Perfect Matchings in Statistical Physics and Chemistry

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Abstract

A perfect matching of a graph is a collection of vertex-disjoint edges that are collectively incident to all vertices of G. Problems involving enumeration of perfect matchings have been examined extensively not only by mathematicians but also by physicists and chemists. In this talk, we introduce two methods for enumerating perfect matchings— Pfaffian method and transfer matrix method. Some of our recent results on enumeration of matchings are also introduced.

Outline

- Introduction
- Enumeration of perfect matchings by Pfaffians
- Enumeration of perfect matchings by transfer matrix
- Matching polynomials

1. Introduction

Suppose G is a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$.

A set M of edges in G is a matching if every vertex of G is incident with at most one edge in M; it is a perfect matching if every vertex of G is incident with exactly one edge in M. $\phi_k(G)$: the number of matchings of G with k edges. $\phi_0(G) = 1$.

$M(G)$–number of perfect matchings of G,

$m(G, x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k \phi_k(G) x^{n-2k}$–matching polynomial of G.

Problems involving enumeration of perfect matchings have been examined extensively not only by mathematicians (see for example [2-6]) but by physicists and chemists (see for example [7-10]). The dimer problem (or monomer-dimer problem) in statistical physics and enumeration of Kekulé structures of molecular graphs in quantum chemistry are equivalent with the problem involving enumeration of perfect matchings of graphs. In 1961, Kasteleyn [9] introduced the Pfaffian method and Found a formula for the number of perfect matchings of an $m \times n$ quadratic lattice graph. Temperley and Fisher [10] used a different method and arrived at the same result at almost exactly the same time. Both lines of calculation showed the logarithm of the number of perfect matchings, divided by $\frac{mn}{2}$, converges to $2c/\pi \approx 0.58$ (here c is Catalan's constant). This limit is called the entropy per dimer of the quadratic lattice graph by statistical physicists in the lattice gass model.

The computation of $M(G)$ and $m(G,x)$ is difficult: NP-hard (Jerrum, 1987). But it is easy to compute $M(G)$ for the plane graph. How to compute for plane graphs? We need to introduce the concept of the Pfaffian orientation.

2. Enumeration of perfect matchings by Pfaffians

Suppose G^e is an orientation of a simple graph G. Let $A(G^e) = (b_{ij})_{n\times n}$ be the matrix of order n defined as follows:

$$b_{ij} = \begin{cases} 1 & \text{if } (v_i, v_j) \text{ is an arc in } G^e, \\ -1 & \text{if } (v_j, v_i) \text{ is an arc in } G^e, \\ 0 & \text{otherwise.} \end{cases}$$

$A(G^e)$–skew adjacency matrix of G^e. Obviously, $(A(G^e))^T = -A(G^e)$.

If G^e is an orientation of a graph G and C is a cycle of even length, we say that C is oddly oriented in G^e if C contains odd number of edges that are directed in G^e in the direction of each orientation of C. Called G^e a Pfaffian orientation of G if every nice cycle of even length of G is oddly oriented in G^e.

Theorem. If G^e is a Pfaffian orientation of a graph G, then

$$M(G) = \sqrt{\det(A(G^e))},$$

where $A(G^e)$ is the skew adjacency matrix of G^e.

Problem: Does there exist a Pfaffian orientation for every graph? which graphs have a Pfaffian orientation? If a graph has a Pfaffian orientation, then how to orient it?

Pólya's Permanent Problem (in 1913): Given a (0,1) matrix $A = (a_{ij})_{n\times n}$, is there a $B = (b_{ij})_{n\times n}$ such that

$$Per(A) = \det(B)?$$

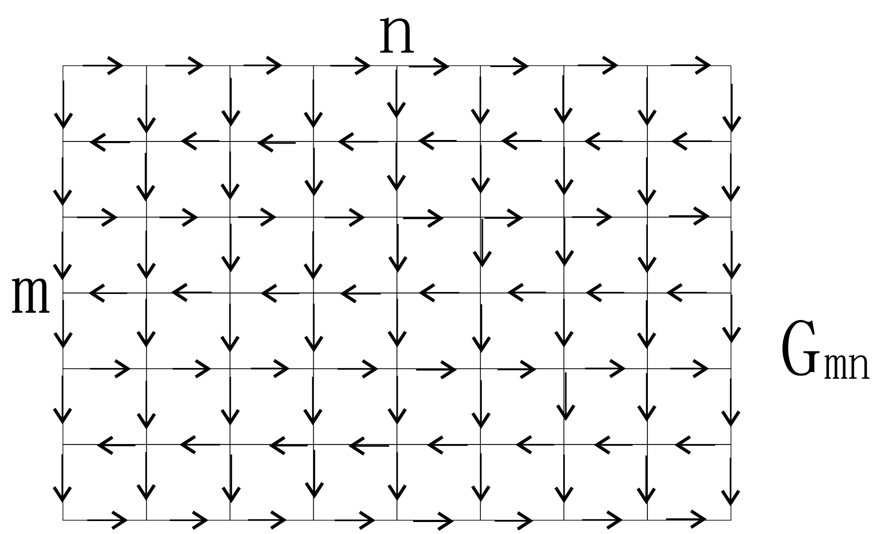
where $b_{ij} = a_{ij}$ or $-a_{ij}$.

The Polyá Permanent Problem is equivalent to:

When does a bipartite graph have a Pfaffian orientation?

Robertson, Seymour and Thomas (Ann. Math., 1999) proved a structural characterization of the feasible instances, which implies a polynomial-time algorithm to solve all of the above problems. Thomas (Pfaffian orientations of graphs, 45 minutes lecture in 2006 ICM) gives a survey of Pfaffian orientations and considers the case of general graphs.

Theorem (Kasteleyn, Fisher, Temperley, 1961):
Every plane graph G has a Pfaffian orientation G^e: Every boundary face—except possible the infinite face—has an odd number edges oriented clockwise. Such G^e can be constructed in polynomial time.



Pfaffian Orientation

Theorem (Fisher, Kasteleyn, and Temperley, 1961) Let G_{mn} be the $m \times n$ square grid graph. Then

$$M(G_{mn}) = 2^{mn/2} \prod_{k=1}^{m} \prod_{l=1}^{n} \left(\cos^2 \frac{k\pi}{n+1} + \cos^2 \frac{l\pi}{m+1} \right)^{\frac{1}{4}},$$

and the entropy, $i.e.,$ $\lim_{m,n \to \infty} \frac{2}{mn} \ln M(G_{mn}) =$

$$\frac{1}{16\pi^2} \int_0^{2\pi} \int_0^{2\pi} \log[4 - 2\cos x - 2\cos y] dx dy \approx 0.58.$$

Symmetric graphs

A plane graph G is called to be reflective symmetric if it is invariant under the reflection across some straight line.

Let G be a reflective symmetric plane bipartite graph with symmetry axis ℓ, which we consider to be horizontal. Let $s_1, t_1, s_2, t_2, \cdots, s_k, t_k$ be the vertices lying on ℓ as they occur from left to right. Let us color the vertices of G in two bipartition classes black and white. For definiteness, choose the leftmost vertex lying on the symmetric axis ℓ to be white. We define two subgraphs G_+ and G_- as follows. Perform cutting operations above all white s_i's and black t_i's and below all black s_i's and white t_i's. Reduce the weight of each such edge by half, leave all other weights unchanged. Two parts– one lying above ℓ, denoted by G_+, and another lying below ℓ, denoted by G_-, are obtained.

Theorem (Ciucu, JCTA, 77(1997), 67-97) Let G be a plane weighted bipartite graph of order $2n$ with reflective symmetry, which splits into two parts G_+ and G_- after removing the vertices on the symmetry axis. Then

