Merrifield-Simmons index and its entropy of the 4-8-8 lattice

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Abstract

The Merrifield-Simmons index is a topological index used in structural chemistry for quantifying relevant properties of molecular structure. This index, in different names, has been studied on the square, triangular and hexagonal lattices by using the method of transfer matrix. To compute the Merrifield-Simmons index of more complicated lattices such as the 4-8-8 and triangular kagomé lattices, the use of multi-step transfer matrices is needed. In this paper we introduce the concept of transfer multiplicity and use multi-step transfer matrices to derive a rigorous upper and lower bound for the entropy of Merrified-Simmons index of the 4-8-8 lattice. We show that this method can be used to deal with other complex 2-dimensional lattices.

1 Introduction

In the study of structural chemistry, Merrifield and Simmons defined a topological space for the chemical graphs [15]; the cardinality of this topological space is called the Merrified-Simmons index. In the context of combinatorics, for a graph G , the Merrifield-Simons index is the number of vertex independent sets of G . The properties of Merrifield-Simmons index of some types of benzenoids and polyominoes have been studied in [8, 22, 24, 25]. In statistical mechanics, an essentially same problem is to count the ways of putting particles in the sites of a 2-dimensional lattice such that no two share the same site or are in adjacent sites [2–4, 6, 7, 16].

The 4-8-8 lattice is an Archimedean tiling which has been used to describe phase transitions in the layered hydrogen-bonded $\text{SnCl}_2 \cdot 2\text{H}_2\text{O}$ crystal [18] in physical systems. The triangular kagomé lattice corresponds to the positions of Cu atoms in the fabricated materials $\text{Cu}_9\text{X}_2(\text{cpa})_6 \cdot x\text{H}_2\text{O}$ (cpa= 2-carboxypentonic acid, an derivative of asorbic acid; X-F,Cl,Br) [14]. Various physical models such as the spanning trees, dimer covering and bond percolation have been studied on these two lattices [1, 9, 12, 13, 18–21]. To compute the Merrifield-Simmons index and its entropy of such complicated lattices, using single-step transfer matrix as in [5] is not compatible. In this paper, we propose the concept of transfer multiplicity and use multi-step transfer matrices to overcome such limitation. We demonstrate our method on the 4-8-8 lattice, provide numerical results of the Merrified-Simmons index and a rigorous bound of its entropy.

2 Transfer matrix

Let $G_{m,n}$ (where m and n always denote positive integers) denote a finite section of the 4-8-8 lattice whose hexagons are arranged in m rows and n columns as shown in Fig.1.

Fig. 1: $G_{m,n}$

Given an independent set S of $G_{m,n}$, a portion of S that lies in a fixed column of $G_{m,n}$ can be represented by either an $(m+1)$ -vector or a $2m$ -vector of 0's and 1's, where a 1 indicates that the vertex is in S and a 0 indicates that the vertex is not in S . Thus, any independent set of $G_{m,n}$ can be represented by $3n+1$ column vectors.

Example 2.1. Fig.2 below shows an independent set S in $G_{3,4}$. The portions of S that lie in each of the columns are represented by the respective vectors $(1, 0, 0, 0, 1, 0)$, $(0, 1, 0, 1)$, $(1, 0, 1, 0)$, $(0, 0, 1, 0, 0, 1)$, $(0, 0, 1, 0)$, $(0, 1, 0, 1)$, $(1, 0, 0, 1, 1, 0)$, $(0, 0, 0, 0)$, $(1, 1, 1, 1)$, $(0, 0, 0, 0, 0, 0)$, $(0, 1, 0, 0)$, $(0, 0, 1, 1)$, $(0, 1, 1, 0, 0, 0)$.

Fig. 2: An independent set of $G_{3,4}$.

