\alpha\alpha\alpha\alpha$	524	$\alpha \alpha \beta \alpha \alpha \alpha$	664	$\alpha\beta\beta\alpha\alpha\alpha$	848
	$\alpha \alpha \alpha \beta \alpha \alpha$	664	$\alpha\beta\alpha\beta\alpha\alpha$	1498	$\alpha \alpha \beta \beta \alpha \alpha$	1008	$\alpha\beta\beta\beta\alpha\alpha$	909
	$\alpha \alpha \alpha \alpha \beta \alpha$	524	$\alpha\beta\alpha\alpha\beta\alpha$	1588	$\alpha \alpha \beta \alpha \beta \alpha$	1498	$\alpha\beta\beta\alpha\beta\alpha$	1669
	$\alpha \alpha \alpha \beta \beta \alpha$	848	$\alpha\beta\alpha\beta\beta\alpha$	1669	$\alpha \alpha \beta \beta \beta \beta \alpha$	909	$\alpha\beta\beta\beta\beta\alpha$	680
	$\alpha \alpha \alpha \alpha \alpha \alpha \beta$	300	$\alpha\beta\alpha\alpha\alpha\beta$	1086	$\alpha \alpha \beta \alpha \alpha \beta$	1196	$\alpha\beta\beta\alpha\alpha\beta$	1437
	$\alpha \alpha \alpha \beta \alpha \beta$	946	$\alpha\beta\alpha\beta\alpha\beta$	2037	$\alpha \alpha \beta \beta \alpha \beta$	1277	$\alpha\beta\beta\beta\alpha\beta$	1086
	$\alpha \alpha \alpha \alpha \beta \beta$	456	$\alpha\beta\alpha\alpha\beta\beta$	1277	$\alpha \alpha \beta \alpha \beta \beta$	1117	$\alpha\beta\beta\alpha\beta\beta$	1196
	$\alpha \alpha \alpha \beta \beta \beta$	517	$\alpha\beta\alpha\beta\beta\beta$	946	$\alpha \alpha \beta \beta \beta \beta \beta$	456	lphaetaetaetaetaeta	300

The numerical results of $\mathcal{K}(\mathcal{H}_{m,n})$ for n = 3 and $m \leq 7$.

张 橘 基(合作者: 任海珍,钱建国) Dimer coverings on random multiple chains of planar honeycon

т	р	$\mathbb{E}(K(H_{m,3}))$	р	$\mathbb{E}(K(H_{m,3}))$	р	$\mathbb{E}(K(H_{m,3}))$
1	$\in [0,1]$	4				
2	$\in [0,1]$	10				
3	0,1	20	0.1, 0.9	21.8	0.2, 0.8	23.2
	0.3, 0.7	24.2	0.4, 0.6	24.8	0.5	25
4	0, 1	35	0.1, 0.9	44.9	0.2, 0.8	52.6
	0.3, 0.7	58.1	0.4, 0.6	61.4	0.5	62.5
5	0,1	56	0.1, 0.9	90.4196	0.2, 0.8	118.49
	0.3, 0.7	139.236	0.4, 0.6	151.962	0.5	156.25
6	0, 1	84	0.1, 0.9	180.647	0.2, 0.8	266.502
	0.3, 0.7	333.551	0.4, 0.6	376.07	0.5	390.625
7	0,1	120	0.1, 0.9	360.08	0.2, 0.8	599.236
	0.3, 0.7	799.	0.4, 0.6	930.676	0.5	976.562

The numerical results of $\mathbb{E}(\mathcal{K}(\mathcal{H}_{m,n}))$ for n = 3 and $m \leq 7$.

