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PI indices of nanotubes $SC_4C_8[q, 2p]$ covering by C_4 and C_8[1]

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Abstract

The Padmakar-Ivan (PI) index of a graph $G = (V, E)$ is defined as $PI(G) = \sum_{e \in E}(n_u(e) + n_v(e))$, where $e = uv$, $n_u(e)$ is the number of edges of G lying closer to u than to v and $n_v(e)$ is the number of edges of G lying closer to v than to u. In this paper, a formula for calculating the PI index of a nanotube $SC_4C_8[q, 2p]$ is given.

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1 Introduction

Since the Wiener index was introduced by Wiener [1] in the study of paraffin boiling points, many topological indices have been designed [2]. Such a proliferation is still going on and is becoming counter productive. In 1990s, Gutman [3] and coworkers [4] introduced a generalization of the Wiener index (W) for cyclic graphs called Szeged index (Sz). The main advantage of the Szeged index is that it is a modification of W; otherwise, it coincides with the Wiener index. In [5,6] another topological index was introduced and it was named Padmakar-Ivan index, abbreviated as PI. This new topological index, PI, does not coincide with the Wiener index. Deng [7,8] gave the formulas for calculating the PI indices of $TUVC_6[2p, q]$ and catacondensed hexagonal systems, and characterized the extremal catacondensed hexagonal systems with the minimum or maximum PI index. Ashrafi and Loghman [9] computed the PI index of zig-zag polyhex nanotubes. Recently, Deng [10] computed the PI index of a torus covering by C_4 and C_8.

Following [10], the primary aim of this article is to introduce the method for calculation of PI index for a nanotube covering by C_4 and C_8. Throughout this paper $G = SC_4C_8[q, 2p]$ denotes a nanotube covering by C_4 and C_8 with q rows and $2p$ columns in its cutting, see Figure 1. A nanotube $G = SC_4C_8[q, 2p]$ is called the type-I (or the type-II) if all the edges on the open ends are the edges of C_8 (or C_4); otherwise, it is called the type-III. Note that $G = SC_4C_8[q, 2p]$ is a type-III nanotube if and only if q is odd.

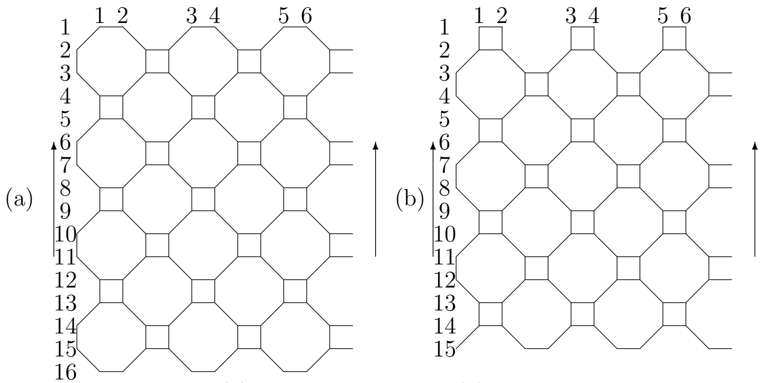


Figure 1. (a) a type-I nanotube; (b) a type-III nanotube.

2 The number of edges equidistant to the both ends of an edge

Let G be a connected and undirected graph without multiple edges or loops. By $V(G)$ and $E(G)$ we denote the vertex and edge sets, respectively, of G. If $e = xy \in E(G)$, then $n_1(e)$ is the number of edges nearer to x than y and $n_2(e)$ is the number of edges nearer to y than x. The PI index of G is defined as

$$PI(G) = \sum_{e \in E(G)} [n_1(e) + n_2(e)]$$

In all cases of cyclic graphs, there are edges equidistant to the both ends of the edges. Such edges are not taken into account. Let X be the subset of vertices of $V(G)$ which are closer to x than y and Y the subset of vertices which are closer to y than x. $[X, Y]$ denotes the subset of edges between X and Y, $n(e) = |[X, Y]|$. Then $n(e) = |E(G)| - (n_1(e) + n_2(e))$ is the number of edges equidistant to the both ends of e for a bipartite connected graph G (It includes the current edge e in $n(e)$). And

$$PI(G) = |E(G)|^2 - \sum_{e \in E(G)} n(e)$$

Therefore, for computing the PI index of a bipartite connected graph G, it is enough to calculate $n(e)$ for each $e \in E(G)$.

For the horizontal and vertical edges, we can observe the following results by the symmetry of the nanotube $SC_4C_8[q, 2p]$.

