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ORIGINAL PAPER

On k-resonance of grid graphs on the plane, torus and cylinder

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Abstract Grid graphs on the plane, torus and cylinder are finite 2-connected bipartite graphs embedded on the plane, torus and cylinder, respectively, whose every interior face is bounded by a quadrangle. Let k be a positive integer, a grid graph is k-resonant if the deletion of any $i \leq k$ vertex-disjoint quadrangles from G results in a graph either having a perfect matching or being empty. If G is k-resonant for any integer $k \geq 1$, then it is called maximally resonant. In this study, we provide a complete characterization for the k-resonance of grid graphs $P_m \times P_n$ on plane, $C_m \times C_n$ on torus and $P_m \times C_n$ on cylinder.

Keywords Grid graphs · k-Resonant · Maximally resonant

Mathematics Subject Classification 05C70, 05C90

1 Introduction

The concept of resonance originates from the conjugated circuits method which was early found in [29] and [8,9] and Clar's aromatic sextet theory [4] and Randić's conjugated circuit model [21–24]. Then Klein [12] clarified the connection of Clar's aromatic sextet theory with the conjugated circuits method. In mathematics [19], a conjugated circuit is named an alternating cycle. A matching (resp. perfect matching)

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of a graph is a set of its edges such that every vertex of the graph is incident with at most (resp. exactly) one edge in this set. For a graph G with a matching M, an M-alternating cycle is a cycle of which the edges appear alternately in and out of M.

The k-resonance of plane molecular graphs have been investigated extensively [6,13,15,17,32,35]. In the investigation of the resonance of some molecular graphs, it was found that the k-resonance of the molecular graphs indicates the stability of the corresponding moleculars a great deal. On the other hand, the k-resonance of graphs seems relating to the study of matchings problems. Besides the plane molecular graphs, graphs on sphere, cylinder, torus and Klein-bottle were also studied extensively [16,26,27,30,31]. We focus on the k-resonance of grid graphs on plane, torus and cylinder in this study.

A plane grid graph is a finite plane 2-connected bipartite graph whose every interior face is bounded by a quadrangle. It is also called polyomino graphs [1], square-cell configurations [7] or chess-boards [5]. Polyomino graphs have useful applications in statistical physics and in modeling problems of surface chemistry (please refer to ref. [7] and the references therein). They are also modelings of many interesting combinatorial subjects, such as hypergraphs [1], domination problem [5], rook polynomials [20], etc. In fact, problems based on perfect matchings was extensively studied on fragments of the square-planar net [2,10,14,25,34]. Also, Kivelson developed the conjugated circuits method for the polyomino graphs [11].

A toroidal grid graph (a grid graph on the surface torus) is the product $C_m \times C_n$ embedded on the torus such that each face is bounded by a quadrangle. A grid graph on the cylinder is a grid graph embedded on the cylinder such that each face, except the two infinite open ends, is bounded by a quadrangle. Let k be a positive integer, a plane grid graph or a toroidal grid graph or a grid graph on cylinder G is k-resonant if the deletion of any i $(\leq k)$ vertex-disjoint quadrangles from G results in a graph either having perfect matchings or being empty.

If G is k-resonant for any integer $k \geq 1$, then it is called maximally resonant. In the paper [17], all maximally resonant plane grid graphs were characterized. In fact, the least integer k such that a k-resonant graph is maximally resonant was determined for all the considered molecular graphs, such as benzenoid systems [35], coronoid systems [3], open-end nanotubes [31], toroidal polyhexes [26,33], Klein-bottle polyhexes [27], fullerene graphs [30], B-N fullerene graphs [32] and other graphs [18,28].

In this paper, we provide a complete characterization for the k-resonance of grid graphs $P_m \times P_n$ on plane, $C_m \times C_n$ on torus and $P_m \times C_n$ on cylinder. As plane grid graphs, the least integer k such that a k-resonant grid graph on torus or cylinder is maximally resonant is 4.

