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 $\alpha$ 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
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 (2011), and establish a one-to-one correspondence between the nice perfect matchings of $G$ and the edge-involutions of $G$. In Section 2, we provide a proof to Theorem 1.2, obtain an equivalent condition for the nice perfect matching of $G$, and show 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 $G$.

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). Deng and Zhang (2017b) showed that its maximum forcing number equals its Clar number, respectively. 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, $Af(G) \leq r(G)$.

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

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

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. Let $\Phi^*(G)$ denote the number of nice perfect matchings of a graph $G$. For a Cartesian decomposition $G = G_1 \Box \cdots \Box G_k$, 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 $M$ (“$\times$”).](image)

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 2.2. 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. 1 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. 1. 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 $M$. 

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
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 2.2** For any perfect matching $M$ of $G$, let $A$ be a vertex subset of $G$ consisting of one end vertex for each edge of $M$, $A := V(G) \setminus A$. Then $G' := G(A, \overline{A})$ 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 $S' \cup E(\overline{A})$ are anti-forcing sets of $M$ in $G$. Hence

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

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

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, $c'(M) \geq \binom{n}{2} = \frac{m^2 - m}{2}$. 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 $af(K_{2n}, M') \geq c'(M') \geq 2 \times \frac{n^2}{2} = n^2 - n$. 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 $\overline{x} := 1 - x$. The edge connecting the two vertices $x_1 \cdots x_{i-1}x_i x_{i+1} \cdots x_n$ and $x_1 \cdots x_{i-1} \overline{x}_i x_{i+1} \cdots x_n$ 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 $\Theta_{Q_n}$-class of $Q_n$. We can show the following result for $Q_n$.

**Lemma 2.4.** $\Theta_{Q_n}$-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 $y = \overline{x}_1x_2 \cdots x_n$, 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 $af(Q_n, E_1) = Af(Q_n) = (n - 1)2^{n-2}$. \hfill $\Box$

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 $d_G(v)$. 

![Figure 2](https://via.placeholder.com/150) 

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

![Diagram](https://via.placeholder.com/150) 

C1, C2, C3, e1, e2, e3, C

1e
2e
3e
1C
2C
3C
C

C1, C2, C3, e1, e2, e3, C

1e
2e
3e
1C
2C
3C
C

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 $yu \in E(G)$, obviously, any two distinct $M$-alternating 4-cycles are compatible. Then

$$
\begin{align*}
    c'(M) & \geq \frac{1}{2} \sum_{wz \in M} c'_{wz}(M) \\
    & = \frac{1}{2} \sum_{wz \in M} \left( (d_G(w) - 1) + (d_G(z) - 1) \right) \\
    & = \frac{1}{2} \sum_{w \in V(G)} (d_G(w) - 1) \\
    & = \frac{e(G) - v(G)}{2}.
\end{align*}
$$

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 $\omega$ 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 $\omega$ 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

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

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

Since $G - E^\omega_A \cup E(A)$ has a unique perfect matching $M$, $E^\omega_A \cup E(A)$ is an anti-forcing set of $M$ in $G$. Similarly, $E^\omega_{\bar{A}} \cup E(\bar{A})$ 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 $|E^\omega_A \cup E(A)| \geq \frac{2e(G) - v(G)}{4}$, $|E^\omega_{\bar{A}} \cup E(\bar{A})| \geq \frac{2e(G) - v(G)}{4}$. Since $|E^\omega_A \cup E(A)| + |E^\omega_{\bar{A}} \cup E(\bar{A})| = e(G) - |M| = e(G) - \frac{v(G)}{2}$, $|E^\omega_A \cup E(A)| = |E^\omega_{\bar{A}} \cup E(\bar{A})| = \frac{2e(G) - v(G)}{4}$. Hence $E^\omega_A \cup E(A)$ 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 $\omega_2 \mid_{M \setminus \{e_1, e_2\}} = \omega_1 \mid_{M \setminus \{e_1, e_2\}}$. As the above extension of $\omega$, we extend the weight functions $\omega_1$ and $\omega_2$ 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 $A' := A \setminus \{x, u\}$, $\bar{A}' := \bar{A} \setminus \{y, v\}$, $E^\omega_A' := \{wz \in E(G) : \omega_1(w) > \omega_1(z), w \in A' \text{ and } z \in \bar{A}'\}$. Then

$$
E^\omega_{A'} \cup E(A) = \{xv\} \cup E(\{y, v\}, A') \cup E_0 \cup E(A) = \{xv\} \cup E^\omega_{A'} \cup E(A).
$$