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Asymptotic behavior



Figure 3 The asymptotic behavior of $\frac{2}{M} \log(\mathbb{E}(K(H_{m,n})))$

In a planar honeycomb lattice, all dimers can be distinguished to be three classes corresponding to the three orientations: x-dimers, y-dimers and z-dimers. Dimers in the same class are all parallel. Let H be a honeycomb lattice with M sites. Denote by $g_H(n_x, n_y, n_z)$ the number of ways placing n_x , n_y and n_z $(2n_x + 2n_y + 2n_z = M)$ independently x-, y- and z-dimers on H so that each site of H is occupied exactly once. The partition function of H with three types of dimers is defined as the generating function [18]

$$Z_{x,y,z}(H) = \sum_{n_x,n_y,n_z} g_H(n_x,n_y,n_z) x^{n_x} y^{n_y} z^{n_z},$$

where, x, y and z are thermodynamically the activities of x-dimers, y-dimers and z-dimers, respectively. In graph theory, $Z_{1,1,1}(H)$ is the number of perfect matchings of H.

The free energy per dimer of H is defined as

$$f_H(x, y, z) = \lim_{M \to \infty} \frac{2}{M} \log Z_{x,y,z}(H)$$

and the entropy per dimer of H, denoted by E(H), is defined as

$$E(H)=f_H(1,1,1)$$

by physicists [23, 22, 25, 24, 26, 27].

Let *H* be a honeycomb lattice with a pure dimer covering *K*. The dimers in *K* can be partitioned into three subsets K_x , K_y and K_z such that in each subset all the dimers are mutually parallel [28]. Zhang *et al.* [29] introduced the concept of *Z*-transformation graph and proved that *Z*-transformation graph is connected. This result implies that all the pure dimer coverings of *H* have the same number of dimers in K_x , K_y and K_z , respectively. Hence, Yan *et al.* obtained the following Lemmas [18]. **Lemma 3.1.**([18]) If H is a planar honeycomb lattice of M sites with three activities x, y and z respectively, then

$$Z_{x,y,z}(H) = Z_{1,1,1}(H) x^{n_x} y^{n_y} z^{n_z},$$

where n_x , n_y and n_z are the numbers of x-dimers, y-dimers and z-dimers in an arbitrary pure dimer covering of H. And the free energy per dimer

$$f_H(x, y, z) = \lim_{M \to \infty} \frac{2}{M} \log Z_{1,1,1}(H) x^{n_x} y^{n_y} z^{n_z}$$

= $E(H) + \lim_{M \to \infty} \frac{2n_x \log x}{M} + \lim_{M \to \infty} \frac{2n_y \log y}{M} + \lim_{M \to \infty} \frac{2n_z \log z}{M}$

if these limits exist.

Lemma 3.2.([18]) Let *H* be a planar honeycomb lattice with *M* sites and let the numbers of dimers belonging to the three different orientations be simply n_x , n_y and n_z . If there exists one (say n_x) among n_x , n_y and n_z such that $n_x = o(\frac{M}{\log m_x})$, where m_x is the maximum number of hexagons intersected by one of the cut segments which are perpendicular to x-dimers of $H_{m,n}$. Then the entropy per dimer of *H*

$$E(H) = \lim_{M \to \infty} \frac{2}{M} \log Z_{1,1,1}(H) = 0.$$

In the following, we consider H as a random multiple chain $H_{m.n} \in \mathcal{H}(m, n, p)$ and determine its expected value of the free energy per dimer. Without loss of generality, we assume that the x-dimers in $H_{m,n}$ are vertical, the y-dimers and z-dimers are then parallel with the other two directions of the hexagon, respectively, as illustrated in Figure 4. As we pointed out in section 2, any dimer covering K contains exactly one vertical dimer edge in each layer. Hence, we have $n_x = m$. On the other hand, one can see that $m_x = n$ and, therefore, $n_x = m = o(\frac{M}{\log m_x})$. So by Lemma 3.2, the entropy per dimer of $H_{m,n}$ is zero, i.e., $E(H_{m,n}) = 0$. Hence, by Lemma 3.1,