$$M^*(G) = 2^k M^*(G_+) M^*(G_-).$$

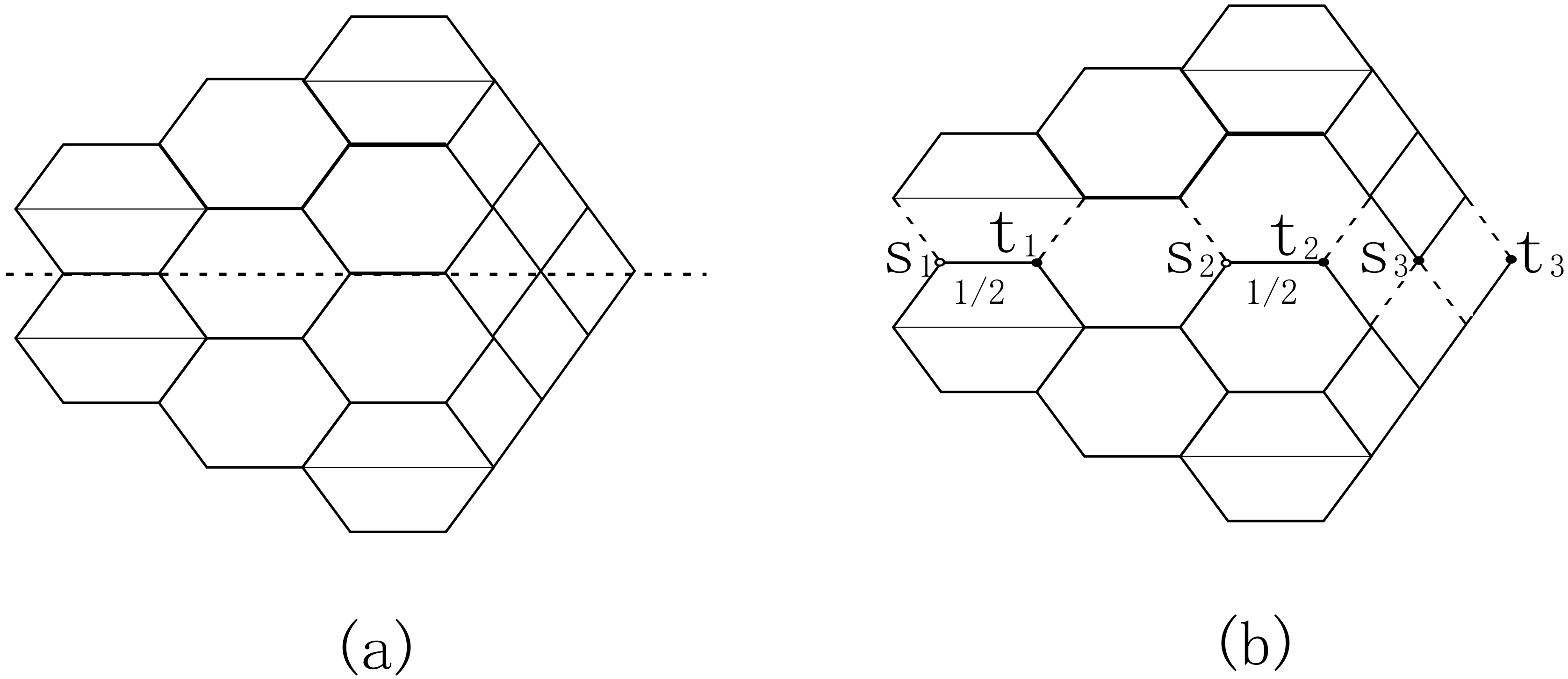
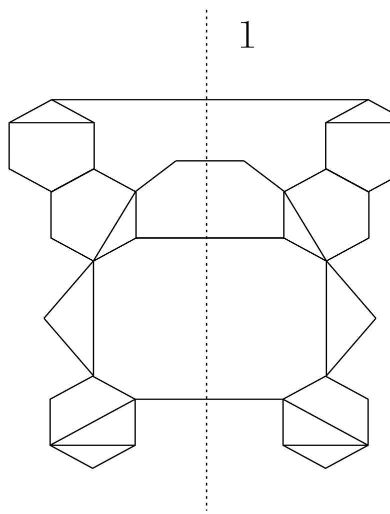
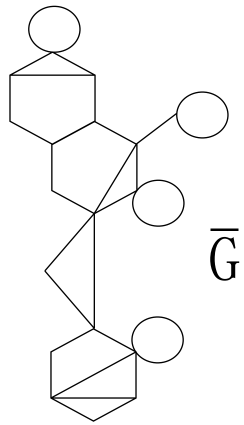


Figure 1: (a) A reflective symmetric graph G. (b) The above part G_+ and the below part G_-.

Let G be a simple connected graph with the symmetry axis ℓ and assume that there are no vertices lying on ℓ (we consider ℓ to be vertical). Then the set of edges of G crossing ℓ forms an edge cut B of G. Define $\bar{G}$ to be the graph obtained from G by adding a loop to each vertex in the left half of G which is an end vertex of an edge in edge cut B.





Theorem (Yan and Zhang, Adv. Appl. Math., 32(2004),655-668) Let G be a symmetric connected plane simple graph with no vertices lying on the symmetry axis l, and let $\bar{G}$ be the graph described above. Then there exists an orientation $\bar{G}^e$ of $\bar{G}$ such that $M^*(G) = |\det A(\bar{G}^e)|$, where $A(\bar{G}^e)$ denotes the skew adjacency matrix of $\bar{G}^e$.

As applications of the above theorem, we proved the following:

$\star$ If G contains no subgraph which is, after the contraction of at most one cycle of odd length, and even subdivision of $K_{2,3}$, then there exists an orientation G^e of G s.t.

$$M(G \times P_2) = \det(A(G^e) + I).$$

⋆ If G is a bipartite graph without cycle of length $4k$, then

$$M(G \times P_2) = \prod_{\theta}(1+\theta^2),$$

where θ ranges over all non negative eigenvalues of G.

⋆ If T is a tree, then

$$M(T \times C_4) = \prod_{\theta}(2+\theta^2), \tag{1}$$

$$M(T \times P_4) = \prod_{\theta}(1+3\theta^2+\theta^4), \tag{2}$$

where the first product (resp. second product) ranges over all eigenvalues (resp. all non-negative eigenvalues) of T.

$\star$ If T contains a perfect matching, then

$$M(T \times P_3) = \prod_{\alpha} (2 + \alpha^2), \tag{3}$$

where α ranges over all non negative eigenvalues of T. Hence $M(T \times C_4) = [M(T \times P_3)]^2$.

Let G be a plane weighted graph with $2n$ vertices. Let vertices $a_1, b_1, \dots, a_k, b_k (2 \le k \le n)$ appear in a cyclic order on a face of G, and let $A = \{a_1, a_2, \cdots, a_k\}$, $B = \{b_1, b_2, \cdots, b_k\}$.

Theorem 5 (Yan, Yeh, and Zhang, TCS, 349(2005), 452-461) For an arbitrary $j = 1, 2, \cdots, k$, we have

$$M(G)M(G-A-B) = \sum M(G-a_j-Y)M(G-A\backslash\{a_j\}-\overline{Y})$$

$$-\sum M(G-W)M(G-A-\overline{W}).$$

where the first sum is over all odd subsets Y of B and the second sum ranges over all non empty even subsets W of B, $\overline{Y} = B\backslash Y$ and $\overline{W} = B\backslash W$.

Corollary 1 (Propp, TCS, 303(2003), 267-301) Let $G = (U, V)$ be a plane bipartite graph in which $|U| = |V|$. Let vertices a, b, c, and d form a $4-$cycle face in G, $a, c \in U$, and $b, d \in V$. Then

$$M(G)M(G - \{a, b, c, d\}) =$$

$$M(G - \{a, b\})M(G - \{c, d\}) +$$
$$M(G - \{a, d\})M(G - \{b, c\}).$$

Corollary 2 (Kuo, TCS, 319(2004), 29-57) Let $G = (U, V)$ be a plane bipartite graph in which $|U| = |V|$. Let vertices $a, b, c,$ and d appear in a cyclic order on a face of G.

(1) If $a, c \in U$, and $b, d \in V$, then

$$M(G)M(G - \{a, b, c, d\}) =$$

$$M(G - \{a, b\})M(G - \{c, d\}) + M(G - \{a, d\})M(G - \{b, c\});$$

(2) If $a, b \in U$, and $c, d \in V$, then

$$M(G - \{a, d\})M(G - \{b, c\}) =$$

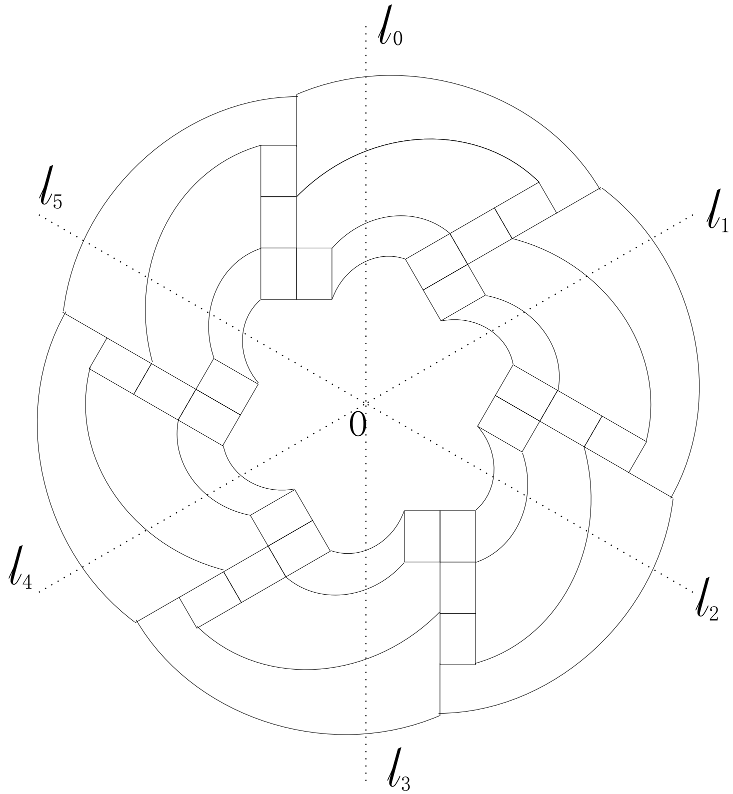
$$M(G)M(G - \{a, b, c, d\}) + M(G - \{a, c\})M(G - \{b, d\}).$$

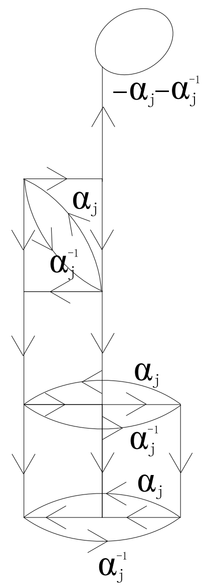
A graph G is called to be n-rotation symmetric if the cyclic group of order n is a subgroup of the automorphism group of G.

Theorem (Yan, Yeh, and Zhang) Let G be a simple connected plane bipartite graph of order N with $2n$-rotation symmetry.