Lemma 1. (1) Let e be any horizontal edge between columns j and j+1 in $G = SC_4C_8[q, 2p]$. If G is a type-I, then $n(e) = q$; If G is a type-II, then

$$n(e) = \begin{cases} q, & q \equiv 0(mod4); \\ q, & q \equiv 2(mod4) \text{ and p is odd;} \\ q+2, & q \equiv 2(mod4) \text{ and p is even, j is odd;} \\ q-2, & q \equiv 2(mod4) \text{ and p is even, j is even.} \end{cases}$$

If G is a type-III, then $n(e) = \begin{cases} q, & \text{p is odd;} \\ q+1, & \text{p is even and j is odd;} \\ q-1, & \text{p is even and j is even.} \end{cases}$

(2) Let E_h be the set of horizontal edges in $G = SC_4C_8[q, 2p]$, $H = \sum_{e \in E_h} n(e)$.

If G is a type-I, then $H = pq^2$; If G is a type-II, then

$$H = \begin{cases} pq^2, & q \equiv 0(mod4); \\ pq^2, & q \equiv 2(mod4) \text{ and p is odd;} \\ pq^2 + 4p, & q \equiv 2(mod4) \text{ and p is even.} \end{cases}$$

If G is a type-III, then $H = \begin{cases} pq^2, & \text{p is odd;} \\ pq^2 + p, & \text{p is even.} \end{cases}$

Proof. (1) Since e is a horizontal edge between columns j and j+1 in $G = SC_4C_8[q, 2p]$, $1 \leq j \leq 2p$, where $2p + 1 \equiv 1(mod2p)$, all the edges equidistant to the both ends of e are the edges between columns j and j+1 or between columns p+j and p+j+1 by the symmetry. If G is a type-II and $q \equiv 2(mod4)$, there are $\frac{q}{2} + 1$ edges between columns j and j+1 when j is odd; there are $\frac{q}{2} - 1$ edges between columns j and j+1 when j is even. If G is a type-III, there are $\frac{q+1}{2}$ edges between columns j and j+1 when j is odd; there are $\frac{q-1}{2}$ edges between columns j and j+1 when j is even. Otherwise, there are $\frac{q}{2}$ edges between columns j and j+1. So, (1) holds.

(2) If G is a type-II, $q \equiv 2(mod4)$ and p is even, then $H = (q + 2)(\frac{q}{2} + 1)p + (q - 2)(\frac{q}{2} - 1)p = pq^2 + 4p$; If G is a type-III and p is even, then $H = (q+1)(\frac{q+1}{2})p + (q-1)(\frac{q-1}{2})p = pq^2 + p$. Otherwise, $H = pq^2$ since there are pq horizontal edges in $G = SC_4C_8[q, 2p]$.

Lemma 2. (1) Let e be any vertical edge in $G = SC_4C_8[q, 2p]$, then $n(e) = 2p$.

(2) Let E_v be the set of horizontal edges in $G = SC_4C_8[q, 2p]$, $K = \sum\limits_{e \in E_h} n(e)$. Then

$$K = \begin{cases} 2p^2(q-2), & \text{if } G \text{ is a type-I;} \\ 2p^2 q, & \text{if } G \text{ is a type-II;} \\ 2p^2(q-1), & \text{if } G \text{ is a type-III.} \end{cases}$$

Proof. (1) Let e be any vertical edge between rows i and i+1 in $G = SC_4C_8[q, 2p]$, $1 \leq i \leq q - 1$. Then all the edges equidistant to the both ends of e are the edges between rows i and $i + 1$. So, $n(e) = 2p$.

(2) The number of vertical edges in $G = SC_4C_8[q, 2p]$ is

$$|E_v| = \begin{cases} p(q-2), & \text{if } G \text{ is a type-I;} \\ pq, & \text{if } G \text{ is a type-II;} \\ p(q-1), & \text{if } G \text{ is a type-III.} \end{cases}$$

So, (2) holds.

To calculating $PI(G)$, we need calculate $n(e)$ for all oblique edges e in . We first note that: (1) if $G = SC_4C_8[q, 2p]$ is a type-II nanotube, then $G' = SC_4C_8[q - 2, 2p]$ is a type-I, where G' is obtained from G by deleting the first and the last rows; (2) if $G = SC_4C_8[q, 2p]$ is a type-III nanotube, then $G'' = SC_4C_8[q - 1, 2p]$ is a type-I, where G'' is obtained from G by deleting the first or the last row. And G and G' (G'') have the same oblique edges. So, we suppose that $G = SC_4C_8[q, 2p]$ is a type-I in the following, then q is even. For the oblique edge $e = x_{11}x_{21}$ in G, we will give a formula for calculating the distances from x_{11} (or x_{21}), and find the subset X of vertices which are closer to x_{11} than x_{21} and the subset Y of vertices which are closer to x_{21} than x_{11} in $V(G)$.

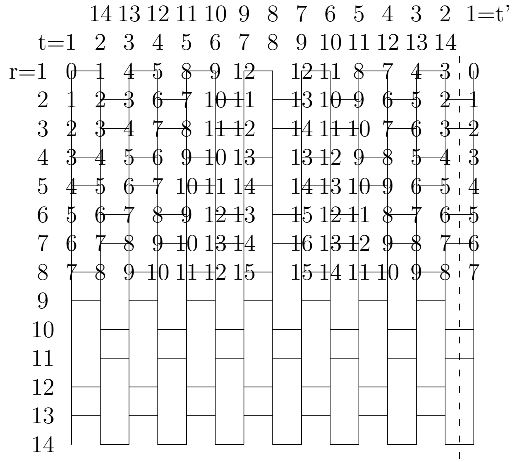


Figure 2. Some distances from the vertex x_{11} in G_1 and G_2.

