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Original Article

k -Resonance of the Cartesian Product Graph $P_3 \times C_n$

Yanfei Ma [1], Rui Yang [2]

School of Mathematics and Information Science, Henan Polytechnic University, Henan, China.

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Abstract *- For $n \geq 4$, the cartesian product $P_3 \times C_n$ is a polyhedral graph, where P_3 is a 3-path and C_n is a n -cycle. A set $\mathcal{H}$ of disjoint even faces of $P_3 \times C_n$ is called resonant pattern if $P_3 \times C_n$ has a perfect matching M such that the boundary of every even face in $\mathcal{H}$ is M -alternating. Let k be a positive integer, $P_3 \times C_n$ is k -resonant if any $i \leq k$ disjoint even faces of $P_3 \times C_n$ form a resonant pattern. Moreover, if graph $P_3 \times C_n$ is k -resonant for any integer k, then it is called maximally resonant. In this study, we provide a complete characterization for the k-resonance of $P_3 \times C_n$. We show that every graph $P_3 \times C_n$ is 1-resonant, 2- resonant, 3- resonant and it is not k -resonant$(k \geq 4)$except for $P_3 \times C_4$, $P_3 \times C_6$, $P_3 \times C_8$. Moreover, we get a corollary that $P_3 \times C_n$ is maximally resonant if and only if it is 4-resonant.*

Keywords *- Perfect matching, $P_3 \times C_n$, k - Resonance, Cartesian product graph, Maximally resonant.*

1. Introduction

Resonance is an important topic in mathematical chemistry with a rapidly growing literature. Its originlies in the work of Clar on the aromatic sextet theory [1] and the work of Randić's on the conjugated circuit model [2,3,4]. This concept of the "aromatic sextet" used in resonant theory explains very well π-electronic properties, i.e., relative stabilities, aromaticities, and reactivities of isomeric benzenoid hydrocarbons. In Randić's theory, the conjugated hexagon has the largest contribution to the resonance energy among all $(4n+2)$-length conjugated circuits which contribute positively to the resonance energy of molecule.

In mathematics [5], a conjugated circuit is named an alternating cycle. A *matching* in a graph G is a set M of edges of G such that no two edges in M have a vertex in common. A matching M of G is *perfect* if any vertex of G is incident with an edge of M. For a graph G with a matching M, a cycle C of G is called an$M$ *-alternating* cycle if the edges of C appear alternately in and off M. A set $\mathcal{H}$ of disjoint even faces of a graph G is called *resonant pattern* if G has a perfect matching M such that the boundary of every even face in $\mathcal{H}$ is M -alternating, equivalently, if $G - \mathcal{H}$ has a perfect matching, where $G - \mathcal{H}$ represents the subgraph obtained from$G$ by deleting all vertices of $\mathcal{H}$ together with their incident edges. A graph G is k *-resonant*, if every i $(0 \leq i \leq k)$ pairwise disjoint even faces form a resonant pattern. Obviously, if a graph is k -resonant, it is also $(k-1)$-resonant for integer $k \geq 1$. If the graph G is k -resonant for any positive integer k $(k \geq 1)$, then the graph is *maximally resonant*.

The discussion of some molecular graphs has made the study of resonance theory very important and common. The resonance of molecular graphs was firstly studied in benzene systems [6]. Later, Zhang and Chen [7] gave some sufficient necessary conditions for 1-resonant benzenoid systems.

Theorem 1.1. *[7] Every hexagon of a hexagonal system H is resonant if and only if there exists a perfect matching M of Hsuch that the boundary of H is an M -alternating cycle.*

Soon after, Zhang and Zheng [8] gave a similar characterization for generalized hexagonal systems. Moreover, Zheng [9] first proposed k -resonant when studying hexagonal systems. Further, Zheng [10] characterized general k -resonant benzenoid systems and obtained the following results.

Theorem 1.2. *[10] Every 3-resonant benzenoid systems is also k -resonant for any integer $k \geq 3$.*

The same results are still held for coronoid systems [11], open-ended carbon nanotube [12], toroidal polyhexes [13,14] , Klein-bottle polyhexes [15], fullerene graphs [16], boron-nitrogen fullerenes [17], polygonal systems [18], cubic bipartite polyhedral graphs [19], (3,6)-fullerenes [20]. In fact, these molecular graphs are maximally resonant if and only if they are 3-

resonant. In recent years, Liu et al. [21,22] provided the k -resonance of grid graphs. Not long ago, Yang et al. [23] discussed the resonance of the graph $P_2 \times C_n$ (i.e. n -prism, $n \geq 3$) and obtained that it is k -resonant for any positive integer k $(k \geq 1)$.

