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. (2015)] introduced 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 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 graph as the smallest number of edges whose removal results in a subgraph with a unique perfect matching.
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, 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, $Af(G) \leq r(G)$.

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 $M$ (“×”).](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 2.3.

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 $G - (S \setminus \{e_1\})$ 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 $M$.

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 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 $M$, $A := V(G) \setminus A$. 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 $x_1 \cdots x_{i-1}x_i x_{i+1} \cdots x_n$ and $x_1 \cdots x_{i-1} \bar{x_i} x_{i+1} \cdots x_n$ 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 $y = \bar{x_1}x_2 \cdots x_n$, 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 $d_G(v)$. 
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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 $yu \in E(G)$, and $xv \in E(G)$ if and only if $yv \in E(G)$.

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 $yu \in E(G)$, and $xv \in E(G)$ if and only if $yv \in E(G)$ if and only if $yu \in E(G)$. Obviously, any two distinct $M$-alternating 4-cycles are compatible. Then

$$c'(M) \geq \frac{\sum_{wz \in M} c'_{wz}(M)}{2} = \frac{1}{2} \left[ (d_G(w) - 1) + (d_G(z) - 1) \right] = \frac{1}{2} \sum_{w \in V(G)} (d_G(w) - 1) = \frac{e(G) - \nu(G)}{2}.$$  

(2)

(1) $c'(M) \leq a_f(G, M) \leq A_f(G) \leq \frac{2e(G) - \nu(G)}{4}$. So $a_f(G, M) = \frac{2e(G) - \nu(G)}{4}$, 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 $\tilde{A} := V(G) \setminus A$. Then $(A, \tilde{A})$ is a partition of $V(G)$. Given any bijection $\omega : M \rightarrow \{1, \ldots, |M|\}$, 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 $A \cup \tilde{A}$. Clearly, if $e = xy \in M$, then $\omega(x) = \omega(y)$, otherwise, $\omega(x) \neq \omega(y)$. Set

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

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

Since $G - E_\omega^\tilde{A} \cup E(A)$ has a unique perfect matching $M$, $E_\omega^\tilde{A} \cup E(A)$ is an anti-forcing set of $M$ in $G$. Similarly, $E_\omega^\omega \cup E(\tilde{A})$ is also an anti-forcing set of $M$ in $G$. Since $M$ is a nice perfect matching of $G$, $a_f(G, M) = \frac{2e(G) - \nu(G)}{4}$. So $|E_\omega^\tilde{A} \cup E(A)| \geq \frac{2e(G) - \nu(G)}{4}$, $|E_\omega^{\omega} \cup E(\tilde{A})| \geq \frac{2e(G) - \nu(G)}{4}$. Since $|E_\omega^{\tilde{A}} \cup E(A)| + |E_\omega^{\omega} \cup E(\tilde{A})| = \nu(G) - |M| = e(G) - \nu(G) + \nu(G) = e(G)$. Hence $E_\omega^{\tilde{A}} \cup E(A)$ 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 $yu \in E(G)$, and $xv \in E(G)$ if and only if $yv \in E(G)$. It is sufficient to show that $xv \in E(G)$ implies $yu \in E(G)$. Given two bijections $\omega_1 : M \rightarrow \{1, \ldots, |M|\}$ and $\omega_2 : M \rightarrow \{1, \ldots, |M|\}$ 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 $\omega$, 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 $A' := A \setminus \{x, u\}$, $\tilde{A}' := \tilde{A} \setminus \{y, v\}$, $E_1^\omega := \{wz \in E(G) : \omega_1(w) > \omega_1(z), w \in A' \text{ and } z \in \tilde{A}'\}$. Then

$$E_1^\omega \cup E(\tilde{A}) = \{xv\} \cup E(\{y, v\}, A') \cup E_1^\omega \cup E(A) = \{xv\} \cup E_1^\omega \cup E(\tilde{A}) = (3)$$

By the above proof we know that both $E_1^{\tilde{A}} \cup E(A)$ and $E_1^{\omega} \cup E(\tilde{A})$ 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 \( yu \in E(G) \).

\[
\begin{align*}
M_1 & \quad M_2 & \quad H
\end{align*}
\]

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 \( Af(G) < \frac{2v(G)-v(G)}{4} \) 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 \( xy \alpha_M(x) \) and \( yx \alpha_M(y) \) 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 \( \alpha_M \) 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 \( G_i \) 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) \( G := G_1 + e + e' \), 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 \( \phi \) from \( V(M'_1) \) to \( V(M'_2) \) with \( w \in M'_1 \) 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 \( \phi \), 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 \( E' := \{u\phi(u) : u \in V(M'_1)\} \).

