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Merrifield-Simmons index of generalized Aztec diamonds and related graphs

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Abstract

Using the transfer matrix method, we compute the Merrifield-Simmons index (the number of independent sets) of the generalized Aztec diamonds and a type of related graphs which are obtained from the weak directed product (tensor product) of paths. In our approach two transfer matrices need to be introduced, each of which is the transpose of the other. Some numerical results obtained by using Matlab are tabulated, which suggest the statement that the generalized Aztec diamonds and a type of related graphs have equal entropy constant. Then we prove the statement.

1. Introduction

Merrifield and Simmons defined a topological space for the chemical graphs which had been used in structural chemistry [1]; the cardinality of the topological space is called the Merrifield- Simmons index. For a graph G the Merrifield-Simmons index is the number of independent sets of G. The properties of the Merrifield-Simmons index of some type of benzenoids and polyominoes have been studied in [2,3,4,5]. The enumeration of the perfect matchings of Aztec diamonds has been studied by several authors. An elegant formula was given in [6] and four proofs were given. Some recurrent relations were given in [7,8,9], which in turn imply the results in [6]. The weighted Aztec diamonds were also considered in [7]. The enumeration of spanning trees of Aztec diamonds was considered in [11] in which the spanning trees of Aztec diamonds were tabulated for $n \leq 6$. Based on the numerical result Stanley conjectured that Aztec diamonds contain exactly 4 times as many spanning trees as a type of related graphs. This conjecture was proved in [12,13,14] by using the spectral theory of graphs.

In this paper, we consider the generalized Aztec diamonds as in [11], which are a type of chemical graphs including Aztec diamonds as a special case. An interesting problem is to compute the Merrifield-Simmons index of such graphs. We will deal with this problem by using the transfer matrix method.

Let Li be the path with i vertices 1, 2,..., i . The tensor product of two paths $L_n * L_m$ is the graph on $n \times m$ vertices {(x, y): $1 \le x \le n$, $1 \le y \le m$}, with (x, y) adjacent to (x', y') if and only if $|x-x'| = |y-y'| = 1$. Obviously this graph consists of two connected components:

one denoted O($L_n * L_m$) has the vertices {(x, y)| x+ y is odd}, and the other denoted E($L_n * L_m$) has the vertices {(x, y)| x+ y is even}.

The graph O($L_{2n+1} * L_{2n+1}$) is called the Aztec diamond of order n. The more general O($L_{2n+1} * L_{2m+1}$) is called the generalized Aztec diamond of order $n \times m$. We attempt to enumerate the independent sets of O($L_{2n+1} * L_{2m+1}$) as well as the independent sets of E($L_{2n+1} * L_{2m+1}$). As an illustrative example, $L_9 * L_9$ is depicted in Fig 1 and the two components of $L_9 * L_9$ are shown in Fig 2 where an independent set is indicated by bigger dots.

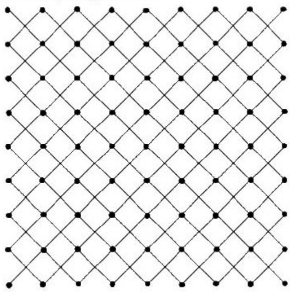

Fig 1

$L_9 * L_9$

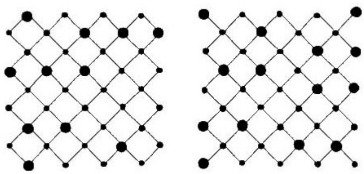

Fig 2

O($L_9 * L_9$) E($L_9 * L_9$)

To enumerate the independent sets of generalized Aztec diamonds we need to introduce two transfer matrices T_1 and T_2, each of which is the transpose of the other. The matrices T_1, T_2 can also be employed to enumerate the independent sets of E($L_{2n+1} * L_{2m+1}$) in a similar way. The numerical results for n$\leq$6 and m$\leq$10 are tabulated. The data shows that the number of independent sets of O($L_{2n+1} * L_{2m+1}$) and that of E($L_{2n+1} * L_{2m+1}$) are not proportional, which is different from the case on the numbers of spanning trees. However, the numerical results supports my conjecture that O($L_{2n+1} * L_{2m+1}$) and E($L_{2n+1} * L_{2m+1}$) have the same entropy constant.

