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Dimers Belonging to Three Orientations on Plane Honeycomb Lattices

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Abstract It is well known that there are three types of dimers belonging to the three different orientations in a honeycomb lattice, and in each type all dimers are mutually parallel. Based on a previous result, we can compute the partition function of the dimer problem of the plane (free boundary) honeycomb lattices with three different activities by using the number of its pure dimer coverings (perfect matchings). The explicit expression of the partition function and free energy per dimer for many types of plane honeycomb lattices with fixed shape of boundaries is obtained in this way (for a shape of plane honeycomb lattices, the procedure that the size goes to infinite, corresponds to a way that the honeycomb lattice goes to infinite). From these results, an interesting phenomena is observed. In the case of the regions of the plane honeycomb lattice has zero entropy per dimer—when its size goes to infinite—though in the thermodynamic limit, there is no freedom in placing a dimer at all, but if we distinguish three types of dimers with nonzero activities, then its free energy per dimer is nonzero. Furthermore, a sufficient condition for the plane honeycomb lattice with zero entropy per dimer (when the three activities are equal to 1) is obtained. Finally, the difference between the plane honeycomb lattices and the plane quadratic lattices is discussed and a related problem is proposed.

Keywords Honeycomb lattice · Partition function · Dimers · Free energy

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1 Introduction

The dimer problem has a long history. In 1927 Fowler and Rushbrooke [14] introduced it in order to describe the absorption of diatomic molecules on crystal surface. After more than thirty years, three authors, Kasteleyn [20], Fisher [13], and Temperley and Fisher [37] solved independently the case of an $m \times n$ plane quadratic lattice simultaneously. The starting point is a special plane quadratic lattice. Based on this result they obtained the exact formula of the partition function and the bulk limit of the entropy (free energy per dimer). To solve the dimer problem in this way is usually called the dimer problem with free boundary condition. Kasteleyn [20] also obtained the solution of the dimer problem of the quadratic lattice with toroidal boundary condition. In their work dimers are distinguished to be two types and then got its bulk limit of entropy. The variability of this problem is discovered in 1996 by Cohn et al. [4] and they studied the dimer problem of the plane regions called Aztec diamonds and got the partition function. The different methods for counting partition function of Aztec diamonds had been considered by many authors (see for example [11, 41]). In [11, 41] dimers are distinguished to be more than four types and the partition function was obtained. Using this result we can easily to get the partition function which distinguishes the activities of two types of dimers according to their two orientations. The dimer problem of another type of quadratic lattices with the different boundary condition had been studied by Sachs and Zeritz [35]. The free energy per dimer was also obtained. From these results we can say that, for the plane quadratic lattices with variant fixed shape of boundaries (for a shape of plane quadratic lattices, the procedure that the size goes to infinite, corresponds to a way that the quadratic lattice goes to infinite), the free energies can be obtained by going to infinite for plane quadratic lattice with fixed shape of boundaries. For these three cases their free energies per dimer are different.

Similarly, for the plane honeycomb lattices variant boundaries can be considered. In this case each dimer has one of three possible orientations, that is, three types of dimers, x-dimers, y-dimers, and z-dimers, can be distinguished. For the case of a hexagonal-shaped region $H(k,l,m)$ shown in Fig. 3(b) (which is a plane honeycomb lattice), Elser [12] found its partition function and showed that the number of dimers belonging to the three orientations are simply kl, lm, and km, in general the bulk limit of the entropy does not exist. But as pointed out in Example 3.2, the free energy per dimer exists when k, l, and m go to infinite in a special way. The dimer problem on hexagonal-shaped region $H(k,l,m)$ was also considered for example in [7, 10, 42]. Klein [23] considered the long-range order for spin pairing in valence bond theory in which three types of dimers are distinguished, and Klein et al. [26, 27] found some further results for the honeycomb lattice strips of arbitrary widths, arbitrary lengths, and arbitrary long-range-order values. Kasteleyn [20], Baxter [1], and Wu et al. [40] also treated the dimers with the three different orientations for double periodic boundary and they showed that when the three activities of dimers satisfy a triangular inequality the partition function is smoothly function of the three activities. Otherwise the free energy per dimer may be frozen. But in [15] and some other previous work coming from the Ising model (see [38]) and chemistry (see [7, 10, 16, 42] and the references cited therein) did not distinguish three types of dimers to compute the free energy per dimer. In fact, these works concentrated on the case in which all dimers have the same activity 1. On the other hand, the Nobel Prize in Physics 2010 has been awarded to Geim and Novoselov for groundbreaking experiments regarding the two-dimensional material graphene which form finite honeycomb lattice (see [31] and [9] and reference cited therein). This fact stimulated a lots of work on the physical properties of two-dimensional material graphene.