Partition function on random multiple chains



Figure 4

Partition function on random multiple chains

$$f_{H_{m,n}}(x,y,z)$$

$$= E(H_{m,n}) + \lim_{M \to \infty} \frac{2n_x \log x}{M} + \lim_{M \to \infty} \frac{2n_y \log y}{M} + \lim_{M \to \infty} \frac{2n_z \log z}{M}$$

$$= \lim_{M \to \infty} \frac{2m \log x}{M} + \lim_{M \to \infty} \frac{2(n+mn-n_z) \log y}{M} + \lim_{M \to \infty} \frac{2n_z \log z}{M}$$

$$= \log y + \lim_{M \to \infty} \frac{2n_z (\log z - \log y)}{M}.$$

Therefore,

$$\mathbb{E}(f_{H_{m,n}}(x,y,z)) = \log y + \lim_{M \to \infty} \mathbb{E}\left(\frac{2n_z}{M}\right) (\log z - \log y).$$

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Recall that any two dimer coverings of $H_{m,n}$ have the same number n_z of dimers in K_z . So, in order to determine the value $\lim_{M\to\infty} \mathbb{E}(2n_z/M)$, it would be convenient to choose the first vertical edge in each layer as the dimer edge of K. Thus, one can check that $n_z = (k+1)n$, where k is the number of the α -type layers, see Figure 4 for an example. In other word, n_z depends only on the number of the α -type layers in $H_{m,n}$. On the other hand, there are exactly $\binom{m-1}{k}$ random multiple chains with k α -type layers, each of which has probability $p^k(1-p)^{m-k-1}$. Thus,

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Partition function on random multiple chains

$$\begin{split} \lim_{M \to \infty} \mathbb{E}\left(\frac{2n_{z}}{M}\right) &= \lim_{m,n \to \infty} \frac{1}{mn+m+n} \sum_{k=0}^{m-1} {m-1 \choose k} p^{k} (1-p)^{m-k-1} (k+1) m \\ &= \lim_{m,n \to \infty} \frac{n(1-p)^{m-1}}{mn+m+n} \left(t \sum_{k=0}^{m-1} {m-1 \choose k} \left(\frac{pt}{1-p} \right)^{k} \right)' \Big|_{t=1} \\ &= \lim_{m,n \to \infty} \frac{(m-1)np}{mn+m+n} = p. \end{split}$$

Therefore,

$$\mathbb{E}(f_{H_{m,n}}(x,y,z)) = (1-p)\log y + p\log z.$$
(3)

Partition function on random multiple chains

Remark. The (k, h, n)-chevron region C(k, h, n) is a particular type of (non-random) multiple chains consisting of k + h - 1 layers whose *i*-th layers with $i \in \{2, 3, \dots, k\}$ are of α -type and the last h - 1 layers are of β -type. The (4, 3, 5)-chevron region is depicted in Figure 4, for an example. It has been known [18] that the free energy per dimer of the (at, bt, ct)-chevron region with a + b + c = 1, c > 0 and $t \to \infty$ is

$$f_{C(bt,at,ct)}(x,y,z)) = \frac{b}{a+b}\log y + \frac{a}{a+b}\log z.$$

Combining with (3), we have

$$\mathbb{E}(f_{H_{m,n}}(x, y, z)) = f_{C(bt,at,ct)}(x, y, z) = (1-p)\log y + p\log z,$$

where $a = \frac{p}{1+c}, b = \frac{1-p}{1+c}$ and $t \to \infty$.

Zdeborová L and Mézard M, *The number of matchings in random graphs*, 2006 *J. Stat. Mech.* **5** 1-17

- Frieze A and Pittel B, Perfect matchings in random graphs with prescribed minimal degree, 2003 ACM-SIAM Symp. on Discrete Algorithms 148-57
- Lovász L and Plummer M D, 1986 *Matching Theory* (Amsterdam, New York: North-Holland)
- Gutman I and Cyvin S J, 1988 *Kekulé structures in Benzenoid Hydrocarbons* (Springer, Berlin)
- M. S. Dresselhaus, G. Dresselhaus, P. Avouris, Carbon Nanotubes: Synthesis, Structure, Properties, and Applications, Springer-Verlag Berlin 2001