Table 1. The values of $d_1(x_{11}, x_{rt}) - t$.

	1	2	3	4	5	6	7	8	9	10	11	12
1	-1	-1	1	1	3	3	5	5	7	7	9	9
2	0	0	0	2	2	4	4	6	6	8	8	10
3	1	1	1	3	3	5	5	7	7	9	9	11
4	2	2	2	2	4	4	6	6	8	8	10	10
5	3	3	3	3	5	5	7	7	9	9	11	11
6	4	4	4	4	4	6	6	8	8	10	10	12
7	5	5	5	5	5	7	7	9	9	11	11	13
8	6	6	6	6	6	6	8	8	10	10	12	12
9	7	7	7	7	7	7	9	9	11	11	13	13

We first consider two graphs G_1 and G_2, where G_1 is obtaining from $G = SC_4C_8[q, 2p]$ by deleting the horizontal edges between columns 1 and 2p (see Figure 2), G_2 is obtaining from $G = SC_4C_8[q, 2p]$ by deleting the horizontal edges between columns 1 and 2. And the distances from x_{11} (or x_{21}) in G is the minimum of the ones in G_1 and G_2.

Now, we calculate the distances from x_{11} in G_1 as showing in Figure 2. And Table 1 lists the values of $d_1(x_{11}, x_{rt}) - t$, where $d_1(x_{11}, x_{rt})$ is the distance between x_{11} and x_{rt} in G_1.

From Table 1, we can see that

$$d_1(x_{11}, x_{rt}) - t = \begin{cases} r - 2, & 1 \le t \le [\frac{r}{2}] + 2; \\ 2[\frac{2t+r+1}{4}] - 3, & t \ge [\frac{r}{2}] + 3 \text{ and r is odd}; \\ 2[\frac{2t+r-2}{4}] - 2, & t \ge [\frac{r}{2}] + 3 \text{ and r is even}. \end{cases}$$

where $[x]$ denotes the maximum integer not larger than x throughout this paper. So, we have

Lemma 3. $d_1(x_{11}, x_{rt}) = t + \begin{cases} r-2, & 1 \le t \le [\frac{r}{2}]+2; \\ 2[\frac{2t+r+1}{4}]-3, & t \ge [\frac{r}{2}]+3 \text{ and r is odd;} \\ 2[\frac{2t+r-2}{4}]-2, & t \ge [\frac{r}{2}]+3 \text{ and r is even.} \end{cases}$

Lemma 3 can be easily proved by the inductive method on t, we omit here.

Table 2. The values of $d_2(x_{11}, x_{rt'}) - t'$.

	1	2	3	4	5	6	7	8	9	10	11	12
1	-1	1	1	3	3	5	5	7	7	9	9	11
2	0	0	2	2	4	4	6	6	8	8	10	10
3	1	1	3	3	5	5	7	7	9	9	11	11
4	2	2	2	4	4	6	6	8	8	10	10	12
5	3	3	3	5	5	7	7	9	9	11	11	13
6	4	4	4	4	6	6	8	8	10	10	12	12
7	5	5	5	5	7	7	9	9	11	11	13	13
8	6	6	6	6	6	8	8	10	10	12	12	14
9	7	7	7	7	7	9	9	11	11	13	13	15

Similarly, we calculate the distances from x_{11} in G_2 as showing in Figure 2. And Table 2 lists the values of $d_2(x_{11}, x_{rt'}) - t'$, where $d_2(x_{11}, x_{rt'})$ is the distance between x_{11} and $x_{rt'}$ in G_2 and

$$t' = \begin{cases} 1, & t = 1 \\ 2p+2-t, & t \ge 2 \end{cases}$$

From Table 2, we can see that

$$d_2(x_{11}, x_{rt'}) - t' = \begin{cases} r-2, & 1 \le t' \le [\frac{r}{2}]+1; \\ 2[\frac{2t'+r}{4}]-1, & t' \ge [\frac{r}{2}]+2 \text{ and r is odd;} \\ 2[\frac{2t'+r}{4}]-2, & t' \ge [\frac{r}{2}]+2 \text{ and r is even.} \end{cases}$$

So, we have

Lemma 4. $d_2(x_{11}, x_{rt'}) = t' + \begin{cases} r-2, & 1 \le t' \le [\frac{r}{2}]+1; \\ 2[\frac{2t'+r}{4}]-1, & t' \ge [\frac{r}{2}]+2 \text{ and r is odd;} \\ 2[\frac{2t'+r}{4}]-2, & t' \ge [\frac{r}{2}]+2 \text{ and r is even} \end{cases}$

Since the vertices x_{rt} in G_1 and $x_{rt'}$ in G_2 are identical, we have

Lemma 5. (i)If $t = 1$, then $d_1(x_{11}, x_{rt}) = d_2(x_{11}, x_{rt'})$;
(ii) If $2 \le t \le p+1$, then $d_1(x_{11}, x_{rt}) \le d_2(x_{11}, x_{rt'})$;
(iii) If $p+2 \le t \le 2p$, then $d_1(x_{11}, x_{rt}) \ge d_2(x_{11}, x_{rt'})$;

Proof. (i) It is immediate from Lemmas 3 and 4.