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 \( \phi' \), 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 \( M = \{e_1, e_2, \ldots, e_n\} \). 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 \( u_nv_i \) and \( v_nv_i \) for some \( i \in \{1, \ldots, n-1\} \), where \( u_iv_i = e_i \in M \). Let \( G'' = G' \circledast K_2 \) over

![Fig. 4.](image-url)
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 \( G \in \mathcal{P}' \).

\[ \square \]

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 \( \bar{E} := \{ \bar{x} : x = x_1x_2\ldots x_n, \bar{x} = \bar{x}_1\bar{x}_2\ldots \bar{x}_n \} \), \( \bar{x}_i := 1 - x_i \). 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 \( C := uxvyu \). 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. \( \square \)

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 \((x_i, v_j)\) of \( G \square H \), the subgraphs of \( G \square H \) induced by the vertex set \( \{(x, u) : x \in V(G)\} \) and the vertex set \( \{(x_i, v) : v \in V(H)\} \) are called a \( G \)-layer and an \( H \)-layer of \( G \square H \), and denoted by \( G^v \) and \( H^x \), respectively.
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 $\rho_{vi}$ from $G_1$ to $G_1^{vi}$ and an isomorphism $\sigma_{xj}$ from $G_2$ to $G_2^{xj}$: $\rho_{vi}(x) := (x, v_i)$ for any vertex $x$ of $G_1$ and $\sigma_{xj}(v) := (x, j)$ for any vertex $v$ of $G_2$. For any nice perfect matching $M_i$ of $G_i$, $i = 1, 2$, let

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

(4)

By Theorem 2.5, $\rho_{vi}(M_1)$ is a nice perfect matching of $G_1^{vi}$ 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 $E(G_1^{vi}), \ldots, E(G_1^{v_{n_2}}), E(G_2^{x1}), \ldots, E(G_2^{x_{n_1}})$ 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 $M \cap E(G_1^{x_j}) \neq \emptyset$ or $M \cap E(G_2^{v_i}) \neq \emptyset$. If $M \cap E(G_2^{v_i}) \neq \emptyset$ for some $x_i$, then we have the following Claim.

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

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

Take an edge $f = (x_1, v_1)(x_2, v_2) \in M \cap E(G_2^{v_1})$. Then $v_1v_2 \in E(G_2)$. If $n_2 = 2$, then $M \cap E(G_2^{v_1}) = \{f\}$ is a nice perfect matching of $G_2^{v_1}$. 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 $(x_1, v_2)(x_1, v_3) \in E(G_2^{v_1})$. Let $g$ be an edge of $M$ with an end-vertex $(x_1, v_3)$. Since $M$ is a nice perfect matching of $G$, the other end-vertex of $g$ must be adjacent to $(x_1, v_1)$ by Theorem 2.5. So the other end-vertex of $g$ belongs to $V(G_2^{v_3})$ (see Fig. 6), that is, $g \in E(G_2^{v_3})$. Since $G_2^{v_3} \cong G_2$ is a connected graph, we can obtain that $M \cap E(G_2^{v_i})$ is a perfect matching of $G_2^{v_i}$ in the above way. So $M \cap E(G_2^{v_i})$ is a nice perfect matching of $G_2^{v_i}$ 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 $(x_i', v_1) \notin G_2^{v_1}$ 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 2.5. So $f' = (x_i', v_1)(x_i', v_2) \in M \cap E(G_2^{v_1'})$. As the above proof, we can similarly show that $M \cap E(G_2^{v'_i})$ is a nice perfect matching of $G_2^{v'_i}$. Since $G_1$ is connected, in an inductive way we can show that $M \cap E(G_2^{v_i'})$ is a nice perfect matching of $G_2^{v_i'}$ for any $x_i \in V(G_1)$.

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
Theorem 5.2. Let \( g' \in E(G_2^{1'}) \). This implies that \( \sigma_{x_i}^{-1}(g') = v_3v_4 = \sigma_{x_i}^{-1}(g) \). In an inductive way, we can show that \( \sigma_{x_i}^{-1}(M \cap E(G_2^{1'})) = \sigma_{x_i}^{-1}(M \cap E(G_2^{1})) \). Similarly, we also have \( \sigma_{x_i}^{-1}(M \cap E(G_2^{3})) = \sigma_{x_i}^{-1}(M \cap E(G_2^{3})) \) for any \( x \in V(G_1) \).