Let $\mathbf{P}_m$ denote the set of all possible $(m+1)$ -vectors which may represent a column in an independent set of $G_{m,n}$. The $(3k+2)$ -th and $(3k+3)$ -th columns of an independent set of $G_{m,n}$ are chosen from $\mathbf{P}_m$, where $0 \leq k \leq n-1$. Clearly, $\mathbf{P}_m$ is a collection of $(m+1)$ -vectors of 0's and 1's, and the cardinality of $\mathbf{P}_m$ is 2^{m+1} . Similarly, let $\mathbf{Q}_m$ denote the set of all possible $2m$ -vectors which may represent a $(3k+1)$ -th column in an independent set of $G_{m,n}$, where $0 \leq k \leq n$. It's easy to see that $\mathbf{Q}_m$ consists of $2m$ -vectors of 0's and 1's in which no consecutive 1's occupy the positions of the $(2k-1)$ -th and $2k$ -th entries, for $1 \leq k \leq m$. Since there are

three possibilities at each pair of consecutive $(2k - 1)$ -th and $2k$ -th positions, the set Q_m has 3^m vectors.

Let $\mathbf{v}(i)$ denote the i -th element of a vector $\mathbf{v}$. Note that two column vectors $\mathbf{v}, \mathbf{v}'$ need to fit into one of the following two cases to be a possible consecutive pair of columns in an independent set of $G_{m,n}$,

- (i) $\mathbf{v}$ and $\mathbf{v}'$ are chosen from $\mathbf{P}_m$ and they are orthogonal to each other.
- (ii) $\mathbf{v}, \mathbf{v}'$ are chosen from $\mathbf{P}_m$ and $\mathbf{Q}_m$ respectively and they satisfy the following conditions
 - (a) $\mathbf{v}(1) \cdot \mathbf{v}'(1) = 0$,
 - (b) $\mathbf{v}(i) \cdot \mathbf{v}'(2i - 2) = 0$ and $\mathbf{v}(i) \cdot \mathbf{v}'(2i - 1) = 0$ for $i = 2, 3, \dots, m$,
 - (c) $\mathbf{v}(m + 1) \cdot \mathbf{v}'(2m) = 0$.

For fixed m and n , all possible independent sets S of $G_{m,n}$ can be obtained by a gluing process described below. First, take a vector from $\mathbf{Q}_m$ such that it corresponds to the first column of S , and denote it as $\mathbf{u}$. Second, to the right of $\mathbf{u}$ we glue a vector $\mathbf{v}$ selected from $\mathbf{P}_m$, making sure that $\mathbf{u}$ and $\mathbf{v}$ satisfy (ii). Third, we glue a vector $\mathbf{v}'$ from $\mathbf{P}_m$ to the right of $\mathbf{v}$ under the condition that $\mathbf{v}$ and $\mathbf{v}'$ satisfy (i). Then, we glue $\mathbf{u}'$ to the right of $\mathbf{v}'$ such that $\mathbf{v}'$ and $\mathbf{u}'$ satisfy (ii). Repeat the above procedure until the $(3n + 1)$ -th column is glued.

Let us call the gluing of the $(i + 1)$ -th column v_{i+1} to the right of i -th column v_i as step i . Thus the transfer matrix representing step one, denoted $T_{m_1} = (T_{v_1, v_2})$, is a $3^m \times 2^{m+1}$ matrix whose rows are indexed by vectors of Q_m and columns are indexed by vectors of P_m , where $T_{v_1, v_2} = 1$ if v_1 and v_2 represent possible consecutive pair of columns in an independent set of $G_{m,n}$ and $T_{v_1, v_2} = 0$ otherwise. Note that the matrix depends only on n .

Similarly, the transfer matrix for step two is a $2^{m+1} \times 2^{m+1}$ matrix T_{m_2} whose rows and columns are indexed by vectors of P_m . T_{m_2} 's entry in position (α, β) is 1 if the vectors represented by α, β are orthogonal, and is 0 otherwise. The transfer matrix, T_{m_3} , for step three is the transpose of T_{m_1} . Note that T_{m_1} is the transfer matrix for every step i when $i = 3k + 1$ ($0 \leq k \leq n - 1$), T_{m_2} is the transfer matrix for every step i when $i = 3k + 2$ ($0 \leq k \leq n - 1$) and T_{m_3} is the transfer matrix for every step i when $i = 3k + 3$ ($0 \leq k \leq n - 1$). Thus, if we take the transfer matrix of $G_{m,n}$ to be $T_m = T_{m_1} T_{m_2} T_{m_3}$, then it is well known that for the Merrified-Simmons index of $G_{m,n}$, we have

$$f(m, n) = \mathbf{1} \cdot T_m^n \mathbf{1},$$

where $\mathbf{1}$ denotes the all one column vector. We call T_m a triple-step transfer matrix since it is given as the product of three transfer matrices.