By the above proof we know that both $E^\omega_A \cup E(A)$ and $E^\omega_{A'} \cup E(A)$ 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 \( yu \in E(G) \).

\[ \begin{array}{c}
M_1 \\
M_2 \\
H
\end{array} \]

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 \( \text{Af}(G) < \frac{2e(G) - v(G)}{4} \) 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 \( \alpha \) 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 \( \alpha \) 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 \( \alpha_M \) 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 \( xo_M(x) \) and \( yo_M(y) \) 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 \( \alpha_M \) is an automorphism of \( G \). Thus \( \alpha_M \) is an edge-involution of \( G \).
Conversely, let \( \alpha \) be an edge-involution of \( G \). Then for any vertex \( y \) of \( G \), \( y\alpha(y) \in E(G) \). Since \( \alpha \) 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 \( M' \), \( y_1, y_2 \in E(G) \) 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 \( \alpha \) 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 \( G_1 \) 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) \( G := G_1 + e + e' \), where \( e, e' \notin E(G) \) 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 \( \phi \) from \( V(M'_1) \) to \( V(M'_2) \) with \( w \in E(G) \) if and only if \( \phi(u)\phi(v) \in E(G) \), \( G_1 \) joins \( G_2 \) over matchings \( M'_1 \) and \( M'_2 \) about bijection \( \phi \), denoted by \( G_1 \otimes G_2 \), 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 = H1 ⊕ H2 over matchings M1 and M2 about bijection φ'.](image)

For example, in Fig. 4 graph \( H \) is \( H_1 \otimes H_2 \) over matchings \( M'_1 \) of \( H_1 \) and \( M'_2 \) of \( H_2 \) about bijection \( \phi' \), where \( M'_1 = \{e_1, e_2, e_3\}, M'_2 = \{f_1, f_2, f_3\} \), \( \phi'(u_1) = v_1, \phi'(b_1) = u_2, i = 1, 2, 3 \). \( H \) 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 \( M = \{e_1, e_2, \ldots, e_n\} \). 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 \( \{e_1, \ldots, e_{n-1}\} \) 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 \( u_nv_n \) and \( v_nv_i \) for some \( i \in \{1, \ldots, n - 1\} \), where \( u_iv_i = e_i \in M \). Let \( G'' = G' \oplus K_2 \) over
matchings \{e_i\} and \{e_n\} about bijection \(\phi : \{u_i, v_i\} \rightarrow \{u_n, v_n\}\). So \(G'' \in \mathcal{P}'\). Then \(G\) can be constructed from \(G''\) by implementing several times operations (i). So \(G \in \mathcal{P}'\).

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 2.3 \(xy \in E(G)\). 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 \(G \square H\) 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 \((x, v)\) of \(G \square H\), the subgraphs of \(G \square H\) induced by the vertex set \(\{(x, v) : x \in V(G)\}\) and the vertex set \(\{(x, v) : v \in V(H)\}\) are called a \(G\)-layer and an \(H\)-layer of \(G \square H\), and denoted by \(G^v\) and \(H^v\), respectively.
Tight upper bound on the maximum anti-forcing numbers of graphs

For any graph $H$, let $E'$ be the set of edges of all $K_2$-layers of $H \square K_2$. Clearly, $E'$ is a perfect matching of $H \square K_2$. Define a bijection $\alpha$ on $V(H \square K_2)$ as follows: for every edge $uv \in E'$, $\alpha(u) := v$ and $\alpha(v) := u$. Then $\alpha$ is an edge-involution of $H \square K_2$. So $H \square K_2$ 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 $\varphi$ 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

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

**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 $\rho_i$ from $G_1$ to $G_1^i$ and an isomorphism $\sigma_i$ from $G_2$ to $G_2^i$ : $\rho_i(x) := (x, v_i)$ for any vertex $x$ of $G_1$ and $\sigma_i(v) := (x, v)$ for any vertex $v$ of $G_2$. For any nice perfect matching $M_i$ of $G_i$, $i = 1, 2$, let

$$\rho(M_1) := \bigcup_{v_i \in V(G_2)} \rho_i(M_1), \quad \sigma(M_2) := \bigcup_{x_j \in V(G_1)} \sigma_i(M_2),$$

By Theorem 2.8, $\rho_i(M_1)$ is a nice perfect matching of $G_1^i$ and $\rho(M_1)$ is a nice perfect matching of $G_1 \square G_2$. Similarly, $\sigma(M_2)$ is also a nice perfect matching of $G_1 \square G_2$.