Since the k -resonance of the molecular graphs indicates the stability of the corresponding moleculars, in this paper, we consider the k -resonance of the cartesian product graph $P_3 \times C_n$. In section 2, we give some basic notations and preliminary results. In section 3, we prove that all cartesian product graphs $P_3 \times C_n$ are 1-resonant, 2-resonant, 3-resonant and the only k -resonant $(k \geq 4)$graphs $P_3 \times C_n$ are $P_3 \times C_4$, $P_3 \times C_6$ and $P_3 \times C_8$. Furthermore, we come to the conclusion that a cartesian product graph $P_3 \times C_n$ is maximally resonant if and only if it is 4-resonant.

2. Definitions and Preliminary Results

Definition 2.1. *[23] Let G_1 be a simple graph with vertex-set $V(G_1) = \{v^1, v^2, v^3, \cdots, v^m\}$, edge-set $E(G_1)$ and G_2 be another simple graph with vertex-set $V(G_2) = \{v_1, v_2, v_3, \cdots, v_n\}$, edge-set $E(G_2)$. The cartesian product of simple graphs G_1 and G_2 is the graph $G_1 \times G_2$, which is defined as follows:*
(1) $V(G_1 \times G_2) = V(G_1) \times V(G_2) = \{(v_i^j)|1 \leq j \leq m, 1 \leq i \leq n\}$;
(2) $E(G_1 \times G_2) = \{(v_p^a v_q^b)|v^a v^b \in E(G_1), v_p = v_q$; or $v_p v_q \in E(G_2), v^a = v^b\}$.

Definition 2.2. *A path is a non-empty simple graph $P = (V, E)$ such that $V(P) = \{v_1, v_2, v_3, \cdots, v_m\}$ and $E(P) = \{v_1v_2, v_2v_3, \cdots, v_{m-1}v_m\}$, where all the vertices $v_1, v_2, v_3, \cdots, v_m$ are pairwise distinct. We always denote a path with m vertices by P_m, and say P_m a m -path . Sometimes, we also call $P = v_1v_2v_3 \cdots v_m$ an v_1-v_m path. If $P = v_1v_2v_3 \cdots v_m$ is a path with $m \geq 3$, then we call the graph C consisting of P together with the edge v_1v_m a cycle. As with paths, denote by C_m. $C_m = v_1v_2v_3 \cdots v_mv_1$ represents a cycle with m vertices, and say C_m a m -cycle.*

Definition 2.3. *When $n \geq 3$, the cartesian product graph $P_3 \times C_n$ is a polyhedral graph, where P_3 is a 3-path and C_n is a n -cycle.*

Definition 2.4. *[24] A graph is said to be embeddable in the plane, or planar, if it can be drawn in the plane so that its edges intersect only at their ends. Such a drawing is called a planar embedding of the graph.*

In this paper, the graphs considered are all plane.

Definition 2.5. *For a face f of a plane graph G, its boundary is a closed walk and $\partial(f)$ represents for the boundary of f. we often represent a face f by its boundary if unconfused.*

Definition 2.6. *In a planar embedding, a face is said to be an even face if its boundary is an even cycle, and an odd face if its boundary is an odd cycle.*

Definition 2.7. *Vertices and edges contained in the boundary of a face f are said to belong to f or to be on f, and denoted the sets of vertices and edges on $\partial(f)$by $V(f)$ and $E(f)$, respectively.*

Definition 2.8. *A face of a plane graph G is called resonant if its boundary is an M -alternating cycle with a perfect matching $M$of G.*

Definition 2.9. *Two different faces f_1,$f_2$of a plane graph G are disjoint if $V(f_1) \cap V(f_2) = \emptyset$, and we say f_1 is a neighboring face of f_2 if $V(f_1) \cap V(f_2) \neq \emptyset$.*

Definition 2.10. *The symmetric difference of two finite sets A and $B$is denoted as $A \oplus B = (A \cup B) - (A \cap B)$.*

For more terminologies used in this paper, please see literatures [24, 25].