A k-resonant grid graph should have even vertices. Hence in the grid graphs $P_m \times P_n$, $C_m \times C_n$ and $P_m \times C_n$ considered here, at least one of m and n is even.

2 k-Resonance of plane grid graphs $P_m \times P_n$

Note that a graph $P_m \times P_n$ $(m, n \geqslant 2,\ n \bmod 2 = 0)$ has perfect matchings. Then the k-resonance of plane grid graphs $P_m \times P_n$ $(m, n \geqslant 2,\ n \bmod 2 = 0)$ can be obtained by the following facts.

Fig. 1 $P_3 \times P_n$, where $n \geq 6$

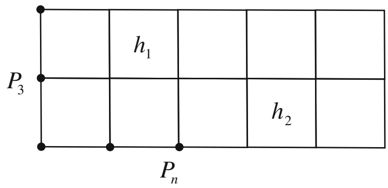
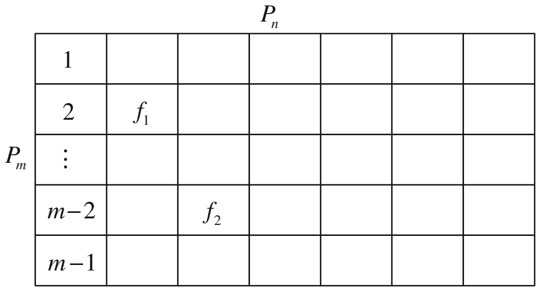


Fig. 2 $P_m \times P_n$, where $m \geq 5,\ n \geq 6$



Lemma 2.1 *$P_m \times P_n$ $(m, n \geqslant 2,\ n \bmod 2 = 0)$ is 1-resonant.*

Proof Let f_1 be an arbitrary square of $P_m \times P_n$. Then it belongs to a subgraph isomorphic to $P_2 \times P_n$, which is k-resonant $(k \geqslant 1)$ [17]. The leaving graph has perfect matchings. Hence $P_m \times P_n$ is 1-resonant. □

Lemma 2.2 *$P_m \times P_n$ $(m, n \geqslant 2,\ n \bmod 2 = 0)$ is not 2-resonant if and only if $m = 3$ and $n \geq 6$.*

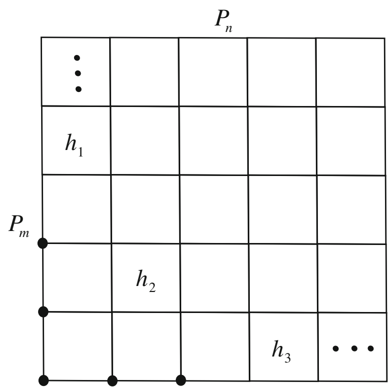
Proof $P_2 \times P_n$ and $P_4 \times P_n$ are maximally resonant [17]. Now we should only consider the cases of $P_3 \times P_n$ $(n \geq 6)$ and $P_m \times P_n$ $(m \geq 5, n \geq 6)$. Clearly, by Fig. 1, one can see that $P_3 \times P_n$ $(n \geq 6)$ is not 2-resonance since $(P_3 \times P_n) - h_1 - h_2$ leaves an odd component with five vertices.

Now we consider $H \cong P_m \times P_n$ $(m \geq 5,\ n \geq 6)$ with $m - 1$ rows of squares. Let f_1 and f_2 be any two disjoint quadrangles in H. Suppose that $r_1,\ r_2$ are the rows that $f_1,\ f_2$ lie, respectively (see Fig. 2). If $|r_1 - r_2| \leq 1$, consider a subgraph H' of H isomorphic to $P_4 \times P_n$, which contains both f_1 and f_2. Certainly, $H' - f_1 - f_2$ has a perfect matching. On the other hand, $H - H'$ has perfect matchings, since its every component is isomorphic to $P_k \times P_n$ with $k \geqslant 1$ and n even. Hence $H - f_1 - f_2$ has perfect matchings. If $|r_1 - r_2| \geqslant 2$, then f_1 and f_2 are contained in two disjoint subgraphs of H isomorphic to $P_2 \times P_n$, which are k-resonant $(k \geqslant 1)$. And the leaving graph has perfect matchings. Hence $H \cong P_m \times P_n$ $(m \geq 5,\ n \geq 6)$ is 2-resonant. □