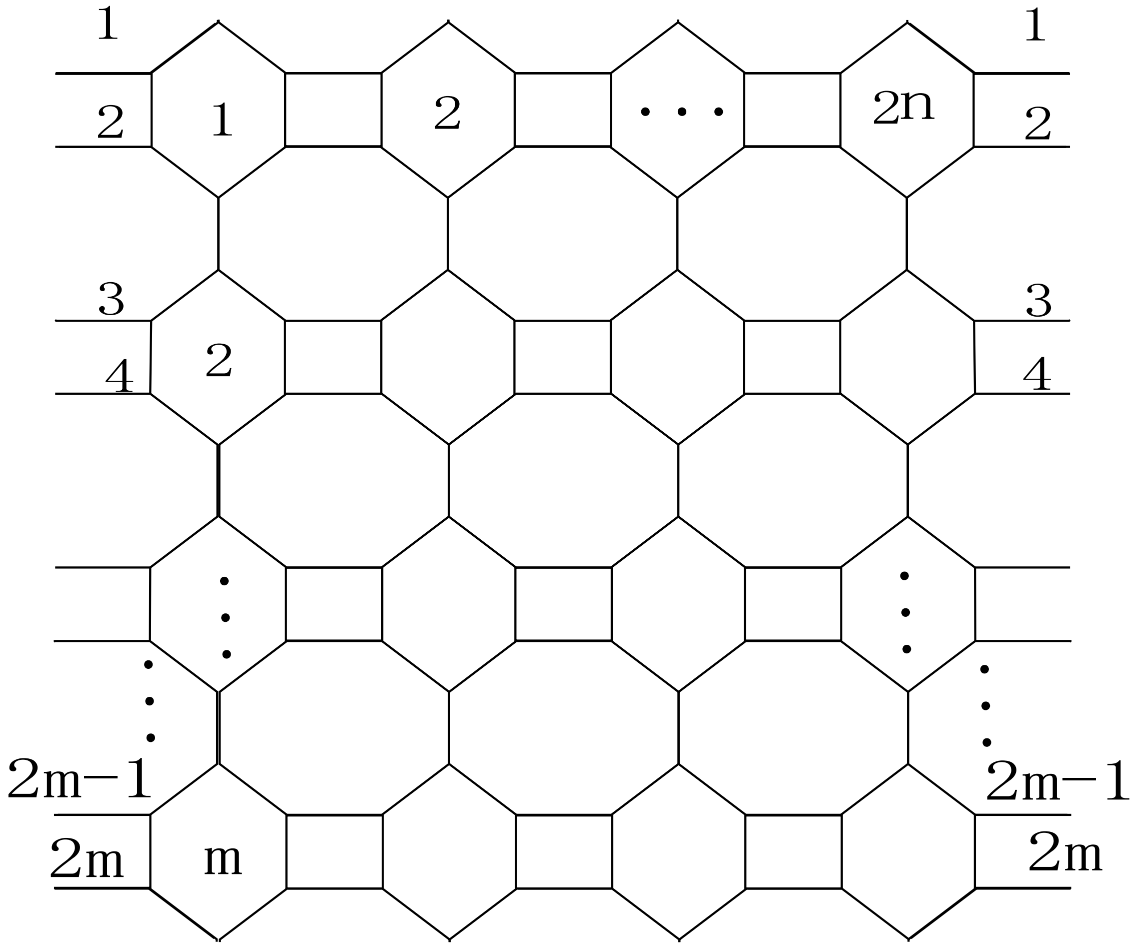
$$M(G) = \prod_{j=0}^{n-1} |\det(A_j)|,$$

where $\alpha_j = \cos\frac{j\pi}{n} + i\sin\frac{j\pi}{n}$ if n is odd and $\alpha_j = \cos\frac{(2j+1)\pi}{2n} + i\sin\frac{(2j+1)\pi}{2n}$ otherwise.





As applications of the above theorem, we count perfect matchings of two cylinders as follows.



4-6-8 lattice cylinder $G_{2n,m}$

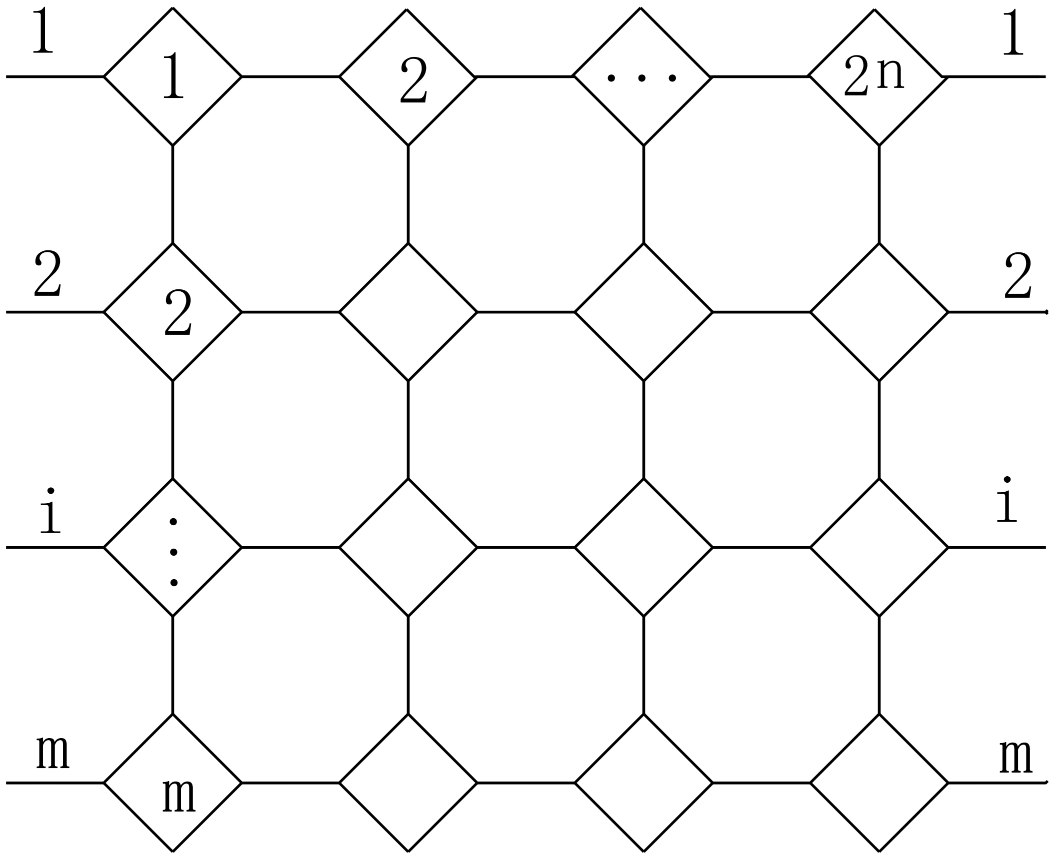
Theorem (Yan, Yeh, Zhang) For the 4-6-8 lattice cylinder $G_{2n,m}$,

$$M(G_{2n,m}) =$$

$$\frac{1}{2^n}\prod_{j=0}^{n-1}\frac{1}{\sqrt{4+\beta_j^2}}\left[\left(\sqrt{4+\beta_j^2}+\beta_j\right)^{2m+1}+\left(\sqrt{4+\beta_j^2}-\beta_j\right)^{2m+1}\right],$$

where $\beta_j = \cos\frac{j\pi}{n}$ if n is odd and $\beta_j = \cos\frac{(2j+1)\pi}{2n}$ otherwise. Hence the entropy equals

$$\frac{2}{3\pi}\int_0^{\frac{\pi}{2}}\log(\cos x+\sqrt{4+\cos^2 x})d_x \approx 0.3344.$$



4-8 Lattice cylinder $G^*_{2n,m}$

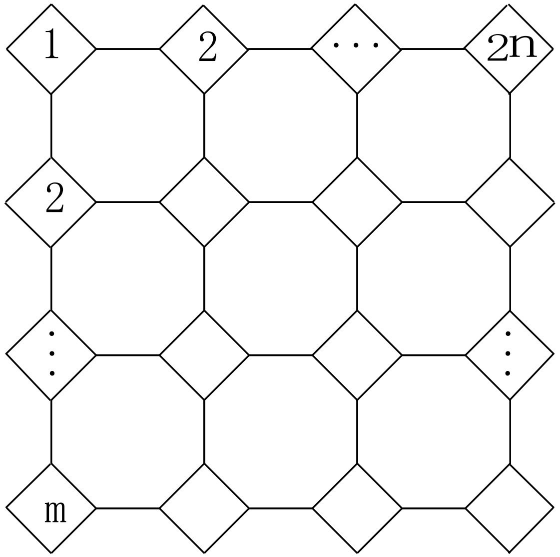
Theorem (Yan, Yeh, Zhang) For the 4-8 lattice cylinder $G^*_{2n,m}$,

$$M(G^*_{2n,m}) = \prod_{j=0}^{n-1}\left[\frac{\sqrt{9+16\beta_j^2}+3}{2\sqrt{9+16\beta_j^2}}\left(\frac{5+\sqrt{9+16\beta_j^2}}{2}\right)^m + \frac{\sqrt{9+16\beta_j^2}-3}{2\sqrt{9+16\beta_j^2}}\left(\frac{5-\sqrt{9+16\beta_j^2}}{2}\right)^m\right],$$

and the entropy equals

$$\frac{1}{8\pi}\int_0^{2\pi}\log(5+\sqrt{9+16\cos^2 x})d_x - \frac{1}{4}\log 2 \approx 0.3770.$$

Where $\beta_j = \cos\frac{j\pi}{n}$ if n is odd and $\beta_j = \cos\frac{(2j+1)\pi}{2n}$ otherwise.



4-8 lattice $G^{**}_{2n,m}$

Theorem (Salinas, Nagle, Phys. Rev. B, 1974) For the 4-8 lattice $G^{**}_{2n,m}$, the entropy is about 0.3770.

Hence both the 4-8 lattice cylinder and the 4-8 lattice have the same entropy!!!

Some of our related papers on Pfaffians:

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6. W. G. Yan, Y. N. Yeh, and F. J. Zhang, Intern. J. Quant. Chem., 105(2005), 124-130.

7. W. G. Yan and Y. N. Yeh, Replacing Pfaffians and applications, to appear in Adv. Appl. Math..

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3. Enumeration of perfect matchings by transfer matrix

The method of transfer matrices is widely used in statstic physics such as the compution of the lattice gass model, partition function etc. Following the experimental discovery of carbon nanotube [4, 5, 6] and the theoretical prediction of the existence of boron-nitride nanotubes, the index Kekulé count of nanotubes has become interesting objects of research.