(ii) $2 \leq t \leq p+1$.

Case 1. $t \geq [\frac{r}{2}]+3$. Then $[\frac{r}{2}]+3 \leq t \leq p+1$ and $[\frac{r}{2}] \leq p-2$, $t' = 2p+2-t \geq p+1 \geq [\frac{r}{2}]+2$.

(a) If r is even, then by Lemmas 3 and 4

$$\begin{aligned} d_2(x_{11}, x_{rt'}) - d_1(x_{11}, x_{rt}) &= (t' + 2[\tfrac{2t'+r}{4}] - 2) - (t + 2[\tfrac{2t+r-2}{4}] - 2) \\ &= 4p + 4 - 2t + 2([\tfrac{-2t+r}{4}] - [\tfrac{2t+r-2}{4}]) \\ &\geq 4p + 4 - 4t \quad (\text{since } [\tfrac{-2t+r}{4}] - [\tfrac{2t+r-2}{4}] \geq -t) \\ &\geq 0. \end{aligned}$$

(b) If r is odd, then by Lemmas 3 and 4

$$\begin{aligned} d_2(x_{11}, x_{rt'}) - d_1(x_{11}, x_{rt}) &= (t' + 2[\tfrac{2t'+r}{4}] - 1) - (t + 2[\tfrac{2t+r+1}{4}] - 3) \\ &= 4p + 6 - 2t + 2([\tfrac{-2t+r}{4}] - [\tfrac{2t+r+1}{4}]) \\ &\geq 4p + 6 - 4t > 0. \end{aligned}$$

Case 2. $2 \leq t \leq [\frac{r}{2}]+2$.

(a) If $t' \leq [\frac{r}{2}]+1$, then by Lemmas 3 and 4

$$\begin{aligned} d_2(x_{11}, x_{rt'}) - d_1(x_{11}, x_{rt}) &= (r + t' - 2) - (r + t - 2) \\ &= t' - t = 2p + 2 - 2t \geq 0. \end{aligned}$$

(b) If $t' \geq [\frac{r}{2}]+2$, i.e., $2p+2-t \geq [\frac{r}{2}]+2$, then $t + [\frac{r}{2}] \leq 2p$.

When r is odd, $[\frac{r}{2}] = \frac{r-1}{2}$. And $2t+r \leq 4p+1$, $r-2t \geq r-2[\frac{r}{2}]-4 = -3$.

By Lemmas 2 and 3, we have

$$\begin{aligned} d_2(x_{11}, x_{rt'}) - d_1(x_{11}, x_{rt}) &= (t' + 2[\tfrac{2t'+r}{4}] - 1) - (r + t - 2) \\ &= 4p + 5 + 2[\tfrac{r-2t}{4}] - (2t + r) \\ &\geq 4p + 5 + 2(-1) - (4p + 1) > 0. \end{aligned}$$

When r is even, $[\frac{r}{2}] = \frac{r}{2}$. And $2t + r \leq 4p$, $r - 2t \geq r - 2[\frac{r}{2}] - 4 = -4$.

By Lemmas 2 and 3, we have

$$\begin{aligned} d_2(x_{11}, x_{rt'}) - d_1(x_{11}, x_{rt}) &= (t' + 2[\tfrac{2t'+r}{4}] - 2) - (r + t - 2) \\ &= 4p + 4 + 2[\tfrac{r-2t}{4}] - (2t + r) \\ &\geq 4p + 5 + 2(-1) - 4p > 0. \end{aligned}$$

(iii) $p+2 \leq t \leq 2p$. Then $2 \leq t' = 2p+2-t \leq p$.

Case 1. $t' \geq [\frac{r}{2}]+2$.

