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Tight upper bound on the maximum anti-forcing numbers of graphs *

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Let G be a simple graph with a perfect matching. Deng and Zhang showed that the maximum anti-forcing number of G is no more than the cyclomatic number. In this paper, we get a novel upper bound on the maximum anti-forcing number of G and investigate the extremal graphs. If G has a perfect matching M whose anti-forcing number attains this upper bound, then we say G is an extremal graph and M is a *nice* perfect matching. We obtain an equivalent condition for the nice perfect matchings of G and establish a one-to-one correspondence between the nice perfect matchings and the edge-involutions of G, which are the automorphisms α of order two such that v and $\alpha(v)$ are adjacent for every vertex v. We demonstrate that all extremal graphs can be constructed from K_2 by implementing two expansion operations, and G is extremal if and only if one factor in a Cartesian decomposition of G is extremal. As examples, we have that all perfect matchings of the complete graph K_{2n} and the complete bipartite graph $K_{n,n}$ are nice. Also we show that the hypercube Q_n, the folded hypercube FQ_n ($n \geq 4$) and the enhanced hypercube $Q_{n,k}$ ($0 \leq k \leq n-4$) have exactly n, $n+1$ and $n+1$ nice perfect matchings respectively.

Keywords: Maximum anti-forcing number, Perfect matching, Edge-involution, Cartesian product, Hypercube, Folded hypercube

1 Introduction

Let G be a finite and simple graph with vertex set $V(G)$ and edge set $E(G)$. We denote the number of vertices of G by $v(G)$, and the number of edges by $e(G)$. For $S \subseteq E(G)$, $G - S$ denotes the subgraph of G with vertex set $V(G)$ and edge set $E(G) \setminus S$. A *perfect matching* of G is a set M of edges of G such that each vertex is incident with exactly one edge of M. A perfect matching of a graph coincides with a Kekulé structure in organic chemistry.

The *innate degree of freedom* of a Kekulé structure was firstly proposed by Klein and Randić (1987) in the study of resonance structure of a given molecule in chemistry. In general, Harary et al. (1991) called the innate degree of freedom as the forcing number of a perfect matching of a graph. The *forcing number* of a perfect matching M of a graph G is the smallest cardinality of subsets of M not contained in other perfect matchings of G. The *minimum forcing number* and *maximum forcing number* of G are the minimum and maximum values of forcing numbers over all perfect matchings of G, respectively. Computing the minimum forcing number of a bipartite graph with the maximum degree three is an NP-complete problem, see Afshani et al. (2004). As we know, the forcing numbers of perfect matchings have been studied for many specific graphs, see Adams et al. (2004); Che and Cheng (2011); Jiang and Zhang (2011, 2016); Lam and Pachter (2003); Pachter and Kim (1998); Shi and Zhang (2016); Zhang and Deng (2015); Zhang et al. (2010, 2015); Zhao and Zhang (2016).

Vukičević and Trinajstić (2007) defined the anti-forcing number of a graph as the smallest number of edges whose removal results in a subgraph with a unique perfect matching. Recently Lei et al. (2016) introduced the anti-forcing

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number of a single perfect matching M of a graph G as follows. A subset $S \subseteq E(G) \setminus M$ is called an *anti-forcing set of* M if $G - S$ has a unique perfect matching M. The *anti-forcing number* of a perfect matching M is the smallest cardinality of anti-forcing sets of M, denoted by $af(G, M)$. Obviously, the anti-forcing number of G is the minimum value of the anti-forcing numbers over all perfect matchings of G. The *maximum anti-forcing number* of G is the maximum value of the anti-forcing numbers over all perfect matchings of G, denoted by $Af(G)$. It is an NP-complete problem to determine the anti-forcing number of a perfect matching of a bipartite graph with the maximum degree four, see Deng and Zhang (2017a). For some progress on this topic, see refs. Vukičević and Trinajstić (2008); Che and Cheng (2011); Deng (2007, 2008); Deng and Zhang (2017a,b,c); Lei et al. (2016); Li (1997); Shi and Zhang (2016); Yang et al. (2015b); Zhang et al. (2011).

For a bipartite graph G, Riddle (2002) proposed the trailing vertex method to get a lower bound on the forcing numbers of perfect matchings of G. Applying this lower bound, the minimum forcing number of some graphs have been obtained. In particular, Riddle (2002) showed that the minimum forcing number of Q_n is 2^{n-2} if n is even. However, for odd n, determining the minimum forcing number of Q_n is still an open problem. For the maximum forcing number of Q_n, Alon proved that for sufficiently large n this number is near to the total number of edges in a perfect matching of Q_n (see Riddle (2002)), but its specific value is still unknown. Afterwards, Adams et al. (2004) generalized Alon's result to a k-regular bipartite graph and for a hexagonal system, a polyomino graph or a $(4, 6)$-fullerene, Xu et al. (2013); Zhang and Zhou (2016); Shi et al. (2017) showed that its maximum forcing number equals its Clar number, respectivey. For a graph G with a perfect matching, Lei et al. (2016) connected the anti-forcing number and forcing number of a perfect matching of G, and showed that the maximum forcing number of G is no more than $Af(G)$. Particularly, for a hexagonal system H, Lei et al. (2016) showed that $Af(H)$ equals the Fries number (see Fries (1927)) of H. Recently, see Shi et al. (2017), we also showed that for a $(4, 6)$-fullerene graph G, $Af(G)$ equals the Fries number of G.

The *cyclomatic number* of a connected graph G is defined as $r(G) = e(G) - v(G) + 1$. Deng and Zhang (2017c) recently obtained that the maximum anti-forcing number of a graph is no more than the cyclomatic number.

Theorem 1.1 (Deng and Zhang (2017c)). *For a connected graph G with a perfect matching, $Af(G) \leq r(G)$.*

Deng and Zhang (2017c) further showed that the connected graphs with the maximum anti-forcing number attaining the cyclomatic number are a class of plane bipartite graphs. In this paper, we obtain a novel upper bound on the maximum anti-forcing numbers of a graph G as follows.

Theorem 1.2. *Let G be any simple graph with a perfect matching. Then for any perfect matching M of G,*

$$af(G, M) \leq Af(G) \leq \frac{2e(G) - v(G)}{4}. \tag{1}$$

In fact, this upper bound is also tight. By a simple comparison we immediately get that the upper bound is better than the previous upper bound $r(G)$ when $3v(G) < 2e(G) + 4$. In next sections we shall see that many non-planar graphs can attain this upper bound, such as complete graphs K_{2n}, complete bipartite graphs $K_{n,n}$, hypercubes Q_n, etc.

We say that a graph G is *extremal* if the maximum anti-forcing number $Af(G)$ attains the upper bound in Theorem 1.2, that is, G has a perfect matching M such that both equalities in (1) hold. Such M is said to be a *nice* perfect matching of G. In Section 2, we give a proof to Theorem 1.2, obtain an equivalent condition for the nice perfect matchings of G, and establish a one-to-one correspondence between the nice perfect matchings of G and the edge-involutions of G. In Section 3, we provide a construction of all extremal graphs, which can be obtained from K_2 by implementing two expansion operations, and show that such a graph is an elementary graph (each edge belongs to some perfect matching). In Section 4, we investigate Cartesian decompositions of an extremal graph. Let $\Phi^*(G)$ denote the number of nice perfect matchings of a graph G. For a Cartesian decomposition $G = G_1 \square \cdots \square G_k$, we obtain $\Phi^*(G) = \sum_{i=1}^{k} \Phi^*(G_i)$. This implies that a graph G is extremal if and only if in a Cartesian decomposition of G one factor is an extremal graph. As applications we show that three cube-like graphs, the hypercubes Q_n, the folded hypercubes FQ_n and the enhanced hypercubes $Q_{n,k}$ are extremal. In particular, in the final section we prove that Q_n has exactly n nice perfect matchings and $Af(Q_n) = (n-1)2^{n-2}$, FQ_n ($n \geq 4$) has exactly $n+1$ nice perfect matchings and $Af(FQ_n) = n2^{n-2}$, and for $0 \leq k \leq n-4$, $Q_{n,k}$ has $n+1$ nice perfect matchings and $Af(Q_{n,k}) = n2^{n-2}$. We also show that FQ_n is a prime graph under the Cartesian decomposition.