Theoretically to say, an open-ended nanotube is mathematically a hexagonal system embedded in a cylinder and a capped nanotube consists of an open-ended nanotube capped at its ends by two hemispherical (trivalent and 2-connected polygonal system) caps. For examples, the caps in a capped carbon nanotube are composed of hexagons and (twelve) pentagons while, in a Boron-Nitride nanotube, the caps are composed of hexagons and (six) squares.

Sachs, Hansen and Zheng have done some significant works on Kekulé counts in the open-ended nanotubes and gave out, in particular, the closed formula for a special capped carbon fullerene tubule which consists of an untwisted (or called zigzag in some other literatures) tubule capped at its ends by two halves of a pentagon-dodecahedron [7]. For the hexagonal system embedding on the torus, Klein bottle and the capped near-benzenoid nanotube (or called the cylindrical near-benzenoid graph in their article), Klein and Zhu established the analytical formulae, in terms of transfer matrix and self-avoiding walk system, to this index. In [8], Lin and Tang set up a recurrence algorithm to the Kekulé count for two types of the boron-nitride zigzag nanotubes and gave out the numerical results for those of length up to 8. From their numerical results, Lin $et.al.$ also observed that the Kekulé counts increase exponentially with respect to the length of the tubule. In [9], the present authors dealt with the capped zigzag nanotubes. A closed expression of the Kekulé count is obtained and the asymptotic behavior is also considered.

In this section, we count the Kekulé structures on two extreme patterns of the twisted tubules (see [7, 10] for details): the capped zigzag and armchair nanotubes, by using the technique of the transfer matrix.

The zigzag tubule [7, 8, 10] is constructed by starting from a suitable rectangular section cut from the honeycomb lattice as shown in Figure 1(a) in which two edges of each hexagon are parallel to the axis y: each dangling bond at the left-side $(x = 0)$ is identified to the corresponding

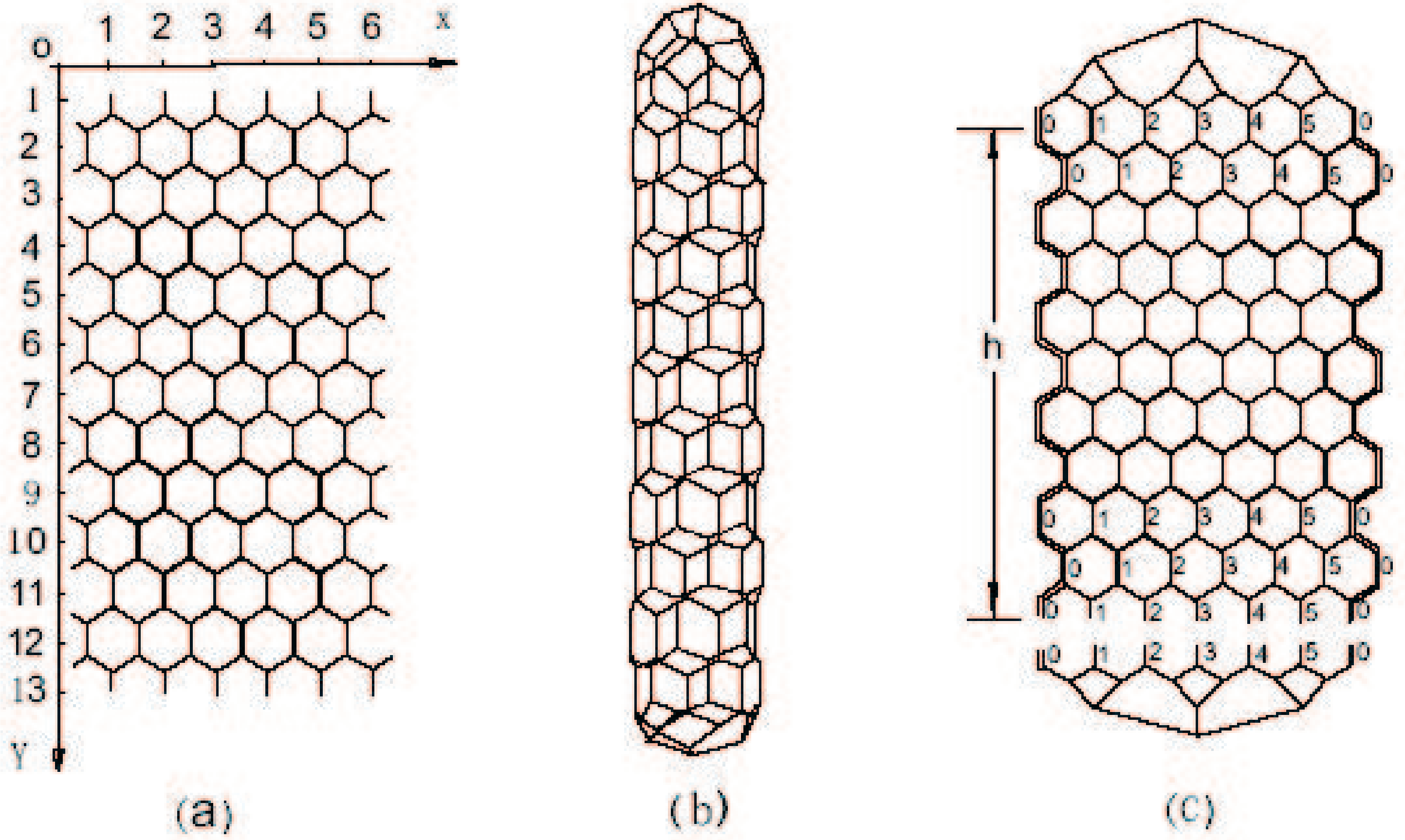

Figure 2: (a). A rectangular section cut from the honeycomb lattice; (b). A capped zigzag nanotube; (c). Draw a semi-capped tubule and a cap in a planar mode.

(with equal-y axis) dangling bond at the right-side($x = w$). The number h ($h \geq 1$) and w measure the length and the circumference of the tubule (in Figure 1(a), we have $h = 13$ and $w = 6$), respectively. In the following, the layers of a tubule of length h are always numbered by $1, 2, \cdots, h$, in an order from the top to the bottom, respectively.

The capped zigzag tubule [8, 10] $T_h(C, C')$ is constructed by adding two suitable caps (i.e., the trivalent and 2-connected polygonal system with some dangling bonds on its boundary) C and C' to the upper and lower open ends of an open-ended zigzag tubule of length h, respectively (i.e., identifying the corresponding dangling bonds of the open tubule with that of the two caps C and C'). To be convenient, we will call a tubule with exactly one end capped with a cap C a semi-capped tubule and denote it by $T_h(C)$. Therefore, a capped tubule $T_h(C, C')$ could be considered to be constructed by joining a cap C' to the semi-capped tubule $T_h(C)$. One can see that the structure of a capped tubule $T_h(C, C')$ is determined uniquely by the way how to join C' with $T_h(C)$. Some examples of caps are shown in Figure 2 and a capped tubule $T_h(C_4, C_4)$ is shown in Figure 1(b). For the further information of caps, we may refer to [8, 11, 12]. Let us draw a semi-capped tubule $T_h(C)$ and a cap C' in a planar mode as shown in Figure 1(c).

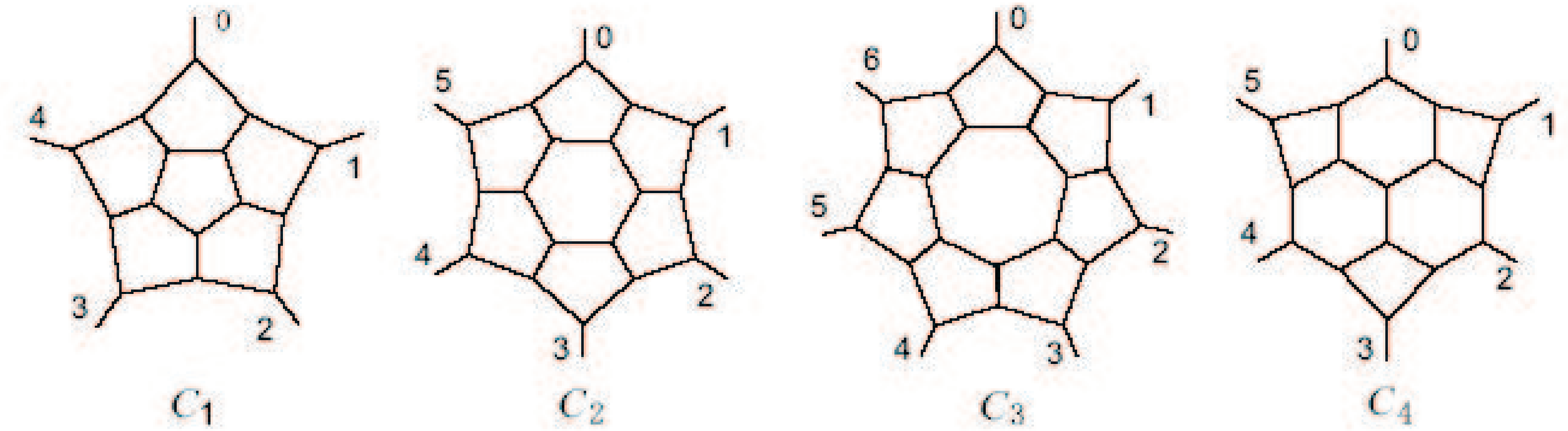

Figure 3: Some examples of caps.

The armchair tubule [7, 8, 10] is constructed by starting from a suitable rectangular section cut from the honeycomb lattice as shown in Fig. 3(a) in which two edges of each hexagon are parallel to the axis x: each dangling bond at the left-side ($x = 0$) is identified to the corresponding (with equal-y axis) dangling bond at the right-side($x = w$). The number h ($h \geq 1$) and w measure the length and the circumference of the tubule (in Fig. 3(a), we have $h = 16$ and $w = 8$), respectively. The capped armchair tubule [10] $T_h(C, C')$ is constructed analogously (see fig 4).