(a) If r is even, then by Lemmas 3 and 4

$$\begin{aligned} d_1(x_{11}, x_{rt}) - d_2(x_{11}, x_{rt'}) &= (t - 2 + 2[\tfrac{2t+r-2}{4}]) - (t' - 2 + 2[\tfrac{2t'+r}{4}]) \\ &= (2p - t' + 2([\tfrac{4p+2-2t'+r}{4}]) - (t' - 2 + 2[\tfrac{2t'+r}{4}]) \\ &= 4p + 2 - 2t' + 2([\tfrac{r-2t'+2}{4}] - [\tfrac{2t'+r}{4}]) \\ &\geq 4p + 2 - 2t' + 2(\tfrac{r-2t'-1}{4} - \tfrac{2t'+r}{4}) \\ &> 4p + 2 - 2t' + 2(t' - 1) \geq 0. \end{aligned}$$

(b) If r is odd, then by Lemmas 3 and 4

$$\begin{aligned} d_1(x_{11}, x_{rt}) - d_2(x_{11}, x_{rt'}) &= (t - 3 + 2[\tfrac{2t+r+1}{4}]) - (t' - 1 + 2[\tfrac{2t'+r}{4}]) \\ &= 4p + 2 - 2t' + 2([\tfrac{r-2t'-1}{4}] - [\tfrac{2t'+r}{4}]) \\ &\geq 4p - 4t' + 2 > 0. \end{aligned}$$

Case 2. $2 \leq t' \leq [\frac{r}{2}]+1$.

(a) If $t \leq [\frac{r}{2}]+2$, then by Lemmas 3 and 4

$$\begin{aligned} d_1(x_{11}, x_{rt}) - d_2(x_{11}, x_{rt'}) &= (r + t - 2) - (r + t' - 2) \\ &= t - t' = 2p + 2 - 2t' > 0. \end{aligned}$$

(b) If $t \geq [\frac{r}{2}] + 3$, then by Lemmas 3 and 4

$$\begin{aligned} d_1(x_{11}, x_{rt}) - d_2(x_{11}, x_{rt'}) &= (t - 2 + 2[\tfrac{2t+r-2}{4}]) - (r + t' - 2) \\ &\geq (t - 2 + 2[\tfrac{2r+4}{4}]) - (r + t' - 2) \\ &= (t + r) - (r + t' - 2) = 2p + 4 - 2t' > 0 \end{aligned}$$

when r is even; and

$$\begin{aligned} d_1(x_{11}, x_{rt}) - d_2(x_{11}, x_{rt'}) &= (t - 3 + 2[\tfrac{2t+r+1}{4}]) - (r + t' - 2) \\ &\geq (t - 3 + 2[\tfrac{2r+6}{4}]) - (r + t' - 2) \\ &\geq (t - 3 + 2(\tfrac{2r+3}{4})) - (r + t' - 2) \\ &> t - t' = 2p + 2 - 2t' > 0 \end{aligned}$$

when r is odd.

Now by Lemma 5, we can directly give a formula of calculating the distances from x_{11} in $G = SC_4C_8[q, 2p]$.

Theorem 1. (i) $d(x_{11}, x_{rt}) = d_1(x_{11}, x_{rt})$ if $1 \leq t \leq p + 1$;
(ii) $d(x_{11}, x_{rt}) = d_2(x_{11}, x_{rt})$ if $p + 2 \leq t \leq 2p$.

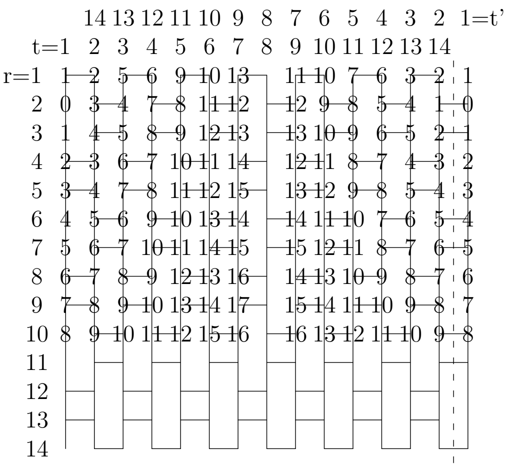


Figure 3. Some distances from the vertex x_{21} in G_1 and G_2.

Next, we consider the distances from x_{21}. Using the same methods as above, we can calculate the distances from x_{21} in G_1 and G_2 (see Figure 3.)

Table 3. The values of $d_1(x_{21}, x_{rt}) - t$.

	1	2	3	4	5	6	7	8	9	10	11	12
1	0	0	2	2	4	4	6	6	8	8	10	10
2	-1	1	1	3	3	5	5	7	7	9	9	11
3	0	2	2	4	4	6	6	8	8	10	10	12
4	1	1	3	3	5	5	7	7	9	9	11	11
5	2	2	4	4	6	6	8	8	10	10	12	12
6	3	3	3	5	5	7	7	9	9	11	11	13
7	4	4	4	6	6	8	8	10	10	12	12	14
8	5	5	5	5	7	7	9	9	11	11	13	13
9	6	6	6	6	8	8	10	10	12	12	14	14

We can see from Table 3 that

$$d_1(x_{21}, x_{rt}) - t = \begin{cases} r-3, & 1 \le t \le [\frac{r}{2}]; \\ 2[\frac{2t+r-2}{4}] - 1, & t \ge [\frac{r}{2}] + 1 \text{ and r is even;} \\ 2[\frac{2t+r-3}{4}], & t \ge [\frac{r}{2}] + 1 \text{ and r is odd.} \end{cases}$$

So, we have

Lemma 6. $d_1(x_{21}, x_{rt}) = t + \begin{cases} r-3, & 1 \le t \le [\frac{r}{2}]; \\ 2[\frac{2t+r-2}{4}] - 1, & t \ge [\frac{r}{2}] + 1 \text{ and r is even;} \\ 2[\frac{2t+r-3}{4}], & t \ge [\frac{r}{2}] + 1 \text{ and r is odd.} \end{cases}$

Table 4. The values of $d_2(x_{21}, x_{rt'}) - t'$.

