國 立 陽 明 交 通 大 學

應 用 數 學 系

博 士 論 文

A general version of Kelmans transformation and its applications on graphs and matrices

廣 義 凱 爾 曼 斯 轉 換 與 其 於 圖 與 矩 陣 之 應 用

研究生 ： 高至芃

指導教授 ： 翁志文 教授

中 華 民 國 一 百 一 十 一 年 六 月

A general version of Kelmans transformation and its applications on graphs and matrices
廣 義 凱 爾 曼 斯 轉 換 與 其 於 圖 與 矩 陣 之 應 用

Student: Louis Kao　　Advisor: Chih-wen Weng

研究生: 高至芃　　指導教授：翁志文 教授

國 立 陽 明 交 通 大 學
應 用 數 學 系

博 士 論 文

A Thesis
Submitted to Department of Applied Mathematics
College of Science
National Yang Ming Chiao Tung University
in Partial Fulfillment of Requirements
for the Degree of Doctor
in Applied Mathematics

June 2022
Hsinchu, Taiwan, Republic of China

中 華 民 國 一 百 一 十 一 年 六 月

廣義凱爾曼斯轉換
與其於圖與矩陣之應用

研究生: 高至芃　　　　　　　　指導教授: 翁志文 教授

國立陽明交通大學

應用數學系

摘要

簡單無向圖 G 的凱爾曼斯轉換是一個將點 b 的鄰居中不與點 a 相鄰的點改為連接至點 a 所形成的新圖 G_b^a。我們定義了廣義凱爾曼斯轉換，使其能夠被應用於非負矩陣上。我們證明了非負矩陣之廣義凱爾曼斯轉換的最大實特徵值不小於原矩陣的最大實特徵值。

混合圖是一種可同時包含有向邊與無向邊的簡單圖，因此其鄰接矩陣是不一定對稱的非負矩陣。運用廣義凱爾曼斯轉換，我們可以定義出混和圖 G 之凱爾曼斯轉換 G_b^a。在給定點數 n 與邊值 m 的混合圖所形成的集合 $\mathcal{G}(n,m)$ 中我們將大小關係 $G \leq G_b^a$ 拓展至一個偏序集 $(\mathcal{G}(n,m), \leq)$，並且給出此偏序集的一些子偏序集和弱子偏序集中的極大元素與極小元素。

我們也研究了可以涵蓋傳統鄰接矩陣理論和無號拉普拉斯矩陣理論的 A_α 矩陣理論。對於所有介於零和一之間的 α 值，我們給出了 $\mathcal{G}(n,m)$ 中一個混合樹 T 的 α 圖譜半徑 $\rho_\alpha(T)$ 的上界：

$$\rho_\alpha(T) \leq \frac{1}{2}\left(\alpha n + \sqrt{\alpha^2 n^2 - 4\alpha^2(n-1) + 4(1-\alpha)^2(m-n+1)}\right)$$

並分別刻畫出那些有最大及最小 α 圖譜半徑的混合樹。

在論文的最後部分我們使用了論文中提到的參數與工具，找出一些關於圖的漢彌爾頓性的充分條件。首先，我們證明了除了某些特定圖以外，只要 α 圖譜半徑足夠大就能保證一個圖為漢彌爾頓圖。另外對於笛卡爾積圖 $G_1 \Box G_2$，我們也給出兩組與 G_1 和 G_2 有關的條件去保證其漢彌爾頓性。我們可以完全決定偏序集 $\mathcal{G}(n,m)$ 中哪些極大圖具有漢彌爾頓性。最後，我們證明了在特定條件之下，圖 $P_n \Box H$ 的漢彌爾頓性可藉由 $P_n \Box H_b^a$ 的漢彌爾頓性獲得。

關鍵字: 凱爾曼斯轉換，混和圖，α 圖譜半徑，漢彌爾頓圖，笛卡爾積。

A general version of Kelmans transformation and its applications on graphs and matrices

Student: Louis Kao Advisor: Chih-wen Weng

Department of Applied Mathematics

National Yang Ming Chiao Tung University

abstract

A Kelmans transformation of a simple undirected graph G is a new graph G_b^a obtained from picking two vertices a, b in G and moving the edges incident on b and not on a to be incident on a. We generalize this concept to nonnegative matrices. With minor constraints, the first result of this thesis shows that the largest real eigenvalue of a nonnegative matrix will not decrease after a Kelmans transformation.

A mixed graph is a simple graph whose edges are either directed or undirected, and hence has a nonnegative adjacency matrix which is not necessary symmetric. The general version of the Kelmans transformation is applicable on the adjacency matrix of a mixed graph and this helps us to define the Kelmans transformation G_b^a of a mixed graph G. We extend the relation $G \leq G_b^a$ into a partial order on the set $\mathcal{G}(n, m)$ of the isomorphism classes of mixed graphs of order n and size m; then characterize the maximal/minimal elements in some of the subposets and weak subposets of $(\mathcal{G}(n, m), \leq)$.

We also apply the general version of the Kelmans transformation on the researches of the spectral theory of A_α-matrices, which combines the spectral theories of adjacency matrix and signless Laplacian matrix. In particular, we show that for $\alpha \in [0, 1]$ and a mixed tree T of order n and size m, the A_α-spectral radius $\rho_\alpha(T)$ satisfies

$$\rho_\alpha(T) \leq \frac{1}{2}\left(\alpha n + \sqrt{\alpha^2 n^2 - 4\alpha^2(n-1) + 4(1-\alpha)^2(m-n+1)}\right).$$

Base on the knowledges and tools we introduced, we give new sufficient conditions of the Hamiltonicity of graphs. First we prove that except some specific graphs, if the A_α-spectral radius of a graph is large enough, then the graph is Hamiltonian. Next, conditions for the graphs G_1 and G_2 are given to ensures that the Cartesian product graph $G_1 \square G_2$ is Hamiltonian. The Hamiltonicity of the maximal graphs in $\mathcal{G}(n, m)$ is also characterized. Finally, we show that with given constraints, the graph $P_n \square H$ is Hamiltonian whenever the graph $P_n \square H_b^a$ is Hamiltonian.

Keywords: Kelmans transformation, mixed graphs, A_α-spectral radius, Hamiltonian graphs, Cartesian product.

Contents

1 Introduction

Extremal graph theory is a branch of graph theory that studies the properties of graphs which are maximal or minimal in some prescribed parameters. For example, it is an old and famous problem to characterize the graphs with largest/smallest spectral radius within a specific family of graphs. The study of the adjacency matrix is called the *A-spectral theory* and the study of the signless Laplacian matrix is called the *Q-spectral theory*. In 2017, Nikiforov [33] introduced the theory of the A_α-matrix. The spectral theory of the A_α-matrix merges the A- and Q-spectral theories.

Many tools are used in the study of extremal graph theory. A tool called "Kelmans transformation" has been used frequently. Kelmans transformation of graphs reduces the possibilities of candidates of graphs with desired properties [29]. However, although the Kelmans transformation has been introduced [27] for about 40 years, it is only applied on a specific type of matrices associated to a specific type of graphs. This thesis studies a general version of the Kelmans transformation that applies to matrices.

1.1 Main results

In this section, we will state the main results of this thesis.

Let $C = (c_{ij})$ be a nonnegative square matrix of order n and the notation $[n]$ denote $\{1, 2, \ldots, n\}$. For $k \subseteq [n]$, let $C[k]$ denote the principal submatrix of C restricted to the entries in $|k| \times |k|$. Fix a 2-subset $\{a, b\}$ of $[n]$, and assume that C is symmetric on $\{a, b\}$, that is

$$C[a, b] = \begin{pmatrix} s & t \\ t & u \end{pmatrix}$$

for some scalars s, t, u. The Kelmans transformation of C from b to a is the following matrix of order n :

$$
\begin{array}{cc}
 & \begin{array}{ccccc} & j & & a & b \end{array} \\
C_b^a = \begin{array}{c} \\ i \\ \\ a \\ b \end{array} & \begin{bmatrix}
 & \vdots & & \vdots & \vdots \\
\cdots & c_{ij} & \cdots & c_{ia} + t_i & c_{ib} - t_i \\
 & \vdots & & \vdots & \vdots \\
\cdots & c_{aj} + s_j & \cdots & c_{aa} + k & c_{ab} \\
\cdots & c_{bj} - s_j & \cdots & c_{ba} & c_{bb} - k
\end{bmatrix},
\end{array}
$$

when t_i, s_j and k are nonnegative with some constraints. See Section 3.1 for details. We prove the following theorem in Chapter 3.

- **Theorem 3.1 :** *The largest real eigenvalue of C is no larger than the largest real eigenvalue of C_b^a.*

A *mixed graph* is a simple graph whose edges are either directed or undirected. When C is the adjacency matrix of a mixed graph G, in Section 4.1 we show that C_b^a is unique and is denoted by G_b^a. We show in Proposition 4.3 that the relation $G \le G_b^a$ extends to a partial order on the set $\mathcal{G}(n, m)$ of the isomorphism classes $[G]$, where G is a mixed graph of order n and size m. Let $\mathcal{T}(n, m)$ denote the subposet of $\mathcal{G}(n, m)$ restricting to mixed trees. We determined the maximal elements of $\mathcal{T}(n, m)$ in Proposition 4.5 and use this to show the following two theorems.

- **Theorem 5.6 :** *If $\alpha \in [0, 1]$ and $[T] \in \mathcal{T}(n, m)$, then the largest real eigenvalue $\rho_\alpha(T)$ of the A_α-matrix of T satisfies*

$$\rho_\alpha(T) \le \frac{1}{2}\left(\alpha n + \sqrt{\alpha^2 n^2 - 4\alpha^2(n-1) + 4(1-\alpha)^2(m-n+1)}\right).$$

Moreover, the mixed star of order n and size m with maximum out-degree $n-1$ attains the above upper bound.

- **Theorem 5.8 :** *Let* $[T] \in \mathcal{T}(n, m)$*, and set* $k = \lceil \frac{n}{2n-m-1} \rceil$*. Then*

$$\rho_\alpha(T) \geq \rho_\alpha(P_k),$$

where P_k *is a path of order* k*.*

The Kelmans transformation of undirected graphs defined by A.K. Kelmans [27] is a special case of our definition. Here we list our results related to the Kelmans transformation G_b^a from vertex b to a of a simple undirected graph G. Let $\mathcal{UG}(n, m)$ denote the subposet of $\mathcal{G}(n, 2m)$ restricting to undirected graphs. A version of Kelmans transformation restricted on trees is considered in Chapter 4.4. Denoted by $\partial_G(a, b)$ the distance of vertices a, b in G. Let $\mathcal{UT}(n)$ denote the subposet of $\mathcal{UG}(n, n-1)$ restricting to trees. We prove the following proposition.

- **Proposition 4.9 :** *Let* $[T] \in \mathcal{UT}(n)$*. Then* $[T]$ *is minimal in* $\mathcal{UT}(n)$ *if and only if the subgraph* T_ℓ *of* T *induced by* $\{v : \partial_T(v, \ell) \leq 3\}$ *is a path for each leaf* ℓ *in* T*.*

We consider another restricted version of the Kelmans transformation that each transformation G_b^a is applied only when the distance between a, b is 2. Let $(\mathcal{UG}(n, m), \leq_2)$ denote the weak subposet of $(\mathcal{UG}(n, m), \leq)$ restricting to the above version of the Kelmans transformation. We show that the maximal elements in $(\mathcal{UG}(n, m), \leq_2)$ do not contain six given induced subgraphs. The forbidden graphs are shown in Figure 5 in Chapter 4.4.

- **Proposition 4.11 :** *Let* $[G] \in \mathcal{UG}(n, m)$*. Then* $[G]$ *is maximal in* $(\mathcal{UG}(n, m), \leq_2)$ *if and only if* G *is* $\{P_5, C_5, K_1 \vee 2K_2, K_1 \vee P_4, \overline{P_5}, H_1\}$*-free.*

Based on the knowledges and tools we introduced in the first five chapters on the thesis, we give new sufficient conditions of the Hamiltonicity of graphs in Chapter 6.

The first one is a condition using A_α-spectral radius $\rho_\alpha(G)$ of a graph G.

- **Proposition 6.9 :** *If G is a graph on $n \geq 3$ vertices, $G \neq K_1 \vee (K_1 \cup K_{n-2})$, $G \neq K_2 \vee \overline{K_3}$, and the A_α-spectral radius $\rho_\alpha(G)$ satisfies*

$$\begin{cases} \rho_\alpha(G) > n - 1 - 2\alpha, & \text{if } \alpha \in [0, 1/2); \\ \rho_\alpha(G) > n - 3 + 2\alpha, & \text{if } \alpha \in [1/2, 1], \end{cases}$$

then G is Hamiltonian.

We prove the following theorem on the Cartesian product graph $G_1 \square G_2$.

- **Theorem 6.11 :** *Let G_1 be a traceable graph and G_2 a connected graph with maximum degree $\Delta(G_2)$. Statements (a) and (b) are given as following:*

  (a) G_2 has a perfect matching and G_1 contains at least $\Delta(G_2)$ vertices.

  (b) G_2 has a path factor and the order of G_1 is an even integer which is at least $4\Delta(G_2) - 2$.

  If one of (a), (b) holds, then the Cartesian product $G_1 \square G_2$ of G_1 and G_2 has a Hamiltonian cycle.

It will be explained in Chapter 6 that after reordering the vertices, the adjacency matrix of a maximal element in $\mathcal{UG}(n, m)$ is *stepwise*, i.e. $a_{i(j+1)} = 0$ if $a_{ij} = 0$ for $i \neq j$. Let M_n be the n-by-n binary matrix with $M_n(i, j) = 1$ if and only if $i \neq j, i + j \leq n + 2$. Then M_n is an example of stepwise adjacency matrix with $\frac{n^2+2n-3}{2}$ 1's when n is odd, and $\frac{n^2+2n-4}{2}$ 1's when n is even.

Write $A \geq B$ when the matrix $A - B$ is non-negative. An equivalent condition of Hamiltonicity of maximal elements in $\mathcal{UG}(n, m)$ is given as follows in Chapter 6.

- **Proposition 6.30 :** *Let $[G]$ be a maximal element in $\mathcal{UG}(n, m)$ with a stepwise adjacency matrix A. Then G is Hamiltonian if and only if $A \geq M_n$.*

We use the knowledges of Kelmans transformation and Cartesian product graph to deduce the following corollary.

- **Corollary 6.34 :** *Let H be a connected bipartite graph. Let n be an even integer and $n \geq 4\Delta(H) - 2$. If there exist $a, b \in V(H)$ such that $P_n \square H_b^a$ is Hamiltonian, then $P_n \square H$ is Hamiltonian.*

The contents of the following papers are included in this thesis :

1. L. Kao, C.-W. Weng, A note on the largest real eigenvalue of a nonnegative matrix, *Appl. Math. Sci.* 15(12) (2021) 553–557.

2. L. Kao, C.-W. Weng, The relation between Hamiltonian and 1-tough properties of the Cartesian product graphs, *Graphs Combin.* 37(3) (2021) 933-943.

3. L. Kao, Hamiltonian properties of Cartesian product graphs, Master Thesis, National Chaio Tung University, (2016) < https://hdl.handle.net/11296/q89fq7 >.

2 Preliminaries

In this chapter, we recall some definitions, notations and results on which our study is based.

