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Semi-cartesian product of graphs

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Abstract In this paper, we define a kind of new product graphs with hexagonal inner faces, called semi-cartesian products, so that they directly link with hexagonal system, e.g., the semi-cartesian product of an even cycle and a path is a zigzag polyhex nanotube, a path and an even cycle is an armchair polyhex nanotube, two even cycles is a polyhex nanotorus and two paths is a polyhex lattice. Then we consider the distance in a semi-cartesian product and show two formulas to calculate the distance of two vertices and the sum of all pair of distances. Moreover we illustrate that the applying of the semi-cartesian products would be greatly simplifies the calculation of the distances in the carbon nanotubes and polyhex nanotorus by presenting some examples.

1 Introduction

A graph product of two graphs G and H most commonly means a graph on the vertex set $V(G) \times V(H)$, while its edges are determined by a function on the edges of the factors. Many properties of structural models can be obtained by considering the properties of their factors [1]. This simplifies many complicated calculations and makes it possible to find the topological properties of the models in a much easier manner

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employing the topological properties of their factors. As an example, the eigen solution of the adjacency and Laplacian matrices of the models can easily be obtained using those of their factors. The eigenvalues and eigenvectors of these matrices facilities certain combinatorial optimization problems such as ordering and partitioning for parallel computing [2,3].

In this paper, we define and characterize a new kind of product graphs with hexagonal inner faces, call them as semi-cartesian products, such that they directly link with the hexagonal systems. In Sect. 2, we define the semi-artesian product of two connected bipartite graphs and drove a picture of a zigzag polyhex nanotube to display that it is an example of a semi-cartesian product of an even cycle and a path. In Sect. 3, we consider the distance in the semi-cartesian products and show two formulas to calculate the distance of two vertices and the sum of all pair of distances. In the last section, presenting some examples we illustrate that the application of the semi-cartesian products how greatly simplifies the calculation of the distance in the carbon nanotubes and polyhex nanotorus.

2 Definition

For terminology and notation not defined here we refer to [1,2,4]. Let $G = (V(G), E(G))$ be a connected graph with the vertex set $V(G)$ and edge set $E(G)$. An orientation of a connected graph G is called connected cycle preserving if there is a directed $u - v$ path for any $u, v \in V(G)$ and any induced cycle of G is a directed cycle.

Definition 1 ([1,5]) Cartesian product (Sum graph) $G \square H$:

$V(G \square H) = V(G) \times V(H)$,
$E(G \square H) = \{(u, v)(u', v') : v = v' \text{ and } uu' \in E(G) \vee u = u' \text{ and } vv' \in E(H)\}$.

Definition 2 Let G and H be two connected bipartite graphs with the white and black color partition sets and G symmetric subject to the partition and H connected cycle preserving orientable. Then the semi-cartesian product (semi-sum) of the graphs G and H, denoted by $G \sqcup H$, defined as:

$V(G \sqcup H) = V(G) \times V(H)$,
$E(G \sqcup H) = \{(u, v)(u', v') : v = v' \text{ and } uu' \in E(G) \vee u = u' \text{ and } vv' \in E(H) \text{ and } u \text{ and } v \text{ colored with same color}\}$, where $v \to v'$ on a fixed connected cycle preserving orientation of H.

Since G and H are connected bipartite graphs and G has a symmetric bipartition, the disjoint union of $G \cup H$ is uniquely two colorable, the vertex set of $G \cup H$ is uniquely partitioned into two classes such that no two vertices are adjacent in a same class, and it is in turn implies that the semi-cartesian products of such two graphs are unique even if we switch the white and black colors of any factor and choose different connected cycle preserving orientation.

It is clear from Definition 2 that this modified cartesian product of two graphs is a subgraph of the corresponding cartesian product, i.e., we obtain the modified cartesian product of two graphs by deleting about $|V(G)| \left\lceil \frac{|E(H)|}{2} \right\rceil$ edges from the

cartesian product of this two graphs, thus we name the modified cartesian product graphs as semi-cartesian product graphs.