Lemma 2.3 *$P_n \times P_m$ $(m, n \geqslant 2)$ is 3-resonant if and only if it is isomorphic to $P_2 \times P_m$ $(m \geq 2)$ or $P_4 \times P_m$ $(m \geq 3)$.*

Proof $P_2 \times P_m$ and $P_4 \times P_m$ are 3-resonant [17]. By lemma 2.2, we know that $P_3 \times P_m$ $(m \geq 6)$ is not 2-resonant. Hence it is not 3-resonant. By Fig. 3, it can be seen that $P_m \times P_n$ $(m, n \geq 5)$ is not 3-resonant, since by deleting $h_1,\ h_2$ and h_3 there will be an odd component with five vertices. □

Fig. 3 $P_m \times P_n$, where $m,\ n \geq 5$



By Theorems 2.1 in [17], we know that $P_2 \times P_n$ and $P_4 \times P_m$ $(m, n \geq 2)$ is k-resonant for any integer $k \geqslant 1$ and $P_3 \times P_m$ $(m \geq 6)$, $P_m \times P_n$ $(m, n \geq 5)$ are not k-resonant for $k \geqslant 4$. Together with Lemmas 2.1 and 2.2, k-resonance of plane grid graphs $P_m \times P_n$ $(m, n \geq 2)$ is obtained.

Theorem 2.4 *The k-resonance of plane grid graphs $P_m \times P_n$ $(m, n \geqslant 2$ and at least one of them is even) is given in the following table.*

	$P_2 \times P_n,\ P_4 \times P_n$	$P_3 \times P_n$ $(n \geq 6)$	$P_m \times P_n$ $(m, n \geq 5)$
1-Resonant	Yes	Yes	Yes
2-Resonant	Yes	No	Yes
3-Resonant	Yes	No	No
$\geqslant$ 4-Resonant	Yes	No	No

3 *k*-Resonance of grid graphs on torus

A toroidal grid graph $C_m \times C_n$ embedded on the torus such that each face is bounded a quadrangle can be also obtained from $P_m \times P_n$ by gluing the pendent half edges with the same labels into one as shown in Fig. 4.

On the other hand, note that for a set F of disjoint faces of a graph G, if $G - F$ has a spanning subgraph with a perfect matching, then $G - F$ has a perfect matching.

Lemma 3.1 *A toroidal grid graph $C_m \times C_n$ $(m, n \geq 5)$ is not k-resonant for any integer $k \geqslant 4$.*

Proof Let h_1, h_2, h_3 and h_4 be the four vertex-disjoint quadrangles as shown in Fig. 5. Then $C_m \times C_n - h_1 - h_2 - h_3 - h_4$ has an isolated vertex v when $m, n \geq 5$. So it is not k-resonant for any integer $k \geqslant 4$. □

Lemma 3.2 *A toroidal grid graph $C_4 \times C_m$ $(m \geq 2)$ is k-resonant $(k \geqslant 1)$.*

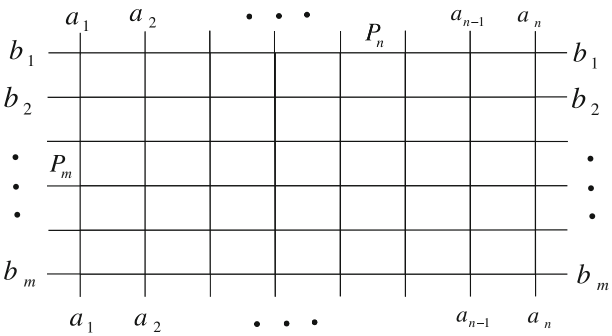
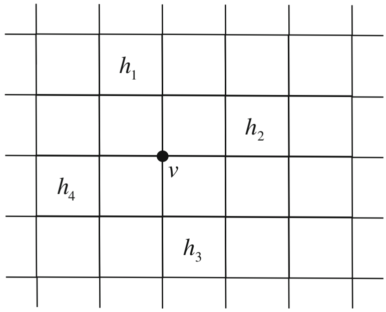