2 Upper bound and nice perfect matchings

2.1 The proof of Theorem 1.2

Let G be a graph with a perfect matching M. A cycle of G is called an *M-alternating cycle* if its edges appear alternately in M and $E(G) \setminus M$. If G has not M-alternating cycles, then M is a unique perfect matching since the symmetric difference of two distinct perfect matchings is the union of some M-alternating cycles. So M is a unique perfect matching of G if and only if G has no M-alternating cycles. Lei et al. obtained the following characterization for an anti-forcing set of a perfect matching.

Lemma 2.1 (Lei et al. (2016))**.** *A set $S \subseteq E(G) \setminus M$ is an anti-forcing set of M if and only if S contains at least one edge of every M-alternating cycle of G.*

A *compatible M-alternating set* of G is a set of M-alternating cycles such that any two members are either disjoint or intersect only at edges in M. Let $c'(M)$ denote the maximum cardinality of compatible M-alternating sets of G. By Lemma 2.1, the authors obtained the following theorem.

Theorem 2.2 (Lei et al. (2016))**.** *For any perfect matching M of G, we have $af(G, M) \geq c'(M)$.*

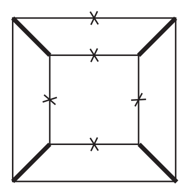

Fig. 1. A perfect matching M of Q_3 (thick edges) and an anti-forcing set S of M ("$\times$").

In general, for any anti-forcing set S of a perfect matching M of G, the edge set $E(G) \setminus (M \cup S)$ may not be an anti-forcing set of M (see Fig. 1). However, for any minimal anti-forcing set in a bipartite graph, we have Lemma 2.3. Here an anti-forcing set is *minimal* if its any proper subset is not an anti-forcing set. Recall that for an edge subset E of a graph G, $G[E]$ is an edge induced subgraph of G with vertex set being the vertices incident with some edge of E and edge set being E.

Lemma 2.3. *Let G be a simple bipartite graph with a perfect matching M, and S a minimal anti-forcing set of M. Then $S^* := E(G) \setminus (M \cup S)$ is an anti-forcing set of M.*

Proof: Clearly, M is a perfect matching of $G[M \cup S]$. It is sufficient to show that $G[M \cup S]$ has no M-alternating cycle by Lemma 2.1. By the contrary, we suppose that C is an M-alternating cycle of $G[M \cup S]$. Then the edges of C appear alternately in M and S. Let $E(C) \cap S = \{e_1, e_2, \ldots, e_k\}$ (see Fig. 2 for $k = 3$). Since S is a minimal anti-forcing set of M in G, the subgraph $G - (S \setminus \{e_i\})$ has an M-alternating cycle C_i such that $E(C_i) \cap S = \{e_i\}$, $i = 1, 2, \ldots, k$. Then $G - S$ has a closed M-alternating walk $W = G[\bigcup_{i=1}^{k} (E(C_i) \setminus \{e_i\})$ as depicted in Fig. 2. Since G is a bipartite graph, W contains an M-alternating cycle C'. So $G - S$ has an M-alternating cycle C'. This implies that S is not an anti-forcing set of M, a contradiction. So S^* is an anti-forcing set of M. $\square$

Let X and Y be two vertex subsets of a graph G. We denote by $E(X, Y)$ the set of edges of G with one end in X and the other end in Y. The subgraph induced by $E(X, Y)$, for convenience, is denoted by $G(X, Y)$. For a vertex

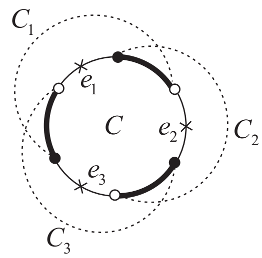

Fig. 2. Example of $k = 3$.

subset X of G, $G[X]$ is a vertex induced subgraph of G with vertex set X and any two vertices are adjacent if and only if they are adjacent in G. The edge set of $G[X]$ is denoted by $E(X)$.

Proof of Theorem 1.2. For any perfect matching M of G, let A be a vertex subset of G consisting of one end vertex for each edge of M, $\bar{A} := V(G) \setminus A$. Then $G' := G(A, \bar{A})$ is a bipartite graph and M is a perfect matching of G'. Let S be a minimum anti-forcing set of M in G'. By Lemma 2.3, $S^* := E(G') \setminus (M \cup S)$ is an anti-forcing set of M in G'. So both $S \cup E(A)$ and $S^* \cup E(\bar{A})$ are anti-forcing sets of M in G. Hence

$$2af(G, M) \leq |S \cup E(A)| + |S^* \cup E(\bar{A})| = e(G) - |M| = e(G) - \frac{v(G)}{2}.$$

Then $af(G, M) \leq \frac{2e(G)-v(G)}{4}$. By the arbitrariness of M, $Af(G) \leq \frac{2e(G)-v(G)}{4}$. □

For any perfect matching M of a complete bipartite graph $K_{m,m}$ ($m \geq 2$), any two edges of M belong to an M-alternating 4-cycle. Since any two distinct M-alternating 4-cycles are compatible, $c'(M) \geq \binom{m}{2} = \frac{m^2-m}{2}$. By Theorems 2.2 and 1.2, we obtain $af(K_{m,m}, M) = \frac{m^2-m}{2} = Af(K_{m,m})$. Let M' be any perfect matching of a complete graph K_{2n}. For any two edges e_1 and e_2 of M', there are two distinct M'-alternating 4-cycles each of which simultaneously contains edges e_1 and e_2. So $af(K_{2n}, M') \geq c'(M') \geq \binom{n}{2} \times 2 = n^2 - n$. By Theorem 1.2, we know that $af(K_{2n}, M') = Af(K_{2n}) = n^2 - n$. Hence every perfect matching of $K_{m,m}$ and K_{2n} is nice.

Recall that the *n-dimensional hypercube* Q_n is the graph with vertex set being the set of all 0-1 sequences of length n and two vertices are adjacent if and only if they differ in exactly one position. For $x \in \{0, 1\}$, set $\bar{x} := 1 - x$. The edge connecting the two vertices $x_1 \cdots x_{i-1}x_ix_{i+1} \cdots x_n$ and $x_1 \cdots x_{i-1}\bar{x}_ix_{i+1} \cdots x_n$ of Q_n is called an *i-edge* of Q_n. We denote by E_i the set of all the i-edges of Q_n, $i = 1, 2, \ldots, n$. In fact, E_i is a Θ_{Q_n}-class of Q_n. We can show the following result for Q_n.

Lemma 2.4. *Θ_{Q_n}-class E_i of Q_n is a nice perfect matching, that is,* $af(Q_n, E_i) = Af(Q_n) = (n-1)2^{n-2}$.

Proof: It is sufficient to discuss E_1. Clearly, E_1 is a perfect matching of Q_n. For vertices $x = x_1x_2 \cdots x_n$ and $y = \bar{x}_1x_2 \cdots x_n$, the edge $xy \in E_1$ belongs to $n-1$ E_1-alternating 4-cycles. Over all edges of E_1, since each E_1-alternating 4-cycle is counted twice, there are $\frac{(n-1)2^{n-1}}{2} = (n-1)2^{n-2}$ distinct E_1-alternating 4-cycles in Q_n. Since any two distinct E_1-alternating 4-cycles are compatible, $c'(E_1) \geq (n-1)2^{n-2}$. So $af(Q_n, E_1) \geq c'(E_1) \geq (n-1)2^{n-2}$ by Theorem 2.2. Since $Af(Q_n) \leq (n-1)2^{n-2}$ by Theorem 1.2, $af(Q_n, E_1) = Af(Q_n) = (n-1)2^{n-2}$. □

The above three examples show that the upper bound in Theorem 1.2 is tight.