Since the inner faces of most familiar graph products are triangles or quadrangles, there is no direct relations between hexagonal system and them. For this purpose some modified product graphs were defined, for instance, the type 3 directed graph product of a spacial direct graph and a path like graph with some regular loops is a polyhex lattice [3], and the F-sum product of P_{n+1} and P_2 is the linear chain L_n [6].

Carbon nanotubes are the super fibers with light weight and a perfectly connected hexagonal cylindrical structure. It is well-known that these cylindrical carbon molecules have many unusual properties, which are valuable for nanotechnology, electronics, optics and other fields of material science and technology. Owing to their extraordinary properties, they had a broad application prospects and aroused widespread attention and enthusiasm.

It is commonly believe that the honeycomb cells are an example of geometric efficiency, they are composed of hexagons rather than any other shape, and the hexagon tiles the plane with minimal surface area so that a hexagonal structure uses the least material to create a lattice of cells.

One of the most pleasing features of the semi-cartesian product is that every inner face of it is a hexagon. Notice that the semi-cartesian product of an even cycle and a path is a zigzag polyhex nanotube, a path and an even cycle is an armchair polyhex nanotube, two even cycles is a polyhex nanotorus, and the semi-cartesian product of an odd path and an even path could be two different graphs according to the choice of colors, since an odd path has no symmetric bipartition, and one of them is a polyhex lattice, for instance see Fig. 1, in which the vertices with even subscript are belong to the white class and other are black class and $v_i \rightarrow v_{i+1}$.

Although $G \sqcup H \ncong H \sqcup G$, it is can be checked that $G \sqcup H$ also has a symmetric bipartition. So we can easily generalize the definition of the semi-cartesian product of two graphs to n graphs by setting that each G_i is a connected bipartite graph and G_1 has a symmetric bipartition and G_i has a connected cycle preserving orientation for $2 \leq i \leq n$, but $G_1 \sqcup G_2 \sqcup \cdots \sqcup G_n$ is neither commutative nor associative, we only operate it in the proper order from the left to the right.

3 Distance in semi-cartesian product

In this section, we need some extra notations. The symbol $d_G(u, u')$ denotes the distance between the vertices u and u' of G defined as the length (number of edges) of a shortest $u - u'$ path in G. Let $E\lceil x \rceil$ be the maximal even number no bigger than x and $E\lfloor x \rfloor$ be the minimal even number no less than x, and set $E\lceil x \rceil = E\lfloor x \rfloor = 0$ for $x \leq 0$ and put $E\langle x \rangle = E\lceil x \rceil + E\lfloor x \rfloor$.