Fig. 4 A grid graph $C_m \times C_n$ on torus

Fig. 5 $C_5 \times C_6$ on torus



Proof Let F be any set of vertex-disjoint quadrangles of $C_4 \times C_m$ and H denote the subgraph of $C_4 \times C_m$ induced by all the columns of quadrangles containing at least one element of F. Then write H'=$C_4 \times C_m - H$. Clearly, every component of H or H' is isomorphic to a $C_4 \times P_{m_i}$ for some $m_i \geq 1$. H' has perfect matchings. We shall show in what follows that for any component H_1 of H, either $H_1 - F$ is empty or it has perfect matchings and so the lemma follows.

If H_1 consists of one column, then $H_1 - F$ is empty or is a quadrangle with perfect matchings. Now consider the case when H_1 consists of at least two columns. It is not difficult to see that each column of H_1 contains a unique quadrangle of F and that all these quadrangles must lie in two separating rows alternatively as in Fig. 6. No matter whether H_1 has an odd or even number of columns, $H_1 - F$ consists of two disjoint edges e' and e'' as is illustrated in Fig. 6. These two edges enter into a perfect matching of $H_1 - F$. □

Lemma 3.3 *A toroidal grid graph* $C_3 \times C_m$ $(m \geq 10)$ *is not k-resonant for any integer* $k \geqslant 4$.

Proof Let h_1, h_2, h_3 and h_4 be the four vertex-disjoint quadrangles of $C_3 \times C_m$ $(m \geq 10)$ as in Fig. 7. Then $C_3 \times C_m - h_1 - h_2 - h_3 - h_4$ contains a component with seven vertices, so it has no perfect matchings. □

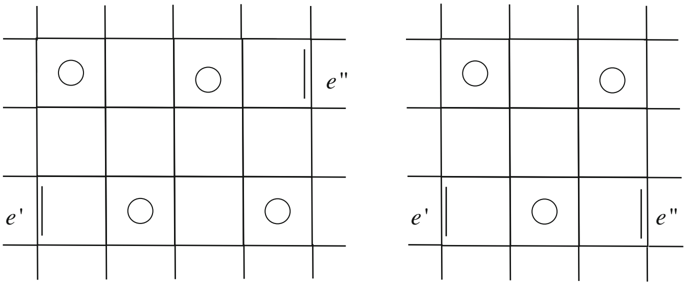


Fig. 6 $H_1 - F$ has a perfect matching $\{e', e''\}$, where the quadrangles inserted cycles belong to F

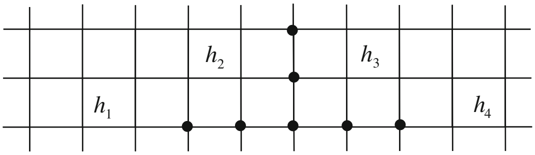


Fig. 7 A toroidal grid graph $C_3 \times C_m$ with $m \geq 10$

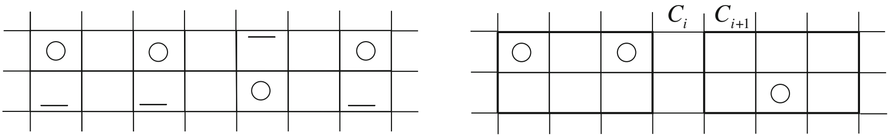


Fig. 8 An illustration for the proof of Lemma 3.4

Lemma 3.4 *A toroidal grid graph* $C_3 \times C_m$ $(m = 6, 8)$ *is* k*-resonant* $(k \geqslant 1)$.