2. Transfer matrices

The transfer matrices used to enumerate the independent sets of O($L_{2n+1} * L_{2m+1}$) and E($L_{2n+1} * L_{2m+1}$) can be introduced similarly.

Given an independent set S of the graph under our consideration. For each column of vertices of the graph there is a corresponding vector of 0's and 1's where 1 indicates the corresponding vertex is in S and 0 indicates that the corresponding vertex is not in S. Let V_i denote the vector corresponding to the i-th column of vertices. Note that for O($L_{2n+1} * L_{2m+1}$) the vector V_i is of dimension n when i is odd and V_i is of dimension n+1 when i is even, while for E($L_{2n+1} * L_{2m+1}$) the V_i is of dimension n+1 when i is odd and it is of dimension n when i is even. This can be illustrated by using the example in Fig.2, where O($L_9 * L_9$) and E($L_{2n+1} * L_{2m+1}$) are shown with a given independent set S. For O($L_9 * L_9$) with the given S, we have the following corresponding 9 vectors { V_i }: (0, 1, 0, 0), (1, 0, 0, 1, 1), (0, 1, 0, 0), (0, 0, 0, 1, 0), (1, 1, 0, 0), (0, 0, 0, 0, 0,), (1, 0, 0, 1), (0, 0, 0, 0, 0), (1, 0, 0, 0). For E($L_9 * L_9$) with the given S, the corresponding 9 vectors are: (1, 0, 0, 1, 1), (0, 1, 0, 0), (0, 0, 0, 1, 0), (1, 1, 0, 0), (0, 0, 0, 0, 0), (0, 0, 0, 1), (0, 1, 1, 0, 0), (0, 0, 0, 1), (1, 1, 1, 0, 0).

Note that each independent set S of the graph O($L_{2n+1} * L_{2m+1}$) or E($L_9 * L_9$) can be obtained by assembling the columns of S one by one in the natural order. During the process of assembling, when an additional column is assembled to the right hand side of existed structure, we only need to make sure that the new column does not clash with the rightmost column. No matter what the new column is, its addition never clashes with the other existed columns. This is the so called Markov property.