$d_{G \square H}((u, v), (u', v')) = d_G(u, u') + d_H(v, v')$ (distance lemma) is a well-known property of the cartesian product graphs. By this result and careful observing, one can obtain the following lemma. Indeed, since $G \sqcup H$ is a subgraph of $G \square H$, if $d_G(u, u') \geq d_H(v, v')$, then we can easily find a shortest $(u, v) - (u', v')$-path of length $d_G(u, u') + d_H(v, v')$ in $G \sqcup H$. Thus we only consider the case $d_G(u, u') < d_H(v, v')$. In this case, same number of alternative edges of every shortest $(u, v) - (u', v')$-path in $G \square H$ are replaced by P_4 in $G \sqcup H$ for $d_H(v, v') - d_G(u, u')$, and so that the length of
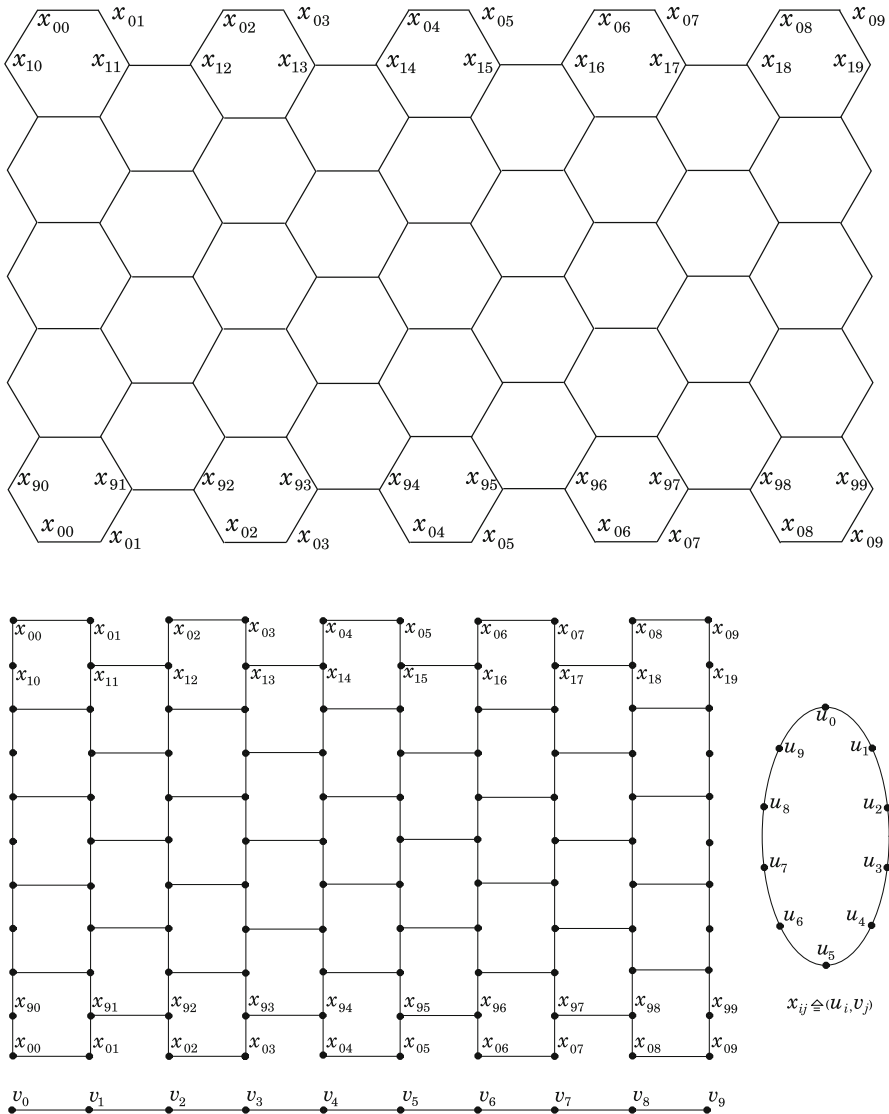
Fig. 1 The profile of the semi-cartesian product $C_{10} \sqcup P_{10} = TUHC_6[10, 10]$

a shortest $(u, v) - (u', v')$-path in $G \sqcup H$ is calculated simultaneously with $d_G(u, u')$ and $d_H(v, v')$.

Lemma 1 *Let G and H be two connected bipartite graphs with the white and black color partition sets and G symmetric subject to the partition and H connected cycle preserving orientable. Then the distance of two vertices in the semi-cartesian product $G \sqcup H$ is given as:*

$$d_{G \sqcup H}\left((u, v), (u', v')\right) = d_G(u, u') + d_H(v, v') + M\left(d_H(v, v') - d_G(u, u')\right),$$

where (u, v) lies on the left end of a shortest $(u, v) - (u', v')$-path and

$$M(d_H(v, v') - d_G(u, u')) = \begin{cases} E\lceil d_H(v, v') - d_G(u, u') \rceil, & u \text{ and } v \text{ are same color;} \\ E\lfloor d_H(v, v') - d_G(u, u') \rfloor, & \text{otherwise.} \end{cases}$$

One can also easily determine $M(d_H(v, v') - d_G(u, u'))$ in the following way. Set $G_v = \{(u, v) \mid u \in V(G)\}$, where $v \in V(H)$. If the neighbor of (u, v) or (u', v') lies on a shortest $(u, v) - (u', v')$-path is belong to G_v or $G_{v'}$ respectively, then

$$M(d_H(v, v') - d_G(u, u')) = E\lfloor d_H(v, v') - d_G(u, u') \rfloor;$$

otherwise

$$M(d_H(v, v') - d_G(u, u')) = E\lceil d_H(v, v') - d_G(u, u') \rceil.$$

Obviously both formula can be applied for a case in the same time and we use them convertibly in the next section. In the end of this section, we discuss the sum of all pair of distance, which known as Wiener index, in the semi-cartesian product graphs.