Conversely, since $E(G_1^i), \ldots, E(G_1^{n_1}), E(G_2^2), \ldots, E(G_2^{n_2})$ is a partition of $E(G_1 \square G_2)$, for any nice perfect matching $M$ of $G_1 \square G_2$ there is some $x_i$ or $v_j$ such that $M \cap E(G_2^j) \neq \emptyset$ or $M \cap E(G_1^i) \neq \emptyset$. If $M \cap E(G_2^j) \neq \emptyset$ for some $x_i$, then we have the following Claim.

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

![Fig. 6. Illustration for the proof of the Claim in Theorem 4.1](image)

Take an edge $f = (x_i, v_1)(x_i, v_2) \in M \cap E(G_2^j)$. Then $v_1v_2 \in E(G_2)$. If $n_2 = 2$, then $M = E(G_2^2) = \{f\}$ is a nice perfect matching of $G_2^j$. 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 $(x_i, v_2)(x_i, v_3) \in E(G_2^j)$. 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 2.8. So the other end-vertex of $g$ belongs to $V(G_2^2)$ (see Fig. 6), that is, $g \in E(G_2^2)$. Since $G_2^j \cong G_2$ is a connected graph, we can obtain that $M \cap E(G_2^j)$ is a perfect matching of $G_2^j$ in the above way. So $M \cap E(G_2^j)$ is a nice perfect matching of $G_2^j$ 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 $(x_i', v_1) \notin G_2^j$ is adjacent to $(x_i, v_1)$ in $G_1 \square G_2$ (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 $G_1 \square G_2$, the other end-vertex of $f'$ must be adjacent to $(x_i, v_2)$ by Theorem 2.8. So $f' = (x_i', v_1)(x_i, v_2) \in M \cap E(G_2^j)$. As the above proof, we can similarly show that $M \cap E(G_2^j)$ is a nice perfect matching of $G_2^j$. Since $G_1$ is connected, in an inductive way we can show that $M \cap E(G_2^j)$ is a nice perfect matching of $G_2^j$ for any $x_j \in V(G_1)$.

Notice that $\sigma_j^{-1}(f) = v_1v_2 = \sigma_j^{-1}(f')$. 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 2.8. So
\[ g' = (x'_1, v_3)(x'_4, v_4) \] since \( g' \in E(G_{2}^{2}) \). This implies that \( \sigma_g^{-1}(g') = v_3v_4 = \sigma_g^{-1}(g) \). In an inductive way, we can show that \( \sigma_g^{-1}(M \cap E(G_{2}^{2})) = \sigma_g^{-1}(M \cap E(G_{2}^{2})) \). Similarly, we also have \( \sigma_g^{-1}(M \cap E(G_{2}^{2})) = \sigma_g^{-1}(M \cap E(G_{2}^{2})) \) for any \( x_j \in V(G_1) \).

By this Claim, \( M_2 := \sigma_g^{-1}(M \cap E(G_{2}^{2})) \) is a nice perfect matching of \( G_2 \) with \( M = \sigma(M_2) \). If \( M \cap E(G_{2}^{2}) \neq \emptyset \), then we can similarly show that \( G_1 \) has a nice perfect matching \( M_1 \) with \( M = \rho(M_1) \). So \( \Phi^*(G_1 \square G_2) = \Phi^*(G_1) + \Phi^*(G_2) \).

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 \( G'_1 \square \cdots \square G'_k \) 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 [Zeng and Wei (1991)]( ), is the graph with vertex set \( V(Q_n,k) = V(Q_n) \) and edge set \( E(Q_n,k) = E(Q_n) \cup \{ (x_1x_2 \cdots x_{n-1}x_n, x_1x_2 \cdots x_{n-k}x_{n-k+1}x_{n-k+2} \cdots x_n : x_1x_2 \cdots x_n \in V(Q_n,k) \} \), 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 \( Q_n,k \cong FQ_{n-k} \), 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 \( Ad(Q_n,k) = n2^{n-2} \).