2.2 Nice perfect matchings

In the following, we will characterize the nice perfect matchings of a graph. The set of neighbors of a vertex v in G is denoted by $N_G(v)$. The degree of a vertex v is the cardinality of $N_G(v)$, denoted by $d_G(v)$.

Theorem 2.5. *For any perfect matching M of a simple graph G, M is a nice perfect matching of G if and only if for any two edges $e_1 = xy$ and $e_2 = uv$ of M, $xu \in E(G)$ if and only if $yv \in E(G)$, and $xv \in E(G)$ if and only if $yu \in E(G)$.*

Proof: Here we only need to consider simple connected graphs. To show the sufficiency, we firstly estimate the value of $c'(M)$ for such perfect matching M of G. Let $c'_{wz}(M)$ be the number of M-alternating 4-cycles that contain edge wz. Since for any two edges $e_1 = xy$ and $e_2 = uv$ of M, $xu \in E(G)$ if and only if $yv \in E(G)$, and $xv \in E(G)$ if and only if $yu \in E(G)$, $c'_{wz}(M) = d_G(w) - 1 = d_G(z) - 1$ for any edge wz of M. Obviously, any two distinct M-alternating 4-cycles are compatible. Then

$$\begin{aligned} c'(M) &\geq \frac{\sum\limits_{wz\in M} c'_{wz}(M)}{2} \\ &= \frac{\sum\limits_{wz\in M} \frac{1}{2}[(d_G(w)-1)+(d_G(z)-1)]}{2} \\ &= \frac{\sum\limits_{w\in V(G)} \frac{1}{2}(d_G(w)-1)}{2} \\ &= \frac{e(G)-\frac{v(G)}{2}}{2}. \end{aligned} \tag{2}$$

By Theorems 1.2 and 2.2, $c'(M) \leq af(G, M) \leq Af(G) \leq \frac{2e(G)-v(G)}{4}$. So $af(G, M) = \frac{2e(G)-v(G)}{4}$, that is, M is a nice perfect matching of G.

Conversely, suppose that M is a nice perfect matching of G. Let A be a vertex subset of G consisting of one end vertex for each edge of M and $\bar{A} := V(G) \setminus A$. Then $(A, \bar{A})$ is a partition of $V(G)$. Given any bijection $\omega : M \to \{1, \ldots, |M|\}$, we extend weight function ω on M to the vertices of G: if $v \in V(G)$ is incident with $e \in M$, then $\omega(v) := \omega(e)$. This weight function ω gives a natural ordering of the vertices in A ($\bar{A}$). Clearly, if $e = xy \in M$, then $\omega(x) = \omega(y)$, otherwise, $\omega(x) \neq \omega(y)$. Set

$$E_A^\omega := \{xy \in E(G) : \omega(x) > \omega(y), x \in A \text{ and } y \in \bar{A}\},$$

$$E_{\bar{A}}^\omega := \{xy \in E(G) : \omega(x) < \omega(y), x \in A \text{ and } y \in \bar{A}\}.$$

Since $G - E_A^\omega \cup E(A)$ has a unique perfect matching M, $E_A^\omega \cup E(A)$ is an anti-forcing set of M in G. Similarly, $E_{\bar{A}}^\omega \cup E(\bar{A})$ is also an anti-forcing set of M in G. Since M is a nice perfect matching of G, $af(G, M) = \frac{2e(G)-v(G)}{4}$. So $|E_A^\omega \cup E(A)| \geq \frac{2e(G)-v(G)}{4}$, $|E_{\bar{A}}^\omega \cup E(\bar{A})| \geq \frac{2e(G)-v(G)}{4}$. Since $|E_A^\omega \cup E(A)| + |E_{\bar{A}}^\omega \cup E(\bar{A})| = e(G) - |M| = e(G) - \frac{v(G)}{2}$, $|E_A^\omega \cup E(A)| = |E_{\bar{A}}^\omega \cup E(\bar{A})| = \frac{2e(G)-v(G)}{4}$. Hence $E_A^\omega \cup E(A)$ is a minimum anti-forcing set of M in G.

Now we show that for any two edges $e_1 = xy$ and $e_2 = uv$ of M, $xu \in E(G)$ if and only if $yv \in E(G)$, and $xv \in E(G)$ if and only if $yu \in E(G)$. It is sufficient to show that $xv \in E(G)$ implies $yu \in E(G)$. Given two bijections $\omega_1 : M \to \{1, \ldots, |M|\}$ and $\omega_2 : M \to \{1, \ldots, |M|\}$ with $\omega_1(e_1) = 1$, $\omega_1(e_2) = 2$, $\omega_2(e_1) = 2$, $\omega_2(e_2) = 1$ and $\omega_2|_{M\setminus\{e_1,\, e_2\}} = \omega_1|_{M\setminus\{e_1,\, e_2\}}$. As the above extension of ω, we extend the weight functions ω_1 and ω_2 on M to the vertices of G.

We first consider the case that $x, u \in A$. Suppose to the contrary that $xv \in E(G)$ but $yu \notin E(G)$. Set $A' := A \setminus \{x, u\}$, $\bar{A}' := \bar{A} \setminus \{y, v\}$, $E'_1 := \{wz \in E(G) : \omega_1(w) > \omega_1(z), w \in A' \text{ and } z \in \bar{A}'\}$. Then

$$E_A^{\omega_2} \cup E(A) = \{xv\} \cup E(\{y, v\}, A') \cup E'_1 \cup E(A) = \{xv\} \cup E_A^{\omega_1} \cup E(A). \tag{3}$$

By the above proof we know that both $E_A^{\omega_1} \cup E(A)$ and $E_A^{\omega_2} \cup E(A)$ are minimum anti-forcing sets of M in G, it contradicts to the equation (3). Thus $yu \in E(G)$.

For the case that $x \in A$ and $u \in \bar{A}$, set $U := (A \setminus \{v\}) \cup \{u\}$, $\bar{U} := (\bar{A} \setminus \{u\}) \cup \{v\}$. Then each edge in M is incident with exactly one vertex in U. Substituting the partition $(A, \bar{A})$ of $V(G)$ with the partition $(U, \bar{U})$, by a similar argument as the above case, we can also show that $xv \in E(G)$ implies $yu \in E(G)$. □

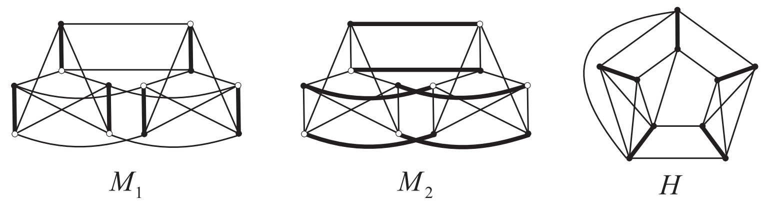

Fig. 3. Two nice perfect matchings M_1 and M_2 of G' and a nice perfect matching of H.

By Theorem 2.5, we can easily check whether a perfect matching of a graph is nice. For example, in Fig. 3, the two perfect matchings M_1 and M_2 of the bipartite graph G' are nice, and the perfect matching of the non-bipartite graph H is also nice.

Proposition 2.6. *Let M be a nice perfect matching of G and S a subset of $V(G)$. Then $M \cap E(S)$ is a nice perfect matching of $G[S]$ if $M \cap E(S)$ is a perfect matching of $G[S]$.*

Proof: By Theorem 2.5, it holds. □

In the proof of Theorem 2.5, we notice that $d_G(u) = d_G(v)$ for every edge uv of a nice perfect matching of G. So we have the following necessary but not sufficiency condition for the upper bound in Theorem 1.2 to be attained.