Let $V(P_3) = \{v^1, v^2, v^3\}$,$V(C_n) = \{v_1, v_2, \cdots v_n\}$, where v_i is adjacent to $v_{i+1}$for $i = 1,2,3 \cdots n$, $v_{n+1} = v_1$. Set $P_3 = v^1v^2v^3$,$C_n = v_1v_2v_3 \cdots v_nv_1$. According to the definition of cartesian products, $V(P_3 \times C_n) = \{v_i^j|1 \leq j \leq 3,1 \leq i \leq n\}$. Let the planar embedding of $P_3 \times C_n$ be shown in Figure 1. It is easy to know that $P_3 \times C_n$ consists of $(2n + 2)$ faces, of which two n -sided faces and $2n$ quadrilateral faces. The number of vertices of the graph $P_3 \times C_n$ is $3n$. A k -resonant graph $P_3 \times C_n$ should have even vertices, so n is even. Moreover, C_n is a n -cycle, $n \geq 3$. Thus, we always suppose $n \geq 4$ in the next discussion. The labeling for $P_3 \times C_n$ is shown in Figure 1.

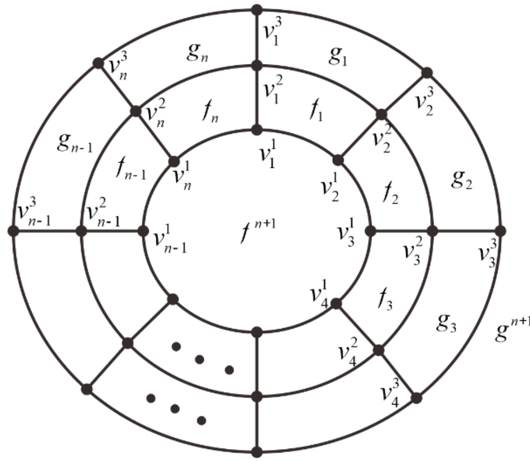
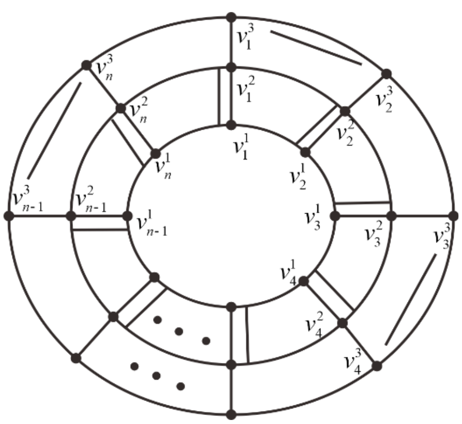


Fig. 1 The graph $P_3 \times C_n$.

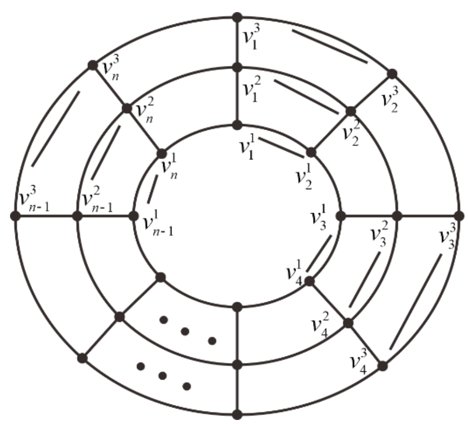
We denote the quadrilateral face with the boundary $v_a^1 v_{a+1}^1 v_{a+1}^2 v_a^2 v_a^1$ as f_a and the quadrilateral face with the boundary $v_a^2 v_{a+1}^2 v_{a+1}^3 v_a^3 v_a^2$ as g_a, where $a = 1,2,3 \cdots n$, $v_{n+1}^1 = v_1^1, v_{n+1}^2 = v_1^2$, $v_{n+1}^3 = v_1^3$. Faces with the boundaries of $\boldsymbol{v_1^1 v_2^1 v_3^1 \cdots v_n^1 v_1^1}$ and $v_1^3 v_2^3 v_3^3 \cdots v_n^3 v_1^3$ are represented as f^{n+1} and g^{n+1}, respectively. (See the labelling of faces of the graph$P_3 \times C_n$ in Figure 1).