Definition 3 Wiener index $\mathcal{W}(G)$ ([7])

$$\mathcal{W}(G) = \sum_{\{u, u'\} \subset V(G)} d(u, u') = \frac{1}{2} \sum_{u, u' \in V(G)} d(u, u').$$

Lemma 2 *Let G and H be two connected bipartite graphs with the white and black color partition sets and G symmetric subject to the partition and H connected cycle preserving orientable. Then*

$$\mathcal{W}(G \sqcup H) = |V(H)|^2 \mathcal{W}(G) + |V(G)|^2 \mathcal{W}(H) + \frac{1}{2} \mathcal{M}_{H,G}$$

where $\mathcal{M}_{H,G} = \sum_{u, u' \in V(G)} \sum_{v, v' \in V(H)} M(d_H(v, v') - d_G(u, u'))$.

Proof By Definition 3 and Lemma 1, we have

$$\mathcal{W}(G \sqcup H) = \frac{1}{2} \sum_{u, u' \in V(G)} \sum_{v, v' \in V(H)} d_{G \sqcup H}((u, v), (u', v'))$$

$$= \frac{1}{2} \sum_{u, u' \in V(G)} \sum_{v, v' \in V(H)} d_G(u, u') + \frac{1}{2} \sum_{u, u' \in V(G)} \sum_{v, v' \in V(H)} d_H(v, v')$$

$$+ \frac{1}{2} \sum_{u, u' \in V(G)} \sum_{v, v' \in V(H)} M\left(d_H(v, v') - d_G(u, u')\right)$$

$$= |V(H)|^2 \mathcal{W}(G) + |V(G)|^2 \mathcal{W}(H) + \frac{1}{2} \mathcal{M}_{H,G}.$$

$\square$

Though this lemma seams awkward, it still reduce the calculation of the distance sum in a semi-cartesian product to their factors and moreover in most of the cases $M(d_H(v, v') - d_G(u, u')) = 0$ so that many calculations related to the distance in a polyhex system would be subtracted and we will demonstrate it in the next section.

4 Some applications

Application of the semi-cartesian graph products may greatly simplifies many complicated tedious calculations in the study of carbon nanotubes and polyhex nanotorus. For example, we first calculate the Wiener index of an arbitrary zigzag polyhex nanotube $TUHC_6[2p, q]$ in the terms of its circumference $2p$ and its length q for the general case $p \leq q$. We numerate the vertices of C_{2p} and P_q as in Fig. 1 and set $V_1 = V(C_{2p}) = \{u_0, u_1, \ldots, u_{2p-1}\}$, $V_2 = V(P_q) = \{v_0, v_1, \ldots, v_{q-1}\}$, $v_i \rightarrow v_{i+1}$, and we view V_i as the number set of subscripts when no ambiguous arise. It is clear that $d_{C_{2p}}(u_i, u_s) = \min\{s - i, i + 2p - s\}$ for $i \leq s$, $d_{P_q}(v_j, u_t) = |t - j|$ in this numeration. Since $TUHC_6[2p, q] = C_{2p} \sqcup P_q$,

$$\mathcal{W}(C_{2p}) = \tfrac{1}{2} \times 2p[2\textstyle\sum_{k=1}^{p-1} d_{C_{2p}}(u_0, u_k) + d_{C_{2p}}(u_0, x_p)] = p[2 \binom{p}{2} + p] = p^3$$

and $\mathcal{W}(P_q) = \sum_{0 \leq j < t < q}(t - j) = \binom{q + 1}{3}$, and by Lemma 2, we only need to calculate

$$\mathcal{M}_{P_q, C_{2p}} = \sum_{i, s \in V_1} \sum_{j, t \in V_2} M\left(d_{P_q}(v_j, v_t) - d_{C_{2p}}(u_i, u_s)\right).$$