	1	2	3	4	5	6	7	8	9	10	11	12
1	0	0	0	2	2	4	4	6	6	8	8	10
2	-1	-1	1	1	3	3	5	5	7	7	9	9
3	0	0	2	2	4	4	6	6	8	8	10	10
4	1	1	1	3	3	5	5	7	7	9	9	11
5	2	2	2	4	4	6	6	8	8	10	10	12
6	3	3	3	3	5	5	7	7	9	9	11	11
7	4	4	4	4	6	6	8	8	10	10	12	12
8	5	5	5	5	5	7	7	9	9	11	11	13
9	6	6	6	6	6	8	8	10	10	12	12	14

We can see from Table 4 that$(r \ge 2)$

$$d_2(x_{21}, x_{rt'}) - t' = \begin{cases} r-3, & 1 \le t' \le [\frac{r}{2}] + 1; \\ 2[\frac{2t'+r}{4}] - 3, & t' \ge [\frac{r}{2}] + 2 \text{ and r is even;} \\ 2[\frac{2t'+r-1}{4}] - 2, & t' \ge [\frac{r}{2}] + 2 \text{ and r is odd.} \end{cases}$$

So, we have

Lemma 7. If $r=1$, then $d_2(x_{21},x_{rt'})=\begin{cases}0, & t'=1;\\ t'+2[\frac{t'}{2}]-2, & t'\geq 2.\end{cases}$

If $r\geq 2$, then $d_2(x_{21},x_{rt'})=t'+\begin{cases}r-3, & 1\leq t'\leq[\frac{r}{2}]+1;\\ 2[\frac{2t'+r}{4}]-3, & t'\geq[\frac{r}{2}]+2 \text{ and r is even};\\ 2[\frac{2t'+r-1}{4}]-2, & t'\geq[\frac{r}{2}]+2 \text{ and r is odd}.\end{cases}$

As in Lemma 5, we can prove the following result by using Lemmas 6 and 7

Lemma 8. (i)If $t=1$, then $d_1(x_{21},x_{rt})=d_2(x_{21},x_{rt'})$;
(ii) If $2\leq t\leq p$, then $d_1(x_{21},x_{rt})\leq d_2(x_{21},x_{rt'})$;
(iii) If $p+1\leq t\leq 2p$, then $d_1(x_{21},x_{rt})\geq d_2(x_{21},x_{rt'})$.

And now, we can give a formula of calculating the distances from x_{21} in $G=SC_4C_8[q,2p]$ by Lemma 8.

Theorem 2. (i) $d(x_{21},x_{rt})=d_1(x_{21},x_{rt})$ if $1\leq t\leq p$;
(ii) $d(x_{21},x_{rt})=d_2(x_{21},x_{rt})$ if $p+1\leq t\leq 2p$.

In the following, we first find the subset X of vertices of $V(G)$ which are closer to x_{11} than x_{21} and the subset Y of vertices which are closer to x_{21} than x_{11} in G, and give the formula of calculating $n(e)$ for the oblique edge $e=x_{11}x_{21}$.

Let $X=\{x_{rt}|x_{rt}\in G, d(x_{11},x_{rt})<d(x_{21},x_{rt})\}$, and $Y=\{x_{rt}|x_{rt}\in G, d(x_{11},x_{rt})>d(x_{21},x_{rt})\}$. Since G is a bipartite graph, $Y=V(G)-X$.

Let $D=d(x_{11},x_{rt})-d(x_{21},x_{rt})$. Then $x_{rt}\in X$ if and only if $D<0$.

Case I. $1\leq t\leq p$.

By Theorems 1 and 2, we have $D=d_1(x_{11},x_{rt})-d_1(x_{21},x_{rt})$, and

(i) $D<0$ for $1\leq r\leq 2t-1$;

(ii) $D>0$ for $2t\leq r\leq q$.

Case II. $p+2\leq t\leq 2p$.

By Theorems 1 and 2, we have $D=d_2(x_{11},x_{rt'})-d_2(x_{21},x_{rt'})>0$.

Case III. $t=p+1$ ($t'=p+1$).

By Theorems 1 and 2, we have $D=d_1(x_{11},x_{rt})-d_2(x_{21},x_{rt'})$.