We can divide the faces of $P_3 \times C_n$ into four classes, one type is the internal n-sided face f^{n+1}, one is the outer n-sided face g^{n+1}, one is quadrilateral faces f_a $(a = 1,2,3 \cdots n)$, and the other is quadrilateral faces g_a $(a = 1,2,3 \cdots n)$. Let the set of quadrilateral facesf_a $(a = 1,2,3 \cdots n)$ be $\mathscr{F}_1$ and the set of quadrilateral faces g_a be $\mathscr{F}_2$, then $\mathcal{F}_1 = \{f_a | a = 1,2,3 \cdots n\}$ and $\mathscr{F}_2 = \{g_a | a = 1,2,3 \cdots n\}$. From the structural properties of the graph $P_3 \times C_n$, we can see that f^{n+1} and g^{n+1} are symmetrical, $\mathscr{F}_1$ and $\mathscr{F}_2$ are symmetrical.

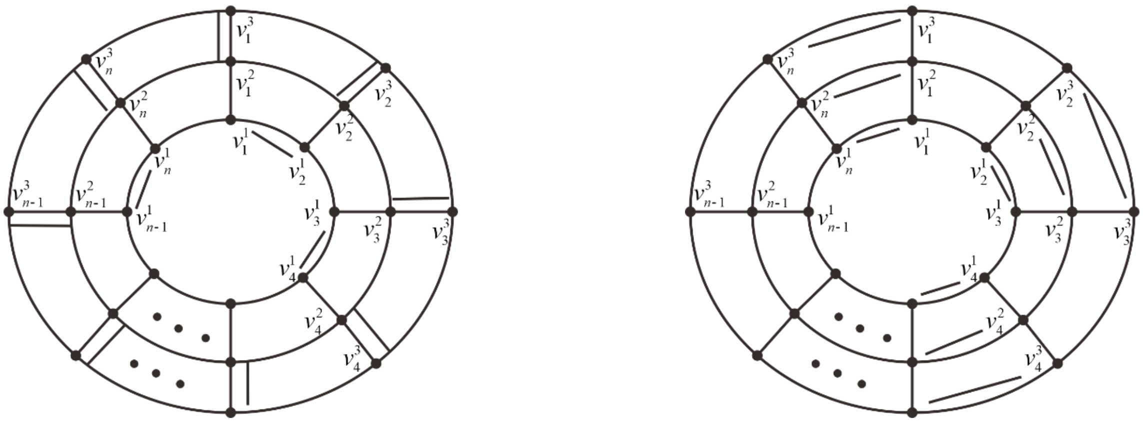
Next we give four perfect matchings for $P_3 \times C_n$,$M_1 = \{v_1^1 v_1^2, v_2^1 v_2^2, v_3^1 v_3^2 \cdots v_n^1 v_n^2, v_1^3 v_2^3, v_3^3 v_4^3 \cdots v_{n-1}^3 v_n^3\}$,$M_2 = \{v_1^1 v_2^1, v_1^2 v_2^2, v_1^3 v_2^3,$ $v_3^1 v_4^1, v_3^2 v_4^2, v_3^3 v_4^3 \cdots v_{n-1}^1 v_n^1, v_{n-1}^2 v_n^2, v_{n-1}^3 v_n^3\}$, $M_3 = \{v_1^2 v_1^3, v_2^2 v_2^3, v_3^2 v_3^3 \cdots v_n^2 v_n^3, v_1^1 v_2^1, v_3^1 v_4^1 \cdots v_{n-1}^1 v_n^1\}$, $M_4 = \{v_2^1 v_3^1, v_2^2 v_3^2, v_2^3 v_3^3, v_4^1 v_5^1, v_4^2 v_5^2, v_4^3 v_5^3$ $\cdots v_n^1 v_1^1, v_n^2 v_1^2, v_n^3 v_1^3\}$, as shown in Figure 2 (double edges).



M_1 (a)



M_2 (b)



M_3 (c) M_4 (d)

Fig. 2 The $P_3 \times C_n$ with four perfect matchings M_1 (a) , M_2 (b), M_3 (c) and M_4 (d).

3. Main results

Lemma 3.1. $P_3 \times C_n$ $(n \geq 4)$ *is 1-resonant.*

Proof. Let h be any face in $P_3 \times C_n$. If h is a quadrilateral face, by symmetry, suppose $h \in \mathscr{F}_1$, we can get the boundary of every quadrilateral face in $\mathscr{F}_1$ is M_1 -alternating, i.e. h is a resonant face. If h is an n -sided face, then $h \in \{f^{n+1}, g^{n+1}\}$, we can find that $\partial(h)$ is M_2-alternating cycle. Each face of the graph $P_3 \times C_n$ is resonant, hence the graph $P_3 \times C_n$ $(n \geq 4)$ is 1-resonant.