Zhang et al. [44] proved that for each pure dimer covering (perfect matching) of a general plane finite honeycomb lattice, the numbers of x-dimers, y-dimers, and z-dimers are three constants (but the statement is not true for the honeycomb with periodic boundary condition). Using this result, in this paper, we get the partition functions of a plane honeycomb lattice whose three types of dimers have different activities (weights) in terms of the number of its pure dimer covering (perfect matching). This problem was proposed by F.Y. Wu to one of the present authors. As pointed out in [15, 23, 27], results in this paper for many plane honeycomb lattices show that the shape of the boundary of a honeycomb lattice has a strong effect on its free energy per dimer. This phenomenon also happens in the previous three cases of plane quadratic lattices (see [11], [20] and [35]). Another similar phenomenon pointed out in [24, 33] is that the shape of the boundary of a finite sub-region of a quadratic plane lattice has a strong effect on the local entropy and local statistics (frequencies of local patterns) of a random dimer configuration. In this paper the examples of the plane honeycomb lattices with zero free energy per dimer—when the three activities are equal to 1—are further discussed. We find that if we distinguish three types of dimers with nonzero activities, then its free energy per dimer is nonzero though in the thermodynamic limit, no freedom in placing a dimer at all. Furthermore, we obtain a new sufficient condition of plane honeycomb lattices which have zero entropy per dimer when the three activities are equal to 1.

Note that for a finite plane quadratic lattice there are x-dimers and y-dimers. But the numbers of x-dimers and y-dimers are not two constants. This fact shows an essential difference between the plane honeycomb lattice and the quadratic lattice. But are there any other essential differences between the plane honeycomb lattice and the quadratic lattice? Finally, at the end of this paper, a new open problem about this is posed.

Some related works see for example [2, 8, 19, 22, 25, 28–30, 32, 36, 43, 46].

2 The Partition Function

A honeycomb lattice or hexagonal system can be defined as a connected plane graph in which every interior face is bounded by a regular hexagon of side length one. In a plane honeycomb lattice, each dimer can be identified to one of the three classes: 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 of placing N_x, N_y, and N_z independently x-, y-, and z-dimers on H so that each site of H is occupied exactly once $(2N_x + 2N_y + 2N_z = M)$. The partition function of H with three types of dimers is defined as the generating function

$$Z_{x,y,z}(H) = \sum_{N_x, N_y, N_z} g_H(N_x, N_y, N_z) x^{N_x} y^{N_y} z^{N_z}, \tag{1}$$

where, thermodynamically, x, y, and z are 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. For many types of honeycomb lattices H, the closed forms of $Z_{1,1,1}(H)$ were obtained by chemists (see for example the book [16]). In chemistry the honeycomb lattice is called the benzenoid system and the pure dimer covering (perfect matching) is called the Kekulé structure. For a type of honeycomb lattices with some boundary condition, let H be an element in this type with M sites. The free energy per dimer of H, denoted by $f_H(x, y, z)$, is defined as

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

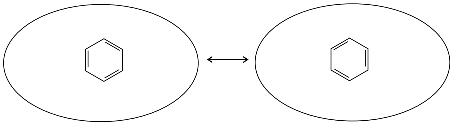


Fig. 1 A sextet rotation for the Z-transformation graph

if the limit exists and is independent of the choice of H. The entropy per dimer of H, denoted by $E(H)$, is defined as

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

by physicists [12, 21, 29, 38–40]. Elser [12] obtained the formula of $Z_{x,y,z}(H)$ for a finite hexagonal region H (see Fig. 3(b)) and showed that the limit of the right-hand side of (2) does not exist in general and is dependent on the shape of H. Grensing et al. [15] obtained the entropy per dimer for some other types of honeycomb lattices.

We would like to mention that the dimer problem on honeycomb lattices is equivalent to the lozenge tiling problem of triangle lattices [12]. Hence, from our point of view, three classes of lozenges can be distinguished and the enumeration problem can go further.

In order to compute the partition function $Z_{x,y,z}(H)$ of honeycomb lattices, we need to use the following basic fact that was found in [44]:

Let H be a honeycomb lattice with a pure dimer covering (perfect matching). For an arbitrary 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. Zhang et al. [45] defined the Z-transformation graph as follows. Its vertex set is the set of pure dimer coverings (perfect matchings) of a honeycomb lattice, where two pure dimer coverings are joined by an edge if and only if they are different only in a hexagon (equivalently the symmetric difference of these two pure dimer coverings is just a hexagon). In chemistry, this idea originates from Herndon's resonance theory [17, 18]. In mathematics, Zhang et al. [45] proved that the Z-transformation graph of a honeycomb lattice H is connected, i.e., any two perfect matchings of H can be joined by a path in the Z-transformation graph. In other words, any pure dimer covering of H can be obtained from another pure dimer covering of H by successive sextet rotations shown in Fig. 1. It is clear that any two adjacent pure dimer coverings in the Z-transformation graph have the same number of dimers in K_x, K_y, and K_z, respectively. Hence the cardinalities $n_x = |K_x|$, $n_y = |N_y|$, and $n_z = |N_z|$ are three invariants for the honeycomb lattice H. Thus the formula (1) has the following elegant form:

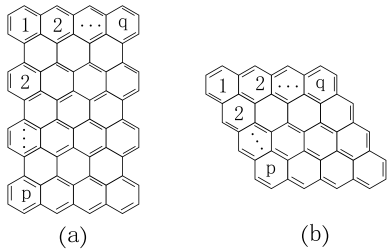
$$Z_{x,y,z}(H) = Z_{1,1,1}(H)x^{n_x} y^{n_y} z^{n_z}. \tag{3}$$

Hence, if H is a plane honeycomb lattice of M sites with three activities x, y, and z respectively, then the free energy per dimer

$$\begin{aligned} f_H(x, y, z) &= \lim_{M\to\infty} \frac{2}{M} \log Z_{1,1,1}(H)x^{n_x} y^{n_y} z^{n_z} \\ &= E(H) + \lim_{M\to\infty} \frac{2n_x \log x}{M} + \lim_{M\to\infty} \frac{2n_y \log y}{M} + \lim_{M\to\infty} \frac{2n_z \log z}{M} \end{aligned} \tag{4}$$

if these limits exist. From (4), we can see that there is an elegant relation between the entropy $E(H)$ per dimer and the free energy $f_H(x, y, z)$ per dimer of the plane honeycomb lattice H (but this result does not hold for the honeycomb lattices with periodic boundaries). That is, for an arbitrary plane honeycomb lattice H the free energy $f_H(x, y, z)$ per dimer can be

Fig. 2 (**a**) A (p,q)-rectangle prolate region $R(p,q)$. (**b**) A (p,q)-parallelogram region $P(p,q)$



expressed completely in terms of the entropy $E(H)$ per dimer and n_x, n_y, and 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.

3 Some Examples and Remarks

Example 3.1 (Rectangle prolate region $R(p,q)$) A (p,q)-rectangle prolate region, denoted by $R(p,q)$, is illustrated in Fig. 2(a) (see [16]), which is a plane honeycomb lattice. The number of pure dimer coverings (perfect matchings) of $R(p,q)$ is $(q+1)^p$ (see [6, 16]). It is not difficult to see that the numbers of dimers belonging to the three orientations are simply p, pq, and pq, respectively. Suppose the corresponding three activities are x, y, and z, respectively. Then, using (4), the free energy per dimer is

$$\lim_{p,q\to\infty}\frac{1}{p+2pq}\log(q+1)^p+\lim_{p,q\to\infty}\frac{p\log x}{p+2pq}+\lim_{p,q\to\infty}\frac{pq\log y}{p+2pq}+\lim_{p,q\to\infty}\frac{pq\log z}{p+2pq}$$
$$=\frac{1}{2}(\log y+\log z).$$

Example 3.2 (Parallelogram regions $P(p,q)$) Figure 2(b) illustrates a (p,q)-parallelogram region, denoted by $P(p,q)$ (see [15] and [16]). This is a plane honeycomb lattice. The number of pure dimer coverings (perfect matchings) of $P(p,q)$ equals $\binom{p+q}{p}$ (see [15, 16]). It is not difficult to show that the numbers of dimers belonging to the three orientations are simply p, q, and pq, respectively. Suppose the corresponding three activities are x, y, and z, as we shall use without comment later. Then, by (4), its free energy per dimer is

$$\lim_{p,q\to\infty}\frac{1}{p+q+pq}\log\frac{(p+q)!}{p!\,q!}+\lim_{p,q\to\infty}\frac{p\log x}{p+q+pq}+\lim_{p,q\to\infty}\frac{q\log y}{p+q+pq}$$
$$+\lim_{p,q\to\infty}\frac{pq\log z}{p+q+pq}=\log z.$$