Now we consider the graph O($L_{2n+1} * L_{2m+1}$). For simplicity, the assembling of the $(i+1)$th column v_{i+1} to the i th column v_i is simply called Step i. It is clear that the generation of each independent set of the graph O(L_{2n+1} * L_{2m+1}) involves 2m assembling Steps after the first column v_1 is established. Step 1 is to assemble v_2 to the right side of v_1. The transfer matrix representing Step 1, denoted T_1 , can be constructed as follows. Let R_n be the set of all possible vectors v_1. Clearly R_n consists of all n-dimensional vectors of 0's and 1's , so R_n has 2^n vectors. Similarly, the set of all possible v_2 is the set R_{n+1} of all (n+1)-dimensional vectors of 0's and 1's, and R_{n+1} has 2^{n+1} vectors. Then the transfer matrix $T_1 = [T_{v_1 \cdot v_2}]$ is a $2^n \times 2^{n+1}$ matrix whose rows are indexed by vectors of R_n and columns are indexed by vectors of R_{n+1} (Note that for any n > 0, R_n can be easily ordered), where $T_{v_1 \cdot v_2} = 1$ if v_1 and v_2 represent possible consecutive pair of columns in an independent set of O(L_{2n+1} * L_{2m+1}), and $T_{v_1 \cdot v_2} = 0$ otherwise. That is, $T_{v_1 \cdot v_2} = 1$ if and only if each selected vertex (according to v_1) in the first column of O(L_{2n+1} * L_{2m+1}) is not adjacent to any selected vertex (according to v_2) in the second column of O(L_{2n+1} * L_{2m+1}). In other words, if we let $v_1 = (v_{11}, v_{12}, \ldots, v_{1n})$ and $v_2 = (v_{21}, v_{22}, \ldots, v_{2,n+1})$, then $T_{v_1 \cdot v_2} = 1$ if and only if $v_{1,i} \cdot v_{2,i} = 0$ and $v_{1,i} \cdot v_{2,i+1} = 0$ for i=1,2,..., n. Similarly, the transfer matrix for Step 2 is a $2^{n+1} \times 2^n$ matrix $T_2 = [T_{v_2 \cdot v_3}]$. For $v_2 = (v_{21}, v_{22}, \ldots, v_{2,n+1})$ and $v_3 = (v_{31}, v_{32}, \ldots, v_{3n})$, $T_{v_2, v_3} = 1$ if and only if $v_{3,i} \cdot v_{2,i} = 0$ and $v_{3,i} \cdot v_{2,i+1} = 0$ for i=1,2,...,n. It is easily seen that T_1 is the transfer matrix for every Step i where i is odd and that T_2 is the transfer matrix for every Step i where i is even. It is also obvious that T_2 is the transpose of T_1, i.e., $T_2 = T_1^t$. So, $T = T_1 T_2$ is a $2^n \times 2^n$ symmetric matrix and $\widetilde{T} = T_2 T_1$ is a $2^{n+1} \times 2^{n+1}$ symmetric matrix.

Let $f(m,n)$ ($\widetilde{f}(m,n)$, resp.) denote the number of independent sets of O(L_{2n+1} * L_{2m+1}) (E(L_{2n+1} * L_{2m+1}), resp.) . It is not difficult to see that $f(m,n)$ equals the sum of the entries of the matrix T^m. So $f(m,n) = \mathbf{1}^t T^m \mathbf{1}$ where $\mathbf{1}$ denotes the 2^n-dimensional column vector whose entries are all 1's. Similarly, $\widetilde{f}(m,n) = \mathbf{1}^t \widetilde{T}^m \mathbf{1}$ where $\mathbf{1}$ denotes the 2^{n+1}-dimensional column vector whose entries are all 1's.

Now we will describe the technical details to generate a transfer matrix. All subsets of a given set N with n elements 0,1,2,..,n-1 can be generated with an algorithm given in [10]. For any given subset $P \subseteq N$, the characteristic vector of P is the n-tuple $\chi(P) = [p_1, p_2, \ldots, p_n]$, where $p_i = 1$ if $n-i \in P$ and $p_i = 0$ otherwise. We can use the characteristic vectors to index the rows and columns of the transfer matrix. Let $a_1, a_2, \ldots, a_{2^{n+1}}$ denote all (n+1)-dimensional characteristic vectors. Let $b_1, b_2, \ldots, b_{2^n}$ denote all n-dimensional characteristic vectors, where b_1 is the zero vector of dimension n and $b_2, b_3, \ldots, b_{n+1}$ are the n unit vectors of dimension n. Then it is easily seen that the first row of T_1 indexed by b_1 is the 2^{n+1}-dimensional vector u_1 of all 1's. Starting from the second row, the n rows of T_1, $u_2, u_3, \ldots, u_{n+1}$ are indexed by $b_2, b_3, \ldots, b_{n+1}$, respectively. It is not difficult to see that $u_2, u_3, \ldots, u_{n+1}$ are 2^{n+1}-dimensional vectors and that they can be generated by the following algorithm.

for j $\leftarrow$ 2 to n+1

do { for i $\leftarrow$ 1 to 2^{n+1}

do { if the *jth* and the (j+1)*th* entries of a_i are 0 then the *ith* entry of u_j is 1

else the *ith* entry of u_j is 0.}

Note that for all other b_j, $n+2 \le j \le 2^n$, each can be obtained by combining some of the unit vectors $b_2, b_3, \ldots, b_{n+1}$ so that the corresponding rows of the transfer matrix T_1 can be obtained by logical operations. The details are illustrated below with n=3.