2.1 Spectral theory

For a square matrix M over real numbers, the polynomial $\mathrm{char}(M) := \det(\lambda I - M)$ in λ is called the *characteristic polynomial* of M, where $\det(\lambda I - M)$ is the determinant of $\lambda I - M$. The following lemma is immediate from the definition of characteristic polynomial of M.

Lemma 2.1. *For an $n \times n$ nonnegative matrix M, if*

$$M = \begin{pmatrix} M_1 & M_2 \\ 0 & M_3 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} M_1 & 0 \\ M_2 & M_3 \end{pmatrix},$$

where M_1, M_3 are square matrices, then $\mathrm{char}(M) = \mathrm{char}(M_1) \cdot \mathrm{char}(M_2)$. ■

A *submatrix* of M restricted to the entries in $R \times L$ is a matrix obtained from M by removing rows and columns which are not in R and L, respectively. If $R = L$, then the submatrix is a *principal submatrix*, denoted by $M[R]$. For an $n \times n$ matrix M and a partition $\Pi = \{\pi_1, \pi_2 \dots, \pi_\ell\}$ of $\{1, 2, \dots, n\}$, the $\ell \times \ell$ matrix $\Pi(M) = (m'_{ab})$, where

$$m'_{ab} = \frac{1}{|\pi_a|} \sum_{i \in \pi_a, j \in \pi_b} m_{ij} \qquad (1 \le a, b \le \ell),$$

is called the *quotient matrix* of M with respect to Π. That is, the entries m'_{ab} of $\Pi(M)$ are equal to the average row sum of the $|\pi_a|$-by-$|\pi_b|$ submatrix of M restricted to the entries in $\pi_a \times \pi_b$. Furthermore, if $\sum_{j \in \pi_b} m_{ij} = m'_{ab}$ for all $1 \le a, b \le \ell$ and $i \in \pi_a$, then $\Pi(M)$ is called the *equitable quotient matrix* of M with respect to Π. For instance, the matrix

$$M' = \begin{pmatrix} 2 & 1 & 0 \\ 3 & 0 & 2 \\ 0 & 1 & 1 \end{pmatrix}$$

is the equitable quotient matrix of

$$M = \left(\begin{array}{ccc|c|cc} 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ \hline 1 & 1 & 1 & 0 & 1 & 1 \\ \hline 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{array}\right)$$

with respect to $\Pi = \{\{1,2,3\},\{4\},\{5,6\}\}$.

The *spectral radius* $\rho(M)$ of a square matrix M is defined to be the largest absolute value of its eigenvalues. Perron-Forbenius theorem shows that the spectral radius of a nonnegative square matrix is equal to its largest real eigenvalue. The following lemma is useful on the calculating of spectral radius. See [2, 8, 41] for recent proofs.

Lemma 2.2. *([2, Theorem 2.5]) If $\Pi(M)$ is an equitable quotient matrix of a nonnegative matrix M, then $\rho(M) = \rho(\Pi(M))$.* ■

For two matrices M, N of the same size, we use the notation $M \leq N$ if the matrix $N - M$ is nonnegative. The following is a well-known consequence of Perron−Frobenius theorem [6, Theorem 2.2.1].

Lemma 2.3. *If N is a nonnegative square matrix and M is a nonnegative matrix of the same size with $M \leq N$, or M is a nonnegative submatrix of N, then $\rho(M) \leq \rho(N)$.* ■

2.2 Graphs

A *graph G* is a triple consisting of a *vertex set $V(G)$*, an *edge set $E(G)$* and a relation that associates with each edge two vertices (not necessary distinct), called its *endpoints*. Based on different situations, the endpoints of an edge are either ordered or unordered. A *loop* is an edge that associates with only one endpoint. *Multiple edges* are edges associating with the same ordered/unordered pair of endpoints. A *simple graph* is a graph without loops and multiple edges. The graphs throughout this thesis are all simple. If the pair of the endpoints of an edge is an unordered pair $\{u, v\}$, then it is an *undirected edge*, denoted by uv. We say that u is *adjacent* to v if uv is an edge. If the pair of the endpoints of an edge is an ordered pair (u, v), then it is called a *directed edge* or an *arc*, denoted by $\overrightarrow{uv}$.

The *order* of a graph G is defined to be the number of vertices of G. A graph G is *isomorphic* to a graph H if there exists a bijection f between the vertex set of G and H such that u, v are endpoints of an undirected edge in $E(G)$ if and only if $f(u), f(v)$ are endpoints of an undirected edge in $E(H)$; and (u, v) is an ordered pair of the endpoints of a directed edge in $E(G)$ if and only if $(f(u), f(v))$ is an ordered pair of the endpoints of a directed edge in $E(H)$. Let $[G]$ denote the class of graphs that are isomorphic to G.

A *subgraph* of a graph G is a graph whose vertex set and edge set are subset of $V(G)$ and $E(G)$, respectively. For convenience, sometimes we use the edge $E(H)$ to denote the subgraph H of G. An *induced subgraph* H of a graph G is a subgraph of G such that $E(H)$ contains all the edges of G that have endpoints in $V(H)$. A graph G is called H*-free* if H is a graph and G doesn't contain an induced subgraph which is isomorphic to H. A *spanning subgraph* H of G is a subgraph H of G with $V(H) = V(G)$.

A graph is a *mixed graph* if for each pair of vertices u, v, at most one of $\overrightarrow{uv}, \overrightarrow{vu}$ and uv belongs to $E(G)$. From now on, for simplicity uv is referred to as an edge and $\overrightarrow{uv}$ as an arc. We define the *size* of a mixed graph G to be the number of arcs in $E(G)$ plus twice the number of undirected edges in $E(G)$.

Matrices are nice tools to represent graphs. For a graph with finite order n with vertex set $V(G)$ and edge set $E(G)$, the *adjacency matrix* $A = (a_{ij})$ is defined to be an n-by-n binary matrix with rows and columns indexed by $V(G)$ such that $a_{ij} = 1$ if and only if $ij \in E(G)$ or $\overrightarrow{ij} \in E(G)$. Notice that the adjacency matrix of a mixed graph is not always symmetric and the size of a mixed graph is the number of 1's in its adjacency matrix.

The *eigenvalues* of a graph is defined to be the eigenvalues of its adjacency matrix.

2.3 Undirected graphs

An *undirected graph* (or graph for short) is a mixed graph without arcs. The *complete graph* of order n, denote as K_n, is a graph whose vertices are pairwisely adjacent. The *complement* $\overline{G}$ of a graph G is a graph with vertex set $V(G)$ and $uv \in E(\overline{G})$ if and only if $uv \notin E(G)$ for distinct $u, v \in V(G)$.

Two vertices $u, v \in V(G)$ are called *connected* if there exists a sequence $u, v_1, \ldots, v_k = v$ of vertices in G such that every two consecutive vertices in the sequence are adjacent. If $u, v \in V(G)$ are connected, the smallest k above is called the *distance* of u and v, denoted by $\partial_G(u, v)$. Write $\partial_G(u, v) = \infty$ if u, v are not connected.

We call a graph to be *connected* if its vertices are pairwisely connected. A disconnected graph G contains several connected subgraphs and a connected subgraph is called a *component* of G if it is not a proper subgraph of any connected subgraph of G. The number of components in G is denoted by $c(G)$.

The *diameter* of G is defined to be $\max_{a,b\in V(G)} \partial(a, b)$. Note that the diameter of a disconnected graph is ∞. The *neighbor set* $N_G(v)$ of vertex v in G is the set $\{u : u \in V(G), \partial_G(u, v) = 1\}$ and the *closed neighbor set* $N_G[v]$ is defined to be $N_G(v) \cup \{v\}$. The *degree* $\deg_G(v)$ of vertex v in G is the number of neighbors of v in G, that is, $|N_G(v)|$. A vertex of degree 1 is called a *leaf*. The symbol $\partial(u, v), N(v), N[v]$ and $\deg(v)$ may also appear if the graph we discuss has no confusion.

A connected graph G with $|V(G)| - 1$ edges is a *tree*. A *path* of order n, denoted as P_n, is a graph whose vertices can be ordered such that two vertices are adjacent if and only if they are consecutive in the ordering. A path $v_1, v_2, \ldots, v_n$ together with an edge v_nv_1 is called a *cycle*. A graph G is *bipartite* if $V(G)$ is the union of two disjoint vertex sets X and Y, called *partite sets* of G, such that the subgraphs of G induced by X and

Y contain no edges, respectively. The *complete bipartite graph* is a bipartite graph such that two vertices are adjacent if they belong to different partite sets. Denote by $K_{n,m}$ the complete bipartite graph of partition sizes n and m. In particular, $K_{1,n-1}$ is called a *star* of order n.

The *join* of graphs G and H, denoted as $G \vee H$, is the graph obtained from G and H with vertex set $V(G \vee H) = V(G) \cup V(H)$, and edge set $E(G \vee H) = E(G) \cup E(H) \cup \{uv : u \in V(G), v \in V(H)\}$. The *Cartesian product graph* $G_1 \Box G_2$ of graphs G_1 and G_2 is a graph with vertex set $V(G_1 \Box G_2) = \{v_u \mid v \in V(G_1), u \in V(G_2)\}$, and edge set $E(G_1 \Box G_2) = \{v_u v_w \mid v \in V(G_1), uw \in E(G_2)\} \cup \{v_u w_u \mid u \in V(G_2), vw \in E(G_1)\}$.

The *underlying graph* of a mixed graph G is the undirected graph obtained from G by removing the directions of arcs. The *distance* $\partial(a, b)$ for vertices a, b in G is their distance in the underlying graph of G. The *mixed tree*, *mixed path*, *mixed star* are defined to be the mixed graphs whose underlying graphs are tree, path, and star, respectively.

2.4 Hamiltonicity and toughness

A graph is *Hamiltonian* if it contains a spanning cycle, and is *traceable* if it contains a spanning path.

For $S \subseteq V(G)$, let $G - S$ denote the subgraph of G induced on $V(G) - S$. To discuss the Hamiltonicity of graphs, another measure of graphs is usually considered. A graph G is *t-tough* if t is a rational number such that $|S| \geq t \cdot c(G - S)$ for any *cut set* S of G, i.e. $S \subseteq V(G)$ such that $G - S$ has $c(G - S)$ components with $c(G - S) \geq 2$. If G is not complete, the largest t makes G to be t-tough is called the *toughness* of G, denoted by $\tau(G)$. For convenience, we set $\tau(K_n) = \infty$.

Toughness is a non-decreasing (with respect to the number of edges) graph property. Therefore, a Hamiltonian graph is 1-tough since it contains a spanning cycle which is 1-tough. However, not all 1-tough graphs are Hamiltonian. Figure 1 gives a 1-tough

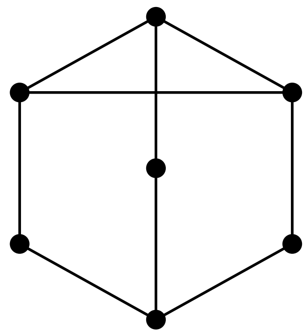


Figure 1: A 1-tough non-Hamiltonian graph with 7 vertices.

non-Hamiltonian graph of order 7.

The idea of graph toughness was first introduced by V. Chvátal in his 1973's seminal paper [11]. He conjectured that there exists a real number t_0 such that all t_0-tough graphs are Hamiltonian. This conjecture is still open. From papers [21] and [3], there are examples of non-Hamiltonian graphs with toughness greater than 1.25 and 2, respectively. On the other hand, for specific graph classes, there may exist a toughness bound to ensure the Hamiltonicity. For instance, [23] shows that every 10-tough chordal graphs are Hamiltonian.

Chvátal's Conjecture holds trivially for bipartite graphs by choosing $t_0 = 1 + \varepsilon$ for any $\varepsilon > 0$ since a bipartite graph has toughness at most 1. Hence the Hamiltonicity of a 1-tough bipartite graph deserves a further study. Contents related to Hamiltonicity are discussed in Chapter 6.

2.5 Partially ordered set

A *partially ordered set* (or called *poset*) $(P, \leq_P)$ is a set P with a relation $\leq_P$ on P satisfying:

- **Reflexivity :** $x \leq_P x$ for all $x \in P$.

- **Antisymmetry :** For all $x, y \in P$, if $x \leq_P y$ and $y \leq_P x$ then $x = y$.

- **Transitivity :** For all $x, y, z \in P$, if $x \leq_P y$ and $y \leq_P z$ then $x \leq_P z$.

When we call $(Q, \leq_Q)$ a *subposet* of $(P, \leq_P)$, we mean that for $x, y \in Q$ we have $x \leq_P y$ in P if and only if $x \leq_Q y$ in Q. A *weak subposet* $(Q, \leq_Q)$ of the poset $(P, \leq_P)$ is a poset such that $Q \subseteq P$ and if $x \leq_Q y$ then $x \leq_P y$ for $x, y \in Q$.

3 Kelmans transformations on nonnegative matrix

The Kelmans transformation, or called “shift transformation”[4, 7] or “compression operator”[24] is a transformation between undirected graphs, which is first defined by A.K. Kelmans [27]. In this chapter, we introduce a general version of the Kelmans transformation which is not limited on adjacency matrices of undirected graphs. The main theorem of the contents of this Chapter is Theorem 3.1.

3.1 Kelmans transformation of a nonnegative matrix

Use the notation $[n] = \{1, 2, \dots, n\}$. Let $C = (c_{ij})$ be a nonnegative square matrix of order n such that $c_{ab} = c_{ba}$ for some $a, b \in [n]$. For every $i, j \in [n] - \{a, b\}$, choose t_i and s_j such that $\max(0, c_{ib} - c_{ia}) \le t_i \le c_{ib}$ and $\max(0, c_{bj} - c_{aj}) \le s_j \le c_{bj}$ and choose k such that $\max(0, c_{bb} - c_{aa}) \le k \le c_{bb}$. We define a new matrix C_b^a of order n from C by shifting the portion t_i of c_{ib} to c_{ia}, the portion s_j of c_{bj} to c_{aj} and the portion k of c_{bb} to c_{aa} such that in the new matrix $C_b^a = (c'_{ij})$ have $c'_{ia} \ge c'_{ib}$ and $c'_{aj} \ge c'_{bj}$, where $i, j \in [n] - \{a, b\}$ and $c'_{aa} \ge c'_{bb}$. The following is an illustration of C_b^a:

$$C_b^a = \begin{array}{cc} & \begin{array}{ccccc} & j & & a & b \end{array} \\ \begin{array}{c} \\ i \\ \\ a \\ b \end{array} & \begin{bmatrix} & \vdots & & \vdots & \vdots \\ \cdots & c_{ij} & \cdots & c_{ia} + t_i & c_{ib} - t_i \\ & \vdots & & \vdots & \vdots \\ \cdots & c_{aj} + s_j & \cdots & c_{aa} + k & c_{ab} \\ \cdots & c_{bj} - s_j & \cdots & c_{ba} & c_{bb} - k \end{bmatrix} \end{array} \left\{ \begin{array}{l} c_{ab} = c_{ba}, \\ i, j \in [n] - \{a, b\}, \\ \max(0, c_{ib} - c_{ia}) \le t_i \le c_{ib}, \\ \max(0, c_{bj} - c_{aj}) \le s_j \le c_{bj}, \\ \max(0, c_{bb} - c_{aa}) \le k \le c_{bb}. \end{array} \right. \tag{1}$$

Formally, the matrix $C_b^a = (c'_{ij})$ is defined from $C = (c_{ij})$ by setting

$$c'_{ij} = \begin{cases} c_{ij}, & \text{if } i,j \in [n]-\{a,b\} \text{ or } (i,j) \in \{(a,b),(b,a)\}; \\ c_{ia}+t_i, & \text{if } j=a \text{ and } i \in [n]-\{a,b\}; \\ c_{ib}-t_i, & \text{if } j=b \text{ and } i \in [n]-\{a,b\}; \\ c_{aj}+s_j, & \text{if } i=a \text{ and } j \in [n]-\{a,b\}; \\ c_{bj}-s_j, & \text{if } i=b \text{ and } j \in [n]-\{a,b\}; \\ c_{aa}+k, & \text{if } i=j=a; \\ c_{bb}-k, & \text{if } i=j=b. \end{cases}$$

In the above setting, if $C = (c_{ij})$ is the adjacency matrix of an undirected graph G of order n (i.e., C is a symmetric binary matrix with zero diagonals), $t_i = \max(0, c_{ib} - c_{ia})$, $s_j = \max(0, c_{bj} - c_{aj})$ and $k = 0$ are uniquely determined, then the Kelmans transformation C' of C from b to a, independent of t_i, s_j and k, is essentially the Kelmans transformation of G defined by A.K. Kelmans [27]. The contents related to the Kelmans transformation on undirected graphs will be further discussed in Chapter 4.4.