Proposition 2.7. *Let G be a graph with a perfect matching. Then $Af(G) < \frac{2e(G)-v(G)}{4}$ if there are an odd number of vertices of the same degree in G.*

Proposition 2.7 is not sufficient. For example, for a hexagonal system with a perfect matching, it does not have a nice perfect matching by Theorem 2.5, that is, its maximum anti-forcing number can not be the upper bound in Theorem 1.2, but it has an even number of vertices of degree 3 and an even number of vertices of degree 2.

Abay-Asmerom et al. (2010) introduced a *reversing involution* of a connected bipartite graph G with partite sets X and Y as an automorphism α of G of order two such that $\alpha(X) = Y$ and $\alpha(Y) = X$. Here we give the following definition of a general graph.

Definition 2.8. *Suppose that G is a simple connected graph. An edge-involution of G is an automorphism α of G of order two such that v and $\alpha(v)$ are adjacent for any vertex v in G.*

Hence an edge-involution of a bipartite graph is also a reversing involution, but a reversing involution of a bipartite graph may not be an edge-involution. In the following, we establish a relationship between a nice perfect matching and an edge-involution of G.

Theorem 2.9. *Let G be a simple connected graph. Then there is a one-to-one correspondence between the nice perfect matchings of G and the edge-involutions of G.*

Proof: For a nice perfect matching M of G, we define a bijection α_M of order 2 on $V(G)$ as follows: for any vertex v of G, there is exactly one edge e in M such that v is incident with e, let $\alpha_M(v)$ be the other end-vertex of e. Let x and y be any two distinct vertices of G. If $xy \in M$, then $\alpha_M(x) = y$, $\alpha_M(y) = x$ and $\alpha_M(x)\alpha_M(y) = yx \in E(G)$. If $xy \notin M$ (x may not be adjacent to y), then both $x\alpha_M(x)$ and $y\alpha_M(y)$ belong to M. Since M is a nice perfect matching, $xy \in E(G)$ if and only if $\alpha_M(x)\alpha_M(y) \in E(G)$ by Theorem 2.5. This implies that α_M is an automorphism of G. Thus α_M is an edge-involution of G.

Conversely, let α be an edge-involution of G. Then for any vertex y of G, $y\alpha(y) \in E(G)$. Since α is a bijection of order 2 on $V(G)$, $M' := \{y\alpha(y) : y \in V(G)\}$ is a perfect matching of G. For any two distinct edges $y_1\alpha(y_1)$ and $y_2\alpha(y_2)$ of M', $y_1y_2 \in E(G)$ if and only if $\alpha(y_1)\alpha(y_2) \in E(G)$, and $y_1\alpha(y_2) \in E(G)$ if and only if $\alpha(y_1)y_2 \in E(G)$ since α is an automorphism of order 2 of G. So M' is a nice perfect matching of G by Theorem 2.5. We can also see that $\alpha_{M'} = \alpha$. This establishes a one-to-one correspondence between the nice perfect matchings of G and the edge-involutions of G. $\square$

3 Construction of the extremal graphs

In the following, we will show that every extremal graph can be constructed from a complete graph K_2 by implementing two expansion operations.

Definition 3.1. *Let G_i be a simple graph with a nice perfect matching M_i, $i = 1, 2$ (note that $V(G_1) \cap V(G_2) = \emptyset$). We define two expansion operations as follows:*

(i) *$G := G_i + e + e'$, where $e, e' \notin E(G_i)$ and there are edges $e_1, e_2 \in M_i$ such that the four edges e, e', e_1, e_2 form a 4-cycle.*

(ii) *For $M_1' \subseteq M_1$ and $M_2' \subseteq M_2$ with $|M_1'| = |M_2'|$, given a bijection ϕ from $V(M_1')$ to $V(M_2')$ with $uv \in M_1'$ if and only if $\phi(u)\phi(v) \in M_2'$. G_1 joins G_2 over matchings M_1' and M_2' about bijection ϕ, denoted by $G_1 \circledast G_2$, is a graph with vertex set $V(G_1) \cup V(G_2)$ and edge set $E(G_1) \cup E(G_2) \cup E'$, where $E' := \{u\phi(u) : u \in V(M_1')\}$.*

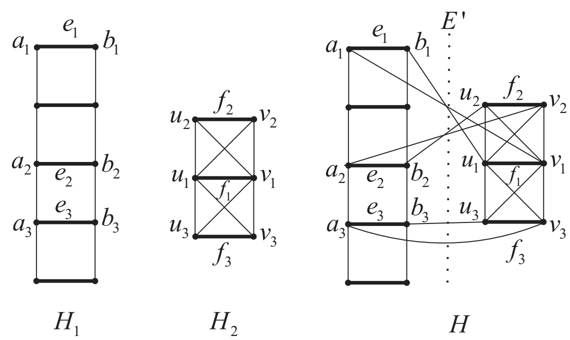

Fig. 4. $H = H_1 \circledast H_2$ over matchings M_1' and M_2' about bijection ϕ'.

For example, in Fig. 4 graph H is $H_1 \circledast H_2$ over matchings M_1' of H_1 and M_2' of H_2 about bijection ϕ', where $M_1' = \{e_1, e_2, e_3\}$, $M_2' = \{f_1, f_2, f_3\}$, $\phi'(a_i) = v_i$, $\phi'(b_i) = u_i$, $i = 1, 2, 3$. H has a nice perfect matching which is marked by thick edges in Fig. 4. Recall that nK_2 is the disjoint union of n copies of K_2.

Theorem 3.2. *A simple graph G is an extremal graph if and only if it can be constructed from K_2 by implementing operations (i) or (ii) in Definition* 3.1 *(regardless of the orders).*

Proof: Let $\mathcal{P}'$ be the set of all the graphs that can be constructed from K_2 by implementing operations (i) or (ii). For any graph $G \in \mathcal{P}'$, G is a simple graph with a nice perfect matching by the definition of the two operations.

Conversely, we suppose that G is an extremal graph, that is, G has a nice perfect matching $M = \{e_1, e_2, \dots, e_n\}$. If $n = 1$, or 2, then G must be isomorphic to K_2, $2K_2$, C_4 or K_4. So $G \in \mathcal{P}'$. Next, we suppose that $n \geq 3$ and it holds for $n-1$. Let $G' := G[\bigcup_{i=1}^{n-1} V(e_i)]$. Then $\{e_1, \dots, e_{n-1}\}$ is a nice perfect matching of G' by Proposition 2.6. So $G' \in \mathcal{P}'$ by the induction. If e_n is an isolated edge in G, then $G = G' \cup \{e_n\} \in \mathcal{P}'$. Otherwise, $e_n = u_nv_n$ has adjacent edges u_nv_i and v_nu_i, or u_nu_i and v_nv_i for some $i \in \{1, \dots, n-1\}$, where $u_iv_i = e_i \in M$. Let $G'' = G' \circledast K_2$ over matchings $\{e_i\}$ and $\{e_n\}$ about bijection $\phi : \{u_i, v_i\} \to \{u_n, v_n\}$. So $G'' \in \mathcal{P}'$. Then G can be constructed from G'' by implementing several times operations (i). So $G \in \mathcal{P}'$. □

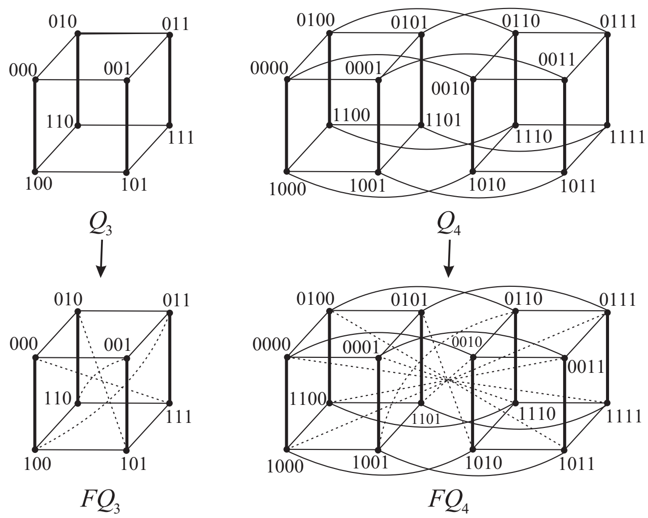

Fig. 5. The nice perfect matchings E_1 of Q_3 and Q_4 are depicted by thick edges; the dashed edges are the complementary edges.