The 3-dimensional vectors are

(0, 0, 0),(1, 0, 0),(0, 1, 0),(0, 0, 1), (1, 1, 0),(1, 0, 1),(0, 1, 1),(1, 1, 1).

The 4-dimensional vectors are

(0, 0, 0, 0), (1, 0, 0, 0), (0, 1, 0, 0), (0, 0, 1, 0), (0, 0, 0, 1), (1, 1, 0, 0), (1, 0, 1, 0), (1, 0, 0, 1), (0, 1, 1, 0), (0, 1, 0, 1), (0, 0, 1, 1), (1, 1, 1, 0), (1, 1, 0, 1), (1, 0, 1, 1), (0, 1, 1, 1), (1, 1, 1, 1).

The transfer matrix T_1 is an 8×16 matrix with u_1=(1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1).

By the algorithm the rows of T_1 correspond to (1, 0, 0), (0, 1, 0), (0, 0, 1) are

u_2 = (1,0,0,1,1,0,0,0,0,0,1,0,0,0,0,0), u_3 = (1,1,0,0,1,0,0,1,0,0,0,0,0,0,0,0),

$u_4 = (1,1,1,0,0,1,0,0,0,0,0,0,0,0,0,0)$.

For $v_1 = (v_{11}, v_{12}, \ldots, v_{1n})$, $v_2 = (v_{21}, v_{22}, \ldots, v_{2n})$, we define

$v_1 * v_2 = (v_{11} \times v_{21}, v_{12} \times v_{22}, \cdots, v_{1n} \times v_{2n})$. Then

$u_5 = u_2 * u_3$, $u_6 = u_2 * u_4$, $u_7 = u_3 * u_4$, $u_8 = u_2 * u_3 * u_4$.

Thus we get

$$T_1 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

$$T_2 = T_1^t.$$

3. Numerical results

By MATLAB we can calculate the Merrifield - Simmons indices of the graphs considered in this paper.

Now we tabulate the results for $2 \leq n \leq 6$ and $1 \leq m \leq 10$ below.

The Merrifield - Simmons index of O ($L_{2n+1} * L_{2m+1}$):

f (m, n)

n=2

m=1 29

m=2 257

m=3 2408

m=4 22873

m=5 217969

m=6 2078716

m=7 19827701

m=8 189133073

m=9 1804125632

m=10 17209452337

n=3

m=1 124

m=2 2408

m=3 50128

m=4 1064576
m=5 22734496
m=6 486248000
m=7 10404289216
m=8 222647030144
m=9 4764694602112
m=10 101966374503680

n=4
m=1 533
m=2 22873
m=3 1064576
m=4 50796983
m=5 2441987149
m=6 117656540512
m=7 5672528575545
m=8 273541357254277
m=9 13191518965300160
m=10 636171495829068288

n=5
m=1 2293
m=2 217969
m=3 22734496
m=4 2441987149
m=5 264719566561
m=6 28778500622048
m=7 3131382012183077
m=8 340819280011906496
m=9 37097936406550224896
m=10 4038192819517828628480

n=6
m=1 9866
m=2 2078716
m=3 486248000
m=4 117656540512
m=5 28778500622048
m=6 7063448084710944
m=7 1735575086258267136
m=8 426602245391808593920
m=9 104870171042459653505024
m=10 25780811901305521409359872

The Merrifield - Simmons index of E ($L_{2n+1} * L_{2m+1}$) :