3.2 The largest real eigenvalue of a nonnegative matrix

It is well known that a nonnegative matrix has a real eigenvalue. P. Csikvári [13] proved that the largest real eigenvalue will not be decreased after a Kelmans transformation of an undirected graph. His method uses the Rayleigh quotient and can be directly extended to any symmetric matrices. Here we give a generalization of this result to a nonnegative matrix which is not necessary to be symmetric.

Theorem 3.1. *Let $C = (c_{ij})$ denote a nonnegative square matrix of order n such that $c_{ab} = c_{ba}$ for some $1 \le a, b \le n$. Choose k, t_i, s_j for $i, j \in [n] - \{a, b\}$ that satisfying (1). Let $C' = C_b^a(t_i; s_j; k)$ be the Kelmans transformation from b to a with respect to $(t_i; s_j; k)$. Then the largest real eigenvalue of C is no greater than the largest real eigenvalue of C'.*

Before proving Theorem 3.1, we first observe that the symmetric condition for C on $\{a, b\}$ in Theorem 3.1 is necessary by the following counterexample.

Example 3.2. Consider the 4×4 matrices

$$C = \begin{pmatrix} 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \end{pmatrix}, \quad C' = \begin{pmatrix} 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \end{pmatrix}.$$

The matrix C' is obtained from C by applying Kelmans transformation from 4 to 3 with respect to $t_1 = 0$, $t_2 = 1$ and $s_1 = s_2 = 0$, while the matrix C is not symmetric on $\{3, 4\}$. By direct computing, the largest real eigenvalue of C is closed to 2.234 which is strictly greater than 2.148, the approximate of the largest real eigenvalue of C'.

It is well-known that the largest real eigenvalue of a nonnegative matrix is associated with a nonnegative eigenvector, called *Perron vector*. Moreover, if the matrix is irreducible then its Perron vector is positive (e.g., [6, Theorem 2.2.1]). Our proof of Theorem 3.1 utilizes Perron vectors in a way inspired by [9].

Now we shall introduce a few basic properties of Kelmans transformation of nonnegative matrices for later use. Recall that for a nonnegative square matrix M, $\rho(M)$ is the largest real eigenvalue of M.

Let I_n denote the identity matrix of order n and E_{ij} denote the binary matrix of order n which has a unique 1 in the position ij. Note that $(I_n + E_{ij})^{-1} = I_n - E_{ij}$ and $((I_n + E_{ij})^{-1})^t = ((I_n + E_{ij})^t)^{-1}$.

Lemma 3.3. *Let $C = (c_{ij})$ denote a nonnegative square matrix of order n such that C is symmetric on $\{a, b\}$ for some $1 \leq a, b \leq n$. For every pair $i, j \in [n] - \{a, b\}$, choose t'_i, s'_j such that $\max(0, c_{ib} - c_{ia}) \leq t'_i \leq c_{ib}$ and $\max(0, c_{bj} - c_{aj}) \leq s'_j \leq c_{bj}$, and set $t''_i = c_{ia} - c_{ib} + t_i$ and $s''_j = c_{aj} - c_{bj} + s_j$. Choose k' such that $\max(0, c_{bb} - c_{aa}) \leq k' \leq c_{bb}$ and set $k'' = c_{aa} - c_{bb} + k'$. Then the following (i)-(iii) hold.*

(i) $\max(0, c_{ia} - c_{ib}) \leq t''_i \leq c_{ia}$, $\max(0, c_{aj} - c_{bj}) \leq s''_j \leq c_{aj}$ *and* $\max(0, c_{aa} - c_{bb}) \leq k'' \leq c_{aa}$*;*

(ii) If C' (resp. C'') is the Kelmans transformation from b to a (resp. from a to b) with respect to t'_i,s'_j and k' (resp. with respect to t''_i,s''_j and k''''), then $\rho(C') = \rho(C'')$;

(iii) As the notation C' in (ii), we have $(I_n + E_{ba})C(I_n + E_{ba})^t \leq (I_n + E_{ba})C'(I_n + E_{ba})^t$.

Proof. (i) Since $t''_i = c_{ia} - c_{ib} + t'_i$ and

$$\max(0, c_{ia} - c_{ib}) = c_{ia} - c_{ib} + \max(0, c_{ib} - c_{ia}) \leq c_{ia} - c_{ib} + t'_i \leq c_{ia},$$

we have $\max(0, c_{ia} - c_{ib}) \leq t''_i \leq c_{ia}$. Similarly, we have $\max(0, c_{aj} - c_{bj}) \leq s''_j \leq c_{aj}$ and $\max(0, c_{aa} - c_{bb}) \leq k'' \leq c_{aa}$.

(ii) From the definition of $C' = (c'_{ij})$ and $C'' = (c''_{ij})$, we know $C''[b, a] = C'[a, b]$, $C''[[n] - \{a, b\}] = C'[[n] - \{a, b\}]$,

$$\begin{aligned} c''_{ib} =& c_{ib} + t''_i = c_{ib} + c_{ia} - c_{ib} + t_i = c'_{ia}, \\ c''_{ia} =& c_{ia} - (c_{ia} - c_{ib} + t_i) = c'_{ib}, \end{aligned}$$

and similarly $c''_{bj} = c'_{aj}$, $c''_{aj} = c'_{bj}$ for $i, j \in [n] - \{a, b\}$. This shows that $C'' = P^{-1}C'P$, where $P = I - E_{aa} - E_{bb} + E_{ab} + E_{ba}$. Thus $\rho(C') = \rho(C'')$.

(iii) The Kelmans transformation from b to a moves a nonnegative portion of row b of C to row a, but the multiplication of $(I_n + E_{ba})$ from the left will add the whole row a into the row b. Similarly for the column part. Hence (iii) follows. ■

3.3 The proof of Theorem 3.1

Let C and C' be as described in the assumption of Theorem 3.1. Recall that C is symmetric on $\{a, b\}$, which means

$$C[a, b] = \begin{pmatrix} s & t \\ t & u \end{pmatrix}.$$

To prove $\rho(C) \leq \rho(C')$ we might assume $\min(s,u) \geq t$, since if we know this and $\min(s,u) < t$ then applying the matrix $C + (t - \min(s,u))I_n$ as the role of C and considering the corresponding Kelmans transformation $C' + (t - \min(s,u))I_n$, we still have

$$\begin{aligned}\rho(C) &= \rho(C + (t - \min(s,u))I_n) - (t - \min(s,u)) \\ &\leq \rho(C' + (t - \min(s,u))I_n) - (t - \min(s,u)) = \rho(C').\end{aligned}$$

Let row vector $w^t = (w_i)$ denote the left Perron vector for $\rho(C)$ of C. We first assume $w_a \geq w_b$. Set $v^t = w^t Q^{-1}$, where $Q = I_n + E_{ba}$. Thus

$$v^t QC = w^t C = \rho(C) w^t = \rho(C) v^t Q. \tag{2}$$

Note that v is nonnegative since $v_i = w_i \geq 0$ for $i \neq a$ and $v_a = w_a - w_b \geq 0$.

For $\varepsilon > 0$, let $C'^{\varepsilon} = C' + \varepsilon J_n$, where J_n is the matrix of order n with entries all 1's. By Lemma 3.3(iii) and using $QC'Q^t \leq QC'^{\varepsilon}Q^t$, we have

$$QCQ^t \leq QC'^{\varepsilon}Q^t. \tag{3}$$

From the constriction of C'^{ε} and the assumption $\min(s,u) \geq t$ in the beginning, the matrix $(Q^t)^{-1}C'^{\varepsilon}Q^t$ is nonnegative. Let u^{ε} denote a right Perron vector for $(Q^t)^{-1}C'^{\varepsilon}Q^t$. Since C'^{ε} and $(Q^t)^{-1}C'^{\varepsilon}Q^t$ are similar, we have $\rho(C'^{\varepsilon}) = \rho((Q^t)^{-1}C'^{\varepsilon}Q^t)$ and $(Q^t)^{-1}C'^{\varepsilon}Q^t u^{\varepsilon} = \rho(C'^{\varepsilon})u^{\varepsilon}$, which implies

$$C'^{\varepsilon}Q^t u^{\varepsilon} = \rho(C'^{\varepsilon})Q^t u^{\varepsilon}. \tag{4}$$

Because of the irreducibility of C'^{ε}, $Q^t u^{\varepsilon} > 0$.

Multiplying the nonnegative vector u^{ε} from the right to both terms of (3) and applying (4),

$$QCQ^t u^{\varepsilon} \leq QC'^{\varepsilon}Q^t u^{\varepsilon} = \rho(C'^{\varepsilon})QQ^t u^{\varepsilon}. \tag{5}$$

Multiplying the nonnegative row vector v^t from the left to the first and last terms in (5) and using (2), we have

$$\rho(C)v^t QQ^t u^{\varepsilon} = v^t QCQ^t u^{\varepsilon} \leq \rho(C'^{\varepsilon})v^t QQ^t u^{\varepsilon}. \tag{6}$$

As $w^t = v^t Q$ nonnegative and $Q^t u^\varepsilon$ positive, $v^t Q Q^t u^\varepsilon$ is positive. Deleting the positive term $v^t Q Q^t u^\varepsilon$ from both sides of (6), we have $\rho(C) \leq \rho(C'^\varepsilon)$ for any $\varepsilon > 0$ and by continuity

$$\rho(C) \leq \lim_{\varepsilon \to 0^+} \rho(C'^\varepsilon) = \rho(C').$$

Next assume $w_b \geq w_a$. Let C'' denote the Kelmans transformation of C from a to b with respect to $c_{ia} - c_{ib} + t_i$ and $c_{aj} - c_{bj} + s_j$. By the previous case, we have $\rho(C) \leq \rho(C'')$, and by Lemma 3.3(ii), $\rho(C'') = \rho(C')$. Hence $\rho(C) \leq \rho(C')$. ∎

4 Kelmans transformations on mixed graphs

In this chapter, the general Kelmans transformation is applied on mixed graphs. We use the general Kelmans transformation to define poset structures on mixed graphs and mixed trees.

4.1 Kelmans transformations on mixed graphs

As in the case of undirected graph, if C in Theorem 3.1 is the adjacency matrix of a mixed graph G and assume that C_b^a is also an adjacency matrix of some mixed graph, then $t_i, s_i \in \{0,1\}$ and $k = 0$ are uniquely determined from C. We use G_b^a to denote the mixed graph whose adjacency matrix is C_b^a and called G_b^a the *Kelmans transformation* of mixed graph G from b to a. Notice that when the notation G_b^a appears, we always assume that $a, b \in V(G)$ are distinct and have no arc, i.e. $\overrightarrow{ab} \notin E(G)$ and $\overrightarrow{ba} \notin E(G)$.

For a mixed graph G, let $N_G^+(u) := \{v\colon \overrightarrow{uv} \in E(G) \text{ or } uv \in E(G)\}$ be the set of *out-neighbors* of u, $N_G^-(u) := \{v\colon \overrightarrow{vu} \in E(G) \text{ or } uv \in E(G)\}$ be the set of *in-neighbors* of u, and $N_G(u) := N_G^+(u) \cup N_G^-(u)$ be the set of *neighbors* of u. The number $d_G^+(u) := |N_G^+(u)|$ is called the *out-degree* of u in G, and the number $d_G(u) := |N_G^+(u)| + |N_G^-(u)|$ is called the *degree* of u in G. The sequence $d(G) := (d_G(u))_{u \in V(G)}$ in descending order is called the *degree sequence* of G.

For the Kelmans transformation G_b^a of a mixed graph G,

$$N_{G_b^a}^+(a) = N_G^+(a) \cup N_G^+(b), \quad N_{G_b^a}^-(a) = N_G^-(a) \cup N_G^-(b),$$

$$N_{G_b^a}^+(b) - \{a\} = N_G^+(a) \cap N_G^+(b), \quad N_{G_b^a}^-(b) - \{a\} = N_G^-(a) \cap N_G^-(b).$$

Figure 2 shows how the Kelmans transformation on mixed graphs works.

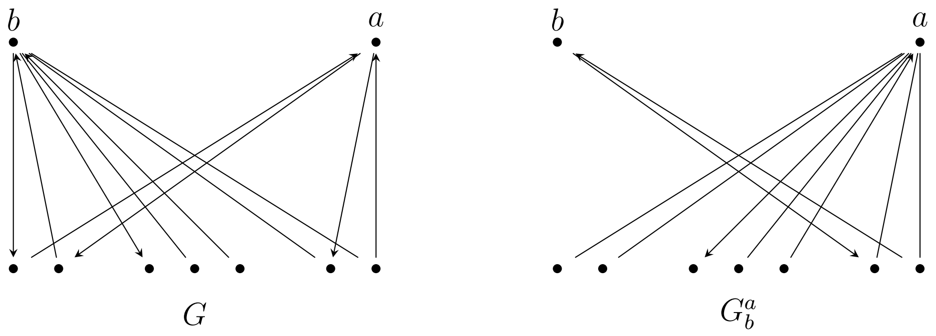


Figure 2: Kelmans transformation on mixed graph G.

Lemma 4.1. *Let G be a mixed graph and distinct $a, b \in V(G)$ have no arc. Then the following (i)–(ii) hold.*

(i) The involution $f : V(G_b^a) \to V(G_a^b)$ defined by

$$f(x) = \begin{cases} a, & \text{if } x = b; \\ b, & \text{if } x = a; \\ x, & \text{otherwise} \end{cases}$$

is a graph isomorphism from G_b^a to G_a^b.

(ii) In dictionary order, $d(G_b^a) \geq d(G)$. Moreover, the following (a)–(c) are equivalent.

(a) $d(G_b^a) = d(G)$;

(b) G is isomorphic to G_b^a;

(c) $N_G^+(a) - \{b\} \subseteq N_G^+(b) - \{a\}$ and $N_G^-(a) - \{b\} \subseteq N_G^-(b) - \{a\}$; or $N_G^+(b) - \{a\} \subseteq N_G^+(a) - \{a\}$ and $N_G^-(b) - \{a\} \subseteq N_G^-(a) - \{b\}$.