Lemma 3.2. $P_3 \times C_n$ $(n \geq 4)$ *is 2-resonant.*

Proof. We choose any pair of disjoint faces h_1 and h_2 in $P_3 \times C_n$. To prove that $P_3 \times C_n$ is 2-resonant , it is sufficient to prove that for any pair of disjoint even faces h_1 and h_2, there exists a perfect matching M such that $\partial(h_1)$ and $\partial(h_2)$ are both M -alternating cycles. According to the classification of the faces in $P_3 \times C_n$, we have the following four cases.

Case 1. $h_1, h_2 \in \{f^{n+1}, g^{n+1}\}$.

If $h_1, h_2 \in \{f^{n+1}, g^{n+1}\}$, then we can know that $\partial(h_1)$ and $\partial(h_2)$ are M_2-alternating cycle.

Case 2. One of $h_1, h_2 \in \{f^{n+1}, g^{n+1}\}$, one of h_1 and h_2 is a quadrilateral face.

Without loss of generality, suppose $h_1 = g^{n+1}$, then $h_2 \in \mathscr{F}_1$. Every quadrangle in $\mathscr{F}_1$ is M_1-alternating. Hence $\partial(h_1)$ and $\partial(h_2)$ are both M_1-alternating cycle.

Case 3. Both h_1, h_2 are quadrilateral faces and $h_1, h_2 \in \mathscr{F}_1$ or $h_1, h_2 \in \mathscr{F}_2$.

We can see from Figure 2 that the boundaries of any two disjoint quadrilateral faces in $\mathscr{F}_1$ or $\mathscr{F}_2$ are M_1-alternating or M_3-alternating, respectively. So any two disjoint quadrilateral faces in $\mathscr{F}_1$ or $\mathscr{F}_2$ form a resonant pattern of $P_3 \times C_n$.

Case 4. Both h_1, h_2 are quadrilateral faces and $h_1 \in \mathscr{F}_1$,$h_2 \in \mathscr{F}_2$.

Let's take any quadrilateral face in $\mathscr{F}_1$, without loss of generality, firstly assume $h_1 = f_i$ $(i = 1,3,5, \cdots n-1)$, we have $h_2 \neq \{g_{i-1}, g_i, g_{i+1}\}$ and let $g_0 = g_n$. Then, we find that $\partial(h_2)$ is M_2-alternating cycle or none of the four edges of $E(h_2)$ belong to M_2. If $\partial(h_2)$ is M_2-alternating cycle, then both $\partial(h_1)$ and $\partial(h_2)$ are M_2-alternating cycles, which means $\{h_1, h_2\}$ forms a resonant pattern. Otherwise, let $h_2 = g_a (a \neq i-1, i, i+1)$, set $M_5 := M_2 \oplus E(g_{a-1}) \oplus E(g_{a+1})$. It is clear that M_5 is a perfect matching alternating on both $\partial(h_1)$ and $\partial(h_2)$. Next suppose $h_1 = f_i$ $(i = 2,4,6, \cdots n)$, then $h_2 \neq \{g_{i-1}, g_i, g_{i+1}\}$ and let $g_{n+1} = g_1$. Now we get $\partial(h_1)$is M_4- alternating cycle from Figure 2(d), and we can know $\partial(h_2)$ is M_4-alternating cycle or none of the four edges of $E(h_2)$ belongs to M_4. Then the similar analysis as above we can get both $\partial(h_1)$ and $\partial(h_2)$ are alternating cycles with respect to some perfect matching of $P_3 \times C_n$.

Thus, any two disjoint quadrilateral faces in $P_3 \times C_n$ can form a resonant pattern, that is, $P_3 \times C_n$ $(n \geq 4)$ is 2-resonant.

Lemma 3.3. *$P_3 \times C_n$ $(n \geq 4)$ is 3-resonant.*
Proof. We take any three pairwise disjoint faces in $P_3 \times C_n$, denoted by h_1, h_2, h_3. We distinguish the following three cases according to the number of n -sided faces in $\{h_1, h_2, h_3\}$.

Case 1. There are exactly two n -sided faces in $\{h_1, h_2, h_3\}$.
Without loss of generality, suppose $h_1, h_2 \in \{f^{n+1}, g^{n+1}\}$, then there are not exist three disjoint even faces, which is trivial.