$\widetilde{f}(m,n)$

n=2
m=1 73
m=2 689
m=3 6556
m=4 62501
m=5 596113
m=6 5686112
m=7 54239137
m=8 517383521
m=9 4935293524
m=10 47077513469

n=3
m=1 314
m=2 6556
m=3 139344
m=4 2976416
m=5 63663808
m=6 1362242592
m=7 29151501760
m=8 623849225024
m=9 13350628082560
m=10 285709494797952

n=4
m=1 1351
m=2 62501
m=3 2976416
m=4 142999897
m=5 6888568813
m=6 332097693792
m=7 16014193762579
m=8 772279980131297
m=9 37243762479698920
m=10 1796118644459454976

n=5
m=1 5813
m=2 596113
m=3 63663808

m=4 6888568813
m=5 748437606081
m=6 81422265300608
m=7 8861477326934565
m=8 964548039869458048
m=9 104992603396454170624
m=10 11428754133439767117824

n=6
m=1 25012
m=2 5686112
m=3 1362242592
m=4 332097693792
m=5 81422265300608
m=6 19999400591072512
m=7 4915269393662666752
m=8 1208259557742388969472
m=9 297029594411422458052608
m=10 73020996395192320903872512

4. Theorem on entropy constants

The entropy constant has been of interest to many physicists and combinatorialists (see [14] and the references cited therein). In statistical mechanics the following similar problem has been considered: in how many ways can we put particles on an $m \times n$ rectangular lattice so that no two share the same vertex and at most one particle on every edge? Based on this problem the entropy constant is defined. The lattices we are considering here are the generalized Aztec diamonds

$O(L_{2n+1} * L_{2m+1})$ and $E(L_{2n+1} * L_{2m+1})$. Note that $O(L_{2n+1} * L_{2m+1})$ has $(n+(n+1))m+n=2mn+m+n$ vertices and $E(L_{2n+1} * L_{2m+1})$ has $(n+n+1)m+n+1=2mn+m+n+1$ vertices. Let $f(m,n)$ denote the number of independent sets of $O(L_{2n+1} * L_{2m+1})$ and $\tilde{f}(m,n)$ denote the number of independent sets of $E(L_{2n+1} * L_{2m+1})$. The entropy constants of these graphs are defined to be:

$$C = \lim_{n\to\infty, m\to\infty} f(m,n)^{1/(2mn+m+n)}.$$

and

$$\tilde{C} = \lim_{n\to\infty, m\to\infty} \tilde{f}(m,n)^{1/(2mn+m+n+1)}.$$

Although there is no obvious relation between $f(m,n)^{1/(2mn+m+n)}$ and $\tilde{f}(m,n)^{1/(2mn+m+n+1)}$ in the first glance, we observe that they are near.

$f(20,6)^{1/266} \approx 1.53251705211$

$\tilde{f}(20,6)^{1/267} \approx 1.53604652356$

Furthermore, the following numbers are nearer,

$f(125,6)^{1/1631} \approx 1.52806707348,$

$\tilde{f}(125,6)^{1/1632} \approx 1.5286449987.$

Thus it suggests that $C = \tilde{C}$. This equality is established in the theorem below. In the proof we use a method of Wilf et al [16] to show the existence of a double limit.

Theorem. The generalized Aztec diamonds $O(L_{2n+1} * L_{2m+1})$ and $E(L_{2n+1} * L_{2m+1})$ have equal entropy constants.

Proof. Let C and $\tilde{C}$ denote the entropy constants of $O(L_{2n+1} * L_{2m+1})$ and $E(L_{2n+1} * L_{2m+1})$, respectively. We need to show that $C = \tilde{C}$.

We now explicitly exhibit the size n by the subscript of the transfer matrix.

Since T_n is a real symmetric 2^nx2^n matrix, there is an orthogonal matrix $P = (p_{i,j})$ whose columns are eigenvectors of T_n and $P^t\ T_n\ P = \begin{pmatrix} \lambda_1(n) & & 0 \\ & \ddots & \\ 0 & & \lambda_{2^n}(n) \end{pmatrix}$, where $\lambda_1(n) \geq \lambda_2(n) \geq \cdots \geq \lambda_{2^n}(n)$ are the eigenvalues of T_n.