Obviously $\sum_{s \in V_1; j, t \in V_2} M(|t - j| - d_{C_{2p}}(u_0, u_s)) = \sum_{s \in V_1; j, t \in V_2} M(|t - j| - d_{C_{2p}}(u_{2k}, u_s))$ and $\sum_{s \in V_1; j, t \in V_2} M(|t - j| - d_{C_{2p}}(u_1, u_s)) = \sum_{s \in V_1; j, t \in V_2} M(|t - j| - d_{C_{2p}}(u_{2k-1}, u_s))$ for $0 < k \leq p$. Then thanks to the symmetrical structure of the zigzag polyhex nanotube $C_{2p} \sqcup P_q$, we have

$$\mathcal{M}_{P_q, C_{2p}} = p\Bigg(\sum_{i=0, 0 \leq s \leq p} \sum_{j, t \in V_2} M(|t - j| - (s - 0))$$

$$+ \sum_{i=0, p < s < 2p} \sum_{j, t \in V_2} M(|t - j| - (2p - s))$$

$$+ \sum_{i=1, 1 \leq s \leq p+1} \sum_{j, t \in V_2} M(|t - j| - (s - 1))$$

$$+ \sum_{i=1, p+1 < s \leq 2p} \sum_{j, t \in V_2} M(|t - j| - (1 + 2p - s))\Bigg)$$

$$= p\Bigg(\sum_{j, t \in V_2} E\langle|t - j|\rangle + 2 \sum_{0 < s < p} \sum_{j, t \in V_2} E\langle|t - j| - s\rangle + \sum_{j, t \in V_2} E\langle|t - j| - p\rangle\Bigg).$$

We calculate the following separately to see it clearly.

$$\sum_{j,t \in V_2} E\langle |t-j|-s \rangle = 2 \sum_{j<t \in V_2} E\langle t-j-s \rangle$$

$$= 2 \sum_{s+j<t<q} \sum_{0 \le j < q-s-1} E\langle t-j-s \rangle$$

$$= 4 \binom{q-s+1}{3}.$$

Thus

$$\mathcal{M}_{P_q,C_{2p}} = p \left(4 \binom{q+1}{3} + 8 \sum_{0<s<p} \binom{q-s+1}{3} + 4 \binom{q-p+1}{3} \right)$$

$$= p \left(4 \binom{q+1}{3} + 8 \left(\binom{q+1}{3} - \binom{q-p+2}{4} \right) + 4 \binom{q-p+1}{3} \right)$$

$$= \frac{p}{3} \left(q^2(q^2-1) + (q-p)^2(1-(q-p)^2) \right).$$

Then, by Lemma 2, the Wiener index of zigzag polyhex nanotube $TUHC_6[2p,q]$ for $p \le q$ equals

$$\mathcal{W}(C_{2p} \sqcup P_q) = q^2 \mathcal{W}(C_{2p}) + (2p)^2 \mathcal{W}(P_q) + \frac{1}{2} \mathcal{M}_{P_q,C_{2p}}$$

$$= \frac{qp^2}{3} (4q^2 + 2p^2 - 3) + \frac{p^3}{6} (1-p^2).$$

This result is identical to the formula in [8,9], but it was obtained by such an easier direct method.

Next we determine the Wiener index of an arbitrary armchair polyhex nanotube $TUVC_6[2p,q]$ in the terms of its circumference $2p$ and its length q for the general case $p \le q$. Although P_q may has no symmetric bipartition, C_{2p} is a highly symmetric graph and $P_q \sqcup C_{2p} = TUVC_6[2p,q]$, and Lemmas 1 and 2 are valid for this case. So similarly in the case of $TUHC_6[2p,q]$, we only consider $\mathcal{M}_{C_{2p},P_q}$. Since $\sum_{s \in V_1; j,t \in V_2} M(d_{C_{2p}}(u_0,u_s) - |t-j|) = \sum_{s \in V_1; j,t \in V_2} M(d_{C_{2p}}(u_k,u_s) - |t-j|)$ for $0 \le k < 2p$, we have