As a variant of the n-dimensional hypercube Q_n, the n-dimensional *folded hypercube* FQ_n, proposed first by El-Amawy and Latifi (1991), is a graph with $V(FQ_n) = V(Q_n)$ and $E(FQ_n) = E(Q_n) \cup \bar{E}$, where $\bar{E} := \{x\bar{x} : x = x_1x_2\cdots x_n, \bar{x} = \bar{x}_1\bar{x}_2\cdots\bar{x}_n\}$, $\bar{x}_i := 1 - x_i$. Each edge in $\bar{E}$ is called a *complementary edge*. The graphs shown in Fig. 5 are FQ_3 and FQ_4, respectively.

Corollary 3.3. *FQ_n is an extremal graph and $Af(FQ_n) = n2^{n-2}$.*

Proof: By Lemma 2.4, E_1 is a nice perfect matching of Q_n. FQ_n is constructed from Q_n by applying the operation (i) over the nice perfect matching E_1 of Q_n (see Fig. 5 for $n = 3, 4$). So E_1 is also a nice perfect matching of the folded hypercube FQ_n. □

For any positive integer n, a connected graph G with at least $2n + 2$ vertices is said to be *n-extendable* if every matching of size n is contained in a perfect matching of G.

Proposition 3.4. *Any connected extremal graph G other than K_2 is 1-extendable.*

Proof: Since G is an extremal graph, it has a nice perfect matching M. For any edge uv of $E(G) \setminus M$, there are edges ux and vy of M. By Theorem 2.5, $xy \in E(G)$. So uv belongs to an M-alternating 4-cycle $C := uxyvu$. Then $M \triangle E(C) := (M \cup E(C)) \setminus (M \cap E(C))$ is a perfect matching of G that contains edge uv. So G is 1-extendable. □

By Proposition 3.4, any connected extremal graph except for K_2 is 2-connected.

4 Cartesian decomposition

The *Cartesian product* $G\Box H$ of two graphs G and H is a graph with vertex set $V(G) \times V(H) = \{(x, u) : x \in V(G), u \in V(H)\}$ and two vertices (x, u) and (y, v) are adjacent if and only if $xy \in E(G)$ and $u = v$ or $x = y$ and $uv \in E(H)$. For a vertex (x_i, v_j) of $G\Box H$, the subgraphs of $G\Box H$ induced by the vertex set $\{(x, v_j) : x \in V(G)\}$ and the vertex set $\{(x_i, v) : v \in V(H)\}$ are called a G-layer and an H-layer of $G\Box H$, and denoted by G^{v_j} and H^{x_i}, respectively.

For any graph H, let E' be the set of edges of all K_2-layers of $H\Box K_2$. Clearly, E' is a perfect matching of $H\Box K_2$. Define a bijection α on $V(H\Box K_2)$ as follows: for every edge $uv\in E'$, $\alpha(u):=v$ and $\alpha(v):=u$. Then α is an edge-involution of $H\Box K_2$. So $H\Box K_2$ is an extremal graph by Theorem 2.9. This fact inspires us to consider the Cartesian product decomposition of an extremal graph. Let $\Phi^*(G)$ be the number of all the nice perfect matchings of a graph G. We have Theorem 4.1. Recall that for an edge $e=uv$ of G and an isomorphism φ from G to H, $\varphi(e):=\varphi(u)\varphi(v)$.

Theorem 4.1. *Let G_1 and G_2 be two simple connected graphs. Then*

$$\Phi^*(G_1\Box G_2)=\Phi^*(G_1)+\Phi^*(G_2).$$

Proof: Let $V(G_1)=\{x_1,x_2,\ldots,x_{n_1}\}$ and $V(G_2)=\{v_1,v_2,\ldots,v_{n_2}\}$. Since $\Phi^*(K_1)=0$, we suppose $n_1\geq 2$ and $n_2\geq 2$.

We define an isomorphism ρ_{v_i} from G_1 to $G_1^{v_i}$ and an isomorphism σ_{x_j} from G_2 to $G_2^{x_j}$: $\rho_{v_i}(x):=(x,v_i)$ for any vertex x of G_1 and $\sigma_{x_j}(v):=(x_j,v)$ for any vertex v of G_2. For any nice perfect matching M_i of G_i, $i=1,2$, let

$$\rho(M_1):=\bigcup_{v_i\in V(G_2)}\rho_{v_i}(M_1),\quad \sigma(M_2):=\bigcup_{x_j\in V(G_1)}\sigma_{x_j}(M_2), \tag{4}$$

By Theorem 2.5, $\rho_{v_i}(M_1)$ is a nice perfect matching of $G_1^{v_i}$ and $\rho(M_1)$ is a nice perfect matching of $G_1\Box G_2$. Similarly, $\sigma(M_2)$ is also a nice perfect matching of $G_1\Box G_2$.

Conversely, since $E(G_1^{v_1})$, …, $E(G_1^{v_{n_2}})$, $E(G_2^{x_1})$, …, $E(G_2^{x_{n_1}})$ is a partition of $E(G_1\Box G_2)$, for any nice perfect matching M of $G_1\Box G_2$ there is some x_i or v_j such that $M\cap E(G_2^{x_i})\neq\emptyset$ or $M\cap E(G_1^{v_j})\neq\emptyset$. If $M\cap E(G_2^{x_i})\neq\emptyset$ for some x_i, then we have the following Claim.

Claim: $M\cap E(G_2^{x_j})$ is a nice perfect matching of $G_2^{x_j}$ for each $x_j\in V(G_1)$, and $\sigma_{x_j}^{-1}(M\cap E(G_2^{x_j}))=\sigma_{x_i}^{-1}(M\cap E(G_2^{x_i}))$. So $M\cap E(G_1^{v})=\emptyset$ for each $v\in V(G_2)$.

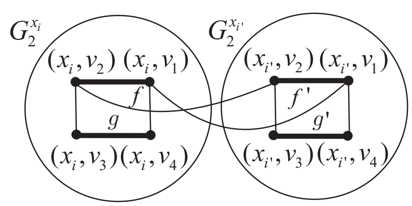

Fig. 6. Illustration for the proof of the Claim in Theorem 4.1.

Take an edge $f=(x_i,v_1)(x_i,v_2)\in M\cap E(G_2^{x_i})$. Then $v_1v_2\in E(G_2)$. If $n_2=2$, then $M\cap E(G_2^{x_i})=\{f\}$ is a nice perfect matching of $G_2^{x_i}$. For $n_2\geq 3$, since G_2 is connected, without loss of generality we may assume that $d_{G_2}(v_2)\geq 2$. Let v_3 be a neighbor of v_2 that is different from v_1. So $(x_i,v_2)(x_i,v_3)\in E(G_2^{x_i})$. Let g be an edge of M with an end-vertex (x_i,v_3). Since M is a nice perfect matching of G, the other end-vertex of g must be adjacent to (x_i,v_1) by Theorem 2.5. So the other end-vertex of g belongs to $V(G_2^{x_i})$ (see Fig. 6), that is, $g\in E(G_2^{x_i})$. Since $G_2^{x_i}\cong G_2$ is a connected graph, we can obtain that $M\cap E(G_2^{x_i})$ is a perfect matching of $G_2^{x_i}$ in the above way. So $M\cap E(G_2^{x_i})$ is a nice perfect matching of $G_2^{x_i}$ by Proposition 2.6.