When $m = 2$, the transfer matrices T_{2_1} , T_{2_2} and T_{2_3} are:

$$T_{2_1} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad T_{2_2} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad T_{2_3} = T_{2_1}^\top.$$

Thus, the triple-step transfer matrix of $G_{m,n}$ is:

$$T_2 = \begin{pmatrix} 27 & 18 & 18 & 18 & 12 & 18 & 18 & 12 & 12 \\ 18 & 9 & 12 & 12 & 6 & 12 & 12 & 6 & 8 \\ 18 & 12 & 9 & 9 & 6 & 9 & 12 & 8 & 6 \\ 18 & 12 & 9 & 9 & 6 & 9 & 12 & 8 & 6 \\ 12 & 6 & 6 & 6 & 3 & 6 & 8 & 4 & 4 \\ 18 & 12 & 9 & 9 & 6 & 9 & 12 & 8 & 6 \\ 18 & 12 & 12 & 12 & 8 & 12 & 9 & 6 & 6 \\ 12 & 6 & 8 & 8 & 4 & 8 & 6 & 3 & 4 \\ 12 & 8 & 6 & 6 & 4 & 6 & 6 & 4 & 3 \end{pmatrix}.$$

By identifying edges (a_i, a_{i+1}) with (a_i^*, a_{i+1}^*) ($1 \leq i \leq 2m-1$) of $G_{m,n}$ respectively, the 4-8-8 lattice with cylindrical boundary condition, denote as $H_{m,n}$, can be obtained. Note that here the graph can be seen as drawn on a vertical cylinder.

Fig. 3: The 4-8-8 lattice $G_{m,n}$ with free boundary condition

Similar to the discussion of $G_{m,n}$, any independent set I of $H_{m,n}$ can be generated by gluing vectors from $\mathbf{P}_{n-1}$ and $\mathbf{Q}_n$. Note that if $\mathbf{v}$ and $\mathbf{v}'$ are chosen from $\mathbf{P}_{n-1}$ and $\mathbf{Q}_n$, they are a possible consecutive pair of vectors in I if and only if

$$\mathbf{v}(1) \cdot \mathbf{v}'(1) + \mathbf{v}(1) \cdot \mathbf{v}'(2n) = 0, \quad \mathbf{v}(i) \cdot \mathbf{v}'(2i-2) = 0 \quad \text{and} \quad \mathbf{v}(i) \cdot \mathbf{v}'(2i-1) = 0 \quad \text{for } i = 2, 3, \dots, n.$$

I can be obtained by the procedure described below. First, take a vector from $\mathbf{Q}_n$ such that it corresponds to the first row of I , and denote it as $\mathbf{u}$. Second, glue a vector $\mathbf{v}$ from $\mathbf{P}_{n-1}$ to the bottom of $\mathbf{u}$, ensuring that $\mathbf{u}$ and $\mathbf{v}$ are legit consecutive vectors in I . Third, glue a vector

$\mathbf{v}'$ from $\mathbf{P}_{n-1}$ to the bottom of $\mathbf{v}$ such that $\mathbf{v}$ and $\mathbf{v}'$ are orthogonal. Then we glue $\mathbf{u}'$ to the bottom of $\mathbf{v}'$, making sure that $\mathbf{v}'$ and $\mathbf{u}'$ are possible consecutive vectors in I . Repeat the above procedure until the $(3m+1)$ -th column is glued.