When $1\leq r\leq 2p-3$, $\begin{cases}D>0, & 2p+r\equiv 1(mod4) \text{ and r is odd};\\ D<0, & 2p+r\equiv 3(mod4) \text{ and r is odd};\\ D>0, & 2p+r\equiv 0(mod4) \text{ and r is even};\\ D<0, & 2p+r\equiv 2(mod4) \text{ and r is even}.\end{cases}$

When $r=2p-2,2p-1$, $D<0$.

When $r\geq 2p$, $D>0$.

So, we have that

Lemma 9. (i) If $2p\leq q$, then

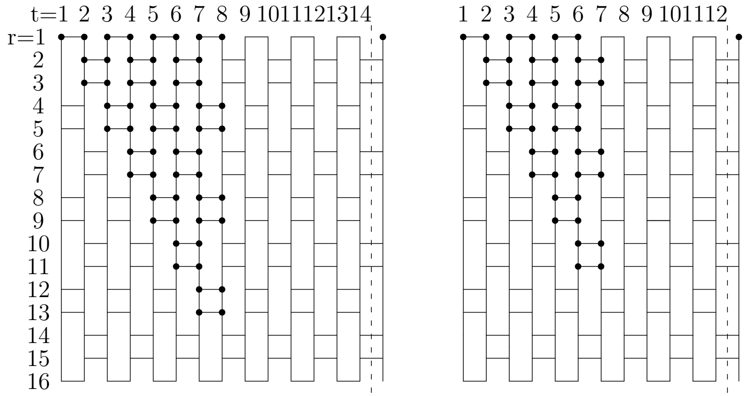
$$X=\{x_{rt}|1\leq r\leq 2t-1 \text{ and } 1\leq t\leq p\}\bigcup\{x_{r,p+1}|2p+r\equiv 2,3(mod4) \text{ and } 1\leq r\leq 2p-1\};$$

(ii) If $2p \geq q+2$, then

$X = \{x_{rt} | 1 \leq r \leq 2t-1 \text{ and } 1 \leq t \leq q\} \bigcup \{x_{r,p+1} | 2p+r \equiv 2, 3 (mod 4) \text{ and } 1 \leq r \leq q\};$

(iii) $n(e) = \begin{cases} 2p, & q \geq 2p \\ q, & q \leq 2p-2, \end{cases}$ where $e = x_{11}x_{21}$.

Two examples are showed in Figure 5, where X is the set of large dots.



In the following, we calculate $n(e)$ for oblique edges $e_r = x_{r1}x_{r+1,1}$ in a type-I nanotube $SC_4C_8[q, 2p]$, where q is even, $r = 2k-1$ is odd and $1 \leq k \leq \frac{q}{2}$. Let $T_1 = SC_4C_8[r+1, 2p]$ be the nanotube consisting of the first $r+1$ rows of $SC_4C_8[q, 2p]$ and $T_2 = SC_4C_8[q-r+1, 2p]$ the one consisting of the last $q-r+1$ rows of $SC_4C_8[q, 2p]$. Then T_1 and T_2 are the type-I ones, and the edge $e_r = x_{r1}x_{r+1,1}$ in $SC_4C_8[q, 2p]$ can be viewed as the oblique edge at row 1 and column 1 in T_1 and also in T_2. By Lemma 9 (iii), we have

$n_1(e_r) = \begin{cases} 2p, & k \geq p \\ 2k, & k \leq p-1, \end{cases}$ in T_1;

$n_2(e_r) = \begin{cases} 2p, & k \leq \frac{q}{2} - p + 1 \\ q - 2k + 2, & k \geq \frac{q}{2} - p + 2, \end{cases}$ in T_2.

And $n(e_r) = n_1(e_r) + n_2(e_r) - 2$ since there are two edges counted twice, $2 \leq k \leq \frac{q}{2} - 1$, and using Lemma 9, we have the following result.

Lemma 10. Let $e = x_{r1}x_{r+1,1}$ be a oblique edge between row r and row $r+1$ in a type-I nanotube $SC_4C_8[q, 2p]$, q is even, $r = 2k-1$, $1 \leq k \leq \frac{q}{2}$.

(i) If $q \leq 2p$, then $n(e) = q$.

(ii) If $2p+2 \leq q \leq 4p-2$, then $n(e) = \begin{cases} 2p + 2k - 2, & 1 \leq k \leq \frac{q}{2} - p; \\ q, & \frac{q}{2} - p + 1 \leq k \leq p-1; \\ 2p + q - 2k, & p \leq k \leq \frac{q}{2}. \end{cases}$

(iii) If $q \geq 4p$, then $n(e) = \begin{cases} 2p+2k-2, & 1 \leq k \leq p-1; \\ 4p-2, & p \leq k \leq \frac{q}{2}-p; \\ 2p+q-2k, & k \geq \frac{q}{2}-p+1. \end{cases}$

Lemma 11. Let N be the sum of $n(e)$ over all oblique edges e in $G = SC_4C_8[q, 2p]$.