Since G_1 is connected and $n_1\geq 2$, there is some vertex $x_{i'}$ of G_1 such that x_i and $x_{i'}$ are adjacent in G_1. So vertex $(x_{i'},v_1)\notin G_2^{x_i}$ is adjacent to (x_i,v_1) in $G_1\Box G_2$ (see Fig. 6). Let f' be an edge of M that is incident with $(x_{i'},v_1)$. Since M is a nice perfect matching of $G_1\Box G_2$, the other end-vertex of f' must be adjacent to (x_i,v_2) by Theorem 2.5. So $f'=(x_{i'},v_1)(x_{i'},v_2)\in M\cap E(G_2^{x_{i'}})$. As the above proof, we can similarly show that $M\cap E(G_2^{x_{i'}})$ is a nice perfect matching of $G_2^{x_{i'}}$. Since G_1 is connected, in an inductive way we can show that $M\cap E(G_2^{x_j})$ is a nice perfect matching of $G_2^{x_j}$ for any $x_j\in V(G_1)$.

Notice that $\sigma_{x_i}^{-1}(f)=v_1v_2=\sigma_{x_i'}^{-1}(f')$. Let g' be the edge of M that is incident with $(x_{i'},v_3)$. Since $(x_{i'},v_3)$ is adjacent to (x_i,v_3), the other end vertex of g' must be adjacent to the other end vertex (x_i,v_4) of g by Theorem 2.5. So

$g' = (x_{i'}, v_3)(x_{i'}, v_4)$ since $g' \in E(G_2^{x_{i'}})$. This implies that $\sigma_{x_{i'}}^{-1}(g') = v_3v_4 = \sigma_{x_i}^{-1}(g)$. In an inductive way, we can show that $\sigma_{x_{i'}}^{-1}(M \cap E(G_2^{x_{i'}})) = \sigma_{x_i}^{-1}(M \cap E(G_2^{x_i}))$. Similarly, we also have $\sigma_{x_j}^{-1}(M \cap E(G_2^{x_j})) = \sigma_{x_i}^{-1}(M \cap E(G_2^{x_i}))$ for any $x_j \in V(G_1)$.

By this Claim, $M_2 := \sigma_{x_i}^{-1}(M \cap E(G_2^{x_i}))$ is a nice perfect matching of G_2 with $M = \sigma(M_2)$. If $M \cap E(G_1^{v_j}) \neq \emptyset$, then we can similarly show that G_1 has a nice perfect matching M_1 with $M = \rho(M_1)$. So $\Phi^*(G_1 \Box G_2) = \Phi^*(G_1) + \Phi^*(G_2)$. □

In fact, we can get the following corollary.

Corollary 4.2. *Let G be a simple connected graph. Then we have $\Phi^*(G) = \sum_{i=1}^{k} \Phi^*(G_i)$ for any decomposition $G_1 \Box \cdots \Box G_k$ of G.*

Now, it is easy to get the following proposition.

Proposition 4.3. *A simple connected graph G is an extremal graph if and only if one of its Cartesian product factors is an extremal graph.*

The *n-dimensional enhanced hypercube* $Q_{n,k}$, see Tzeng and Wei (1991), is the graph with vertex set $V(Q_{n,k}) = V(Q_n)$ and edge set $E(Q_{n,k}) = E(Q_n) \cup \{(x_1x_2\cdots x_{n-1}x_n, \bar{x}_1\bar{x}_2\cdots\bar{x}_{n-k-1}\bar{x}_{n-k}x_{n-k+1}\, x_{n-k+2}\cdots x_n : x_1x_2\cdots x_n \in V(Q_{n,k})\}$, where $0 \leq k \leq n-1$. Clearly, $Q_n \cong Q_{n,n-1}$ and $FQ_n \cong Q_{n,0}$, i.e., the hypercube and the folded hypercube are regarded as two special cases of the enhanced hypercube. By Yang et al. (2015a), we have $Q_{n,k} \cong FQ_{n-k} \Box Q_k$, for $0 \leq k \leq n-1$. Hence we obtain the following result by the Proposition 4.3.

Corollary 4.4. *$Q_{n,k}$ is an extremal graph and $Af(Q_{n,k}) = n2^{n-2}$.*

According to the above discussion, for any graph G, we know that $K_{m,m} \Box G$, $K_{2n} \Box G$, $Q_n \Box G$, $FQ_n \Box G$ and $Q_{n,k} \Box G$ are extremal graphs. Moreover, we can produce an infinite number of extremal graphs from an extremal graph by the Cartesian product operation.

5 Further applications

From examples we already know that $K_{m,m}$, K_{2n}, Q_n, FQ_n and $Q_{n,k}$ are extremal graphs. Two perfect matchings M_1 and M_2 of a graph G are called *equivalent* if there is an automorphism φ of G such that $\varphi(M_1) = M_2$. So we know that all the perfect matchings of $K_{m,m}$ (or K_{2n}) are nice and equivalent. Further in this section we will count nice perfect matchings of the three cube-like graphs.

Theorem 5.1. *Q_n has exactly n nice perfect matchings $E_1, E_2, \ldots, E_n$, all of which are equivalent.*

Proof: By Lemma 2.4, $E_1, E_2, \ldots, E_n$ are n distinct nice perfect matchings of Q_n. Since Q_n is the Cartesian product of n K_2's, Q_n has exactly n nice perfect matchings by Corollary 4.2. So the first part is done. Now, it remains to show that E_i and E_j are equivalent for any $1 \leq i < j \leq n$. Let the automorphism f_{ij} of Q_n be defined as $f_{ij}(x_1\cdots x_{i-1}x_ix_{i+1}\ldots x_{j-1}x_jx_{j+1}\cdots x_n) = x_1\cdots x_{i-1}x_jx_{i+1}\ldots x_{j-1}x_ix_{j+1}\cdots x_n$ for each vertex $x_1x_2\cdots x_n$ of Q_n. Then $f_{ij}(E_i) = E_j$. □

The theorem can be obtained by applying the reversing-involutions of bipartite graphs, see Abay-Asmerom et al. (2010), but the computation is tedious.

Since $FQ_2 \cong K_4$ and $FQ_3 \cong K_{4,4}$, we have $\Phi^*(FQ_2) = 3$ and $\Phi^*(FQ_3) = 24$. For $n \geq 4$, we have a general result as follows.

Theorem 5.2. *FQ_n has exactly $n+1$ nice perfect matchings for $n \geq 4$.*

Proof: By Lemma 2.4, E_i is a perfect matching of Q_n. Then E_i is also a perfect matching of FQ_n. We can easily check that E_i is a nice perfect matching of FQ_n by Theorem 2.5.

Let E_{n+1} be the set of all the complementary edges of FQ_n. Then E_{n+1} is a perfect matching of FQ_n. Let $u\bar{u}$ and $v\bar{v}$ be two distinct edges in E_{n+1}. Since any two distinct complementary edges are independent, the edge linked u to v or $\bar{v}$ (if exist) does not belong to E_{n+1}. We can easily show that $uv \in E_j$ if and only if $\bar{u}\bar{v} \in E_j$ for some $j = 1, 2, \ldots, n$, and $u\bar{v} \in E_s$ if and only if $\bar{u}v \in E_s$ for some $s = 1, 2, \ldots, n$. So E_{n+1} is also a nice perfect matching of FQ_n.