Proof. Excluding the two vertices a, b which are either with an undirected edges or without any directed arcs by the assumption, we have the following three observations of neighbor sets from the definition of Kelmans transformation on G from b to a. (1) the set of out-neighbors (resp. in-neighbors) of b in G_b^a is the union of the set of out-neighbors (resp. in-neighbors) of a in G and the set of out-neighbors (resp. in-neighbors) of b in G; (2) the set of out-neighbors (resp. in-neighbors) of a in G_b^a is the intersection of set of the out-neighbors (resp. in-neighbors) of a in G and the set of out-neighbors (resp. in-neighbors) of b in G; (3) the set of out-neighbors (resp. in-neighbors) of $x \neq a, b$ in G_b^a is the same as that in G. From the above three observations, we find that vertices a, b, x in G_b^a play the role of b, a, x respectively in G_a^b. This proves (i).

(ii) In the proof of (i), we also have $d_G(x) = d_{G_b^a}(x)$ for $x \in V(G) - \{a, b\}$ and in dictionary order $(d_{G_b^a}(a), d_{G_b^a}(b)) \geq (\max(d_G(a), d_G(b)), \min(d_G(a), d_G(b)))$, together implying $d(G_b^a) \geq d(G)$. Next we prove that (a), (b) and (c) are equivalent.

((b) $\Rightarrow$ (a)) This is clear.

((a) $\Rightarrow$ (c)) Suppose $d(G_b^a) = d(G)$. From the proof of (ii) above, we know that $\{d_G(a), d_G(b)\} = \{d_{G_b^a}(a), d_{G_b^a}(b)\}$. If $d_G(a) = d_{G_b^a}(b)$ then $d_G(b) = d_{G_b^a}(a) \geq d_{G_b^a}(b) = d_G(a)$, which implies $N_G^+(a) - \{b\} \subseteq N_G^+(b) - \{a\}$ and $N_G^-(a) - \{b\} \subseteq N_G^-(b) - \{a\}$. If $d_G(a) = d_{G_b^a}(a)$ then $d_G(b) = d_{G_b^a}(b)$, which implies $N_G^+(b) - \{a\} \subseteq N_G^+(a) - \{b\}$ and $N_G^-(b) - \{a\} \subseteq N_G^-(a) - \{b\}$.

((c) $\Rightarrow$ (b)) If $N_G^+(a) - \{b\} \subseteq N_G^+(b) - \{a\}$ and $N_G^-(a) - \{b\} \subseteq N_G^-(b) - \{a\}$ then $G = G_a^b$ and the later is isomorphic to G_b^a by (i). If $N_G^+(b) - \{a\} \subseteq N_G^+(a) - \{b\}$ and $N_G^-(b) - \{a\} \subseteq N_G^-(a) - \{b\}$ then $G = G_b^a$. ∎

4.2 Poset of mixed graphs

For a mixed graph G of order n and size m, let $[G]$ denote the set of mixed graphs that are isomorphic to G. Let

$$\mathcal{G}(n, m) := \{[G] : G \text{ is a mixed graph of order } n \text{ and size } m\}. \tag{7}$$

We will define a reflexive and transitive relation $\leq$ in $\mathcal{G}(n, m)$ as follows.

Definition 4.2. Let $\leq$ be the relation in $\mathcal{G}(n, m)$ such that for all $[G], [H] \in \mathcal{G}(n, m)$,

$[G] \le [H]$ if and only if H is isomorphic to G, or H is isomorphic to a graph which is obtained from G by a finite sequence of Kelmans transformations.

Proposition 4.3. *$(\mathcal{G}(n,m), \le)$ is a partially ordered set (poset).*

Proof. The relation $\le$ is reflexive and transitive from its definition, so we only need to prove the anti-symmetric property. Suppose $[G] \le [H]$ and $[H] \le [G]$, where $[G], [H] \in G(n,m)$. Then $d(G) \le d(H) \le d(G)$ by Lemma 4.1(ii). Hence $d(G) = d(H)$. By Lemma 4.1(ii)(a)$\Rightarrow$(b), we have $[G] = [H]$. ∎

4.3 Poset of mixed trees

Let $n, m \in \mathbb{N}$ with $n-1 \le m \le 2n-2$,

$$\mathcal{T}(n,m) := \{[T] \in \mathcal{G}(n,m) \colon T \text{ is a mixed tree}\}.$$

The set $\mathcal{T}(n,m)$ is not closed under Kelmans transformations. We need the following lemma.

Lemma 4.4. *Let $[T] \in \mathcal{T}(n,m)$ with distinct $a, b \in V(T)$ having no arc. Then $[T^a_b] \in \mathcal{T}(n,m)$ if and only if $ab \in E(T)$ or $\partial(a,b) = 2$ and the unique vertex $x \in V(T)$ with $\partial(a,x) = \partial(x,b) = 1$ satisfying one of the conditions : (i) $ax \in E(T)$ is an undirected edge, (ii) $xb \in E(T)$ is an undirected edge, (iii) $\overrightarrow{ax}, \overrightarrow{bx} \in E(T)$ are arcs or (iv) $\overrightarrow{xa}, \overrightarrow{xb} \in E(T)$ are arcs.*

Proof. The assumption implies $\partial(a,b) \ge 1$ and if $\partial(a,b) = 1$ then $ab \in E(T)$ is an undirected edge. If $\partial(a,b) = 2$ and the necessary condition about x fails, then a, b belong to different components of the underlying graph of T^a_b, so T^a_b is not a mixed tree. If $\partial(a,b) \ge 3$ then the underlying graph of T^a_b contains a cycle of order $\partial(a,b)$, so T^a_b is not a mixed tree.

On the other hand, it is straightforward to observe that $[T^a_b] \in \mathcal{T}(n,m)$ when a, b satisfy the conditions. ∎

We use the notation $a{-}b$, $a{-}x{-}b$, $a{-}x \to b$, $a{-}x \leftarrow b$, $a \leftarrow x{-}b$, $a \to x{-}b$, $a \to x \leftarrow b$ and $a \leftarrow x \to b$ to denote the eight situations in the necessary condition of Lemma 4.4. We give $\mathcal{T}(n,m)$ a poset structure by extending $[T] \leq [T_b^a]$ for any $[T] \in \mathcal{T}(n,m)$ and any $a, b \in V(T)$ that satisfy one of the eight situations.

Proposition 4.5. *Let $[T] \in \mathcal{T}(n,m)$. Then $[T]$ is a maximal element in $\mathcal{T}(n,m)$ if and only if T is a mixed star or T is a mixed tree without undirected edges (i.e. $m = n-1$) and whenever the subgraph $a \to x \leftarrow b$ or $a \leftarrow x \to b$ appears in T, one of a and b is a leaf.*

Proof. ($\Leftarrow$) If T is a mixed star, and one of $a-b$, $a-x \to b$, $a-x \leftarrow b$, $a \leftarrow x-b$, $a \to x-b$, $a \to x \leftarrow b$ and $a \leftarrow x \to b$ appearing in T, then one of a or b is a leaf, so Lemma 4.1(ii,c) with $G = T$ holds, which implies that T_b^a is isomorphic to T. If T is a mixed tree without undirected edges, then we only need to consider $a \to x \leftarrow b$ and $a \leftarrow x \to b$ in T. By the assumption a or b is a leaf and by the same reason as above, T_b^a is isomorphic to T. Hence in both cases, $[T]$ is a maximal element in $\mathcal{T}(n,m)$.

($\Rightarrow$) Let $[T]$ be a maximal element in $\mathcal{T}(n,m)$ such that T is not a mixed star, so T has diameter at least 3. Keeping in mind that the maximality of $[T]$ implies that Lemma 4.1(ii,c) with $G = T$ holds for $a, b \in V(T)$ satisfying the necessary conditions $a-b$, $a-x \to b$, $a-x \leftarrow b$, $a \leftarrow x-b$, $a \to x-b$, $a \to x \leftarrow b$ or $a \leftarrow x \to b$ of Lemma 4.4, thus at least one of a or b is a leaf. To exclude the situations $a-b$, $a-x \to b$, $a-x \leftarrow b$, $a \leftarrow x-b$ and $a \to x-b$, on the contrary, suppose that T contains an undirected edge uv with leaf u. Since the diameter of T is at least 3, we have another two vertices $y, z \in V(T)$ such that $\partial(v,y) = \partial(y,z) = 1$ and $\partial(u,z) = 3$. Since v, y are not leaves in T, they have an arc, say $v \to y$ (similar for $v \leftarrow y$) in $E(T)$. Hence $T_y^u \in \mathcal{T}(n,m)$ is well-defined, $v \in (N_T^+(v) - \{y\}) - (N_T(y) - \{u\})$, and $z \in N_T(y) - N_T(u)$, a contradiction to the maximality of $[T]$. Thus T has no undirected edges. ∎

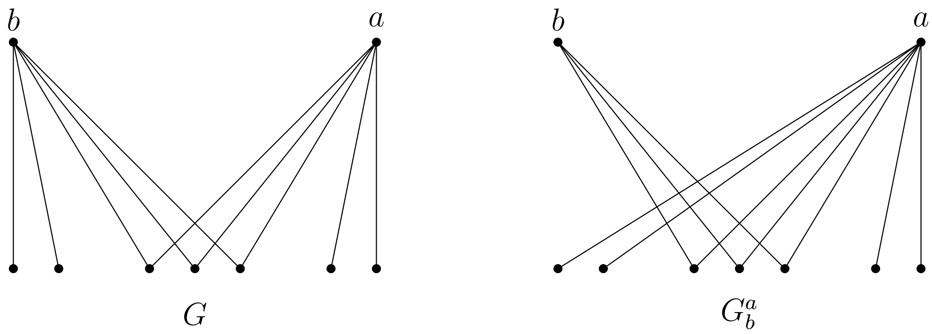


Figure 3: Kelmans transformation on an undirected graph G.

4.4 Kelmans transformations on undirected graphs

Recall that the Kelmans transformation on undirected graphs, defined by A.K. Kelmans [27], is a special case of our definition. In this chapter, we give some combinatorial results about the Kelmans transformation on undirected graphs.

Let G be an undirected graph, then the *Kelmans transformation* G_b^a is an undirected graph with vertex set $V(G)$ and edge set $E(G) \cup \{av : v \in N_G(b) \backslash N_G(a)\} \backslash \{bv : v \in N_G(b) \backslash N_G(a)\}$. Equivalently, $N_{G_b^a}(b) = N_G(b) \cap N_G[a], N_{G_b^a}(a) = N_G(b) \cup N_G(a) \backslash \{a\}$ and $N_{G_b^a}(v) \backslash \{a, b\} = N_G(v) \backslash \{a, b\}$ for all $v \neq a, b$. Figure 3 shows how the Kelmans transformation works.

It has been proved in [13] that the spectral radius of a graph is non-decreasing after any Kelmans transformation. In [24], the affects of Kelmans transformations on parameters of graphs, including vertex connectivity, edge connectivity, toughness, edge toughness, scattering number and binding number have been studied.

As shown in Figure 4, the Kelmans transformation G_b^a of a connected graph G is not necessary connected. In graph theory, the properties of a disconnected graph is usually combined by the properties from each of its components. Hence we focus on connected graphs in the discussions of graphs. To keep the graph connected, we need the following lemma :

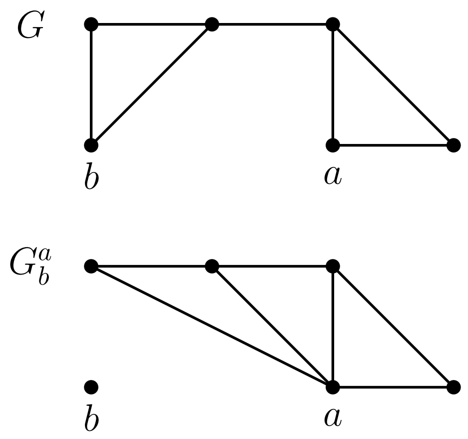


Figure 4: An example that G_b^a is not connected where G is connected.

Lemma 4.6. *If G is connected and $\partial_G(b,a) \leq 2$, then G_b^a is connected.*

Proof. Observe that the degree of each vertex is non-decreasing from G to G_b^a except b. Let G be connected. Since $\deg_{G_b^a}(b) = |N_G(b) \cap N_G(a)| \geq 1$ for $\partial_G(b,a) = 2$ and $a \in N_{G_b^a}(b)$ for $\partial_G(b,a) = 1$, G_b^a is connected. ∎

For an undirected graph G of order n with m edges, let $[G]$ denote the set of undirected graphs that are isomorphic to G. Let

$$\mathcal{UG}(n,m) := \{[G] \;:\; G \text{ is an undirected graph of order } n \text{ with } m \text{ edges}\}.$$

Define a reflexive and transitive relation $\leq$ in $\mathcal{UG}(n,m)$ as follows.

Definition 4.7. Let $\leq$ be the relation in $\mathcal{UG}(n,m)$ such that for all $[G],[H] \in \mathcal{UG}(n,m)$, $[G] \leq [H]$ if and only if H is isomorphic to G, or H is isomorphic to a graph which is obtained from G by a finite sequence of Kelmans transformations.

Since undirected graphs are also mixed graphs, from Proposition 4.3 we know that $(\mathcal{UG}(n,m), \leq)$ forms a subposet of $(\mathcal{G}(n,2m), \leq)$.

Let

$$\mathcal{UT}(n) := \{[T] \,:\, T \text{ is an undirected tree of order } n\}.$$

Then $\mathcal{UT}(n) = \mathcal{T}(n, 2n-2)$ and the following lemma is a straightforward consequence of Lemma 4.4.

Lemma 4.8. *Let* $[T] \in \mathcal{UT}(n)$. *Then* $[T^a_b] \in \mathcal{UT}(n)$ *if and only if* $ab \in E(T)$ *or* $\partial(a,b) = 2$. ■

We then give $\mathcal{UT}(n)$ a poset structure by extending $[T] \leq [T^a_b]$ for any $[T] \in \mathcal{UT}(n)$ and any $a, b \in V(T)$ with $ab \in E(T)$ or $\partial(a,b) = 2$. In particular, Proposition 4.5 shows that the maximal element of $\mathcal{UT}(n)$ is the star $K_{1,n-1}$.

The following proposition gives the minimal elements of $\mathcal{UT}(n)$.

Proposition 4.9. *Let* $[T] \in \mathcal{UT}(n)$. *Then* $[T]$ *is minimal in* $\mathcal{UT}(n)$ *if and only if the subgraph of* T *induced by* $\{v : \partial_T(v,\ell) \leq 3\}$ *is a path for each leaf* ℓ *in* T.

Proof. ($\Rightarrow$) If the subgraph of T induced by $\{v : \partial_T(v,\ell) \leq 3\}$ is not a path for a leaf $\ell \in V(T)$, there are two cases for the unique neighbor u of ℓ : (i) $\deg_T(u) \geq 3$, (ii) $N_T(u) = \{\ell, v\}$ for some $v \in V(T)$ and $\deg_T(v) \geq 3$. In case (i), choose $v \in N_T(u)\backslash\{\ell\}$ and let T' be a tree with $V(T') = V(T)$ and $E(T') = E(T) \cup \{v\ell\} \backslash \{vu\}$. Then $[(T')^u_\ell] = [T]$ and $[T'] \neq [T]$ by Lemma 4.1(ii). In case (ii), choose $w \in N_T(v)\backslash\{u\}$ and let T' be a tree with $V(T') = V(T)$ and $E(T') = E(T) \cup \{w\ell\} \backslash \{wv\}$. Then $[(T')^u_\ell] = [T]$ where $[T'] \neq [T]$ by Lemma 4.1(ii). Hence $[T]$ is not minimal in $\mathcal{UT}(n)$.