Proof Let F be any set of vertex-disjoint quadrangles of $C_3 \times C_m$. Firstly, suppose $m = 8$. $C_3 \times C_8$ contains eight columns consisting of three quadrangles (illustrated in Fig. 8). Since the quadrangles in two adjacent columns are pairwise adjacent, there are at most four quadrangles in F. If there are exactly four quadrangles in F, then $C_3 \times C_8 - F$ has a perfect matching as shown in Fig. 8(1). If there are two adjacent columns containing no quadrangle of F. Then $C_3 \times C_8$ can always be divided into two subgraphs containing all the quadrangles in F which are isomorphic to $P_3 \times P_4$ and thus are k-resonant $(k \geqslant 1)$. Hence $C_3 \times C_8 - F$ has a perfect matching (refer to Fig. 8(2)).

Secondly, we suppose that $m = 6$. $C_3 \times C_6$ consists of six columns of quadrangles. By the similar argument as for $m = 8$, there are at most three quadrangles in F. Similarly, if there are exactly three quadrangles in F, then $C_3 \times C_6 - F$ has a perfect matching. If there are two adjacent columns containing no quadrangle of F. Then divide $C_3 \times C_6$ into a $P_3 \times P_4$ and a $P_3 \times P_2$, which are k-resonant $(k \geqslant 1)$, containing all the quadrangles in F. Hence $C_3 \times C_6 - F$ has a perfect matching.

In all, $C_3 \times C_m$ $(m = 6, 8)$ is k-resonant $(k \geqslant 1)$. □

Lemma 3.5 *Toroidal grid graphs* $C_m \times C_n$ $(m, n \geq 5)$ *and* $C_3 \times C_m$ $(m \geq 10)$ *are* 3*-resonant.*

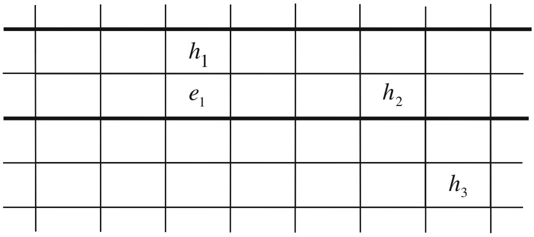


Fig. 9 An illustration for the 3-resonance of $C_m \times C_n$ $(m, n \geq 5)$

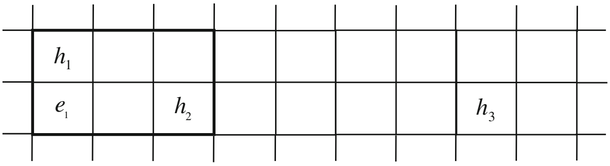


Fig. 10 An illustration for the 3-resonance of $C_3 \times C_m$ $(m \geq 10)$

Proof Firstly, let F be any set of three disjoint quadrangles $\{h_1, h_2, h_3\}$ of $C_m \times C_n$ $(m, n \geq 5)$ which contain m rows and n columns. Suppose n is even. Assume that h_1, h_2 and h_3 lie in the r_1th, r_2th and r_3th rows, respectively.

If $|r_i - r_j| \neq 1$ for any $i, j \in \{1, 2, 3\}$, since $P_2 \times P_n$ is k-resonant $(k \geq 1)$, then both $\cup_{i=1}^{3} r_i - h_1 - h_2 - h_3$ and $C_m \times C_n - (\cup_{i=1}^{3} r_i)$ have perfect matchings.

If h_1, h_2, h_3 are contained in a subgraph $H' \cong P_4 \times C_n$ consisting of three consequent rows, then H' has a spanning subgraph $P_4 \times P_n$ containing h_1, h_2, h_3, which is k-resonant $(k \geqslant 1)$. Hence $H' - F$ and thus $C_m \times C_n - F$ have perfect matchings.

Otherwise, we assume that exactly two of r_1, r_2 and r_3, say r_1 and r_2, satisfy that $|r_1 - r_2| = 1$ and $|r_3 - r_i| > 1$ for $i = 1, 2$. Let $H' = r_1 \cup r_2$ $(\cong P_3 \times C_n)$. See Fig. 9. Note that $H' - h_1 - e$ is isomorphic to $P_3 \times P_{n-2}$ which is 1-resonant by Theorem 2.4. Hence $H' - h_1 - h_2$ has perfect matchings. $C_m \times C_n - H' - h_3$ also has a perfect matching. Thus $C_m \times C_n - F$ has perfect matchings.