Now, we have found $n+1$ nice perfect matchings of FQ_n. Next, we will show that FQ_n has no other nice perfect matchings. By the contrary, we suppose that M is a nice perfect matching of FQ_n that is different from any E_i, $i = 1, 2, \ldots, n+1$. Since $E_1, \ldots, E_{n+1}$ is a partition of the edge set $E(FQ_n)$, there is E_k with $k \neq n+1$ such that $M \cap E_k \neq \emptyset$ and $E_k \neq M$. Clearly, $FQ_n - (E_{n+1} \cup E_k)$ has exactly two components both of which are isomorphic to Q_{n-1}. We notice that the k-th coordinate of each vertex in one component is 0, and 1 in the other component. We denote the two components by Q_n^0 and Q_n^1, respectively. In fact, $V(Q_n^i) = \{x_1 \cdots x_{k-1} i x_{k+1} \cdots x_n : x_j = 0 \text{ or } 1, j = 1, \ldots, k-1, k+1, \ldots, n\}$, $i = 0, 1$. Since $M \cap E_k \neq \emptyset$, there is some edge $vv' \in M \cap E_k$ with $v \in V(Q_n^0)$ and $v' \in V(Q_n^1)$. For any vertex w of Q_n^0 with w and v being adjacent, we consider the edge g of M that is incident with w. By Theorem 2.5, the other end-vertex of g is adjacent to v'. If $g = w\bar{w}$ is a complementary edge of FQ_n, then there are exactly two same bits in the strings of $\bar{w}$ and v'. So the edge $\bar{w}v' \in E(FQ_n)$ is not a complementary edge of FQ_n. Since $\bar{w}$ and v' are adjacent, there is exactly one different bit in the strings of $\bar{w}$ and v'. So $n = 3$, a contradiction. If $g = wz \in E(Q_n^0)$, then there are exactly three different bits in the strings of z and v'. Since z and v' are adjacent in FQ_n, the edge zv' is a complementary edge of FQ_n. So $n = 3$, a contradiction. Hence $g \in E_k$. Since Q_n^0 is connected, using the above method repeatedly, we can show that $M = E_k$, a contradiction. So FQ_n has exactly $n+1$ nice perfect matchings. □

Proposition 5.3. *All the nice perfect matchings of FQ_n $(n \geq 2)$ are equivalent.*

Proof: We notice that $FQ_2 \cong K_4$ and $FQ_3 \cong K_{4,4}$. So all the nice perfect matchings of FQ_n are equivalent for $2 \leq n \leq 3$. Suppose that $n \geq 4$. From the proof of Theorem 5.2 we know that E_1, E_2, $\ldots$, E_{n+1} are all the nice perfect matchings of FQ_n. f_{ij} defined in the proof of Theorem 5.1 is also an automorphism of FQ_n such that $\varphi(E_i) = E_j$ for $1 \leq i < j \leq n$. We will show that E_1 and E_{n+1} are equivalent. Clearly, $FQ_n - (E_1 \cup E_{n+1})$ has exactly two components each isomorphic to Q_{n-1}, denoted by Q_n^0 and Q_n^1. Set $V(Q_n^i) = \{ix_2x_3 \cdots x_n : x_j = 0 \text{ or } 1, j = 2, \ldots, n\}$, $i = 0, 1$. We define a bijection f on $V(FQ_n)$ as follows:

$$f(x_1x_2 \cdots x_n) = \begin{cases} \bar{x}_1 x_2 \cdots x_n, & \text{if } x_1x_2 \cdots x_n \in V(Q_n^0), \\ \bar{x}_1 \bar{x}_2 \cdots \bar{x}_n, & \text{if } x_1x_2 \cdots x_n \in V(Q_n^1). \end{cases}$$

It is easy to check that f is an automorphism of FQ_n. In addition, $f(E_1) = E_{n+1}$. Hence all the nice perfect matchings of FQ_n are equivalent. □

By Corollary 4.2 and Theorems 5.1 and 5.2, we can obtain the following conclusion.

Corollary 5.4. $\Phi^*(Q_{n,n-1}) = n$, $\Phi^*(Q_{n,n-2}) = n+1$, $\Phi^*(Q_{n,n-3}) = n+21$ *and* $\Phi^*(Q_{n,k}) = n+1$ *for any* $0 \leq k \leq n-4$.

Proposition 5.5. *For $0 < k < n-1$, $Q_{n,k}$ has exactly two nice perfect matchings up to the equivalent.*

Proof: Since $Q_{n,k} = FQ_{n-k} \Box Q_k$, by adapting the notations in Eq. (4) and by the proof of Theorem 4.1 we know that all the nice perfect matchings of $Q_{n,k}$ are divided into two classes $\mathcal{M}'$ and $\mathcal{M}''$, where $\mathcal{M}' = \{\rho(M) : M \text{ is a nice perfect matching of } FQ_{n-k}\}$ and $\mathcal{M}'' = \{\sigma(M) : M \text{ is a nice perfect matching of } Q_k\}$.

For $M_1', M_2' \in \mathcal{M}'$, there are two nice perfect matchings M_1 and M_2 of FQ_{n-k} such that $M_i' = \rho(M_i)$, $i = 1, 2$. By Proposition 5.3, there exists an automorphism φ of FQ_{n-k} such that $\varphi(M_1) = M_2$. Let $\varphi'(x, u) := (\varphi(x), u)$ for each vertex (x, u) of $FQ_{n-k} \Box Q_k$. It is easy to check that φ' is an automorphism of $Q_{n,k}$ and $\varphi'(M_1') = M_2'$. By the arbitrariness of M_1' and M_2', we know that all the nice perfect matchings in $\mathcal{M}'$ are equivalent. Similarly, we can show that all the nice perfect matchings in $\mathcal{M}''$ are equivalent.

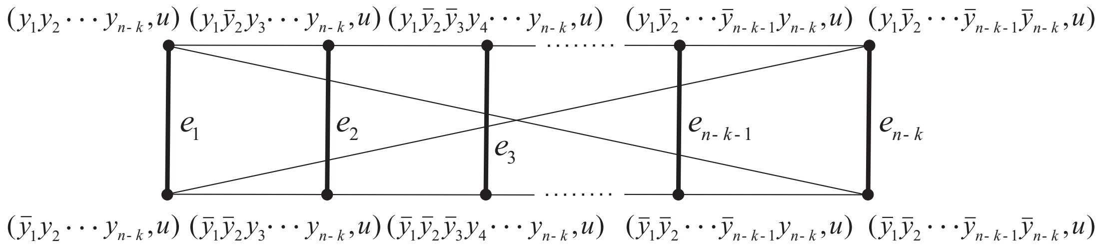

Fig. 7. The graph H.

Let F_1 and E_1 be the sets of all the 1-edges of FQ_{n-k} and Q_k respectively. Then F_1 is a nice perfect matching of FQ_{n-k} and E_1 is a nice perfect matching of Q_k. So $\rho(F_1) \in \mathcal{M}'$ and $\sigma(E_1) \in \mathcal{M}''$. See Fig. 7, we choose a subset $S := \{e_1, \ldots, e_{n-k}\}$ of $\rho(F_1)$. Then all the vertices incident with S induce a subgraph H as depicted in Fig. 7. For any subset $R \subseteq \sigma(E_1)$ of size $n-k$, let G be the subgraph of $Q_{n,k}$ induced by all the vertices incident with R. We note that $Q_{n,k} - \sigma(E_1)$ has exactly two components A and B each of which is isomorphic to $FQ_{n-k}\Box Q_{k-1}$, and $\sigma(E_1) = E(A,B)$. So $G-R$ has at least two components. Clearly $H-S$ is connected. So for any automorphism ψ of $Q_{n,k}$, $\psi(S) \neq R$. By the arbitrariness of R we know that $\rho(F_1)$ and $\sigma(E_1)$ are not equivalent. Then we are done. $\Box$

From Corollary 4.2 it is helpful to give a Cartesian decomposition of an extremal graph. It is known that $Q_n \cong K_2\Box\cdots\Box K_2$ and $Q_{n,k} \cong FQ_{n-k}\Box Q_k$. However we shall see surprisedly that FQ_n is undecomposable.

A nontrivial graph G is said to be *prime* with respect to the Cartesian product if whenever $G \cong H\Box R$, one factor is isomorphic to the complete graph K_1 and the other is isomorphic to G. Clearly, for $m \geq 3$ and $n \geq 2$, $K_{m,m}$ and K_{2n} are prime extremal graphs. In the sequel, we show that FQ_n is a prime extremal graph, too.