Consider the transfer matrix of $H_{m,n}$. The transfer matrix B_{n_1} , which represents every $(3k+1)$ -th ($0 \leq k \leq n-1$) step, can be defined as a $3^n \times 2^n$ matrix of 0's and 1's as follows. The rows of B_{n_1} are indexed by vectors of $\mathbf{Q}_n$ and columns are indexed by vectors of $\mathbf{P}_{n-1}$, and the entry of B_{n_1} in position (α, β) is 1 if α, β represent possible consecutive pair of rows in an independent set of $H_{m,n}$, and is 0 otherwise. Let B_{n_3} denote the transfer matrix that represents every $(3k+3)$ -th ($0 \leq k \leq n-1$) step. It is no difficult to see that B_{n_3} is the transpose of B_{n_1} . The transfer matrix B_{n_2} that represents every $(3k+2)$ -th ($1 \leq k \leq n-1$) step is a $2^n \times 2^n$ matrix whose rows and columns are indexed by vectors of $\mathbf{P}_{n-1}$. The entry of B_{n_2} in position (α, β) is 1 if α, β are orthogonal, and is 0 otherwise. Thus if we take the transfer matrix of $H_{m,n}$ to be $B_n = B_{n_1} B_{n_2} B_{n_3}$, for the Merrified-Simmons index of $H_{m,n}$, we have

$$g(m, n) = \mathbf{1} \cdot B_n^m \mathbf{1},$$

where $\mathbf{1}$ denotes the all one column vector.

When $n = 2$, the transfer matrices B_{2_1} , B_{2_2} and B_{2_3} are

$$B_{2_1} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad B_{2_2} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad B_{2_3} = B_{2_1}^\top.$$

Therefore, the triple-step transfer matrix of $H_{m,n}$ is

$$B_2 = \begin{pmatrix} 9 & 6 & 6 & 6 & 4 & 6 & 6 & 6 & 4 \\ 6 & 3 & 4 & 4 & 2 & 4 & 3 & 3 & 2 \\ 6 & 4 & 3 & 3 & 2 & 3 & 4 & 4 & 2 \\ 6 & 4 & 3 & 3 & 2 & 3 & 4 & 4 & 2 \\ 4 & 2 & 2 & 2 & 1 & 2 & 2 & 2 & 1 \\ 6 & 4 & 3 & 3 & 2 & 3 & 4 & 4 & 2 \\ 6 & 3 & 4 & 4 & 2 & 4 & 3 & 3 & 2 \\ 6 & 3 & 4 & 4 & 2 & 4 & 3 & 3 & 2 \\ 4 & 2 & 2 & 2 & 1 & 2 & 2 & 2 & 1 \end{pmatrix}.$$

The 4-8-8 lattice with toroidal boundary condition, denote as $T_{m,n}$, can be obtained by identifying edges (b_i, b_{i+1}) with (b_i^*, b_{i+1}^*) ($1 \leq i \leq 2n-1$) of $H_{m,n}$ respectively (see Fig.3).

In general, for a lattice $P_{m,n}$ with free boundary condition and transfer matrix T_m , let us denote its corresponding lattices with cylindrical boundary condition and toroidal boundary condition by $C_{m,n}$ (with transfer matrix B_n) and $T_{m,n}$ respectively.

We say that the square lattice is of transfer multiplicity one since computing the Merrifield-Simmons index for it only needs to employ single-step transfer matrices as shown in [5]. This may not hold for other lattices. For example, in [23], for a generalized aztec diamond we need to introduce double-step transfer matrices, therefore the transfer multiplicity of a generalized aztec diamond is two. Based on the discussion above, the 4-8-8 lattice is of transfer multiplicity three. The triangular kagomé lattice has multiplicity four since quadruple-step transfer matrices need to be involved in computing its Merrifield-Simmons index. The entropy constant of a lattice with free boundary condition is defined by $\eta = \lim_{m,n \rightarrow \infty} f(m,n)^{1/k(m,n)}$ where $f(m,n)$ is the Merrifield-Simmons index of $P_{m,n}$ and $k(m,n)$ denotes the number of vertices of $P_{m,n}$. The entropy of the lattices with cylindrical or toroidal boundary conditions can be defined similarly. As in [5], we have that the Merrifield-Simmons index for $P_{m,n}$, $C_{m,n}$ and $T_{m,n}$ are $1 \cdot T_m^n 1$, $1 \cdot B_n^m 1$ and $\text{Trace}(1 \cdot B_n^m 1)$ respectively.