Case 2. There is exactly one n -sided face in $\{h_1, h_2, h_3\}$.
Without loss of generality, suppose $h_1 = g^{n+1}$, then we have $h_2, h_3 \neq f^{n+1}$ and $h_2, h_3 \in \mathscr{F}_1$. Instantly we have all $\partial(h_1)$, $\partial(h_2)$, $\partial(h_3)$ are M_1-alternating cycle. Hence h_1,h_2, and h_3 form a resonant pattern of $P_3 \times C_n$.
Case 3. There are no n -sided faces in h_1, $h_2$and h_3.
We know that h_1, $h_2$and h_3 are all quadrilateral faces, $h_1, h_2, h_3 \in \{\mathcal{F}_1, \mathcal{F}_2\}$. Without loss of generality, let's assume $h_1, h_2 \in \mathscr{F}_1$, $h_3 \in \mathscr{F}_2$. As can be seen from Figure 2(a), the boundaries of any two disjoint quadrilateral faces in $\mathscr{F}_1$ are M_1-alternating cycles. Next we analyze h_3. We can distinguish the following two cases.
Subcase 3.1. None of the edges of $E(h_3)$ belong to M_1.
Let h_3=g_i and g_i $(i = 2,4,6, \cdots, n)$ be the face where none of the four edges of $E(h_3)$ belong to M_1. Let $M_6 := M_1 \oplus E(f_i) \oplus E(g^{n+1})$. It is clear that M_6 is a perfect matching of $P_3 \times C_n$ such that $\partial(h_1)$, $\partial(h_2)$, $\partial(h_3)$ are simultaneously M_6-alternating.
Subcase 3.2. Only one edge of $E(h_3)$ belongs to M_1.
We suppose h_3=g_j. Let g_j $(j = 1,3,5, \cdots, n-1)$ be the face where one edge of $E(g_j)$ belongs to M_1. Let $M_7 := M_1 \oplus E(f_j)$. We can know that M_7 is a perfect matching alternating on $\partial(h_1)$, $\partial(h_2)$ and $\partial(h_3)$.
So h_1, $h_2$and h_3 can form a resonant pattern of $P_3 \times C_n$, we have proofed Lemma 3.3.

Lemma 3.4. *For any positive integer $k \geq 1$,$P_3 \times C_n (4 \leq n \leq 8)$ is k -resonant.*
Proof. According to the Lemmas 3.1-3.3, we show that $P_3 \times C_n$ is 1-resonant, 2-resonant and 3-resonant. No any four pairwise disjoint even faces can be found in $P_3 \times C_4$, so it is trivial, i.e., $P_3 \times C_4$ is maximally resonant. It is easy to prove that $P_3 \times C_6$ is 4-resonant and $P_3 \times C_8$ is 5-resonant. We also know that any five pairwise disjoint even faces in $P_3 \times C_6$ cannot be found and there are no any six pairwise disjoint even faces in $P_3 \times C_8$. Hence $P_3 \times C_n (4 \leq n \leq 8)$ is k -resonant for any positive integer $k \geq 1$.

Lemma 3.5. *For any positive integer $k \geq 4$, $P_3 \times C_n$ $(n \geq 10)$ is not k -resonant.*
Proof. Let h_1, h_2,h_3 and h_4 be the four pairwise disjoint quadrilateral faces in $P_3 \times C_n$ as shown in Figure 3. Then $P_3 \times C_n - \{h_1, h_2, h_3, h_4\}$ consists of an odd component of seven vertices(see Figure 3, the seven black vertices), that is, $P_3 \times C_n$-$\{h_1, h_2, h_3, h_4\}$ does not have a perfect matching. So $P_3 \times C_n$ is not 4-resonant, then it is also not k -resonant ($k \geq 4$).

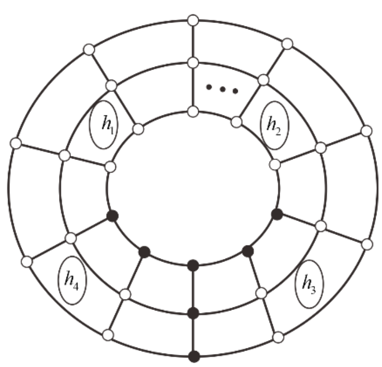


Fig. 3 The illustration for the proof of Lemma 3.5.

From the above proofing process, and combining with Lemmas 3.4-3.5, we can get the following direct result.
Corollary 3.6. *The graph $P_3 \times C_n$ is maximally resonant if and only if it is 4-resonant.*

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