($\Leftarrow$) If $[T]$ is not minimal in $\mathcal{UT}(n)$, then there exists another tree $T' \in \mathcal{UT}(n)$ such that $[T'] \neq [T] = [(T')^w_u]$ for some $u, w \in V(T')$. By Lemma 4.8, $\partial_{T'}(u,w) \in \{1, 2\}$.

If u is a leaf in T', then $N_{T'}(u)\backslash\{w\} \subseteq N_{T'}(v)$ and hence $[T] = [(T')^w_u] = [T']$ by Lemma 4.1(ii), a contradiction. Since $[(T')^w_u] = [(T')^u_w]$ by Lemma 4.1(i), w is not a leaf in T' either. Therefore, there exist $a \in N_{T'}(u)$ and $b \in N_{T'}(w)$ such that $\partial_{T'}(a,w) =$

$\partial_{T'}(b,u) = \partial_{T'}(u,w)+1$. Let $c = u$ if $\partial_{T'}(u,w) = 1$ and c be the unique vertex in $N_{T'}(u) \cap N_{T'}(w)$ if $\partial_{T'}(u,w) = 2$. Then a, b, c are distinct vertices in $N_{(T')^w_u}(w)$.

Notice that u is a leaf in $(T')^w_u$ and the subgraph of $(T')^w_u$ induced by $\{v : \partial_{(T')^w_u}(v,u) \leq 3\}$ is not a path since it contains the vertex v of degree at least 3. We get the proof.

■

From the view of Lemma 4.6, we consider a restricted version of Kelmans transformation, called *distance-*2 *Kelmans transformation*, which is a Kelmans transformation G^a_b of G with $\partial_G(b,a) = 2$. Let $(\mathcal{UG}(n,m), \leq_2)$ denote the weak subposet of $(\mathcal{UG}(n,m), \leq)$ restricting to the distance-2 Kelmans transformation.

We first recall a known result that characterizes the maximal graphs of $\mathcal{UG}(n,m)$.

Proposition 4.10 ([12])**.** *The element $[G]$ is maximal in $(\mathcal{UG}(n,m), \leq)$ if and only if G is $\{2K_2, P_4, C_4\}$-free.*

Let H_1 be a graph with vertex set $V(H_1) = \{v_1, v_2, v_3, v_4, v_5\}$ and edge set $E(H_1) = \{v_1v_2, v_2v_3, v_3v_4, v_4v_5, v_3v_5\}$. The following proposition is a characterization of maximal graphs of the distance-2 Kelmans transformation.

Proposition 4.11. *The element $[G]$ is maximal in $(\mathcal{UG}(n,m), \leq_2)$ if and only if G is $\{P_5, C_5, K_1 \vee 2K_2, K_1 \vee P_4, \overline{P_5}, H_1\}$-free.*

Proof. If G contains any of $P_5, C_5, K_1 \vee 2K_2, K_1 \vee P_4, \overline{P_5}$ and H_1 as an induced subgraph, then there exist four vertices $a, b, u, v \in V(G)$ with $\partial_G(a,b) = 2$ such that $v \in N_G(b) \backslash N_G(a)$ and $u \in N_G(a) \backslash N_G(b)$. Then $[G^a_b] \neq [G]$ by Lemma 4.1(ii), so $[G]$ is not maximal in $(\mathcal{UG}(n,m), \leq_2)$.

If $[G]$ is not maximal in $(\mathcal{UG}(n,m), \leq_2)$, then there exist $a, b \in V(G)$ with $\partial_G(b,a) = 2$ such that $[G^a_b] \neq [G]$. By Lemma 4.1(ii), $N_G(b) \backslash N_G(a) \neq \emptyset$ and $N_G(a) \backslash N_G(b) \neq \emptyset$. Let $x \in N_G(b) \cap N_G(a)$, $v \in N_G(b) \backslash N_G(a)$ and $u \in N_G(a) \backslash N_G(b)$. Let H be the subgraph of G induced on vertices $\{u, v, x, a, b\}$, then H contains edges ax, bx, au, bv and doesn't contain edges ab, bu, av. Furthermore, there are eight possible cases for H between three vertices $\{x, u, v\}$:

(i) All of xu, xv and uv are not edges of H.

(ii) $xu \in E(H), xv \notin E(H), uv \notin E(H)$.

(iii) $xv \in E(H), xu \notin E(H), uv \notin E(H)$.

(iv) $uv \in E(H), xu \notin E(H), xv \notin E(H)$.

(v) $xu \in E(H), xv \in E(H), uv \notin E(H)$.

(vi) $xu \in E(H), xv \notin E(H), uv \in E(H)$.

(vii) $xu \notin E(H), xv \in E(H), uv \in E(H)$.

(viii) All of xu, xv and uv belongs to $E(H)$.

In case (i), $H \cong P_5$. In case (ii), $H \cong C_5$. In case (iii),(iv), $H \cong H_1$. In case (v), $H \cong K_1 \vee 2K_2$. In case (vi),(vii), $H \cong \overline{P_5}$. In case (viii), $H \cong K_1 \vee P_4$. Therefore, G is not $\{P_5, C_5, K_1 \vee 2K_2, K_1 \vee P_4, \overline{P_5}, H_1\}$-free. ■

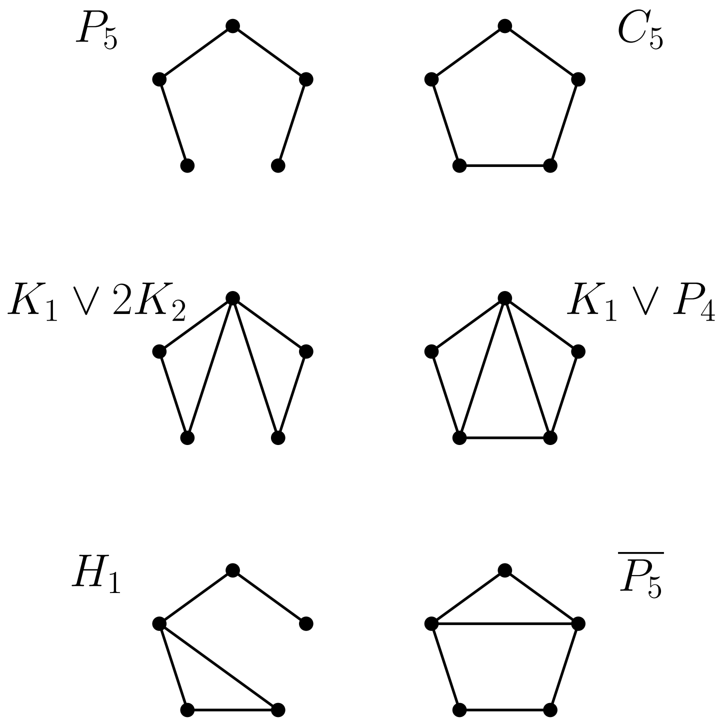


Figure 5: Forbidden subgraphs of the maximal graphs in $(\mathcal{UG}(n,m), \leq_2)$.

5 A_α-spectral radius

In this chapter, we will introduce the "A_α-matrix" and "A_α-spectral radius", which were first introduced by Nikiforov [33] in 2017. The main results of this chapter is Theorem 5.6 and Theorem 5.8 that characterize the mixed trees with maximum/minimum A_α-spectral radius, respectively.

Recall that the adjacency matrix $A = (a_{ij})$ of a mixed graph G is defined by $a_{ij} = 1$ if and only if $ij \in E(G)$ or $\overrightarrow{ij} \in E(G)$. Define the *out-degree matrix* $D^+ = (d^+_{ij})$ of G to be a diagonal matrix of order $|V(G)|$ such that $d^+_{ii} = d^+_G(i)$. The *signless Laplacian matrix* of a mixed graph is defined to be the sum of its adjacency matrix and its out-degree matrix. For real number $\alpha \in [0, 1]$, the matrix $A_\alpha(G)$ of a mixed graph G is defined to be $\alpha D^+ + (1 - \alpha)A$. The concepts of A_α-matrix of graphs were first introduced by Nikiforov [33] in 2017 and then liu et al. [31] start to consider the A_α-matrix for mixed graphs. Notice that when $\alpha = 0$, the A_α-matrix of a mixed graph is its adjacency matrix; when $\alpha = 1/2$, the A_α-matrix is half the signless Laplacian matrix. Therefore, the researches on A_α matrices are generalizations of the researches on adjacency matrices and signless Laplacian matrices. Since A_α matrices are nonnegative and it is well known that a nonnegative matrix has a real eigenvalue, let $\rho_\alpha(G)$ denote the largest real eigenvalue $\rho(A_\alpha(G))$ of the A_α matrix $A_\alpha(G)$ of G, and refer $\rho_\alpha(G)$ to as the *A_α-spectral radius*, or *α-index* of G. For the previous studies on A_α-spectral radii of graphs and mixed graphs, see [19, 20, 30, 35, 38, 40].

5.1 The A_α-matrix of a mixed graph

The following lemma tells that the Kelmans transformation of the A_α-matrix of a mixed graph is equal to the A_α-matrix of the corresponding Kelmans transformation mixed graph.

Lemma 5.1. *Let $\alpha \in [0, 1]$, $[G] \in \mathcal{G}(n, m)$ with distinct vertices $a, b \in V(G)$ having no* *arc, adjacency matrix $A = (c_{ij})$ and A_α-matrix $A_\alpha(G)$ of G. Set $k := \alpha|N_G^+(b) - N_G^+(a)|$, $t_i = (1-\alpha)\max(0, c_{ib} - c_{ia})$ and $s_i = (1-\alpha)\max(0, c_{bi} - c_{ai})$ for $i \in V(G) - \{a, b\}$. Then the Kelmans transformation matrix $A_\alpha(G)_b^a$ of $A_\alpha(G)$ from b to a with respect to $(t_i; s_i; k)$ is the A_α-matrix $A_\alpha(G_b^a)$ of G_b^a, i.e.,*

$$A_\alpha(G)_b^a = A_\alpha(G_b^a).$$

Proof. We only need to check that the ij entries in matrices $A_\alpha(G)_b^a$ and $A_\alpha(G_b^a)$ are equal for one of i, j in $\{a, b\}$. Indeed they are equal from the setting listed in the order aa, bb, ia, ib, aj and bj below:

$$\begin{aligned}
\alpha d_G^+(a) + k =& \alpha d_{G_b^a}^+(a),\\
\alpha d_G^+(b) - k =& \alpha d_{G_b^a}^+(b),\\
(1-\alpha)c_{ia} + t_i =& (1-\alpha)(c_{ia} + \max(0, c_{ib} - c_{ia})),\\
(1-\alpha)c_{ib} - t_i =& (1-\alpha)(c_{ib} - \max(0, c_{ib} - c_{ia})),\\
(1-\alpha)c_{ia} + s_j =& (1-\alpha)(c_{aj} + \max(0, c_{bj} - c_{aj}),\\
(1-\alpha)c_{ib} - s_j =& (1-\alpha)(c_{bj} - \max(0, c_{bj} - c_{aj}),
\end{aligned}$$

where $i, j \in V(G) - \{a, b\}$. ■

Proposition 5.2. *If $\alpha \in [0, 1]$, and $[G], [H] \in G(n, m)$ such that $[G] \leq [H]$, then $\rho_\alpha(G) \leq \rho_\alpha(H)$.*

Proof. We might assume $H = G_b^a$ by Lemma 4.3. Applying Theorem 3.1 and Lemma 5.1, we have

$$\rho_\alpha(G) = \rho(A_\alpha(G)) \leq \rho(A_\alpha(G)_b^a) = \rho(A_\alpha(G_b^a)) = \rho_\alpha(H).$$

■

5.2 The upper bound of A_α-spectral radius

If an arc in a mixed tree T is deleted, then we have two mixed trees. Thus if the arcs in a mixed tree T of order n and size m are all removed, then the remaining is a graph without cycles with $2n - m - 1$ components.

Lemma 5.3. *If $\alpha \in [0,1]$, $[T] \in \mathcal{T}(n,m)$ and C_1, C_2, …, C_{2n-m-1} are the components of the graph obtained from T by removing the arcs, then*

$$\operatorname{char}(A_\alpha(T)) = \prod_{i\in[t]} \operatorname{char}(A_\alpha(T)[C_i]),$$

where $A_\alpha(T)[C_i]$ is the principal submatrix of $A_\alpha(T)$ restricted to C_i.

Proof. If $\overrightarrow{ij} \in E(T)$ is deleted to obtain two mixed trees with vertex sets V and W, then besides $\overrightarrow{ij}$ there is no arc or edge between a vertex in V and a vertex in W. With $M = A_\alpha(T)$, $M_1 = M[V]$, $M_2 = M[W]$, we find that M satisfies the assumption of Lemma 2.1. Hence $\operatorname{char}(M) = \operatorname{char}(M_1) \times \operatorname{char}(M_2)$. We have the lemma by using this process on M_1 and M_2, and repeating again until each matrix is corresponding to a component of T. ∎

Note that $A_\alpha(T)[C_i]$ in Lemma 5.3 is not the A_α-matrix of the component C_i of T.

Corollary 5.4. *If $\alpha \in [0,1]$ and $[T] \in \mathcal{T}(n,n-1)$, then*

$$\operatorname{char}(A_\alpha(T)) = \prod_{i\in[n]} (\lambda - \alpha d_i^+).$$

Proof. For $[T] \in \mathcal{T}(n,n-1)$, the graph obtained from T by removing the arcs is a $\overline{K_n}$. Then $A_\alpha(T)[\{i\}]$ is a 1×1 matrix with entries αd_i^+ and the result is straightforward from Lemma 5.3. ∎

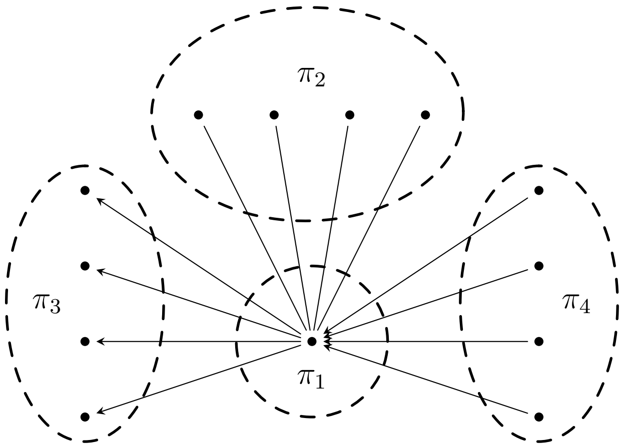


Figure 6: The partition Π of the vertices of a mixed star.

Proposition 5.5. *Let S be mixed star of order n, size m and maximum out-degree $m-n+k+1$ for some $0 \le k \le 2n-m-2$. Then for $\alpha \in [0,1]$, the A_α-spectral radius $\rho_\alpha(S)$ of S is the maximal root of the following quadratic polynomial in λ:*

$$(\lambda-\alpha)(\lambda-\alpha(m-n+k+1))-(1-\alpha)^2(m-n+1). \tag{8}$$

Proof. Note that there are $m-n+1$ edges in S. For convenience, assume that $V(S)=[n]$, the vertex 1 has the maximum degree $n-1$, $N_S^+(1)=[m-n+k+2]-\{1\}$ and $N_S^-(1)=([m-n+2]-\{1\})\cup\{m-n+k+3, m-n+k+4, \ldots, n\}$.