Lemma 2.2. *Let $P_{m,n}$, whose transfer matrix is denoted by T_m , be a lattice with free boundary condition for given positive integers m and n . Let $C_{m,n}$, whose transfer matrix is denoted by B_n , be the corresponding lattice with cylindrical boundary condition and $T_{m,n}$ be the corresponding lattice with toroidal boundary condition. Then the trace of T_m^n is equal to the Merrifield-Simmons index of $C_{m,n}$ and the trace of B_n^m is equal to the Merrifield-Simmons index of $T_{m,n}$.*

Proof. Recall that $C_{m,n}$ can be obtained by identifying the leftmost and the rightmost column of $P_{m,n}$. Thus there is a bijection between the independent sets of $C_{m,n}$ and the independent sets of $P_{m,n}$ whose leftmost and rightmost column vectors are the same. And the latter is the trace of T_m^n .

Similarly, $T_{m,n}$ can be obtained by identifying the top row and the bottom row of $C_{m,n}$. Thus there is a bijection between the independent sets of $T_{m,n}$ and the independent sets of $C_{m,n}$ whose corresponding top and bottom row vectors are the same. And the latter is the trace of B_n^m . $\square$

In [5], Calkin and Wilf proved the existence of the entropy constant of the square lattice and established its upper and lower bounds. Note that the method provided by Calkin and Wilf is valid for the lattices with the same symmetric transfer matrices in both horizontal and vertical directions. Thus, the bounds can be generalized and stated as follows.

Theorem 2.3. *Let $P_{m,n}$ be a lattice with the same real symmetric transfer matrix T_m in both horizontal and vertical directions. Let B_n be the transfer matrix of the corresponding lattice with cylindrical boundary condition. For both lattices, the entropy constant of the Merrifield-Simmons index is lower bounded by $(\frac{\lambda_{p+2q}}{\lambda_{2q}})^{1/p}$ where λ 's are the largest eigenvalues of corresponding T 's. And the upper bound of the entropy constant is $(\xi_{2k})^{1/2k}$ where ξ 's are the largest eigenvalues of corresponding B 's.*

3 Numerical results

Note that the 4-8-8 lattice has the same symmetric transfer matrix in both horizontal and vertical directions. By Lemma 2.2, we can apply Theorem 2.3 to derive the lower and upper bound of entropy constant for the 4-8-8 lattice.

Let $p = 2$, $q = 3$ and $k = 4$ in Theorem 2.3, since the largest eigenvalues of T_6 , T_8 and B_8 are 105606.367915106937..., 3510407.307349548675... and 1220870.544468111359... respectively. We have

$$5.765456527051... \leq \lim_{m,n \rightarrow \infty} f(m,n)^{1/mn} \leq 5.765456529341...,$$

where $f(m,n)$ is the Merrifield-Simmons index of the 4-8-8 lattice $G_{m,n}$. Since the number of vertices of $G_{m,n}$ is $4mn + 2m + 2n$, we can see that the entropy constant of the 4-8-8 lattice is

$$\eta = \lim_{m,n \rightarrow \infty} f(m,n)^{1/4mn+2m+2n},$$

which is between 1.549560101247... and 1.549560101400....

Some numerical results of Merrifield-Simmons index of the 4-8-8 lattice with various boundary conditions are presented in the following tables.

Table 1: The numerical results of Merrifield-Simmons index of the 4-8-8 lattice $G_{m,n}$ with free boundary condition

n	$f(1, n)$	$f(2, n)$	$f(3, n)$	$f(4, n)$
1	47	779	12887	213203
2	779	74753	7144259	682899449
3	12887	7144259	3935795807	2168825644779
4	213203	682899449	2168825644779	6890559309027361
5	3527231	65275954619	1195119855466343	21891571255589181023
6	58354523	6239500931057	658564832936254227	69550417915510873198592
7	965417447	596412129451379	362898854276036750752	220964515515328798010638336
8	15971869859	57008955129453545	199973597225797700796416	702013283095176099770505625600
9	264238674767	5449287169347507444	110194449810190513907695616	
n	$f(5, n)$	$f(6, n)$	$f(7, n)$	$f(8, n)$
1	3527231	58354523	965417447	15971869859
2	65275954619	6239500931057	596412129451379	57008955129453545
3	1195119855466343	658564832936254227	362898854276036750752	199973597225797700796416
4	21891571255589181059	69550417915510873198592	220964515515328798010638336	702013283095176099770505625600
5	400989410760263959456896	7344958142436702598532694016		
6	7344958142436702598532694016			
n	$f(9, n)$			
1	264238674767			
2	5449287169347507444			
3	110194449810190513907695616			

4 Final remark

1. This transfer matrix method for computing Merrifield-Simmons index is also valid for non-planar lattices. For instance, the square lattice with crossed diagonal bonds (obtained by adding two crossed diagonals to each square inner face) is non-planar; its Merrifield-Simmons index can be computed by using multi-step transfer matrix and it can be showed that the entropy constant is between 1.342542258... and 1.342652572....