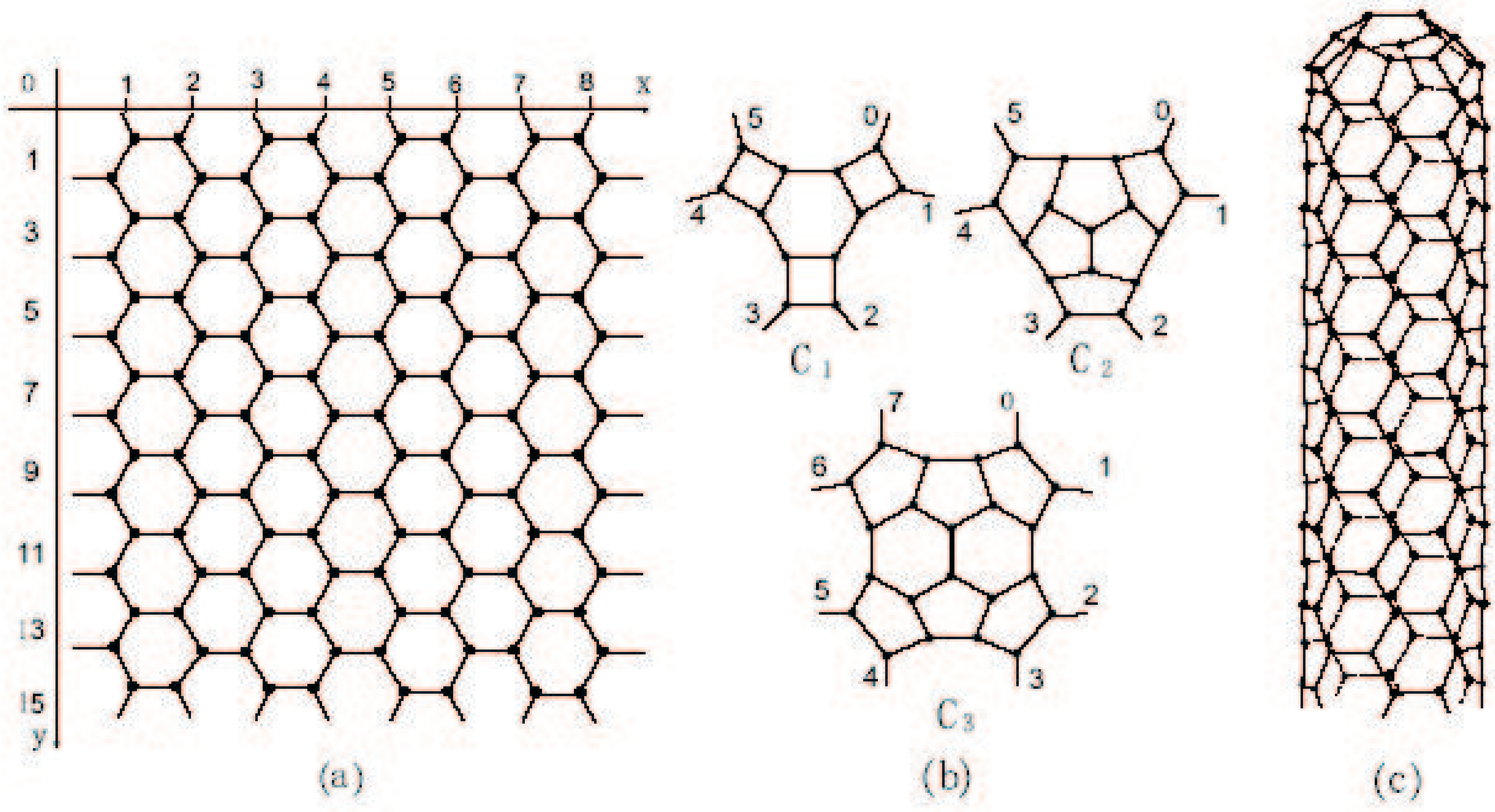

Fig. 4: (a). A rectangular section cut from the honeycomb lattice; (b). Example of caps; (c). An armchair nanotube with one end capped with C_3.

In [16, 17], Qian and Zhang established some formula for zigzag and armchair nanotubes by using the technique of transfer matrix. As an example, in the following, we only discuss the zigzag nanotubes.

For a Kekulé structure M of $T_h(C, C')$, a vertical bond e is said to be a double bond if $e \in M$. It could be observed that there is exactly one double bond between two successive double bonds of the previous layer. So for any Kekulé structure M, the number of double bonds in each layer are the same. Let the bonds in each layer be numbered by $0, 1, 2, \cdots, w$ as illustrated in Figure 1(c). For a layer j and a subset $\{x_1, x_2, \cdots, x_k\} \subseteq \{0, 1, 2, \cdots, w-1\}$, denote by $x_1 x_2 \cdots x_k$

the double-bond structure (or shortly, D-B structure) when the j-th layer has exactly k double bonds, numbered by $x_1, x_2, \cdots, x_k$, respectively. With no loss of generality, we always assume that $x_1 < x_2 < \cdots < x_k$. Arrange all the possible $\binom{w}{k}$ D-B structures in a suitable order, say the lexicographic order:

$$X_1 = 012\cdots(k-2)(k-1), X_2 = 012\cdots(k-2)k,$$

$$X_3 = 012\cdots(k-2)(k+1),$$
$$\cdots, X_{\binom{w}{k}} = (w-k)(w-k+1)\cdots(w-1).$$

Consider the distribution of the double bonds in two neighboring, say the p-th and $(p+1)$-th, layers. A D-B structure X' in the p-th ($p \in \{0, 1, 2, \cdots, h-1\}$) layer is called a successor of the D-B structure X in the $(p+1)$-th layer if X' may immediately follow X. For an example, let $w = 5$ and let the DB-structure $X = 134$, then all the successors of X are 013, 023, 134 and 234 as illustrated in Figure 3. The following result is immediate.

Proposition 1. $x'_1 x'_2 \cdots x'_k$ is a successor of $x_1 x_2 \cdots x_k$ if and only if

1. When $p+1$ is odd, $x_i \leq x'_i \leq x_{i+1} - 1$ for each $i = 1, 2, \cdots, k-1$, and $x_k \leq x'_k \leq w - 1$ or
   $x_{i-1} \leq x'_i \leq x_i - 1$ for each $i = 2, \cdots, k$, and $0 \leq x'_1 \leq x_1 - 1$;

2. When $p+1$ is even, $x_i + 1 \leq x'_i \leq x_{i+1}$ for each $i = 1, 2, \cdots, k-1$, and $x_k + 1 \leq x'_k \leq w - 1$ or $x_{i-1} + 1 \leq x'_i \leq x_i$ for each $i = 2, \cdots, k$, and $0 \leq x'_1 \leq x_1$.

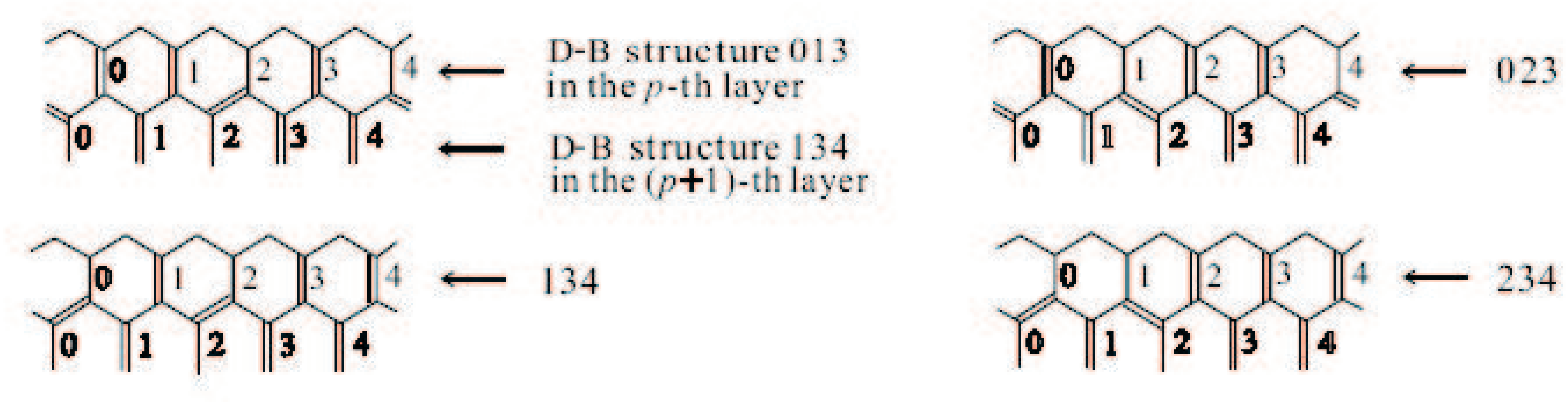

Figure 5: The DB-structure 134 in the $(p+1)$-th layer and its successors.

For a D-B structure X, let $k_h(C, X)$, or $k_h(X)$ if no confusion can occur, be the number of Kekulé structures in the semi-capped tubule $T_h(C)$ when the h-th layer has D-B structure X. In particular, $k_1(C, X)$ is the number of Kekulé structures in the cap C when the dangling bonds of C has the D-B structure X.