Set $\pi_1=\{1\}$, $\pi_2=\{2,3,\ldots,m-n+2\}$, $\pi_3=\{m-n+3, m-n+4, \ldots, m-n+k+2\}$, and $\pi_4=[n]-\pi_1-\pi_2-\pi_3$ as illustrated in Figure 6. With respect to the partition $\Pi=\{\pi_1,\pi_2,\pi_3,\pi_4\}$ of $[m]$, the adjacency matrix A and the diagonal out-degree matrix D^+ of T have equitable quotient matrices

$$\Pi(A)=\begin{pmatrix} 0 & m-n+1 & k & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 1 & 0 & 0 & 0 \end{pmatrix} \text{ and } \Pi(D^+)=\begin{pmatrix} m-n+k+1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 1 \end{pmatrix},$$

respectively, which implies that the A_α-matrix of T has equitable quotient

$$\Pi(A_\alpha) = \begin{pmatrix} \alpha(m-n+k+1) & (1-\alpha)(m-n+1) & (1-\alpha)k & 0 \\ 1-\alpha & \alpha & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1-\alpha & 0 & 0 & \alpha \end{pmatrix}.$$

The characteristic polynomial of $\Pi(A_\alpha)$ is

$$\lambda(\lambda-\alpha)((\lambda-\alpha)(\lambda-\alpha(m-n+k+1))-(1-\alpha)^2(m-n+1)),$$

and the zero in (8) is at least α. By Lemma 2.2, we complete the proof. ∎

The following theorem is the main result of this section.

Theorem 5.6. *If $\alpha \in [0,1]$ and $[T] \in \mathcal{T}(n,m)$, then*

$$\rho_\alpha(T) \le \frac{1}{2}\left(\alpha n + \sqrt{\alpha^2 n^2 - 4\alpha^2(n-1) + 4(1-\alpha)^2(m-n+1)}\right).$$

Moreover, the mixed star of order n and size m with maximum out-degree $n-1$ attains the upper bound.

Proof. By Proposition 5.2, it suffices to show that for each maximal element $[T] \in \mathcal{T}(n,m)$ characterized in Proposition 4.5, $\rho_\alpha(T)$ is at most the upper bound appearing in Theorem 5.6. Suppose T is a mixed star with maximal out-degree $m-n+k+1$. Since the largest root of the quadratic polynomial in (8) increases as lone as k increases, we might assume $k = 2n-m-2$, and find (8) becomes

$$\lambda^2 - \alpha n\lambda + \alpha^2(n-1) - (1-\alpha)^2(m-n+1),$$

which has largest root as the upper bound appearing in Theorem 5.6. For the remaining elements $[T] \in \mathcal{T}(n,n-1)$, from Corollary 5.4 we know that the A_α-matrix of T has characteristic polynomial $\prod_{i\in[n]}(\lambda - \alpha d_i^+)$, so $\rho_\alpha(T) = \alpha \cdot (\max_{i\in[n]} d_i^+) \le \alpha(n-1)$, where the equality holds when T is the mixed star with $n-1$ leaves being out-neighbor of a vertex. Moreover, $\alpha(n-1)$ is equal to the upper bound when $m = n-1$. ∎

5.3 The lower bound of A_α-spectral radius

The mixed tree with smallest A_α-spectral radius is more complicated to characterize. We first state the result on trees.

The following theorem was proved in [35].

Theorem 5.7. *([35]) If T is a tree of order n and $\alpha \in [0,1]$, then*

$$\rho_\alpha(T) \geq \rho_\alpha(P_n).$$

The equality holds if and only if $G = P_n$. ∎

The following theorem gives a lower bound of the A_α-spectral radius of mixed tree of order n and size m.

Theorem 5.8. *Let $[T] \in \mathcal{T}(n,m)$, and set $k = \lceil \frac{n}{2n-m-1} \rceil$, then*

$$\rho_\alpha(T) \geq \rho_\alpha(P_k).$$

Proof. Let T be a mixed tree of order n and size m. Then the graph obtained from T by removing the arcs has $2n-m-1$ components, and there exists a component of order at least $k = \lceil \frac{n}{2n-m-1} \rceil$. Let C_1 be a component with maximum size t. Then $t \geq k \geq 2$ and $A_\alpha(T)[C_1] \geq A_\alpha(C_1)$. Hence by Lemma 2.3, Lemma 5.3 and Theorem 5.7, $\rho_\alpha(T) \geq \rho(A_\alpha(T)[C_1]) \geq \rho(A_\alpha(C_1)) = \rho_\alpha(P_t) \geq \rho_\alpha(P_k)$. ∎

Here we construct a mixed tree to tell that the bound given in Theorem 5.8 may not be reached for some cases. After removing the arcs from a mixed tree of order n and size m, the resulting graph contains $2n-m-1$ components. Let the components be paths with almost equal sizes. That is, the components are all isomorphic to paths $P_{\lceil \frac{n}{2n-m-1} \rceil}$ or $P_{\lfloor \frac{n}{2n-m-1} \rfloor}$. Let the paths be ordered one-by-one in descending order with an arc between each pair of consecutive paths from the last vertex of one path to the first

Figure 7: The mixed tree $P_{(8,12)}$.

vertex of another path. Denote the above mixed tree by $P_{(n,m)}$. An example of $P_{(n,m)}$ where $n = 8, m = 12$ is given in Figure 7.

Let $k = \lceil \frac{n}{2n-m-1} \rceil$. By Lemma 5.3, we deduce that for all $m < 2n-2$, the A_α-spectral radius $\rho_\alpha(P_{(n,m)})$ is equal to $\rho_\alpha(M_k)$, where M_k is the following $k \times k$ matrix :

$$\begin{pmatrix} \alpha & 1-\alpha & & & \\ 1-\alpha & 2\alpha & 1-\alpha & & \\ & \ddots & \ddots & \ddots & \\ & & 1-\alpha & 2\alpha & 1-\alpha \\ & & & 1-\alpha & 2\alpha \end{pmatrix}.$$

Since $[P_{(n,m)}] \in \mathcal{T}(n,m)$, we know that

$$\min_{[T]\in\mathcal{T}(n,m)} \rho_\alpha(T) \leq \rho_\alpha(M_k).$$

Together with Theorem 5.8, we have

$$\rho_\alpha(P_k) \leq \min_{[T]\in\mathcal{T}(n,m)} \rho_\alpha(T) \leq \rho_\alpha(M_k).$$

However, we found that for some $\alpha \in (0,1)$, both of $\rho_\alpha(P_k)$ and $\rho_\alpha(M_k)$ are not the answer of $\min_{[T]\in\mathcal{T}(n,m)} \rho_\alpha(T)$. For example, if $\alpha = 0.9,\ n = 8,\ m = 12$, then $k = \lceil \frac{8}{3} \rceil = 3$. In this case, $\rho_\alpha(P_k) \approx 1.8217$ but this bound cannot be reached by any mixed tree of order 8 and size 12. Meanwhile, $\rho_\alpha(M_k) \approx 1.9051$. However, the mixed tree of order 8 and size 12 with smallest A_α-spectral radius is actually with A_α-spectral radius 1.9, which is given in Figure 8.

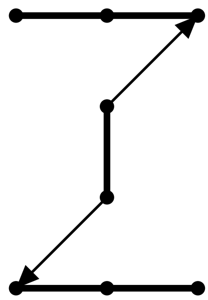


Figure 8: The mixed graph of order 8, size 12 and $A_{0.9}$-spectral radius 1.9.

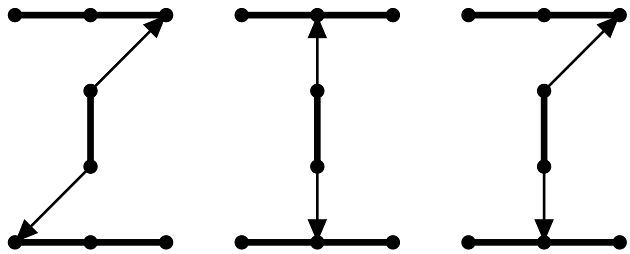


Figure 9: These mixed trees share the same A_α-spectral radius

Notice that the mixed trees with minimum A_α-spectral radius is difficult and in some sense meaningless to characterize since the choice of the out-vertex of each arc doesn't change the A_α-spectral radius. Figure 9 gives 3 mixed trees that share a same A_α-spectral radius.

6 New sufficient conditions of Hamiltonicity

There are many earlier results giving sufficient conditions of Hamiltonicity, like Dirac's theorem [17], Ore theorem [36] and Chvátal's theorem [10]. However, the requirements of above theorems are too strong to reach, so people want to find new approaches for the sufficient conditions of Hamiltonicity. In this chapter, three different approaches are used to find new sufficient conditions of Hamiltonicity. The main results of this chapter are given in Proposition 6.9, Theorem 6.11 and Corollary 6.34.

6.1 Spectral conditions

In 2010, Fiedler and Nikiforov gave the following result.

Theorem 6.1 ([18])**.** *If G is a graph on $n \geq 3$ vertices and with spectral radius $\rho(G) > n-2$, then G is Hamiltonian unless $G = K_1 \vee (K_1 \cup K_{n-2})$.*

Later in 2013, Yu and Fan gave a similar result which uses signless Laplacian spectral radius. Let $q(G)$ be the spectral radius of the signless Laplacian matrix of G.

Theorem 6.2 ([42])**.** *If G is a graph on $n \geq 3$ vertices and with signless Laplacian spectral radius $q(G) > 2(n-2)$, then G is Hamiltonian unless $G = K_1 \vee (K_1 \cup K_{n-2})$ or $G = K_2 \vee \overline{K_3}$.*

We are going to generalize these results into the versions of A_α-spectral radius.

6.1.1 Conditions using A_α-spectral radius

There are several bounds of the A_α-spectral radius $\rho_\alpha(G)$, and here we give a corrected version of an incorrect bound which is given in [28].

Lemma 6.3. *Let n, m, δ, Δ denote the number of vertices, the number of edges, the minimum degree and the maximum degree of a graph G, respectively. Then the A_α-spectral* *radius* $\rho_\alpha(G)$ *of* G *is at most*

$$\frac{\delta-1+\alpha(\Delta-\delta+1)+\sqrt{(\delta-1+\alpha(\Delta-\delta+1))^2+(4-4\alpha)(2m-(n-1)\delta)}}{2},$$

for each $0 \le \alpha \le 1$. ■

Since $\delta \ge 0$ and $\Delta \le n-1$, we have a simpler bound as follow.

Corollary 6.4.

$$\rho_\alpha(G) \le \frac{-1+\alpha n+\sqrt{(-1+\alpha n)^2+8m(1-\alpha)}}{2}.$$

The above bounds are connections between the A_α-spectral radius and the number of edges in graphs. Here we introduce a classic result given by Ore [36] and Bondy [5], independently.

Lemma 6.5. *Let* G *be a graph on* $n \ge 3$ *vertices and* m *edges. If*

$$m \ge \binom{n-1}{2}+1,$$

then G *is Hamiltonian unless* $G = K_1 \vee (K_1 \cup K_{n-2})$ *or* $G = K_2 \vee \overline{K_3}$. ■

The following proposition is a generalization of Theorem 6.1.

Proposition 6.6. *If* G *is a graph on* $n \ge 3$ *vertices and there exists* $0 \le \alpha \le 1$ *such that*

$$\rho_\alpha(G) > n-2+\alpha,$$

then G *is Hamiltonian unless* $G = K_1 \vee (K_1 \cup K_{n-2})$ *or* $G = K_2 \vee \overline{K_3}$.

Proof. Let $n \ge 3$ and $\rho_\alpha(G) > n-2+\alpha$. By Corollary 6.4, we have

$$n-2+\alpha < \rho_\alpha(G) \le \frac{-1+\alpha n+\sqrt{(-1+\alpha n)^2+8m(1-\alpha)}}{2}.$$

Hence

$$(4-4\alpha)n^2+(-12+16\alpha-4\alpha^2)n+(8-12\alpha+4\alpha^2) < (8-8\alpha)m,$$

so the number of edges in G satisfies

$$m > \frac{1}{2}(n^2 + (-3+\alpha)n + (2-\alpha)) \geq \frac{1}{2}(n^2 - 3n + 2) = \binom{n-1}{2}.$$

By Lemma 6.5, G is Hamiltonian unless $G = K_1 \vee (K_1 \cup K_{n-2})$ or $G = K_2 \vee \overline{K_3}$. ■

To give a general version of Theorem 6.2, we first need to generalize a lemma which is applied in the original proof of Theorem 6.2. Here we write down the proof given in [15] for later use.

Lemma 6.7 ([15]). *Let G be a graph of order n with m edges. Then*

$$\max\{d_i + m_i : v_i \in V(G)\} \leq \frac{2m}{n-1} + n - 2,$$

where d_i is the degree of v_i and m_i is the average degree of the neighbors of v_i.

Proof. Let $v_j = \arg\max\{d_i + m_i : v_i \in V(G)\}$. Let T be the sum of the degrees of the neighbors of v_j, then

$$\max\{d_i + m_i : v_i \in V(G)\} = d_j + m_j = d_j + \frac{T}{d_j}.$$

Furthermore,

$$2m = d_j + T + (n - d_j - 1)p_j$$

where p_j is the average degree of the vertices not adjacent to v_j. Hence the inequality we are going to prove is

$$d_j + \frac{T}{d_j} \leq \frac{d_j + T + (n - d_j - 1)p_j}{n-1} + n - 2,$$

which is equivalent to

$$(n - d_j - 1)\left(n - 2 + p_j - \frac{T}{d_j}\right) \geq 0.$$

If $d_j = n-1$, then the equality holds. If not, then $d_j \leq n-2$ and there are two cases: (i) $0 \leq p_j < 1$ (ii) $p_j \geq 1$. For (i), there exists an isolated vertex, which leads to $\frac{T}{d_j} \leq n-2$

and $d_j \leq n-2$, the inequality holds. For (ii), since $\frac{T}{d_j} \leq n-1$ and $d_j \leq n-2$. The inequality holds, too. ∎

The following generalization of Lemma 6.7 has been partially proved in [22], and our version is applicable for all $0 \leq \alpha \leq 1$.

Lemma 6.8. *Let G be a graph of order n with m edges. Then*

$$\begin{cases} \rho_\alpha(G) \leq \frac{2m}{n-1}\alpha + n(1-\alpha) - 1, & \text{if } \alpha \in [0, 1/2), \\ \rho_\alpha(G) \leq \frac{2m}{n-1}(1-\alpha) + n\alpha - 1, & \text{if } \alpha \in [1/2, 1]. \end{cases}$$

Proof. Let d_i be the degree of vertex v_i and m_i be the average degree of the neighbors of v_i. Since the spectral radius of a symmetric matrix is no greater than its largest row sum, we have $\rho_\alpha(G) \leq \max\{\alpha d_i + (1-\alpha)m_i\}$. Let $v_j = \arg\max\{\alpha d_i + (1-\alpha)m_i : v_i \in V(G)\}$. Let T be the sum of the degrees of the neighbor of v_j. For $0 \leq \alpha < \frac{1}{2}$, by Lemma 6.7,

$$\begin{aligned} \alpha d_j + (1-\alpha)m_j &= \alpha(d_j + m_j) + (1-2\alpha)m_j \\ &\leq \alpha\left(\frac{2m}{n-1} + n - 2\right) + (1-2\alpha)m_j \\ &\leq \alpha\left(\frac{2m}{n-1} + n - 2\right) + (1-2\alpha)(n-1) \\ &= \frac{2m}{n-1}\alpha + n(1-\alpha) - 1. \end{aligned}$$

For $\frac{1}{2} \leq \alpha \leq 1$, by Lemma 6.7,

$$\begin{aligned} \alpha d_j + (1-\alpha)m_j &= (1-\alpha)(d_j + m_j) + 2\alpha d_j \\ &\leq (1-\alpha)\left(\frac{2m}{n-1} + n - 2\right) + 2\alpha d_j \\ &\leq (1-\alpha)\left(\frac{2m}{n-1} + n - 2\right) + 2\alpha(n-1) \\ &= \frac{2m}{n-1}(1-\alpha) + n\alpha - 1. \end{aligned}$$

∎

The following proposition generalizes Theorem 6.2.