 Fowler R H and Rushbrooke G S, An attempt to extend the statistical theory of perfect solutions, 1937 Trans. Faraday Soc. 33 1272-1294

- Kasteleyn P W, 1967 Graph Theory and Crystal Physics, (In Graph Theory and Theoretical Physics (Harary F, eds.), pages 43-110. Academic Press, London)
- Kasteleyn P W, The statistics of dimers on a lattice, 1961
 Physica 27 1209-1225
- Temperley H N V and Fisher M E, Dimer problem in statistical mechanics - an exact result, 1961 Phisolophical Magazine 6 1061-1063
- Fisher M E, *Statistical Mechanics of Dimers on a Plane Lattice*, 1961 *Phys.Rev.* **124** 1664-1672

🔋 Elkies N, Kuperberg G, Larsen M and Propp J,

Alternating-sign matrices and domino tilings, 1992 J. Algebraic Combin. **1** 111-132

- Sachs H and Zeritz H, *Remark on the dimer problem*, 1994 *Discrete Appl. Math.* **51** 171-179
- Propp J, Boundary-dependent local behavior for 2-D dimer models, 1997 International Journal of Modern Physics B 11 183-187
- Klein D J and Schmalz T G, Exact enumeration of long-range-ordered dimer coverings on the square-planar lattice, 1990 Phys. Rev. B 41 2244-2248
- Heilmann O J and Lieb E H, Monomers and dimers, 1970 Phys. Rev. Letters 24 1412-1414

- Heilmann O J and Lieb E H, Theory of monomer dimer systems, 1972 Comm. Math. Phys. 25 190-232
- Yan W G, Yeh Y N and Zhang F J, Dimers belonging to three orientations on plane honeycomb lattices, 2011 J. Stat. Phys. 145 1343-1356
- Klein D J, Long-range order for spin pairing in valence bond theory, 1979 Int. J. Quantum Chem. Symp. **13** 293-303
- Klein D J, Hite G E, Seitz W A and Schmalz T G, Dimer coverings and Kekulé structures on honeycomb lattice strips, 1986 Theor. Chim. Acta 69 409-423
- Klein D J, Hite G E and Schmalz T G, Transfer-matrix method for subgraph enumeration: Application to polypyrene fusenes, 1986 J. Comput. Chem. 7 443-456

Kasteleyn P W, Dimer Statistics and Phase Transitions, 1963
 J. Math. Phys. 4 287-293

- Elser V, Solution of the dimer problem on a hexagonal lattice with boundary, 1984 J. Phys. A: Math. Gen. **17** 1509-1513
- Wannier G H, Antiferromagnetism. The Triangular Ising Net, 1950 Phys. Rev. **79** 357-364
- Nagle J F, Critical points for dimer models with 3/2 order transitions, 1975 Phys. Rev. Lett. 34 1150-1153
- Wu F Y, Remarks on the modified KDP model, 1968 Phys. Rev. **168** 539-543
- Wu F Y, Wu X N and Blóte H W J, Critical frontier of the antiferromagnetic Ising model in a nonzero magnetic field: The honeycomb lattice, 1989 Phys. Rev. Lett. 62 2273-2276

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Zhang F J, Chen R S, Guo X F and Gutman I, An invariant of the Kekulé structures of benzenoid hydrocarbons, 1986 J. Serb. Chem. Soc. 51 537-543

Zhang F J, Guo X F and Chen R S, Z-transformation graphs of perfect matchings of hexagonal systems. Proceedings of the First Japan Conference on Graph Theory and Applications (Hakone, 1986), 1988 Discrete Math. **72** 405-415

- Kenyon R, The planar dimer model with boundary: a survey, Directions in mathematical quasicrystals (Michael Baake and Robert V. Moody, eds.), 307-328, CRM Monogr. Ser., Vol. 13, Amer. Math. Soc., Providence, RI, 2000
- Gutman I., Cyvin S.J. (Eds.): Introduction to the Theory of Benzenoid Hydrocarbons. Springer, Berlin (1989)