$$\mathcal{M}_{C_{2p},P_q} = 2p \left(\sum_{i=0,0 \le s \le p} \sum_{j,t \in V_2} M((s-0) - |t-j|) \right.$$

$$\left. + \sum_{i=0,p<s<2p} \sum_{j,t \in V_2} M((0+2p-t) - |t-j|) \right)$$

$$= 2p \left(\sum_{0<s<p} \sum_{j,t \in V_2} E\langle s-|t-j| \rangle + \sum_{j,t \in V_2} E\lceil p - |t-j| \rceil \right),$$

where

$$\sum_{j,t \in V_2} E\langle s - |t - j| \rangle = \sum_{j=t \in V_2} E\langle s \rangle + 2 \sum_{j<t \in V_2} E\langle s - (t - j) \rangle$$

$$= 2qs + 4q \binom{s}{2} - 4 \binom{s+1}{3},$$

$$\sum_{j,t \in V_2} E\lceil p - |t - j| \rceil = \sum_{t=s \in V_2} E\lceil p \rceil + 2 \sum_{j<t \in V_2} E\lceil p - (t - j) \rceil$$

$$= 2q \binom{p}{2} - 2 \binom{p}{3} - \frac{1}{2} \times \begin{cases} (p-1)^2, & p \text{ is odd;} \\ p(p-2), & p \text{ is even.} \end{cases}$$

Thus

$$\mathcal{M}_{C_{2p},P_q} = \frac{1}{3} p^2 (p-1) \big((p+1)(4q - p) + 6 \big) - \begin{cases} p(p-1)^2, & p \text{ is odd;} \\ p^2(p-2), & p \text{ is even.} \end{cases}$$

Then, Again by Lemma 2, the Wiener index of armchair polyhex nanotube $TUVC_6[2p, q]$ for $p \le q$ is equal to

$$\mathcal{W}(P_q \sqcup C_{2p}) = (2p)^2 \mathcal{W}(P_q) + q^2 \mathcal{W}(C_{2p}) + \frac{1}{2} \mathcal{M}_{C_{2p},P_q}$$

$$= \frac{p^2}{6} \big(4q(p^2 - 2) + 2qp(3q + 2p) - p(p^2 - 7) - 6 \big)$$

$$- \frac{1}{2} \times \begin{cases} p(p-1)^2, & p \text{ is odd;} \\ p^2(p-2), & p \text{ is even,} \end{cases}$$

which is found in [10–12] and also obtained by such an easer and direct method. The remaining case $p > q$ (for shorter tubes) in both examples is more easily calculated by a similar method as above.

In the end we compute the Wiener index of an arbitrary polyhex nanotorus $T = T(2p, 2q)$ in terms of its circumference $2q$ and its length $2p$. Set $V_3 = V(C_{2q}) = \{w_0, w_1, \ldots, w_{2q-1}\}$ and assume it is the numeration of the vertices of C_{2q} in the clockwise order as above. Recall that $C_{2p} \sqcup C_{2q} = T(2p, 2q)$. It is easy to observe that

$$\sum_{s \in V_1; t \in V_3} M\big(d_{C_{2q}}(w_0, w_t) - d_{C_{2p}}(u_0, u_s)\big) = \sum_{s \in V_1; t \in V_3} M\big(d_{C_{2q}}(w_r, w_t) - d_{C_{2p}}(u_k, u_s)\big)$$

for any $k \in V_1, r \in V_3$. Therefore

$$\mathcal{M}_{C_{2p},C_{2q}} = 4pq \sum_{i=0, s \in V_1} \sum_{j=0, t \in V_3} M(d_{C_{2q}}(w_t - w_0) - d_{C_{2p}}(u_s - u_0))$$

$$= 4pq \Big(\sum_{i=0, 0 \le s \le p} \sum_{j=0, t \in V_3} M(d_{C_{2q}}(w_t - w_0) - (s - 0))$$

$$+ \sum_{i=0, p < s < 2p} \sum_{j=0, t \in V_3} M(d_{C_{2q}}(w_t - w_0) - (0 + 2p - s)) \Big)$$

$$= 4pq\left(\sum_{t \in V_3} M(d_{C_{2q}}(w_t - w_0)) + 2 \sum_{0<s<p} \sum_{t \in V_3} M(d_{C_{2q}}(w_t - w_0) - s)\right.$$
$$\left. + \sum_{t \in V_3} M(d_{C_{2q}}(w_t - w_0) - p)\right)$$

Now we consider the following two cases separately and bear in mind $i = j = 0$.