Example 3.3 (Chevron regions $C(k,m,n)$) A (k,m,n)-chevron region, denoted by $C(k,m,n)$, is defined to be the plane honeycomb lattice shown in Fig. 3(a) (see [16]). The number of perfect matchings of $C(k,m,n)$ equals

$$\sum_{i=0}^{n}\binom{k+i-1}{i}\binom{m+i-1}{i}$$

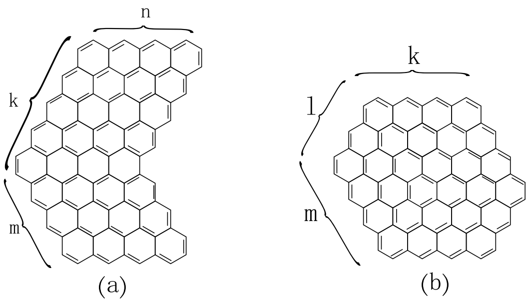


Fig. 3 (**a**) A (k,m,n)-chevron region $C(k,m,n)$. (**b**) A (k,l,m)-hexagonal region $H(k,l,m)$

(see [16]) and we can show easily that the numbers of dimers belonging to the three orientations are simply nk, mn, and $k+m-1$, respectively. Let

$$A=\lim_{k,m,n\to\infty}\frac{1}{nk+mn+(k+m-1)}\log\left[\sum_{i=0}^{n}\binom{k+i-1}{i}\binom{m+i-1}{i}\right];$$

$$B=\lim_{k,m,n\to\infty}\frac{(m+n-1)\log z}{nk+mn+(k+m-1)}.$$

Obviously, $B=0$. Note that for $k,m,n>1$,

$$\sum_{i=0}^{n}\binom{k+i-1}{i}\binom{m+i-1}{i}<n(k+n-1)^{k-1}(m+n-1)^{m-1}.$$

Hence if $\lim_{m,n,k\to\infty}\frac{\log k+\log m}{n}=0$, then $A=0$. Also note that the limits

$$\lim_{k,m,n\to\infty}\frac{nk\log x}{nk+mn+(k+m-1)}\quad\text{and}\quad\lim_{k,m,n\to\infty}\frac{mn\log y}{nk+mn+(k+m-1)}$$

might fail to exist. If we additionally assume the ratios of k, m, and n have limits, say

$$k\sim at,\quad m\sim bt,\quad n\sim ct,\quad (t\to\infty)$$

where $a,b\geq 0$ and $c>0$, and $a+b+c=1$, then the limits all exist. By (4), in this case the free energy per dimer

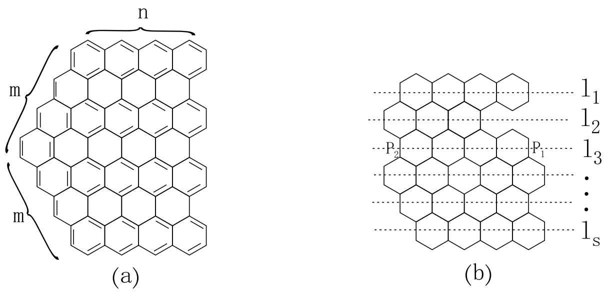
$$f_{H(k,l,m)}(x,y,z)=A+B+\frac{a}{a+b}\log x+\frac{b}{a+b}\log y=\frac{a}{a+b}\log x+\frac{b}{a+b}\log y.$$

In particular, if $m=k$, then the free energy per dimer of the chevron $C(m,m,n)=:C(m,n)$ is exactly $(\log x+\log y)/2$.

Example 3.4 (Hexagonal regions $H(k,l,m)$) For general hexagonal regions $H(k,l,m)$ shown in Fig. 3(b), Elser [12] proved that the bulk limit of the entropy does not exist. But from his result we can see that

$$\lim_{k,l,m\to\infty}\frac{1}{kl+lm+km}\log Z_{1,1,1}(H(k,l,m))$$

Fig. 4 (**a**) An (m, n)-prolate pentagon region $PP(m, n)$. (**b**) A plane honeycomb lattice with cuts $\{l_i | 1 \le i \le s\}$ which are vertical to the x-dimers



$$= \frac{1}{2(ab+bc+ac)}\big[a^2\log a + b^2\log b + c^2\log c$$
$$- (1-a)^2\log(1-a) - (1-b)^2\log(1-b) - (1-c)^2\log(1-c)\big], \qquad (5)$$

when

$$k \sim at, \quad l \sim bt, \quad m \sim ct, \quad (t \to \infty)$$

where $a, b, c \ge 0$, and $a + b + c = 1$. Denote the right-hand side of (5) by $\phi(a, b, c)$. Note that the numbers of dimers belonging to the three orientations are simply kl, lm, and km, respectively. Thus in our case the free energy per dimer of $H(k, l, m)$

$$f_{H(k,l,m)}(x, y, z) = \phi(a, b, c) + \frac{ab\log x + bc\log y + ac\log z}{ab + bc + ac}.$$

Example 3.5 (Prolate pentagon regions $PP(m, n)$) The number of pure dimer coverings of the prolate pentagon regions $PP(m, n)$ as illustrated in Fig. 4(a) (see [16]) equals

$$\prod_{i=1}^{n} \frac{\binom{2m+2i}{m}}{\binom{m+2i-1}{m}}.$$

It is not difficult to see that the numbers of dimers belonging the three different orientations are simply $\frac{1}{2}m(m + 1)$, $(2m - 1)n$, and $(2m - 1)n$, respectively.