Recall that the length of a shortest path between two vertices x and y of G is called the distance between x and y, denoted by $d_G(x,y)$. Let G be a connected graph. Two edges $e = xy$ and $f = uv$ are in the relation Θ_G if $d_G(x,u) + d_G(y,v) \neq d_G(x,v) + d_G(y,u)$. Notice that Θ_G is reflexive and symmetric, but need not to be transitive. We denote its transitive closure by Θ_G^*. For an even cycle C_{2n}, $\Theta_{C_{2n}}$ consists of all pairs of antipodal edges. Hence, $\Theta_{C_{2n}}^*$ has n equivalence classes and $\Theta_{C_{2n}} = \Theta_{C_{2n}}^*$. For an odd cycle C, any edge of C is in relation Θ with its two antipodal edges. So all edges of C belong to an equivalence class with respect to Θ_C^*. By the Cartesian product decomposition Algorithm depicted in Imrich and Klavzar (2000), we have the following lemma.

Lemma 5.6. *If all the edges of a graph G belong to an equivalence class with respect to Θ_G^*, then G is a prime graph under the Cartesian product.*

The *Hamming distance* between two vertices x and y in Q_n is the number of different bits in the strings of both vertices, denoted by $H_{Q_n}(x,y)$.

Theorem 5.7 (Xu and Ma (2006))**.** *For a folded hypercube FQ_n, we have*

(1) *FQ_n is a bipartite graph if and only if n is odd.*

(2) *The length of any cycle in FQ_n that contains exactly one complementary edge is at least $n+1$. If n is even, then the length of a shortest odd cycle in FQ_n is $n+1$.*

(3) *Let u and v be two vertices in FQ_n. If $H_{Q_n}(u,v) \leq \lfloor \frac{n}{2} \rfloor$, then any shortest uv-path in FQ_n contains no complementary edges. If $H_{Q_n}(u,v) > \lceil \frac{n}{2} \rceil$, then any shortest uv-path in FQ_n contains exactly one complementary edge.*

Here we list some known properties of Q_n that will be used in the sequel. For any two vertices x and y in Q_n, $d_{Q_n}(x,y) = H_{Q_n}(x,y)$. For any shortest path P from $x_1x_2\cdots x_n$ to $\bar{x}_1\bar{x}_2\cdots\bar{x}_n$ in Q_n, $|E(P) \cap E_i| = 1$ for each

$i = 1, 2, \ldots, n$. For any integer j $(1 \leq j \leq n)$, there is a shortest path P from $x_1x_2 \cdots x_n$ to $\bar{x}_1\bar{x}_2 \cdots \bar{x}_n$ in Q_n such that the edge in $E(P) \cap E_i$ is the jth edge when traverse P from $x_1x_2 \cdots x_n$ to $\bar{x}_1\bar{x}_2 \cdots \bar{x}_n$.

For every subgraph F of a graph G, the inequality $d_F(u, v) \geq d_G(u, v)$ obviously holds. If $d_F(u, v) = d_G(u, v)$ for all $u, v \in V(F)$, we say F is an *isometric subgraph* of G.

Proposition 5.8 (Hammack et al. (2011))**.** *Let C be a shortest cycle of G. Then C is isometric in G.*

Theorem 5.9. *FQ_n is a prime graph under the Cartesian product.*

Proof: Clearly, FQ_2 and FQ_3 are prime. So we suppose that $n \geq 4$. We recall that E_i is the set of all the i-edges of Q_n, $i = 1, 2, \ldots, n$. Let E_{n+1} be the set of all the complementary edges of FQ_n. Then $E_1, E_2, \ldots, E_{n+1}$ is a partition of $E(FQ_n)$. Since the girth of FQ_n is 4 for $n \geq 4$, any two opposite edges of a 4-cycle are in relation Θ_{FQ_n}. So E_i is contained in an equivalence class with respect to $\Theta^*_{FQ_n}$, $i = 1, 2, \ldots, n + 1$. For any vertex $x_1x_2 \cdots x_n$, it is linked to $\bar{x}_1\bar{x}_2 \cdots \bar{x}_n$ by a complementary edge e in FQ_n. Let P be any shortest path from $x_1x_2 \cdots x_n$ to $\bar{x}_1\bar{x}_2 \cdots \bar{x}_n$ in Q_n. Then the length of P is n and $|P \cap E_i| = 1$ for any $i = 1, 2, \ldots, n$. Set $C := P \cup \{e\}$. Then C is a cycle of length $n + 1$.

If n is even, then the length of any shortest odd cycle in FQ_n is $n + 1$ by Theorem 5.7 (2). So C is a shortest odd cycle in FQ_n. By Proposition 5.8, C is an isometric odd cycle in FQ_n. So all edges of C belong to an equivalence class with respect to $\Theta^*_{FQ_n}$. Since $E(C) \cap E_i \neq \emptyset$ for any $i = 1, 2, \ldots, n + 1$, all edges of $E(FQ_n) = \bigcup_{i=1}^{n+1} E_i$ belong to an equivalence class with respect to $\Theta^*_{FQ_n}$, that is, FQ_n is a prime graph under the Cartesian product by Lemma 5.6.

For n being odd, we first show that C is an isometric cycle in FQ_n. It is sufficient to show that $d_C(u, v) = d_{FQ_n}(u, v)$ for any two distinct vertices u and v of C. By Theorem 5.7 (3), there are two cases for the shortest uv-path in FQ_n. If $H_{Q_n}(u, v) \leq \lfloor \frac{n}{2} \rfloor$, then any shortest uv-path in FQ_n contains no complementary edges. So $d_{FQ_n}(u, v) = d_{Q_n}(u, v) = H_{Q_n}(u, v) = d_C(u, v)$. If $H_{Q_n}(u, v) > \lceil \frac{n}{2} \rceil$, then any shortest uv-path in FQ_n contains exactly one complementary edge. Let P_1 be the uv-path on C that contains the unique complementary edge e. Since $H_{Q_n}(u, v) > \lceil \frac{n}{2} \rceil$ and the length of C is $n + 1$, $d_C(u, v) = |P_1| = n + 1 - H_{Q_n}(u, v) < \lceil \frac{n}{2} \rceil$. Clearly $d_{FQ_n}(u, v) \leq d_C(u, v)$. We suppose that $d_{FQ_n}(u, v) < d_C(u, v)$, that is, P_1 is not a shortest uv-path in FQ_n. Let P_2 be a shortest uv-path in FQ_n. Then P_2 contains exactly one complementary edge by Theorem 5.7 (3). Set $P' := C - (V(P_1) \setminus \{u, v\})$. Then $P' \cup P_2$ is a walk in FQ_n that has exactly one complementary edge. So there is a cycle $C' \subseteq P' \cup P_2$ that contains exactly one complementary edge. We can deduce a contradiction by Theorem 5.7 (2) as follows:

$$n + 1 \leq |C'| \leq |P'| + |P_2| < |P'| + |P_1| = |C| = n + 1.$$

So $d_{FQ_n}(u, v) = d_C(u, v)$.

For any $i \in \{1, 2, \ldots, n\}$, let P^i be a shortest path from $x_1x_2 \cdots x_n$ to $\bar{x}_1\bar{x}_2 \cdots \bar{x}_n$ in Q_n such that the unique edge in $P^i \cap E_i$ is the antipodal edge of e on $C^i := P^i \cup \{e\}$. Since C^i is an isometric even cycle by the above proof, the unique complementary edge e on C^i and its antipodal edge $P^i \cap E_i$ are in relation Θ_{FQ_n}. So E_i and E_{n+1} are contained in an equivalence class with respect to $\Theta^*_{FQ_n}$, $i = 1, 2, \ldots, n$. Hence FQ_n is a prime graph under the Cartesian product by Lemma 5.6. $\square$

Now we know that for $m \geq 3$ and $n \geq 2$, $K_{m,m}$, K_{2n} and FQ_n are prime extremal graphs. From Proposition 4.3, it is interesting to characterize all the prime extremal graphs.

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