Case 1 $p > q$

$$\mathcal{M}_{C_{2p}, C_{2q}} = 4pq\left[\left(\sum_{0<t<q} M(t) + M(q) + \sum_{q<t<2q} M(0 + 2q - t)\right)\right.$$
$$\left. + 2 \sum_{0<s<p}\left(\sum_{0<t<q} M(t-s) + M(q-s) + \sum_{q<t<2q} M(0+2q-t-s)\right)\right]$$
$$= 4pq\left[\sum_{0<t<q} E\langle t\rangle + E\lceil q\rceil + 2 \sum_{0<s<p}\left(\sum_{0<t<q} E\langle t-s\rangle + E\lceil q-s\rceil\right)\right]$$
$$= 4pq\left[2\binom{q}{2} + 4 \sum_{0<s<q-1}\binom{q-s}{2} + \left(E\lceil q\rceil + 2 \sum_{0<s<q-1} E\lceil q-s\rceil\right)\right],$$

where $E\lceil q\rceil + 2\sum_{0<s<q-1} E\lceil q-s\rceil = q(q-1)$ in both cases q is odd and q is even. Then

$$\mathcal{M}_{C_{2p}, C_{2q}} = 4pq\left(q(q-1) + 4\binom{q}{3} + q(q-1)\right)$$
$$= \frac{8}{3}pq^2(q^2 - 1).$$

Case 2 $p \le q$

$$\mathcal{M}_{C_{2p}, C_{2q}} = 4pq\left[\sum_{0<t<q} E\langle t\rangle + E\lceil q\rceil + 2 \sum_{0<s<p}\left(\sum_{0<t<q} E\langle t-s\rangle + E\lceil q-s\rceil\right)\right.$$
$$\left. + \sum_{0<t<q} E\langle t-p\rangle + E\lceil q-p\rceil\right]$$
$$= 4pq\left[2\binom{q}{2} + 4 \sum_{0<s<p}\binom{q-s}{2} + 2\binom{q-p}{2}\right.$$
$$\left. + \left(E\lceil q\rceil + 2 \sum_{0<s<p} E\lceil q-s\rceil + E\lceil q-p\rceil\right)\right].$$

We consider all possible cases such as p & q are odd, p is odd & q is even, p is even & q is odd and p & q are even, and obtain $E\lceil q\rceil + 2\sum_{0<s<p} E\lceil q-s\rceil + E\lceil q-p\rceil = 2pq - p(p+1)$. Thus

$$\mathcal{M}_{C_{2p},C_{2q}} = 4pq\left[2\binom{q}{2} + 4\left(\binom{q}{3} - \binom{q-p+1}{3}\right) + 2\binom{q-p}{2} + 2pq - p(p+1)\right]$$
$$= 8p^2q^2(q-p) + \frac{8}{3}p^2q(p^2-1).$$

Therefore, again by Lemma 2, the Wiener index of a polyhex nanotorus $T[2p, 2q]$ equals

$$\mathcal{W}(C_{2p} \sqcup C_{2q}) = (2q)^2\mathcal{W}(C_{2p}) + (2q)^2\mathcal{W}(C_{2q}) + \frac{1}{2}\mathcal{M}_{C_{2p},C_{2q}}$$
$$= \begin{cases} \frac{4}{3}pq^2(3p^2 + 3pq + 2q^2 - 2), & p > q; \\ \frac{4}{3}p^2q(p^2 + 6q^2 - 1), & p \le q. \end{cases}$$

And it is find as an consequence that the result obtained in [13,14] is only valid for the case $p = q$.

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