(1) If G is a type-I, then $N = \begin{cases} pq^2, & q \leq 2p; \\ 2p(2pq-2p^2-q+2p), & q \geq 2p+2. \end{cases}$

(2) If G is a type-II, then $N = \begin{cases} p(q-2)^2, & q \leq 2p+2; \\ 2p(2pq-2p^2-q-2p+2), & q \geq 2p+4. \end{cases}$

(3) If G is a type-III, then $N = \begin{cases} p(q-1)^2, & q \leq 2p+1; \\ 2p(2pq-2p^2-q+1), & q \geq 2p+3. \end{cases}$

Proof. (1) Let $N_1 = \sum_{k=1}^{\frac{q}{2}} n(e_{2k-1})$ be the sum of $n(e_{2k-1})$ over all oblique edges e_{2k-1} of column 1 in a type-I nanotube $G = SC_4C_8[q, 2p]$. By Lemma 10,

(i) If $q \leq 2p$, then $N_1 = \frac{1}{2}q^2$;

(ii) If $2p+2 \leq q \leq 4p-2$, then

$$\begin{aligned} N_1 &= \sum_{k=1}^{\frac{q}{2}-p}(2p+2k-2) + \sum_{k=\frac{q}{2}-p+1}^{p-1} q + \sum_{k=p}^{\frac{q}{2}}(2p+q-2k) \\ &= (\tfrac{q}{2}-p)(\tfrac{q}{2}+p-1) + q(2p-\tfrac{q}{2}-1) + (\tfrac{q}{2}-p+1)(p+\tfrac{q}{2}) \\ &= 2pq-2p^2-q+2p \end{aligned}$$

(iii) If $q \geq 4p$, then

$$\begin{aligned} N_1 &= \sum_{k=1}^{p-1}(2p+2k-2) + \sum_{k=p}^{\frac{q}{2}-p}(4p-2) + \sum_{k=\frac{q}{2}-p+1}^{\frac{q}{2}}(2p+q-2k) \\ &= (p-1)(3p-2) + (4p-2)(\tfrac{q}{2}-2p+1) + p(3p-1) \\ &= 2pq-2p^2-q+2p \end{aligned}$$

So,

$$N = 2pN_1 = \begin{cases} pq^2, & q \leq 2p; \\ 2p(2pq-2p^2-q+2p), & q \geq 2p+2. \end{cases}$$

(2) and (3) hold, since a type-II $G = SC_4C_8[q, 2p]$ (or a type-III $G = SC_4C_8[q, 2p]$) can be changed into a type-I $G' = SC_4C_8[q-2, 2p]$ (or $G'' = SC_4C_8[q-1, 2p]$) and G and G' (or G'') have the same oblique edges.

3 A formula for calculating PI index of $G = SC_4C_8[q, 2p]$

Using Lemmas 1,2 and 11, we can give a formula for calculating PI index of $G = SC_4C_8[q, 2p]$.

Theorem 3. Let $G = SC_4C_8[q, 2p]$.

(1) If G is a type-I, then

$$PI(G)=\begin{cases}9p^2q^2-14p^2q+8p^2-2pq^2, & q\leq 2p;\\ 9p^2q^2-18p^2q+4p^2+2pq-pq^2+4p^3, & q\geq 2p+2.\end{cases}$$

(2) If G is a type-II, then

$$PI(G)=\begin{cases}9p^2q^2-14p^2q-2pq^2+4pq+4p^2-4p, & q\leq 2p+2, q\equiv 0;\\ 9p^2q^2-14p^2q-2pq^2+4pq+4p^2-4p, & q\leq 2p+2, q\equiv \text{2p is odd};\\ 9p^2q^2-14p^2q-2pq^2+4pq+4p^2-8p, & q\leq 2p+2, q\equiv \text{2p is even};\\ 9p^2q^2-18p^2q-pq^2+4p^3+2pq+8p^2-4p, & q\geq 2p+4, q\equiv 0;\\ 9p^2q^2-18p^2q-pq^2+4p^3+2pq+8p^2-4p, & q\geq 2p+4, q\equiv \text{2p is odd};\\ 9p^2q^2-18p^2q-pq^2+4p^3+2pq+8p^2-8p, & q\geq 2p+4, q\equiv \text{2p is even};\end{cases}$$

(3) If G is a type-III, then

$$PI(G)=\begin{cases}9p^2q^2-14p^2q-pq^2+2pq+6p^2-p, & q\leq 2p+\text{1p is odd};\\ 9p^2q^2-14p^2q-pq^2+2pq+6p^2-2p, & q\leq 2p+\text{1p is even};\\ 9p^2q^2-18p^2q-pq^2+4p^3+2pq+6p^2-2p, & q\geq 2p+\text{3p is odd};\\ 9p^2q^2-18p^2q-pq^2+4p^3+2pq+6p^2-3p, & q\geq 2p+\text{3p is odd}.\end{cases}$$

Proof. It is immediate from Lemmas 1,2 and 11, since $PI(G)=|E(G)|^2-\sum_{e\in E(G)} n(e)=|E(G)|^2-(K+H+N)$ and $|E(G)|=3pq-2p$.

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