2. The 4-8-8 lattice has larger entropy constant of Merrifield-Simmons index comparing to that of the square lattice [5] while the square lattice has larger entropy than that of the square

Table 2: The numerical results of Merrifield-Simmons index of the 4-8-8 lattice $H_{m,n}$ with cylindrical boundary condition

m	$g(m, 1)$	$g(m, 2)$	$g(m, 3)$	$g(m, 4)$
1	15	275	4527	74915
2	81	9223	872817	83484359
3	435	308007	167161419	92210259455
4	2337	10288055	32024704905	101890687050895
5	12555	343638751	6135187215867	112585183506906592
6	67449	11478130575	1175359722363369	124402293749613166592
7	362355	383389471367	225171683166443808	137459739741954729050112
8	1946673	12805873388263	43137676077348913152	151887714595812392365457408
9	10458075	427738384795215	8264179008000619446272	167830070726599585943198367744
m	$g(m, 5)$	$g(m, 6)$	$g(m, 7)$	$g(m, 8)$
1	1239375	20504243	339222255	5612094275
2	7979610641	762745733191	72908185459505	6969039275744391
3	50808099454115	27997712914113532	15427992474894299136	8501518342886229278720
4	323676087966247552	1028340702944578895872	3267078212691260344369152	10379641364400127593513222144
5	2061947765452025364480	37769283626796604821864448	691822641713709142974429921280	
6	13135457408094420540063744	1387206347469407026513191108608		
7	83678274939057768517536317440			

Table 3: The numerical results of Merrifield-Simmons index of the 4-8-8 lattice $S_{m,n}$ with toroidal boundary condition

m	$s(m, 1)$	$s(m, 2)$	$s(m, 3)$	$s(m, 4)$
1	5	29	155	833
2	29	1127	37235	1244819
3	155	37235	7023713	1347121127
4	833	1244819	1347121127	1490864952223
5	4475	41575979	258054952385	1647144129284543
6	24041	1388718947	49437673996703	1820049164089801216
7	129155	46385594795	9471107791983884	2011082476723567853568
8	693857	1549359408899	1814444828776562944	2222168789066396131655680
9	3727595	51751291603979	347605577830867337216	2455410851801241684155564032
m	$s(m, 5)$	$s(m, 6)$	$s(m, 7)$	$s(m, 8)$
1	4475	24041	129155	693857
2	41575979	1388718947	46385594795	1549359408899
3	258054952385	49437673996703	9471107791983884	1814444828776548608
4	1647144129284543	1820049164089801216	2011082476723567853568	2222168789066506995499008
5	10491381016588933120	66835240986806694445056	425767589675573485997391872	2712315179113658136571668332544
6	66835240986806694445056	2454789445716724048587653120	90160437291592209800637701947392	
7	425767589675573485997391872	90160437291592209800637701947392		
8	2712315179113658136571668332544			

lattice with crossed diagonal bonds. Note that the vertices of the 4-8-8 lattice are of degree three while the vertices of the square lattice and square lattice with crossed diagonal bonds are of degree four and eight respectively. Is the entropy constant of Merrifield-Simmons index negatively correlated to the average degree of a lattice? Intuitively, the answer is likely to be a yes but further investigation needs to be made.

3. By straightforward combinatorial arguments, we can see that for Merrifield-Simmons index, the entropy constants of lattices with free boundary condition are the same as the entropy constants of the corresponding cylindrical and toroidal lattices. But this phenomenon may disappear for some other models. For instance, the the boundary condition of a honeycomb lattice has a significant effect on its entropy constant in dimer problem, see [10, 11, 21].

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