Proposition 6.9. *If G is a graph on $n \geq 3$ vertices, $G \neq K_1 \vee (K_1 \cup K_{n-2})$, $G \neq K_2 \vee \overline{K_3}$, and there exists $0 \leq \alpha \leq 1$ such that the A_α-spectral radius $\rho_\alpha(G)$ satisfies*

$$\begin{cases} \rho_\alpha(G) > n - 1 - 2\alpha, & \text{if } \alpha \in [0, 1/2), \\ \rho_\alpha(G) > n - 3 + 2\alpha, & \text{if } \alpha \in [1/2, 1], \end{cases}$$

then G is Hamiltonian.

Proof. If $\rho_\alpha(G) > n - 1 - 2\alpha$ for some $\alpha \in [0, 1/2)$, by Lemma 6.8 we have

$$n - 1 - 2\alpha < \rho_\alpha(G) \leq \frac{2m}{n-1}\alpha + n(1-\alpha) - 1,$$

which implies $m > \binom{n-1}{2}$ and by Lemma 6.5, G is Hamiltonian unless $G = K_1 \vee (K_1 \cup K_{n-2})$ or $G = K_2 \vee \overline{K_3}$.

Similarly, if $\rho_\alpha(G) > n - 3 + 2\alpha$ for some $\alpha \in [1/2, 1]$, by Lemma 6.8 we have

$$n - 3 + 2\alpha < \rho_\alpha(G) \leq \frac{2m}{n-1}(1-\alpha) + n\alpha - 1,$$

which also implies $m > \binom{n-1}{2}$ and by Lemma 6.5, G is Hamiltonian unless $G = K_1 \vee (K_1 \cup K_{n-2})$ or $G = K_2 \vee \overline{K_3}$. ■

6.2 Graph structure conditions

In this section, we focus on the Cartesian product graphs. Recall that the definition of Cartesian product is as follows.

Definition 6.10. The *Cartesian product graph* $G_1 \square G_2$ of graphs G_1 and G_2 is a graph with vertex set

$$V(G_1 \square G_2) = \{v_u \mid v \in V(G_1), u \in V(G_2)\},$$

and edge set

$$E(G_1 \square G_2) = \{v_u v_w \mid v \in V(G_1), uw \in E(G_2)\} \cup \{v_u w_u \mid u \in V(G_2), vw \in E(G_1)\}.$$

Parts of the results are also in the Master thesis [34] of the author. The tools we use here are different from [34] and are more applicable.

Recall that the maximum degree of graph G is denoted as $\Delta(G)$. A *path factor* of a graph is a spanning subgraph of the graph such that each component of the spanning subgraph is isomorphic to a path with order at least two. If each component in a path factor is isomorphic to P_2, the path factor is called a *perfect matching*. The following theorem is the main result of this section.

Theorem 6.11. *Let G_1 be a traceable graph and G_2 a connected graph. Statements (a) and (b) are given as following :*

(a) G_2 has a perfect matching and $|V(G_1)| \geq \Delta(G_2)$.

(b) G_2 has a path factor and $|V(G_1)|$ is an even integer with $|V(G_1)| \geq 4\Delta(G_2) - 2$.

If one of (a),(b) holds, then $G_1 \square G_2$ has a Hamiltonian cycle.

Theorem 6.11 (a) and (b) will be proved in Theorem 6.21 and Theorem 6.24, respectively.

6.2.1 Path factor of a bipartite graph

To introduce properties of a graph with a path factor, we need more notations. First, we say a graph to have a $\{P_2, P_3\}$-factor if it has a spanning subgraph such that each component is isomorphic to P_2 or P_3. Next, we use $i(G)$ to denote the number of isolated vertices of G.

A $\{P_2, P_3\}$-factor is a path factor, and a path with order at least 2 has a $\{P_2, P_3\}$-factor. Therefore, the following lemma follows.

Lemma 6.12. *A graph G has a path factor if and only if G has a $\{P_2, P_3\}$-factor.* ■

The proposition below is from [1].

Proposition 6.13 ([1]). *A graph G has a path factor if and only if $i(G-S) \le 2|S|$ for all $S \subseteq V(G)$.* ∎

Lemma 6.14. *Let G be a graph. If $\delta(G) \ge |V(G)|/3$, then G has a path factor.*

Proof. Suppose G has no path factor. Choose $S \subseteq V(G)$ with $|I| = i(G-S) > 2|S|$ by Proposition 6.13, where I is the set of isolated vertices in $G-S$. As each vertex in I has degree at most $|S|$ in G, we have $|S| < (|S|+|I|)/3 \le |V(G)|/3$, a contradiction to the assumption that $\delta(G) \ge |V(G)|/3$. ∎

Restricted to bipartite graphs, the following proposition is a supplementary of Proposition 6.13.

Proposition 6.15. *If H is a bipartite graph that does not contain a path factor, then there exists a vertex subset S that belongs to a single partite set of H with $i(H-S) > 2|S|$.*

Proof. By Proposition 6.13 there exists $S' \subseteq V(H)$ such that $i(H-S') > 2|S'|$. Let H have partite sets A, B and $S_A := S' \cap A, S_B := S' \cap B$. Note that an isolated vertex in $H-S'$ is either an isolated vertex in $H-S_A$ or an isolated vertex in $H-S_B$. So $i(H-S_A)+i(H-S_B) = i(H-S') > 2|S'| = 2|S_A|+2|S_B|$ which implies $i(H-S_A) > 2|S_A|$ or $i(H-S_B) > 2|S_B|$. ∎

For convenience, assume

$$V(P_n) = \{1, 2, \ldots, n\}, E(P_n) = \{i(i+1) : i = 1, 2, \ldots, n-1\}$$

in the rest part of this section.

Theorem 6.16. *If H be a bipartite graph without path factors, then the Cartesian product $P_n \square H$ is not 1-tough.*

Proof. By Proposition 6.15, there exists a vertex subset S in a single partite set of H such that $i(H-S) > 2|S|$. Let I denote the set of isolated vertices in $H-S$ and $j_S := \{j_s \mid s \in S\}$, $j_I := \{j_u \mid u \in I\}$ for $1 \le j \le n$. Let $V(P_n \square H) = X \cup Y$ be a bipartition of $P_n \square H$ with $|X| \le |Y|$. For the case $|X| = |Y|$, let Y be the partite set which contains 1_S. Note that $1_I, 2_S \subseteq X$, $2_I \subseteq Y$, and $2|1_S| = 2|S| < i(H-S) = |1_I|$. If $|X| < |Y|$, then $c(P_n \square H - X) = |Y| > |X|$, implying that $P_n \square H$ is not 1-tough. Suppose $|X| = |Y|$. Set $X' = (X \cup 1_S) - 1_I$ and $Y' = (Y \cup 1_I) - 1_S$. Now $1_I, 2_I \subseteq Y'$. Since $1_u 2_u$ is the only possible edge in Y' for each $u \in I$, we have $c(P_n \square H - X') \ge |Y'| - |1_I| = |Y| - |1_S| > |X| + |1_S| - |1_I| = |X'|$. Thus $P_n \square H$ is not 1-tough. ■

Considering the special case $n = 1$ in Theorem 6.16, we have the following corollary, which is of independent interest.

Corollary 6.17. *A* 1*-tough bipartite graph has a path factor.*

6.2.2 Trees with perfect matchings

Results about the Hamiltonicity of Cartesian product graphs have been proved in several papers. For instance, the papers [14],[16] and [39] have mentioned the following result.

Theorem 6.18 ([39])**.** *Let T be a tree. If $n \ge \Delta(T)$, then $C_n \square T$ is Hamiltonian.* ■

Motivated by Theorem 6.18, we will prove the Hamiltonicity of $P_n \square T$. Before doing this we comment by the following lemma to show that the assumption $n \ge \Delta(T)$ in Theorem 6.18 is necessary.

Lemma 6.19. *Let G_1 be a connected graph and T be a tree. If $\Delta(T) > |V(G_1)|$, then the Cartesian product $G_1 \square T$ is not* 1*-tough.*

Proof. Find $v \in V(T)$ with $\deg(v) = \Delta(T)$, choose $S = \{u_v : u \in V(G_1)\}$ and note that $|S| = |V(G_1)|$. Now $c(G_1 \Box T - S) = \Delta(T) > |V(G_1)| = |S|$, which means that $G_1 \Box T$ is not 1-tough. ■

Let G be a graph with path factor F. Let G_F be the graph with vertex set F and two components $c_1, c_2 \in F$ are *adjacent* if there exist vertices $u \in c_1, v \in c_2$ such that $uv \in E(G)$. In particular, if T is a tree with path factor F then T_F is a tree, deleting a leaf c in T_F yields a subtree of T_F, and $T - c$ is a subtree of T. Hence we have the following lemma.

Lemma 6.20. *For a tree T with a $\{P_2, P_3\}$-factor F, there exists a component c of F such that $T - c$ is a tree with a $\{P_2, P_3\}$-factor $F - \{c\}$.* ■

For $v \in V(T)$ let $B_v := \{i_v(i+1)_v \mid 1 \leq i < n\} \subseteq E(P_n \Box T)$. Now for $T = P_2$ and $V(T) = \{u, w\}$, the set $\{1_u 1_w\} \cup B_u \cup B_w \cup \{n_u n_w\}$ of edges in $P_n \Box T$ forms a Hamiltonian cycle, and call it the *standard* Hamiltonian cycle for $P_n \Box P_2$. To avoid confusions, the degree of vertex v in G will be denoted by $\deg_G(v)$. To prove Theorem 6.11(a), it is sufficient to find a Hamiltonian cycle of $P_n \Box T$ where $n = |V(G_1)|$ and T is a spanning tree of G_2 that contains perfect matching F of G_2. Note that $n \geq \Delta(G_2) \geq \Delta(T)$. For the convenience of proof, we state a stronger version as follows.

Theorem 6.21. *Let T be a tree with a perfect matching. If $n \geq \Delta(T)$, then there exists a Hamiltonian cycle of $P_n \Box T$ which contains exactly $n - \deg_T(v)$ of the edges from the set B_v for any vertex $v \in V(T)$. In particular, Theorem 6.11 (a) is proved.*

Proof. Apply induction on the number of vertices of T. For $T = P_2$, the standard Hamiltonian cycle for $P_n \Box P_2$ satisfies the requirement since $|B_v| = n - 1 = n - \deg_T(v)$ for $v \in V(P_2)$.

For a tree T with a perfect matching F. By Lemma 6.20, there exists a component (an edge) c in F such that $T - c$ is a tree with a perfect matching. Let $u_1 \in c$ and $u_2 \in V(T - c)$ such that u_1 and u_2 are adjacent. Let H' be the standard Hamiltonian cycles of $P_n \square c$. Since the subtree $T' = T - c$ of T has a perfect matching, $|V(T')| < |V(T)|$ and $n \geq \Delta(T) \geq \Delta(T')$, by the induction hypothesis, there is a Hamiltonian cycle H'' of $P_n \square T'$ which contains exactly $n - \deg_{T'}(v)$ edges from the set B_v for any vertex $v \in V(T')$. Since $n - \deg_{T'}(u_2) = n - (\deg_T(u_2) - 1) \geq n - \Delta(T) + 1 \geq 1$, there exists a j such that $j_{u_2}(j+1)_{u_2} \in H''$. Now

$$H = H' \cup H'' \cup \{j_{u_1} j_{u_2}, (j+1)_{u_1}(j+1)_{u_2}\} - \{j_{u_1}(j+1)_{u_1}, j_{u_2}(j+1)_{u_2}\}$$

is a Hamiltonian cycle of $P_n \square T$.

To check that H satisfies the edge requirement, we only need to check those vertices in T whose incident edges have been changed in the induction step, which are vertices u_1 and u_2. For u_1, all the $n-1$ edges of B_{u_1} are in the cycle H'. We delete one of them, so there are $n - 2 = n - \deg_T(u_1)$ edges from B_{u_1} in H. For u_2, there are $n - \deg_{T'}(u_2) = n - (\deg_T(u_2) - 1)$ edges from B_{u_2} in the cycle H'' by the induction hypothesis. We delete one of them, so there are $n - (\deg_T(u_2) - 1) - 1 = n - \deg_T(u_2)$ edges from B_{u_2} in H. This completes the proof. ■

The paper [14] has proved that $G_1 \square G_2$ is Hamiltonian when G_1 is traceable with $|V(G_1)|$ an even integer no less than $\Delta(G_2) - 1$ and G_2 contains an even 2-factor (i.e. a spanning subgraph consisting of even cycles). Since an even 2-factor must contain a 1-factor, so Theorem 6.11*(a)* is a stronger result apart from the case $|V(G_1)| = \Delta(G_2) - 1$.

The following corollary concludes this section.

Corollary 6.22. *Let T be a tree with a perfect matching and n be a positive integer. The following three statements are equivalent:*

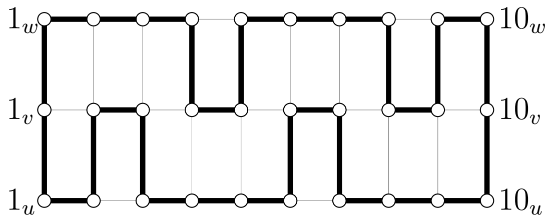


Figure 10: Standard Hamiltonian cycle for $P_{10} \square P_3$

(1) $P_n \square T$ *is Hamiltonian.*

(2) $P_n \square T$ *is* 1*-tough.*

(3) $n \geq \Delta(T)$*.*

Proof. (1) $\Rightarrow$ (2) is clear. (2) $\Rightarrow$ (3) is from Lemma 6.19. (3) $\Rightarrow$ (1) is from Theorem 6.21. ∎

6.2.3 Graphs with path factors

Here we construct a Hamiltonian cycle of $P_n \square G$ where G is connected with a path factor and n is an even integer with $n \geq 4\Delta(G) - 2$. By Lemma 6.12, G has a $\{P_2, P_3\}$-factor F. Let T be the spanning subtree of G that contains F. It suffices to find a Hamiltonian cycle in $P_n \square T$.

For $v \in V(T)$, let $L_v = \{i_v(i+1)_v \mid i \equiv 0, 1, 3 \pmod 4\}, C_v = \{i_v(i+1)_v \mid i \equiv 0, 2 \pmod 4\}, R_v = \{i_v(i+1)_v \mid i \equiv 1, 2, 3 \pmod 4\}$ denote three special subsets of the edge set B_v described in the last section. For $G = P_3$ with $V(G) = \{u, v, w\}$ and $E(G) = \{uv, vw\}$, the set $\{1_u 1_v\} \cup \{n_u n_v, n_v n_w\} \cup L_u \cup C_v \cup R_w \cup \{i_u i_v : i \equiv 2, 3 \pmod 4\} \cup \{i_v i_w : i \equiv 0, 1 \pmod 4\}$ of edges forms a Hamiltonian cycle, and call it the *standard* Hamiltonian cycle for $P_n \square P_3$. See Figure 10 for the standard Hamiltonian cycle for $P_{10} \square P_3$.