For a cap C, we may treat it as a graph including its w dangling bonds. Consider the automorphism group Aut(C) of C. Two D-B structures $x_1 x_2 \cdots x_k$ and $x'_1 x'_2 \cdots x'_k$ of the dangling bonds of C are called equivalent if there is a permutation π on $\{1, 2, \cdots, k\}$ and an automorphism $\rho \in \mathrm{Aut}(C)$ such that

$$\rho(x_{\pi(i)}) = x'_i, i = 1, 2, \cdots, k.$$

In this way, the D-B structures of the dangling bonds of C with cardinality k may be partitioned into some equivalence classes, say $\mathcal{X}_1, \mathcal{X}_2, \cdots, \mathcal{X}_s$. For an example, the equivalence classes of the D-B structures of C_4 with cardinality 2 (see Figure 2) are

$$\mathcal{X}_1 = \{01, 12, 23, 34, 45, 05\}, \mathcal{X}_2 = \{02, 24, 04\}, \mathcal{X}_3 = \{03, 14, 25\},$$

$$\mathcal{X}_4 = \{13, 35, 15\}.$$

From the above definition, one can see that if two D-B structures X and X' are in the same equivalence class, then $k_1(X) = k_1(X')$. It can be observed that $\mathcal{X}_1, \mathcal{X}_2, \cdots, \mathcal{X}_s$, are also the equivalence classes of the D-B structures for each odd layer of $T_h(C)$.

Choose an arbitrary representative D-B structure, say $X_{\alpha(i)}$ ($\alpha(i) \in \{1, 2, \cdots, \binom{w}{k}\}$), from each $\mathcal{X}_i, i = 1, 2, \cdots, s$, respectively. Define the s-dimensional vector $\mathcal{V}_h^k(C)$ for odd h to be

$$\mathcal{V}_h^k(C) = (k_h(X_{\alpha(1)}), k_h(X_{\alpha(2)}), \cdots, k_h(X_{\alpha(s)})).$$

Taking the role of C by $T_2(C)$ and repeating the same discussion as above, we get an equivalence classes, say $\mathcal{Y}_1, \mathcal{Y}_2, \cdots, \mathcal{Y}_t$, for the D-B structures with cardinality k of the second layer of $T_2(C)$. It can also be observed that $\mathcal{Y}_1, \mathcal{Y}_2, \cdots, \mathcal{Y}_t$, are the equivalence classes of the D-B structures for each even layer of $T_h(C)$.

Similarly, choose an arbitrary representative D-B structure, say $X_{\beta(i)}$ $(\beta(i) \in \{1, 2, \cdots, \binom{w}{k}\})$, from each $\mathcal{Y}_i, i = 1, 2, \cdots, t$, respectively. Then $\mathcal{V}_h^k(C)$ for even h is defined analogously to be the t-dimensional vector:

$$\mathcal{V}_h^k(C) = (k_h(X_{\beta(1)}), k_h(X_{\beta(2)}), \cdots, k_h(X_{\beta(t)})).$$

For two representative D-B structures $X_{\alpha(i)}$ and $X_{\beta(i)}$, Let $\mathcal{S}_i$ and $\mathcal{S}_i'$ be the sets of all successors of $X_{\alpha(i)}$ and $X_{\beta(i)}$, respectively. With this notation and recalling that if two D-B structures X and X' are in the same equivalence class then

$k_1(X) = k_1(X')$, when h is odd it can be seen that

$$k_h(X_{\alpha(i)}) = \sum_{X \in \mathcal{S}_i} k_{h-1}(X) = \sum_{j=1}^{t} \sum_{X \in \mathcal{S}_i \cap \mathcal{Y}_j} k_{h-1}(X)$$

$$= \sum_{j=1}^{t} k_{h-1}(X_{\beta(j)}) \cdot |\mathcal{S}_i \cap \mathcal{Y}_j|.$$

Similarly, when h is even, we have

$$k_h(X_{\beta(i)}) = \sum_{X \in \mathcal{S}'_i} k_{h-1}(X) = \sum_{j=1}^{s} \sum_{X \in \mathcal{S}'_i \cap \mathcal{X}_j} k_{h-1}(X)$$

$$= \sum_{j=1}^{s} k_{h-1}(X_{\alpha(j)}) \cdot |\mathcal{S}'_i \cap \mathcal{X}_j|.$$

In terms of transfer matrix [12, 13], the above discussion implies the following result.

Proposition 2 $\mathcal{V}_h^k(C)$ could be expressed by the following recurrence relation

$$\mathcal{V}_h^k(C) = \mathcal{V}_{h-1}^k(C) M_h^k,$$

where the transfer matrix M_h^k is of order $t \times s$ if h is odd; or $s \times t$ if h is even. Furthermore, the entry $t_{i,j}$ at the (i, j)-position of

M_h^k equals

$$t_{i,j} = \begin{cases} \mid \mathcal{Y}_i \cap \mathcal{S}_j \mid, & \text{when } h \text{ is odd} \\ \mid \mathcal{X}_i \cap \mathcal{S}'_j \mid, & \text{when } h \text{ is even.} \end{cases}$$

The above proposition also indicates that $M_l^k = M_h^k$ if l and h have the same parity. So it would be convenient to rewrite M_h^k generally by M_e^k (resp., M_o^k) when h is even (resp., odd).

Thus,

$$\mathcal{V}_h^k(C) = \begin{cases} \mathcal{V}_{h-1}^k M_o^k = \cdots = \mathcal{V}_1^k (M_e^k M_o^k)^{\frac{h-1}{2}}, & \text{when } h \text{ is odd} \\ \mathcal{V}_{h-1}^k M_e^k = \cdots = \mathcal{V}_2^k (M_o^k M_e^k)^{\frac{h}{2}-1}, & \text{when } h \text{ is even.} \end{cases} \tag{1}$$

According to the connecting mode between $T_h(C)$ and the cap C', the D-B structure X of $T_h(C)$ corresponds to a D-B structure, say X^*, of C'. More precisely, let $T_h(C, C')$ be constructed from $T_h(C)$ and C' by identifying the dangling bonds $0, 1, 2, \cdots, w-1$ of $T_h(C)$ with the dangling bonds $q, q+1, q+2, \cdots, q+w-1$ mod$w$ of C', respectively and let

$X = x_1 x_2 \cdots x_k$. Then $X^* = (x_1 + q)(x_2 + q) \cdots (x_k + q)$ mod$w$. Furthermore, we define

$$\mathcal{X}_i^* = \{X^* : X \in \mathcal{X}_i\}.$$

For a D-B structure X in the h-th layer of $T_h(C, C')$, let $k_h(C, C', X)$ denote the number of the Kekulé structures in $T_h(C, C')$ in which the h-th layer of $T_h(C)$ has the D-B structure X. One can verify that

$$k_h(C, C', X) = k_h(C, X) k_1(C', X^*).$$

Let

$$k_h(C, C', \mathcal{X}_i) = \sum_{X \in \mathcal{X}_i} k_h(C, C', X).$$

Let $\mathcal{X}_1, \mathcal{X}_2, \cdots, \mathcal{X}_s$ and $\mathcal{X}'_1, \mathcal{X}'_2, \cdots, \mathcal{X}'_{s'}$ be the equivalence classes of the h-th layer of $T_h(C)$ and the dangling bonds of C', respectively. For any $\mathcal{X}_i \in \{\mathcal{X}_1, \mathcal{X}_2, \cdots, \mathcal{X}_s\}$, define

$$\mathcal{V}_1^k(C')/\mathcal{X}_i = \sum_{j=1}^{s'} |\mathcal{X}'_j \cap \mathcal{X}^*_i| \cdot k_1(C', X'_j),$$

where X'_j is the representative D-B structure of $\mathcal{X}'_j$.

Recall that if two D-B structures X and X' are in the same equivalence class, then $k_p(C, X) = k_p(C, X')$ for any $p \in \{1, 2, \cdots, h\}$. So we have

$$k_h(C, C', \mathcal{X}_i) = \sum_{X \in \mathcal{X}_i} k_h(C, C', X) = \sum_{X \in \mathcal{X}_i} k_h(C, X) k_1(C', X^*)$$

$$= k_h(C, X_i) \cdot \sum_{X \in \mathcal{X}_i} k_1(C', X^*) = k_h(C, X_i) \cdot (\sum_{j=1}^{s'} \sum_{X \in \mathcal{X}'_j \cap \mathcal{X}^*_i} k_1(C', X))$$

$$= k_h(C, X_i) \cdot (\sum_{j=1}^{s'} |\mathcal{X}'_j \cap \mathcal{X}^*_i| \cdot k_1(C', X'_j)) = k_h(C, X_i) \cdot \mathcal{V}_1^k(C')/\mathcal{X}_i,$$

where X_i and X'_j are the representative D-B structures of $\mathcal{X}_i$ and $\mathcal{X}'_j$, respectively.

Let

$$\mathcal{V}_1^k(C')/\mathcal{V}_h^k(C) = (\ \mathcal{V}_1^k(C')/\mathcal{X}_1, \mathcal{V}_1^k(C')/\mathcal{X}_2, \cdots, \mathcal{V}_1^k(C')/\mathcal{X}_s\ ).$$

Then by (1), we have the following result.

Proposition 3 The number of Kekulé structures in $T_h(C, C')$ is

$$K_h(C, C') = \sum_{k=1}^{w} \sum_{i=1}^{s} k_h(C, C', \mathcal{X}_i) = \sum_{k=1}^{w} \sum_{i=1}^{s} k_h(C, X_i) \cdot \mathcal{V}_1^k(C')/\mathcal{X}_i$$

$$= \begin{cases} \sum\limits_{k=1}^{w} \mathcal{V}_1^k(C)(M_e^k M_o^k)^{\frac{h-1}{2}}(\mathcal{V}_1^k(C')/\mathcal{V}_1^k(C))^{\mathrm{T}}, & \text{when } h \text{ is odd} \\ \sum\limits_{k=1}^{w} \mathcal{V}_2^k(C)(M_e^k M_o^k)^{\frac{h}{2}-1}(\mathcal{V}_1^k(C')/\mathcal{V}_2^k(C))^{\mathrm{T}}, & \text{when } h \text{ is even.} \end{cases} \tag{2}$$

For some tubules, for examples, $T_h(C_i, C_i), i \in \{1, 2, 3\}$, the odd layer and the even layer may have the same equivalence classes partition and the same transfer matrix, which implies that (2) could be simplified to be

$$K_h(C, C') = \sum_{k=1}^{w} \mathcal{V}_1^k(C)(M_e^k)^{h-1}(\mathcal{V}_1^k(C')/\mathcal{V}_1^k(C))^{\mathrm{T}}. \tag{3}$$

If the number of vertices in the upper cap is odd ($resp.$, even), then the term for even ($resp.$, odd) k in the summation (1), (2) and (3) will vanish.