Note that if $n \ge 1$ then $n! \sim \sqrt{2\pi n}(\frac{n}{e})^n \exp\frac{1}{12n+\theta_n}$, where $0 < \theta_n < 1$. In particular, $n! \sim (\frac{n}{e})^n$ if $n \to \infty$. Hence if $m, n \to \infty$, then

$$\log\left[\prod_{i=1}^{n} \frac{\binom{2m+2i}{m}}{\binom{m+2i-1}{m}}\right] \sim \log\left[\prod_{i=1}^{n} \frac{(2m+2i)^{2m+2i}(2i-1)^{2i-1}}{(m+2i-1)^{m+2i-1}(m+2i)^{m+2i}}\right]$$
$$+ \sum_{i=1}^{n} \log[\sqrt{2\pi(2i-1)}]\exp\frac{1}{12(2i-1)+\theta_i}$$
$$\sim \int_1^n \big[(2m+2x)\log(2m+2x) - (m+2x-1)\log(m+2x-1)$$
$$+ (2x-1)\log(2x-1) - (m+2x)\log(m+2x)\big]d_x + \frac{n}{2}\log(2\pi)$$

$$
\begin{aligned}
&+\frac{1}{2}\int_1^n \log(2x-1)d_x+\sum_{i=1}^n \frac{1}{12(2i-1)+\theta_i}\\
&=A+B+C+D,
\end{aligned}
$$

where $B=\frac{n}{2}\log(2\pi)$, $C=\frac{1}{2}\int_1^n \log(2x-1)d_x$, $D=\sum_{i=1}^n \frac{1}{12(2i-1)+\theta_i}$, and

$$
\begin{aligned}
A=\int_1^n \big[&(2m+2x)\log(2m+2x)-(m+2x-1)\log(m+2x-1)\\
&+(2x-1)\log(2x-1)-(m+2x)\log(m+2x)\big]\,d_x.
\end{aligned}
$$

Obviously, $C\sim \frac{1}{2}(2n-1)\log(2n-1)$ and $D=o(n)$. Particularly,

$$
\begin{aligned}
A=&\left[\frac{(2m+2x)^2}{4}\log(2m+2x)-\frac{(2m+2x)^2}{8}\right]_{x=1}^n\\
&-\left[\frac{(m+2x-1)^2}{4}\log(m+2x-1)-\frac{(m+2x-1)^2}{8}\right]_{x=1}^n\\
&+\left[\frac{(2x-1)^2}{4}\log(2x-1)-\frac{(2x-1)^2}{8}\right]_{x=1}^n\\
&-\left[\frac{(m+2x)^2}{4}\log(m+2x)-\frac{(m+2x)^2}{8}\right]_{x=1}^n\\
=&\frac{(2m+2n)^2}{4}\log(2m+2n)-\frac{(2m+2)^2}{4}\log(2m+2)-\frac{(2m+2n)^2}{8}+\frac{(2m+2)^2}{8}\\
&-\frac{(m+2n-1)^2}{4}\log(m+2n-1)+\frac{(m+1)^2}{4}\log(m+1)+\frac{(m+2n-1)^2}{8}\\
&-\frac{(m+1)^2}{8}+\frac{(2n-1)^2}{4}\log(2n-1)-\frac{(2n-1)^2}{8}+\frac{1}{8}-\frac{(m+2n)^2}{4}\log(m+2n)\\
&+\frac{(m+2)^2}{4}\log(m+2)+\frac{(m+2n)^2}{8}-\frac{(m+2)^2}{8}\\
\sim&(m+n)^2\log(2m+2n)-m^2\log(2m)-\frac{(m+2n)^2}{4}\log(m+2n)\\
&+\frac{m^2}{4}\log m+n^2\log(2n)-\frac{(m+2n)^2}{4}\log(m+2n)+\frac{m^2}{4}\log m\\
\sim&(m+n)^2\log(2m+2n)-m^2\log 2-\frac{m^2}{2}\log m\\
&-\frac{(m+2n)^2}{2}\log(m+2n)+n^2\log(2n).
\end{aligned}
$$