Then consider $C_3 \times C_m$ $(m \geq 10)$. $F = \{h_1, h_2, h_3\}$ is an arbitrary set of quadrangles of $C_3 \times C_m$, in which any two can not lie in two consequent columns. Refer to Fig. 10. Let c_1, c_2, c_3 be the indices of the columns h_1, h_2, h_3 lie, respectively. If two of them, say c_1 and c_2, satisfying $|c_1 - c_2| = 2$. Let H' be the subgraph isomorphic to $P_3 \times P_4$ containing h_1, h_2, which is 2-resonant. Moreover, $C_3 \times C_m - H'$ is 1-resonant. Hence $C_3 \times C_m - F$ has perfect matchings. If $|c_i - c_j| \geq 3$ for any $i \neq j \in \{1, 2, 3\}$, then $H' = C_3 \times C_m - c_1 \cong C_3 \times P_{m-2}$ where $m - 2$ is even. Since $|c_i - c_j| \geq 3$ for any $i \neq j \in \{1, 2, 3\}$, we can divide H' into two subgraphs isomorphic to $C_3 \times P_s$ and $C_3 \times P_t$, containing h_2 and h_3, respectively, such that s and t are even and $s + t = m - 2$. c_1, $C_3 \times P_s$ and $C_3 \times P_t$ each has a spanning subgraph isomorphic to $P_3 \times P_l$ for $l = 2, s, t$, respectively. By Theorem 2.4, they each has a perfect matching after deleting h_1, h_2 and h_3, respectively. The union of these perfect matchings forms one of $C_3 \times C_m - F$.

If F contains less than three squares, it can be treated as the special case for the above. In all, $C_m \times C_n$ $(m, n \geq 5)$ and $C_3 \times C_m$ $(m \geq 10)$ are 3-resonant. □

By the above lemmas, the resonance of grid graphs on torus is obtained.

Theorem 3.6 *The k-resonance of grid graphs $C_m \times C_n$ ($m, n \geqslant 3$ and at least one of them is even) on torus is given in the following table.*

	1, 2, 3-Resonant	$\geqslant$ 4-Resonant
$C_3 \times C_m (m = 6, 8)$	Yes	Yes
$C_3 \times C_m (m \geq 10)$	Yes	No
$C_4 \times C_m (m \geq 3)$	Yes	Yes
$C_m \times C_n (m, n \geq 5)$	Yes	No

The following corollary is a direct consequence of Theorem 3.6.

Corollary 3.7 *Grid graphs on torus are maximally resonant if and only if they are* 4*-resonant.*

4 k-Resonance of grid graphs on cylinder

In this part, k-resonance of grid graphs on cylinder $P_m \times C_n$ ($m \geqslant 2$, $n \geqslant 3$ and at least one of them is even) are discussed.

$P_m \times C_n$ can be obtained from $C_m \times C_n$ by deleting a set of parallel edges (illustrated in Fig. 11 (1)). In part of the discussion of the k-resonance of $C_m \times C_n$, the existence of these edges do not alter the results. In fact, $P_3 \times C_n$ $(n = 6, 8)$, $P_3 \times C_n$ $(n \geq 10)$ and $P_4 \times C_n$ on cylinder have the same k-resonance and similar proofs as $C_3 \times C_n (n = 6, 8)$, $C_3 \times C_n$ $(n \geq 10)$ and $C_4 \times C_n$ on torus. On the other hand, for an arbitrary non-empty set F of disjoint quadrangles, each component of $P_2 \times C_n - F$ isomorphic to a plane grid graph $P_2 \times P_n$ and hence has perfect matchings. So $P_2 \times C_n$ is k-resonant $(k \geqslant 1)$. For $P_3 \times C_4$, let F be an arbitrary set of disjoint quadrangles. Then at most one quadrangle in F is contained in two adjacent columns. Hence there is a subgraph $P_3 \times P_4 - F$ with a perfect matching which is also one of $P_3 \times C_4 - F$ (illustrated in Fig. 11(1)).