Finally, consider the Boron-Nitride zigzag nanotube $T = T_h(C, C')$. Recall that all the polygons on the caps of T are of even sides and therefore, all the polygons on T are of even sides. So, in terms of graph theory, T is a bipartite graph. Colour the vertices in the upper cap C by using two colors, say black and red, such that any two adjacent vertices have distinct colors. Then it can be observed that the end vertices of the dangling bonds of C must have the same color. Since for any Kekulé structure M, each double bonds in M matches exactly one black vertex and one red vertex, so the dangling bonds of C contains exactly $k = |r - b|$ double bonds which do not depend on the choice of M, where b and r are the numbers of the black and red vertices, respectively. This also implies that each layer of T contains exactly $k = |r - b|$ double bonds. Thus, the formula (2) would be simplified further to be

$$K_h(C, C') =$$

$$\begin{cases} \mathcal{V}_1^k(C)(M_e^k M_o^k)^{\frac{h-1}{2}}(\mathcal{V}_1^k(C')/\mathcal{V}_1^k(C))^{\mathrm{T}}, & \text{when } h \text{ is odd} \\ \mathcal{V}_2^k(C)(M_e^k M_o^k)^{\frac{h}{2}-1}(\mathcal{V}_1^k(C')/\mathcal{V}_2^k(C))^{\mathrm{T}}, & \text{when } h \text{ is even.} \end{cases} \tag{4}$$

An other algebraic expression to the number of Kekulé structures involves the characteristic polynomial of the transfer matrix. Let the characteristic polynomial of the transfer matrix $M_e^k M_o^k$ be

$$p(\lambda) = \lambda^s - d_1\lambda^{s-1} + d_2\lambda^{s-2} - \cdots + (-1)^s d_s, \qquad (5)$$

where the coefficient d_i $(1 \leq i \leq s)$ is the sum of all main minors of order i in the determinant $\det(M_e^k M_o^k)$.

By (1), from a standard result on simultaneous relations, each entry $k_h(X_j)$ of $\mathcal{V}_h^k(C)$ satisfies a common recurrence relation

[13], i.e.

$$k_h(X_j) = \sum_{i=1}^{s} (-1)^{i+1} d_i k_{h-2i}(X_j). \quad (6)$$

Let $\xi_1, \xi_2, \cdots, \xi_p$, $|\xi_1| \geq |\xi_2| \geq \cdots \geq |\xi_p|$, be the roots of (5) (i.e., the eigenvalues of the matrix $M_e^k M_o^k$) with multiplicity $m_1, m_2, \cdots, m_p$, respectively. Then by standard techniques in recursive relation (see [14] for details), we have

$$k_h(X_j) = \sum_{i=1}^{p} (a_{i1}^j h^{m_i-1} + a_{i2}^j h^{m_i-2} + \cdots + a_{im_i}^j) \xi_i^{\frac{h-1}{2}}, \quad (7)$$

where $a_{it}^{j}, i = 1, 2, \cdots, p; t = 1, 2, \cdots, m_p$, are coefficient which could be determined by $k_i(X_j), i = 1, 3, \cdots, 2s-1$, and hence could be calculated from (1). Combining with (2), we get an other expression, by words of eigenvalue, to the number $K_h(C, C')$:

$$K_h(C, C') =$$

$$\sum_{k=1}^{w}\sum_{j=1}^{s}\left((\mathcal{V}_1^k(C')/\mathcal{X}_j)\sum_{i=1}^{p}(a_{i1}^{j}h^{m_i-1} + a_{i2}^{j}h^{m_i-2} + \cdots + a_{im_i}^{j})\xi_i^{\frac{h-1}{2}}\right). \tag{8}$$

Similarly, when h is even we have (the discussion is similar and is omitted)

$$K_h(C, C') =$$

$$\sum_{k=1}^{w} \sum_{j=1}^{t} \left((\mathcal{V}_1^k(C')/\mathcal{Y}_j) \sum_{i=1}^{p} (a_{i1}^j h^{m_i-1} + a_{i2}^j h^{m_i-2} + \cdots + a_{im_i}^j) \xi_i^{\frac{h}{2}-1} \right). \tag{9}$$

The above two algebraic formulae (8) and (9) also provide a way to view the asymptotic behaviour to the number $K_h(C, C')$ which indicates that, in general, the number of Kekulé structures in capped zigzag nanotubes increase exponentially with respect to the length h.

Theorem 1.

$$K_h(C, C') \sim h^{m_1-\delta}\xi^{h/2}, \quad \text{as } h \to +\infty,$$

where ξ is the eigenvalue of greatest modulus among all the matrices $M_e^k M_o^k$ (or $M_3^k M_e^k$), $k = 1, 2, \cdots, w$, satisfying
1). $\mathcal{V}_1^k(C')/\mathcal{V}_1^k(C) \neq (0, 0, \cdots, 0)$ (or $\mathcal{V}_1^k(C')/\mathcal{V}_2^k(C) \neq (0, 0, \cdots, 0)$); and
2). $\delta = \max\{l : a_{1l}^j \neq 0, j = 1, 2, \cdots, t(\text{or } s); l = 1, 2, \cdots, m_1\}$.

The following are the algebraic formula and the enumerating values of $K_h(C_i, C_j)$ for the caps illustrated in Figure 2.

Table 1 The closed expressions of $K_h(C_i, C_i)$, $i = 1, 2, 3, 4$.

tubule	$K_h(C_i, C_i)$
$T_h(C_1, C_1)$	$1 + 5^{h+2} + (2,1)\begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix}^{h-1}\begin{pmatrix} 10 \\ 5 \end{pmatrix}$ $= 1 + 5^{h+2} + 5 \times (\frac{5}{2} + \frac{\sqrt{5}}{2})^h + 5 \times (\frac{5}{2} - \frac{\sqrt{5}}{2})^h$
$T_h(C_2, C_2)$	$1 + 2^{h+3} + (3,4,5)\begin{pmatrix} 2 & 2 & 2 \\ 2 & 4 & 4 \\ 1 & 2 & 3 \end{pmatrix}^{h-1}\begin{pmatrix} 18 \\ 24 \\ 15 \end{pmatrix} + (2,1,0)\begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & 2 \\ 0 & 1 & 2 \end{pmatrix}^{h-1}\begin{pmatrix} 12 \\ 6 \\ 0 \end{pmatrix}$ $= 2 + 2^{h+4} + ((112 + 64\sqrt{3}) \times 2^{h-1} + 7 + 4\sqrt{3})(2 + \sqrt{3})^{h-1}$ $+((112 - 64\sqrt{3}) \times 2^{h-1} + 7 - 4\sqrt{3})(2 - \sqrt{3})^{h-1}$
$T_h(C_3, C_3)$	$1 + 7^{h+2} + (3,2,4,3)\begin{pmatrix} 2 & 1 & 1 & 0 \\ 2 & 4 & 2 & 4 \\ 1 & 1 & 3 & 3 \\ 0 & 2 & 3 & 5 \end{pmatrix}^{h-1}\begin{pmatrix} 21 \\ 28 \\ 28 \\ 21 \end{pmatrix}$ $+(2,1,0)\begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 3 \end{pmatrix}^{h-1}\begin{pmatrix} 14 \\ 7 \\ 0 \end{pmatrix}$ (the second expression is too tedious and is omitted here)

$T_h(C_4, C_4)$ (Type 1)	$(4,8,8,6)\begin{pmatrix} 10 & 16 & 18 & 16 \\ 8 & 16 & 16 & 12 \\ 9 & 16 & 19 & 16 \\ 8 & 12 & 16 & 16 \end{pmatrix}^{\frac{h-1}{2}} \begin{pmatrix} 24 \\ 24 \\ 24 \\ 18 \end{pmatrix}$ (when h is odd) $= 6 \times 4^{\frac{h-1}{2}} + (291 + 168\sqrt{3})(28 + 16\sqrt{3})^{\frac{h-1}{2}} + (291 - 168\sqrt{3})(28 - 16\sqrt{3})^{\frac{h-1}{2}}$ $(28,52,60,32)\begin{pmatrix} 7 & 8 & 9 & 3 \\ 16 & 28 & 32 & 16 \\ 9 & 16 & 19 & 9 \\ 3 & 8 & 9 & 7 \end{pmatrix}^{\frac{h}{2}-1} \begin{pmatrix} 12 \\ 42 \\ 24 \\ 12 \end{pmatrix}$ (when h is even) $= (2172 + 1254\sqrt{3})(28 + 16\sqrt{3})^{\frac{h}{2}-1} + (2172 - 1254\sqrt{3})(28 - 16\sqrt{3})^{\frac{h}{2}-1}$
$T_h(C_4, C_4)$ (Type 2)	$(4,8,8,6)\begin{pmatrix} 10 & 16 & 18 & 16 \\ 8 & 16 & 16 & 12 \\ 9 & 16 & 19 & 16 \\ 8 & 12 & 16 & 16 \end{pmatrix}^{\frac{h-1}{2}} \begin{pmatrix} 24 \\ 18 \\ 24 \\ 24 \end{pmatrix}$ (when h is odd) $= -6 \times 4^{\frac{h-1}{2}} + (291 + 168\sqrt{3})(28 + 16\sqrt{3})^{\frac{h-1}{2}} + (291 - 168\sqrt{3})(28 - 16\sqrt{3})^{\frac{h-1}{2}}$ (The value is the same as that of Type 1 when h is even)