In order to take a limit, let us suppose

$$
m\sim at,\quad n\sim bt,\quad (t\to\infty)
$$

where $a, b > 0$, and $a + b = 1$. In this case, we have

$$\begin{aligned}
E(PP(m,n)) &= \lim_{m,n\to\infty} \frac{1}{\frac{1}{2}m(m+1)+2(2m-1)n} \log Z_{1,1,1}(PP(m,n)) \\
&= \lim_{m,n\to\infty} \frac{1}{\frac{1}{2}m(m+1)+2(2m-1)n} (A+B+C+D) \\
&= \lim_{t\to\infty} \frac{t^2}{\frac{1}{2}a(a+1)t^2+2(2at-1)(bt)} \left\{ \left[\log(2t) - a^2\log 2 - \frac{a^2}{2}\log(at) \right.\right. \\
&\quad \left. - \frac{(a+2b)^2}{2}\log(at+2bt) + b^2\log(2bt) \right] \\
&\quad \left. + \frac{bt}{2}\log(2\pi) + \frac{2bt-1}{2}\log(2bt-1) + o(bt) \right\} \\
&= \lim_{t\to\infty} \frac{t^2}{(\frac{1}{2}a^2+4ab)t^2} \left[(1-a^2+b^2)\log 2 + b^2\log b - \frac{a^2}{2}\log a \right. \\
&\quad \left. - \frac{(1+b)^2}{2}\log(1+b) \right] \\
&= \frac{2}{a(a+8b)} \left[(1-a^2+b^2)\log 2 + b^2\log b - \frac{a^2}{2}\log a \right. \\
&\quad \left. - \frac{(1+b)^2}{2}\log(1+b) \right] \\
&= \frac{2}{a(1+7b)} \left[2b\log 2 + b^2\log b - \frac{a^2}{2}\log a - \frac{(1+b)^2}{2}\log(1+b) \right].
\end{aligned}$$

The limit above depends on a and b. Hence in general the double limit does not exist (when $m, n \to \infty$). If $a = b = \frac{1}{2}$, then the entropy per dimer is $\frac{16}{9}\log 2 - \log 3 \approx 0.13365$. If we assume that $m = ak$ and $n = bk$, and distinguish the three types of dimers, using (4), we need to add the following three terms to the free energy per dimer

$$\frac{a}{1+7b}\log x + \frac{4b}{1+7b}\log y + \frac{4b}{1+7b}\log z.$$

3.1 Some Remarks

Remark 1 In Examples 3.1 and 3.2, if all dimers have the same activity one, then the entropy per dimer is zero. But if we distinguish three types of dimers and give them different activities ($\neq 1$), the free energy per dimer maybe be nonzero. For the free energy per dimer of the parallelogram regions $P(p,q)$, the contribution of the z-dimers is nonzero and that of the other two types of dimers is zero. For the free energy per dimer of the rectangular prolate regions $R(p,q)$, the contribution of the y-dimers and z-dimers is nonzero when both activities are not one. These results are not surprising. Since if the number of dimers in the same type is relatively very few, their activities have nothing to do with the free energy per dimer.

Remark 2 In Example 3.3, if all dimers have the same activity $= 1$, the entropy per dimer is zero. In the general case, if the activities of x-, y-, and z-dimers are $\neq 1$, the triple limit of the entropy does not exist when $m, n, k \to \infty$, whereas it does exist if $k \sim at,\ m \sim bt,\ n \sim ct$ $(t \to \infty)$.

Remark 3 In Examples 3.4 and 3.5, the bulk entropy per dimer does not exist even when $x = y = z = 1$. But if we choose a special boundary the limit exists.

Remark 4 In Example 3.5, we obtained the bulk entropy per dimer of the prolate pentagon regions $PP(n,n)$, which equals $\frac{16}{9}\log 2 - \log 3 \approx 0.13365$. This is maybe the plane honeycomb lattice with the smallest nonzero entropy per dimer which had been computed so far.

4 Honeycomb Lattices with Zero Entropy per Dimer

In Examples 3.1–3.3 in the above section, if $x = y = z = 1$, the bulk entropy per dimer equals zero. In this section we give a sufficient condition for the entropy per dimer of honeycomb lattice H to be equal to zero.

In order to state our result we need to refine the result in Sect. 2 as follows. A straight line segment P_1P_2 is called a cut segment of a plane honeycomb lattice H if P_1P_2 satisfies:

(a) P_1P_2 is perpendicular to one of the three types of dimers of H.
(b) Both P_1 and P_2 are the centers of edges of H lying on the boundary of H.
(c) Deleting all the edges intersected by P_1P_2 from H leaves exactly two components.