Hence we need only discuss the k-resonance of $P_5 \times C_n$ $(n \geqslant 4)$ on cylinder. Consider $P_5 \times C_4$ first. See Fig. 11(2). Let F be an arbitrary set of disjoint quadrangles. If there is a row of quadrangles does not contain any element of F, then there is a subgraph $(P_m \times C_4) \cup (P_n \times C_4) - F$ $(m, n < 5, m + n = 5)$ with a perfect matching which is also one of $P_5 \times C_4 - F$. Otherwise, each row contains a quadrangle of F. That is just the case illustrated in Fig. 11(2) and $P_5 \times C_4 - F$ has just two independent edges. Thus $P_5 \times C_4$ is k-resonant for any positive integer k.

Then consider the k-resonance of $P_5 \times C_n$ $(n \geqslant 6)$. Similar to the case of $C_m \times C_n$ $(m, n \geq 5)$, it is not 4-resonant. Then let F be an arbitrary set of no more than three disjoint quadrangles. If all the quadrangles in F lie in three consequent columns which form a subgraph $P_5 \times P_4$, then $P_5 \times P_4 - F$ together with $P_5 \times P_{n-4}$ have perfect matchings. Otherwise, $P_5 \times C_n$ can be divided into two subgraphs $P_5 \times P_2$ and $P_5 \times P_{n-2}$ $(n - 2 \geqslant 4)$ containing all the quadrangles of F (illustrated in the

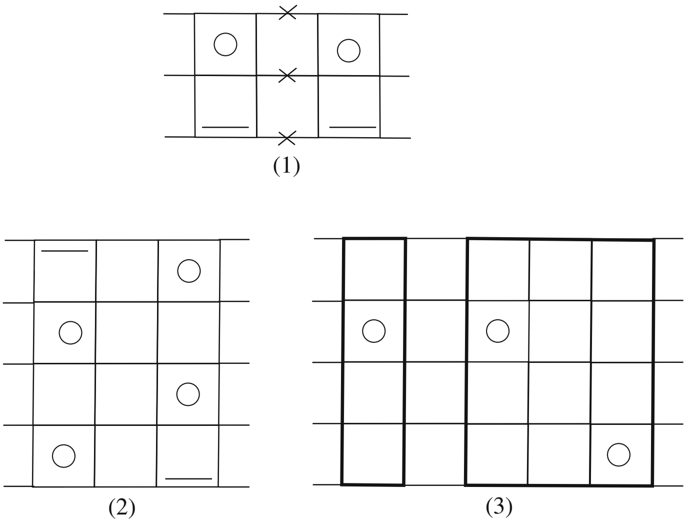


Fig. 11 An illustration for the proof of Theorem 4.1

Fig. 11(3)). By Theorem 2.4, these two subgraphs are all 2-resonant. Hence $(P_5 \times P_2) \cup (P_5 \times P_{n-2}) - F$ has perfect matchings. Hence, $P_5 \times C_n$ is 3-resonant.

In all, the k-resonance of grid graphs on cylinder can be characterized as follows.

Theorem 4.1 *The k-resonance of grid graphs $P_m \times C_n$ ($m \geqslant 2$, $n \geqslant 3$ and at least one of them is even) on cylinder is given in the following table.*

	$P_2 \times C_n,\ P_4 \times C_n,\ P_3 \times C_n (n \leqslant 8),\ P_5 \times C_4$	$P_3 \times C_n\ (n \geq 10),\ P_m \times C_n\ (m, n \geqslant 5)$
1, 2, 3-Resonant	Yes	Yes
$\geqslant$ 4-Resonant	Yes	No

Corollary 4.2 *A grid graph on cylinder is maximally resonant if and only if it is* 4*-resonant.*

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