According to the above discussion, for any graph \( G \), we know that \( K_{m,m} \square G, K_{2m} \square G, Q_n \square G, FQ_n \square G \) and \( Q_n,k \square G \) 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 \( K_{m,m}, K_{2n}, Q_n, FQ_n, Q_n,k \) are extremal graphs. Two perfect matchings \( M_1 \) and \( M_2 \) of a graph \( G \) are called *equivalent* if there is an automorphism \( \varphi \) 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 \( f_{ij}(x_1x_2 \cdots x_{i-1}x_{i+1} \cdots x_{j-1}x_jx_{j+1} \cdots x_n) = x_1x_2 \cdots x_{i-1}x_jx_{i+1}x_{j+1}x_{j+2} \cdots x_n \) 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 2.3.
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 $u\bar{v}$ and $v\bar{u}$ 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 $\bar{u}\bar{v} \in Es$ 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, $V(Q_n^0) = \{x_1 \cdots x_{k-1}ix_{k+1} \cdots x_n : x_j = 0 \text{ or } 1, j = 1, \ldots, k-1, k+1, \ldots, n\}, i = 0, 1$. Since $M \cap E_k \neq \emptyset$, there is some edge $uv \in M \cap E_k$ with $u \in V(Q_n^0)$ and $v \in V(Q_n^1)$ for any vertex $v$ of $Q_n^0$ with $v$ and $w$ 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 $g = w\bar{v}$ 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 $f(E_i) = E_j$ 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 $V(Q_n^0) = \{ix_1x_2 \cdots x_n : x_j = 0 \text{ or } 1, j = 2, \ldots, n\}, i = 0, 1$. We define a bijection $f$ on $V(FQ_n)$ as follows:

$$f(x_1x_2 \cdots x_n) = \begin{cases} \bar{x}_1x_2 \cdots x_n, & \text{if } x_1x_2 \cdots x_n \in V(Q_n^0), \\ \bar{x}_1\bar{x}_2 \cdots \bar{x}_n, & \text{if } x_1x_2 \cdots x_n \in V(Q_n^1). \end{cases}$$

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 $Q_{n,k} = FQ_n \sqcap Q_k$, 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 $M'$ and $M''$, where $M' = \{\rho(M) : M \text{ is a nice perfect matching of } FQ_{n-k}\}$ and $M'' = \{\sigma(M) : M \text{ is a nice perfect matching of } Q_k\}$.

For $M'_1, M'_2 \in M'$, 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 $\varphi$ of $FQ_{n-k}$ such that $\varphi(M_1) = M_2$. Let $\varphi'(x, u) := (\varphi(x), u)$ for each vertex $(x, u)$ of $FQ_{n-k} \sqcap Q_k$. It is easy to check that $\varphi'$ is an automorphism of $Q_{n,k}$ and $\varphi'(M'_1) = M'_2$. By the
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 $FQ_{n-k} \square Q_{k-1}$, and $\sigma(E_1) = E(A, B)$. So $G - R$ has at least two components. Clearly $H - S$ is connected. So for any automorphism $\psi$ 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.

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

A nontrivial graph $G$ is said to be prime with respect to the Cartesian product if whenever $G \cong H \square R$, one factor is isomorphic to the complete graph $K_1$ and the other is isomorphic to $G$. Clearly, for $m \geq 3$ and $n \geq 2$, $K_m \square n$ 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 $\Theta_G$ if $d_G(x,u) + d_G(y,v) \neq d_G(x,v) + d_G(y,u)$. Notice that $\Theta_G$ is reflexive and symmetric, but need not to be transitive. We denote its transitive closure by $\Theta^*_G$. For an even cycle $C_{2n}$, $\Theta^*_C$ consists of all pairs of antipodal edges. Hence, $\Theta^*_C$ has $n$ equivalence classes and $\Theta_{C_{2n}} = \Theta^*_C$. For an odd cycle $C$, any edge of $C$ is in relation $\Theta$ with its two antipodal edges. So all edges of $C$ belong to an equivalence class with respect to $\Theta^*_C$. 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 $\Theta^*_C$, 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
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 \( j \)-th 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 \( \Theta_{FQ_n} \).

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 \ref{Theorem 5.7} (2). So \( C \) is a shortest odd cycle in \( FQ_n \). By Proposition \ref{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 \ref{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 \ref{Theorem 5.7} (3), there are two cases for the shortest \( uv \)-path in \( FQ_n \). If \( H_{Q_n}(u, v) \leq \left\lceil \frac{n}{2} \right\rceil \), then any shortest \( uv \)-path in \( FQ_n \) contains no complementary edges. So \( d_{FQ_n}(u, v) = d_{Q_n}(u, v) = d_{C_n}(u, v) \), \( d_{FQ_n}(u, v) = d_{Q_n}(u, v) = d_{C_n}(u, v) \). 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 \ref{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 \ref{Theorem 5.7} (2) as follows:

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

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 \( \Theta_{FQ_n} \). 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 \ref{Lemma 5.6}.

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 \ref{Proposition 4.3} it is interesting to characterize all the prime extremal graphs.

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