In other words, we consider all minimal edge cuts of H induced by such segments perpendicular to one type of the dimers (see Fig. 4(b)). Let us color the sites of the hexagonal lattice H by two colors black and white. We observe that the sites of edges intersected by a cut segment P_1P_2 in each component have the same color. We call the component containing the white (resp. black) sites to be white (resp. black) bank of P_1P_2. It is not difficult to see that the number of dimers intersected by P_1P_2 in an arbitrary pure dimer covering is equal to the difference between the numbers of white (resp. black) and black (resp. white) sites in the white (resp. black) bank. Thus, for an arbitrary pure dimer covering of a honeycomb lattice, the number of dimers intersected by P_1P_2 is an invariant. This phenomenon was observed by Sachs [34], and in the case of polypyrene fusene strips, this was implied by an earlier result of Klein in his theory of long-range order for spin paring [23]. Now, we can give an accurate mathematical proof to the main result in this section which is also implied by Klein's theory in the case of polypyrene fusene strips.

Now, we can state the main result in this section as follows.

Theorem 4.1 *Let H be a plane 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. Then the entropy per dimer of H*

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

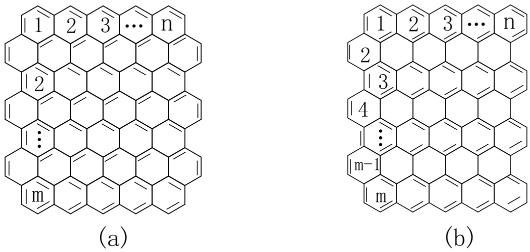


Fig. 5 (**a**) An (m,n)-Oblate rectangle region $PP(m,n)$. (**b**) An (m,n)-multiple zigzag chain region

Proof Without loss of generality, we assume that x-dimers in H are perpendicular. Let α_i be the number of x-dimers intersected by the cut segments l_i in a pure dimer covering of H for $1 \le i \le s$ (see Fig. 4(b)), where $\{l_1, l_2, \dots, l_s\}$ is the set of the cut segments of H intersected x-dimers. Clearly, $\sum_{i=1}^{s} \alpha_i = n_x$. If we select the α_i dimers intersected by l_i in an arbitrary way, there is at most one way to extend it to a pure dimer covering. Therefore

$$Z_{1,1,1}(H) \le \binom{m_x+1}{\alpha_i}\binom{m_x+1}{\alpha_2}\cdots\binom{m_x+1}{\alpha_s} < (m_x+1)^{\sum_{i=1}^{s}\alpha_i} = (m_x+1)^{n_x},$$

and we have

$$\begin{aligned} E(H) &= \lim_{M\to\infty} \frac{2}{M} \log Z_{1,1,1,}(H) \le \lim_{M\to\infty} \frac{2}{M} \log(m_x+1)^{n_x} \\ &= \lim_{M\to\infty} \frac{2n_x}{M} \log(m_x+1) = \lim_{M\to\infty} \frac{2o(\frac{M}{\log m_x})}{\frac{M}{\log(m_x+1)}} = 0. \end{aligned}$$

Then the bulk entropy per dimer of H equals zero, and we have finished the proof of the theorem. □

It is not difficult to check that all of the honeycomb lattices $R(p,q)$, $P(p,q)$, and $C(k,m,n)$ in Examples 3.1–3.3 satisfy the conditions of the above theorem. Hence their bulk entropies per dimer equal zero, as we calculated in Sect. 3. Now we can give another two examples with zero entropy per dimer.

Example 4.2 (Oblate rectangle regions $OR(m,n)$) The formula for the number of pure dimer coverings (perfect matchings) of the plane honeycomb lattice $OR(m,n)$, which is called the oblate rectangle honeycomb lattice ([15] and [16], see Fig. 5(a)), was obtained in [3] as follows:

$$Z_{1,1,1}(OR(m,n)) = \frac{2}{n+2}\sum_{k=1}^{n+1}\left[\cot\frac{k\pi}{2(n+2)}\right]^2 \lambda_k^{m-1},$$

where $\lambda_k = \frac{n+2}{4}[\sin\frac{k\pi}{2(n+2)}]^{-2}$. The numbers of x-dimers, y-dimers, and z-dimers are $n_x = 3m-2$, $n_y = n_z = mn$. The maximum number of hexagons intersected by one of the cut segments perpendicular to x-dimers of $OR(m,n)$ is $m_x = n+1$. Note that

$$\lim_{m,n\to\infty} \frac{n_x \log m_x}{2(3m-2+2mn)} = 0$$

implying $n_x = o(\frac{N}{\log m_x})$. By Theorem 4.1, the entropy per dimer of $OR(m,n)$ equals zero and the free energy per dimer of $OR(m,n)$ equals $\frac{1}{2}(\log y + \log z)$.