By this Claim, \( M_2 := \sigma_{x_i}^{-1}(M \cap E(G_2^{3})) \) is a nice perfect matching of \( G_2 \) with \( M = \sigma(M_2) \). If \( M \cap E(G_2^{3}) \neq \emptyset \), 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 Zeng and Wei [1991], is the graph with vertex set \( V(Q_{n,k}) = V(Q_n) \) and edge set \( E(Q_{n,k}) = E(Q_n) \cup \{(x_1x_2 \cdots x_{n-1}x_n, \bar{x_1x_2 \cdots x_{n-k-1}x_{n-k}x_{n-k+1}x_{n-k+2} \cdots x_n} : x_1x_2 \cdots x_n \in V(Q_{n,k}) \} \), where \( 0 \leq k \leq n - 1 \). Clearly, \( Q_n \cong Q_{n,1} \) 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 \( K_{m,m} \Box G, K_{2m} \Box G, Q_n \Box G, FQ_n \Box G \) 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 \( \varphi \) 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 and Corollary 4.2, \( E_1, E_2, \ldots, E_n \) 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 \( f_{ij}(x_1 \cdots x_{i-1}x_{i+1} \cdots x_{j-1}x_jx_{j+1} \cdots x_n) = x_1 \cdots x_{i-1}x_jx_{i+1} \cdots x_{j-1}x_ix_{i+1} \cdots x_n \) 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 2.3.
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 $v\bar{w}$ be two distinct edges in $E_{n+1}$. Since any two 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 $\bar{u}\bar{w} \in E_s$ if and only if $\bar{u}\bar{w} \in E_s$ 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, $FQ_n \setminus (E_{n+1} \cup E_k)$ 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 in the other component. We denote the two components by $Q_0^n$ and $Q_1^n$, respectively. In fact, $V(Q_0^n) = \{x_1 \cdots x_{k-1}i x_{k+1} \cdots x_n : x_j = 0 \text{ or } 1, j = 1, \ldots, k-1, k+1, \ldots, n\}$, $i = 0, 1$. Since $M \cap E_k \neq \emptyset$, there is some edge $vw' \in M \cap E_k$ with $v \in V(Q_0^n)$ and $v' \in V(Q_1^n)$. For any vertex $w$ of $Q_0^n$ 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 $w\bar{w}'$ is not 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 $g = wz \in E(Q_0^n)$, then there are exactly three different bits in the strings of $z$ and $v'$. Since $\bar{w}$ and $v'$ are adjacent in $FQ_n$, the edge $\bar{w}v'$ is a complementary edge of $FQ_n$. So $n = 3$, a contradiction. Hence $g \in E_k$. Since $Q_0^n$ 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 $2 \leq n \leq 4$. 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, $FQ_n \setminus (E_1 \cup E_{n+1})$ has exactly two components each isomorphic to $Q_{n-1}$, denoted by $Q_0^n$ and $Q_1^n$. Set $V(Q_i^n) = \{i x_1 x_2 \cdots x_n : x_j = 0 \text{ or } 1, j = 2, \ldots, n\}$, $i = 0, 1$. We define a bijection $f$ on $V(FQ_n)$ as follows:

$$f(x_1 x_2 \cdots x_n) = \begin{cases} \bar{x}_1 x_2 \cdots x_n, & \text{if } x_1 x_2 \cdots x_n \in V(Q_0^n), \\ x_1 \bar{x}_2 \cdots \bar{x}_n, & \text{if } x_1 x_2 \cdots x_n \in V(Q_1^n). \end{cases}$$

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 $Q_{n,k} = FQ_{n-k} \sqcup Q_k$, 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 $\varphi$ of $FQ_{n-k}$ such that $\varphi(M_1) = M_2$. Let $\varphi'(x, u) := (\varphi(x), u)$ for each vertex $(x, u)$ of $FQ_{n-k} \sqcup Q_k$. 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 \( FQ_{n-k} \boxtimes Q_{k-1} \), 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. \( \square \)

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

A non-trivial graph \( G \) is said to be prime with respect to the Cartesian product if whenever \( G \cong H \boxtimes R \), 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 \( \Theta_G \) 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 be transitive. We denote its transitive closure by \( \Theta_G^{\ast} \). 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 \( \Theta_{C_{2n}} = \Theta_{C_{2n}}^{\ast} \). 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 \( \Theta^{\ast} \). 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 \( \Theta^{\ast} \), 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 \( H_{Q_n}(u, v) \leq \left\lfloor \frac{n}{2} \right\rfloor \), then any shortest \( uv \)-path in \( FQ_n \) contains no complementary edges. If \( H_{Q_n}(u, v) > \left\lfloor \frac{n}{2} \right\rfloor \), 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 \( Q_n \), let \( d_{Q_n}(x, y) = H_{Q_n}(x, y) \). For any shortest path \( P \) from \( x_1 x_2 \cdots x_n \) 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 \( d_F(u, v) \geq d_C(u, v) \) obviously holds. If \( d_F(u, v) = d_C(u, v) \) 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 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 \( v \) in \( C \). By Theorem 5.7 (3), there are two cases for the shortest \( uv \)-path in \( FQ_n \). If \( H_{Q_n}(u, v) \leq \lceil \frac{n}{2} \rceil \), 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 \( \Theta_{FQ_n} \). 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 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 4.3, it is interesting to characterize all the prime extremal graphs.

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References


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