Table 2 The numerical results of $K_h(C_i, C_i), i = 1, 2, 3, 4$.

h	$k_h(C_1, C_1)$	$k_h(C_2, C_2)$	$k_h(C_3, C_3)$	$k_h(C_4, C_4)$(Type 1)	$k_h(C_4, C_4)$(Type 2)
1	151	272	673	588	576
2	701	1782	4901	4344	– the same as Type 1, herein after
3	3376	12740	38711	32448	32400
4	16501	93654	317864	242016	–
5	81251	694928	2675401	1806528	1806336
6	401876	5174118	22952189	13483392	–
7	1993751	38576900	200041031	100641792	100641024
8	9912501	287790246	1766636593	751197696	–
9	49359376	2147549072	1577299975×10	5607017472	5607014400
10	246062501	1602752348×10	1420811630×10^2	4185133670×10	–
11	1227656251	1196236735×10^2	1288981957×10^3	3123826360×10^2	3123826237×10^2
12	6128671876	8928558289×10^2	1175975363×10^4	2331655692×10^3	–
13	3060859375×10	6664264589×10^3	1077601707×10^5	1740371504×10^4	1740371499×10^4
14	1529171875×10^2	4974236787×10^4	9908269470×10^5	1299030974×10^5	–
15	7641308594×10^2	3712806706×10^5	9134323628×10^6	9696099191×10^5	9696099189×10^5
16	3819007813×10^3	2771271364×10^6	8437762723×10^7	7237266962×10^6	–
17	1908908203×10^4	2068503133×10^7	7806270265×10^8	5401969602×10^7	5401969602×10^7
18	9542385742×10^4	1543951022×10^8	7230457585×10^9	4032085003×10^8	–
19	4770413086×10^5	1152420457×10^9	$6703039330 \times 10^{10}$	3009589219×10^9	3009589219×10^9
20	2384924414×10^6	8601782366×10^9	$6218252628 \times 10^{11}$	$2246387975 \times 10^{10}$	–
21	1192360132×10^7	$6420457382 \times 10^{10}$	$5771447007 \times 10^{12}$	$1676726811 \times 10^{11}$	$1676726811 \times 10^{11}$
22	5961431348×10^7	$4792294489 \times 10^{11}$	$5358794074 \times 10^{13}$	$1251525930 \times 10^{12}$	–

23	2980582056×10^{8}	$3577017250 \times 10^{12}$	$4977081237 \times 10^{14}$	$9341516714 \times 10^{12}$	$9341516714 \times 10^{12}$
24	1490242684×10^{9}	$2669922004 \times 10^{13}$	$4623564470 \times 10^{15}$	$6972602999 \times 10^{13}$	—
25	7451038513×10^{9}	$1992856906 \times 10^{14}$	$4295862613 \times 10^{16}$	$5204421731 \times 10^{14}$	$5204421731 \times 10^{14}$
26	$3725455974 \times 10^{10}$	$1487488643 \times 10^{15}$	$3991880926 \times 10^{17}$	$3884633265 \times 10^{15}$	—
27	$1862705091 \times 10^{11}$	$1110276637 \times 10^{16}$	$3709755288 \times 10^{18}$	$2899529743 \times 10^{16}$	$2899529743 \times 10^{16}$
28	$9313442618 \times 10^{11}$	$8287217635 \times 10^{16}$	$3447811027 \times 10^{19}$	$2164238463 \times 10^{17}$	—
29	$4656691338 \times 10^{12}$	$6185663452 \times 10^{17}$	$3204532118 \times 10^{20}$	$1615409581 \times 10^{18}$	$1615409581 \times 10^{18}$
30	$2328334826 \times 10^{13}$	$4617042056 \times 10^{18}$	$2978537796 \times 10^{21}$	$1205758126 \times 10^{19}$	—
31	$1164163490 \times 10^{14}$	$3446207107 \times 10^{19}$	$2768564474 \times 10^{22}$	$8999901178 \times 10^{19}$	$8999901178 \times 10^{19}$
32	$5820803253 \times 10^{14}$	$2572284003 \times 10^{20}$	$2573451508 \times 10^{23}$	$6717617692 \times 10^{20}$	—
33	$2910396491 \times 10^{15}$	$1919978918 \times 10^{21}$	$2392129754 \times 10^{24}$	$5014098106 \times 10^{21}$	$5014098106 \times 10^{21}$
34	$1455196387 \times 10^{16}$	$1433091774 \times 10^{22}$	$2223612193 \times 10^{25}$	$3742573778 \times 10^{22}$	—
35	$7275975214 \times 10^{16}$	$1069674263 \times 10^{23}$	$2066986098 \times 10^{26}$	$2793495098 \times 10^{23}$	$2793495098 \times 10^{23}$
36	$3637985175 \times 10^{17}$	$7984157392 \times 10^{23}$	$1921406359 \times 10^{27}$	$2085093127 \times 10^{24}$	—
37	$1818991707 \times 10^{18}$	$5959456209 \times 10^{24}$	$1786089718 \times 10^{28}$	$1556334698 \times 10^{25}$	$1556334698 \times 10^{25}$
38	$9094955353 \times 10^{18}$	$4448198671 \times 10^{25}$	$1660309713 \times 10^{29}$	$1161664033 \times 10^{26}$	—
39	$4547476525 \times 10^{19}$	$3320180689 \times 10^{26}$	$1543392181 \times 10^{30}$	$8670778385 \times 10^{26}$	$8670778385 \times 10^{26}$
40	$2273737846 \times 10^{20}$	$2478216604 \times 10^{27}$	$1434711233 \times 10^{31}$	$6471957096 \times 10^{27}$	—
41	$1136868772 \times 10^{21}$	$1849766056 \times 10^{28}$	$1333685614 \times 10^{32}$	$4830734541 \times 10^{28}$	$4830734541 \times 10^{28}$
42	$5684343314 \times 10^{21}$	$1380684180 \times 10^{29}$	$1239775389 \times 10^{33}$	$3605709349 \times 10^{29}$	—
43	$2842171460 \times 10^{22}$	$1030556702 \times 10^{30}$	$1152478915 \times 10^{34}$	$2691338098 \times 10^{30}$	$2691338098 \times 10^{30}$
44	$1421085659 \times 10^{23}$	$7692179944 \times 10^{30}$	$1071330065 \times 10^{35}$	$2008842104 \times 10^{31}$	—
45	$7105428034 \times 10^{23}$	$5741521275 \times 10^{31}$	$9958956683 \times 10^{35}$	$1499420159 \times 10^{32}$	$1499420159 \times 10^{32}$
46	$3552713924 \times 10^{24}$	$4285529822 \times 10^{32}$	$9257731460 \times 10^{36}$	$1119182443 \times 10^{33}$	—
47	$1776356928 \times 10^{25}$	$3198763007 \times 10^{33}$	$8605883332 \times 10^{37}$	$8353691483 \times 10^{33}$	$8353691483 \times 10^{33}$
48	$8881784517 \times 10^{25}$	$2387589212 \times 10^{34}$	$7999934557 \times 10^{38}$	$6235280209 \times 10^{34}$	—
49	$4440892214 \times 10^{26}$	$1782120850 \times 10^{35}$	$7436652590 \times 10^{39}$	$4654076508 \times 10^{35}$	$4654076508 \times 10^{35}$
50	$2220446091 \times 10^{27}$	$1330193111 \times 10^{36}$	$6913032717 \times 10^{40}$	$3473849998 \times 10^{36}$	—

4. Matching polynomials

The matching polynomial was also called the monomer-dimer partition function in statistical physics by Fisher (Phys. Rev., 124(1961), 1664). In his paper Fisher posed the problem: Compute the matching polynomial $m(G_{mn}, x)$ and the entropy $\lim_{m,n\to\infty} \frac{1}{mn} \ln[m(G_{mn}, x)|_{x=1}]$ for the quadratic lattice graph G_{mn}. This is a difficult problem which has not been solved so far!!! Particularly, no exact solutions about the monomer-dimer problem were available (except in one dimension).

It is not difficult to see that all matchings in a graph $G = (V, E)$ form a simplicial complex consisting of subsets of E. In [18], Qian et. al., established a formula to express the matching polynomial depend only on the maximal matching by using techniques of Möbius inversion:

$$M_G(z) = z^n \sum_{\emptyset \neq \mathcal{N} \subseteq \mathcal{M}_{\max}} (-1)^{\#\mathcal{N}-1} (1 - \frac{1}{z^2})^{\#\cap\mathcal{N}}$$

$$= z^n \sum_{k=1}^{q} (-1)^{k-1} \sum_{1 \leq i_1 < i_2 < \cdots < i_k \leq q} (1 - \frac{1}{z^2})^{\# M_{i_1} \cap \cdots \cap M_{i_k}}$$

where $\mathcal{M}_{\max} = \{M_1, M_2, \cdots, M_q\}$ is the set of distinct maximal matchings in G.

Theorem (Yan, Yeh, Zhang, IJQC, 2005) Suppose that G is a simple graph with n vertices having no cycle of even length and G^e is an arbitrary orientation of G. Then

$$m(G, x) = \det(xI_n + iA(G^e)),$$

where $i^2 = -1$.

Theorem (Yan, Yeh, Zhang, IJQC, 2005) Suppose that G is a simple graph with n vertices and ε edges. Then

$$m(G, x) = \frac{1}{2^\varepsilon} \sum_{G^e \in \Phi(G)} \det(xI_n + iA(G^e)),$$

where the summation ranges over all orientations of G.

A related result see (Yan and Yeh, On the number of matchings of graphs formed by a graph operation, Sci. China: Ser. A Math., in press). In this paper, the monomer-dimer problem for infinite many nontrivial lattice graphs was solved.

Remark: No exact solutions about the monomer-dimer problem were available (except in one dimension) before.

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