Example 4.3 (Multiple zigzag regions $MZ(m,n)$) The multiple zigzag region $MZ(m,n)$ is a type of plane honeycomb lattice illustrated in Fig. 5(b) (see [15, 16]). Klein et al. [27] obtained the formula for the number of pure dimer coverings of $MZ(m,n)$ as follows:

$$Z_{1,1,1}(MZ(m,n)) = \frac{2}{2n+3}\sum_{k=1}^{n+1}(-1)^{(m-1)(n+k-1)}\left[\tan\frac{k\pi}{2n+3}\right]^2\left[\sec\frac{k\pi}{2n+3}\right]^{m-1}.$$

The numbers of x-dimers equals exactly m, and the numbers of both y-dimers and z-dimers are approximately $\frac{mn}{2}$. That is, $n_x = m$, $n_y \sim \frac{mn}{2}$ and $n_z \sim \frac{mn}{2}$ $(m,n\to\infty)$. The maximum number of hexagons intersected by a cut segment which is perpendicular to x-dimers of $MZ(m,n)$ is $m_x = n$. Then

$$\lim_{m,n\to\infty}\frac{n_x\log m_x}{m+mn} = 0$$

which implies $n_x = o(\frac{N}{\log m_x})$. By Theorem 4.1, the bulk entropy per dimer of $MZ(m,n)$ equals zero and the free energy per dimer of $MZ(m,n)$ equals $\frac{1}{2}(\log y + \log z)$.

5 An Open Problem

In this paper, for a finite plane honeycomb lattice, based on the fact that for each pure dimer covering the number of dimers belonging to the same orientation is an invariant, we can compute the free energies per dimer of honeycomb lattices in terms of the number of its pure dimer coverings. In fact the free energy per dimer of honeycomb lattices can be obtained from the entropy per dimer by adding extra terms which are easily obtained. Furthermore, using the fact that for an arbitrary pure dimer covering of a honeycomb lattice the number of dimers intersected by P_1P_2 cut is an invariant, we give a new sufficient condition for a honeycomb lattice to have zero entropy per dimer. Note that both these facts are not true for quadratic lattices. Thus this is a notable difference between the thermodynamical properties of the honeycomb lattices and quadratic lattices. Now we turn to another problem: Is there any other notable difference between the thermodynamical properties of the honeycomb lattices and quadratic lattices?

The classical results on the dimer problem were obtained independently by Fisher [13], Temperley and Fisher [37], and Kasteleyn [20] in 1961. They obtained the bulk entropy per dimer of an $m\times n$ rectangular quadratic lattice G_{mn} as follows:

$$E(G_{mn}) = \lim_{m,n\to\infty}\frac{2}{mn}\log Z_{1,1}(G) = \frac{2}{\pi}\left(1-\frac{1}{3^2}+\frac{1}{5^2}-\frac{1}{7^2}+\cdots\right)$$

as well as for an $m\times n$ torus (see [20]). The solution of the dimer problem was seen as insensitive for its boundary. Many years latter some plane quadratic lattices of other shapes, such as the Aztec Diamond [4, 5] and "almost square-shaped" lattices [35], were found, which had different bulk entropies per dimer. From these examples we can see that the free boundary is not unique and it is not suitable to use the word "insensitive" for square lattices in general. But since $E(G_{mn})$ is a double limit, we can still say that for square lattices of a rectangular region, the bulk entropy per dimer is insensitive for the growth ratio of lengths of two sides of the rectangular region. On the contrary, for honeycomb lattices, Elser [12] solved the dimer problem for general hexagonal regions (see Example 3.4). His result implied that the bulk entropy per dimer depends on the growth ratio of the lengths of the three sides of the hexagonal regions, and thus the bulk double limit does not exist. We solved the dimer problem of the pentagon oblate regions in Example 3.5, which has a similar property. A natural question to ask is whether or not there is a honeycomb lattice region whose bulk double limit exist or bulk entropy per dimer is independent of the growth ratio of the lengths of the sides of the region? The honeycomb lattices in Examples 3.1–3.5 and Example 4.2–4.3 have this property. In general, if we assume that all x-, y-, and z-dimers have different activities, the free energy per dimer for the honeycomb lattices in Examples 3.1–3.2 and Examples 4.2–4.3 also have this property (i.e., the free energy per dimer is independent of the growth ratio of the lengths of the sides of the region). But unfortunately in these examples, the entropy per dimer is zero. Hence we would like to pose the following:

Problem 5.1 Does there exist a honeycomb lattice region H with a nonzero entropy, that is independent of the growth ratio of lengths of the sides of the region?

If the answer of Problem 5.1 is negative, i.e., if there is no honeycomb lattice regions with a nonzero entropy, that is independent of the growth ratio of lengths of the sides of the region (as the role of an $m \times n$ rectangular quadratic lattice G_{mn} in plane quadratic lattice), then there is another notable difference between the plane honeycomb lattices and the plane quadratic lattices.

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