Since $f(m,n) = 1^t\, T_n^m\, 1$,

$$\lim_{m\to\infty} f(m,n)^{1/m} = \lim_{m\to\infty} \left(1^t P \begin{pmatrix} \lambda_1^m(n) & & 0 \\ & \ddots & \\ 0 & & \lambda_{2^n}^m(n) \end{pmatrix} P^t 1 \right)^{1/m} =$$

$$= \lim_{m\to\infty} \left(\alpha_1 \lambda_1^m(n) + \alpha_2 \lambda_2^m(n) + \cdots + \alpha_{2^n} \lambda_{2^n}^m(n)\right)^{1/m} = \lambda_1(n)$$

where $\alpha_1 \neq 0$ because the dominant eigenvector of nonnegative matrix T_n can not be orthogonal to **1**.

Thus,

$$\liminf_{n\to\infty} \lambda_1^{1/n}(n) \leq \liminf_{\substack{m\to\infty \\ n\to\infty}} f(m,n)^{1/mn} \leq \limsup_{\substack{m\to\infty \\ n\to\infty}} f(m,n)^{1/mn} \leq \limsup_{n\to\infty} \lambda_1^{1/n}(n) \qquad (1)$$

Let $1^t T_n^r 1 \,/\, 1^t 1$ be the Rayleigh quotient (see [17] p.54) of the $2^n \times 2^n$ real symmetric matrix T_n^r.

Then $\lambda_1^r(n) \geq 1^t T_n^r 1 / 1^t 1$. Clearly, $1^t T_n^r 1 = 1^t T_r^n 1$ since both sides count the independent sets in the same generalized Aztec diamond.

Thus

$$\left(\lambda_1^{1/n}(n)\right)^r \geq (1^t T_r^n 1 / 1^t 1)^{1/n}.$$

Then

$$(\liminf_{n\to\infty} \lambda_1^{1/n}(n))^r \geq \lambda_1(r)/2,$$ where $\lambda_1(r)$ is the dominant eigenvalue of T_r.

Taking the *r*th root, and the limsup as $r \to \infty$, we get

$$\liminf_{n\to\infty} \lambda_1^{1/n}(n) \geq \limsup_{r\to\infty} \lambda_1^{1/r}(r).$$

Since the reverse of this inequality is obvious, we see that $\lim_{n\to\infty} \lambda_1^{1/n}(n)$ exists. By (1) we have

$$\lim_{\substack{m\to\infty \\ n\to\infty}} f(m,n)^{1/mn} = \lim_{n\to\infty} \lambda_1^{1/n}(n).$$

Thus

$$C = \lim_{\substack{m\to\infty \\ n\to\infty}} f(m,n)^{1/2mn+m+n} = (\lim_{n\to\infty} \lambda_1^{1/n}(n))^{1/2},$$ where $\lambda_1(n)$ is the dominant eigenvalue of T_n.

Similarly, $\widetilde{f}(m,n) = 1^t\, \widetilde{T}_n^m\, 1$, and we can show that

$$\widetilde{C} = \lim_{\substack{m\to\infty \\ n\to\infty}} \widetilde{f}(m,n)^{1/2mn+m+n+1} = \lim_{n\to\infty} (\widetilde{\lambda}_1^{1/n}(n))^{1/2},$$ where $\widetilde{\lambda}_1(n)$ is the dominant eigenvalue of $\widetilde{T}_n$.

Since $T_n = T_1 T_2$ and $\widetilde{T}_n = T_2 T_1$, we have $\widetilde{\lambda}_1(n) = \lambda_1(n)$, which implies $C = \widetilde{C}$.

This completes the proof.

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