By direct computation we have the following lemma.

Lemma 6.23. *For even integer* n*,* $|L_v \cap R_v| \geq |R_v \cap C_v| \geq |L_v \cap C_v| = \lceil \frac{n-4}{4} \rceil$*.*

We define the *type* of a vertex v in T as follows. v has type B (resp. C) if v is in an edge in F (resp. if v is the middle vertex in a path of length 3 in F). For the two endpoints of a path of length 3 in F, we arbitrarily assign one endpoint of type L and the other of type R. Let $\delta_X = 1$ if $X \in \{B, L, R\}$ and $\delta_X = 2$ if $X = C$. Note that $\delta_X = \deg_c(v)$ for $c \in F$ and $v \in c$ of type X. The following is a stronger version of Theorem 6.11(b).

Theorem 6.24. *Let T be a connected graph with a $\{P_2, P_3\}$-factor F and n be an even integer. If $n \geq 4\Delta(T) - 2$, then $P_n \square T$ contains a Hamiltonian cycle H such that for any vertex $v \in V(T)$ of type $X \in \{B, L, C, R\}$, we have $H \cap B_v \subseteq X_v$ and $|H \cap B_v| = |X_v| - \deg_T(v) + \delta_X$. In particular, Theorem 6.11(b) holds.*

Proof. We prove by induction on the number of vertices of T. For $T = P_2$, any vertex v of P_2 has type B and the standard Hamiltonian cycle H_1 of $P_n \square P_2$ satisfies $|H_1 \cap B_v| = n - 1 = |B_v| - \deg_{P_2}(v) + 1$ for vertex $v \in P_2$. For $T = P_3$, a vertex v of P_3 has type $X \in \{L, C, R\}$ and the standard Hamiltonian cycle H_2 of $P_n \square P_3$ satisfy $|H_2 \cap B_v| = |X_v| = |X_v| - \deg_{P_3}(v) + \delta_X$.

Now assume $|V(T)| \geq 4$. By Lemma 6.20, there exists a component c of F such that $T - c$ is a tree with the path factor $F - \{c\}$. Let $u_1 \in c$ and $u_2 \in V(T - c)$ such that u_1 and u_2 are adjacent. Assume u_1 has type X and u_2 has type Y. Let H' be the standard Hamiltonian cycle of $P_n \square c$ and $P_n \square T - c$ contains a Hamiltonian cycle H'' that satisfies $H'' \cap B_{u_2} \subseteq Y_{u_2}$ and $|H_2 \cap B_{u_2}| = |Y_{u_2}| - (\deg_T(u_2) - 1) + \delta_Y$ by induction hypothesis. Referring to Lemma 6.23, we have $|H_2 \cap B_{u_2} \cap X_{u_2}| \geq |Y_{u_2} \cap X_{u_2}| - (\deg_T(u_2) - 1) + \delta_Y \geq \lceil \frac{n-4}{4} \rceil - \deg_T(u_2) + 2 \geq \lceil \frac{4\Delta(T)-6}{4} \rceil - \deg_T(u_2) + 2 \geq 1$. Pick $j_{u_2}(j+1)_{u_2} \in H_2 \cap B_{u_2} \cap X_{u_2}$ and then $j_{u_1}(j+1)_{u_1} \in X_{u_1} \subseteq H'$.

Now

$$H = H' \cup H'' \cup \{j_{u_1} j_{u_2}, (j+1)_{u_1}(j+1)_{u_2}\} - \{j_{u_1}(j+1)_{u_1}, j_{u_2}(j+1)_{u_2}\}$$

is a Hamiltonian cycle of $P_n \square T$.

To check H satisfies the edge requirements, we only need to check for $v \in \{u_1, u_2\}$. This follows from $|H \cap X_{u_1}| = |H' \cap X_{u_1}| - 1 = |X_{u_1}| - 1 = |X_{u_1}| - \deg_T(u_1) + \delta_X$ and $|H \cap Y_{u_2}| = |H'' \cap Y_{u_2}| - 1 = |Y_{u_2}| - (\deg_T(u_2) - 1) + \delta_Y - 1 = |Y_{u_2}| - \deg_T(u_2) + \delta_Y$. ■

Similar to Corollary 6.22, another set of equivalent conditions on Hamiltonicity of Cartesian product graphs is given as follows.

Corollary 6.25. *Let H be a connected bipartite graph, n be an even integer and $n \geq 4\Delta(H) - 2$. The following three statements are equivalent :*

(1) $P_n \square H$ is Hamiltonian.

(2) $P_n \square H$ is 1-tough.

(3) H has a path factor.

Proof. (1) $\Rightarrow$ (2) is clear. (2) $\Rightarrow$ (3) is from Theorem 6.16. (3) $\Rightarrow$ (1) is from Theorem 6.24. ■

To show that the assumption $n \geq 4\Delta(H) - 2$ in Corollary 6.25 can not be replaced by $n \geq \Delta(H)$, we provide a 1-tough non-Hamiltonian graph $P_n \square T$ such that T is a tree with a path factor and $n = \Delta(T) + 1$.

Let T_1 be a tree with vertex set $V(T_1) = \{1, 2, 3, 4, 5, 6, 7, 8\}$ and edge set $E(T_1) = \{12, 23, 34, 45, 26, 37, 48\}$.

Proposition 6.26. *The graph $G = P_4 \square T_1$ is 1-tough but not Hamiltonian.*

Proof. If G is Hamiltonian, the edges incident to degree two vertices of G must contained in each Hamiltonian cycle. Therefore the edges

$$1_1 1_2, 1_2 1_6, 1_3 1_7, 1_4 1_5, 1_4 1_8, 1_1 2_1, 1_5 2_5, 1_6 2_6, 1_7 2_7, 1_8 2_8,$$

$$3_1 4_1, 3_5 4_5, 3_6 4_6, 3_7 4_7, 3_8 4_8, 4_1 4_2, 4_2 4_6, 4_3 4_7, 4_4 4_5, 4_4 4_8$$

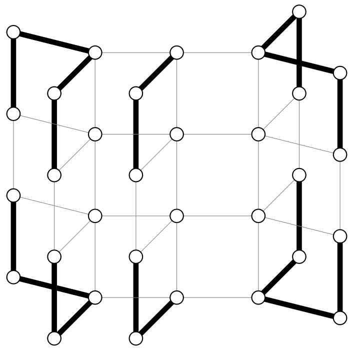
(thick black edges in Figure 11(a)) are chosen. Since each of the vertices $1_2, 1_4$, 4_2 and 4_4 is already incident to two chosen edges, the four edges $1_21_3, 1_31_4, 4_24_3, 4_34_4$ (dotted edges in Figure 11(b)) can not be chosen. Furthermore, this tells that the edges $1_32_3, 3_34_3$ need to be chosen as shown in Figure 11(b). At this time, at least one of $2_22_3, 2_32_4$ can not be chosen to complete the Hamiltonian cycle. Without loss of generality, says the edge 2_22_3 (dashed edges in Figure 11(b)) has not been chosen. Now each of two internal disjoint paths from 2_2 to 2_3 in the Hamiltonian cycle contains the edge 3_23_3, a contradiction. Hence G is not Hamiltonian.

Next we show that G is 1-tough. As G depicted in Figure 11(c), there exists a cycle C of order 30 in G such that $V(G-C)=\{3_5,4_5\}$ and 3_54_5 is an edge of G that is incident to 3 vertices $2_5, 3_4, 4_4$ of C. For a vertex set S, there are 3 cases for $G-S$ to discuss : The set $S\cap\{3_5,4_5\}$ is non-empty; The set $S\cap\{3_5,4_5\}$ is empty and $\{2_5,3_4,4_4\}\subseteq S$; The set $S\cap\{3_5,4_5\}$ is empty and $\{2_5,3_4,4_4\}\not\subseteq S$.

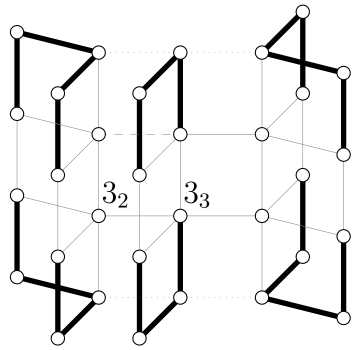
If the set $S\cap\{3_5,4_5\}$ is non-empty, then $c(\{3_5,4_5\}-(S\cap\{3_5,4_5\}))\leq|S\cap\{3_5,4_5\}|$. On the other hand, $c(S\cap C)\leq|C-(S\cap C)|$ since C is 1-tough. Because $G-S\subseteq(C-(S\cap C))\cup(\{3_5,4_5\}-S\cap\{3_5,4_5\})$, we conclude that $c(G-S)\leq c(C-(S\cap C))+c(\{3_5,4_5\}-(S\cap\{3_5,4_5\}))\leq|S\cap C|+|S\cap\{3_5,4_5\}|=|S|$ for all S such that $S\cap\{3_5,4_5\}$ is non-empty.

If the set $S\cap\{3_5,4_5\}$ is empty and $\{2_5,3_4,4_4\}\subseteq S$, then the subgraph induced by $\{3_5,4_5\}$ is a component of $G-S$. As depicted in Figure 11(d), the subgraph G_1 of G induced by $V(G)-\{3_5,4_5,2_5,3_4,4_4\}$ contains a spanning tree such that all vertices has degree at most 2 except an only one degree 3 vertex. This implies $c(G_1-S')\leq|S'|+2$ for $S'=S-\{2_5,3_4,4_4\}$. Therefore, $c(G-S)=c(G_1-S')+1\leq|S'|+3=|S|$ for all S such that the subgraph induced by $\{3_5,4_5\}$ is a component of $G-S$.

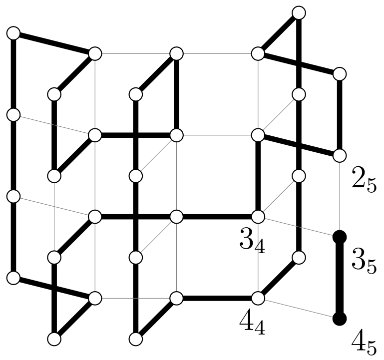
If the set $S\cap\{3_5,4_5\}$ is empty and $\{2_5,3_4,4_4\}\not\subseteq S$, then $S\subseteq C$ and the edge 3_54_5 is adjacent to some vertices of $C-S$. Therefore, $c(G-S)\leq c(C-S)$ for all such S. Since



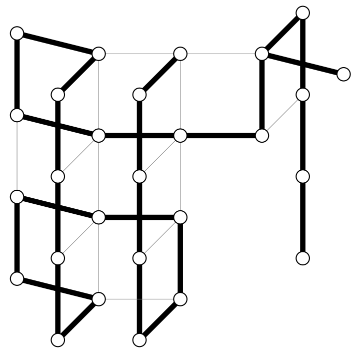
(a) Edges with degree 2 endpoints.



(b) Edges which need to be chosen.



(c) A cycle C and the edge $3_5 4_5$.



(d) Graph G_1 and its spanning tree.

Figure 11: The graph $P_4 \square T_1$ and its subgraphs.

the cycle C is 1-tough, $c(C - S) \leq |S|$. Hence $c(G - S) \leq c(C - S) \leq |S|$.

In conclusion, $c(G - S) \leq |S|$ for all $S \subseteq V(G)$ which means G is 1-tough.

■

6.2.4 More results on the Hamiltonicity of Cartesian product graphs

The well-known Petersen's matching theorem [37] states that a connected 3-regular graph with no cut-edges has a perfect matching, so together with Theorem 6.11(a) we obtain the following corollary.

Corollary 6.27. *Let G_1 be a traceable graph of order at least 3. If G_2 is a connected 3-regular graph with no cut-edge, then $G_1 \square G_2$ has a Hamiltonian cycle.* ■

We use Theorem 6.11(b) to obtain the following two Dirac-type results [17].

Corollary 6.28. *Let G_2 be a connected graph with $2\delta(G_2) \geq \Delta(G_2)$ and G_1 be a traceable graph of even order. If $|V(G_1)| \geq 4\Delta(G_2) - 2$, then $G_1 \square G_2$ has a Hamiltonian cycle.*

Proof. Let S be a vertex subset of $V(G_2)$. Now the number of edges between S and the set of isolated vertices of $G_2 - S$ is at least $i(G_2 - S)\delta(G_2)$ and is at most $|S|\Delta(G_2)$. Since $2\delta(G_2) \geq \Delta(G_2)$, we have $i(G_2 - S) \leq 2|S|$ for all $S \subseteq V(G_2)$. By Proposition 6.13, G_2 has a path factor and by Theorem 6.11(b) we complete the proof. ■

Corollary 6.29. *Let G_2 be a connected graph with $\delta(G_2) \geq |V(G_2)|/3$ and G_1 be a traceable graph of even order. If $|V(G_1)| \geq 4\Delta(G_2) - 2$, then $G_1 \square G_2$ has a Hamiltonian cycle.*

Proof. This is immediate by applying Lemma 6.14 to Theorem 6.11(b). ■

6.3 Conditions using Kelmans transformation

In this section, we focus on the Hamiltonicity of maximal graphs in $\mathcal{UG}(n, m)$ and the Hamiltonicity of the Cartesian product graph of a path and a Kelmans transformation graph. The main results are Proposition 6.30 and Corollary 6.34.

6.3.1 Hamiltonicity of Kelmans transformation graphs

In the Kelmans transformation G_b^a, the vertex a *dominates* the vertex b, which means $(N_{G_b^a}(b)\backslash\{a\}) \subseteq (N_{G_b^a}(a)\backslash\{b\})$. From this property, it is easy to deduce that after reordering the matrix, the adjacency matrix of a maximal element in $\mathcal{UG}(n, m)$ is *stepwise*, i.e.

$a_{i(j+1)} = 0$ if $a_{ij} = 0$ for $i \neq j$. For example, the star $K_{1,n}$ is maximal in $\mathcal{UG}(n+1, n)$ by Proposition 4.5. After reordering the vertices, the adjacency matrix of $K_{1,n}$ is written as:

$$A(K_{1,n}) = \begin{pmatrix} 0 & 1 & 1 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \\ 1 & 0 & \ddots & \vdots & \vdots \\ \vdots & \vdots & \dots & 0 & 0 \\ 1 & 0 & \cdots & 0 & 0 \end{pmatrix}.$$

Stepwise matrices also help us to characterize Hamiltonian maximal graphs. Recall that M_n is the n-by-n binary matrix with $M_n(i,j) = 1$ if and only if $i \neq j, i + j \leq n + 2$. For example,

$$M_6 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}, \ M_7 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

We have the following result.

Proposition 6.30. *Let $[G]$ be a maximal element in $\mathcal{UG}(n, m)$ with a stepwise adjacency matrix A. Then G is Hamiltonian if and only if $A \geq M_n$.*

Proof. Let G_n be the graph with adjacency matrix M_n. When n is even, G_n contains a Hamiltonian cycle $1, n, 2, n-1, 3, n-2, \dots, \frac{n}{2}, \frac{n}{2}+1, 1$. When n is odd, G_n contains a Hamiltonian cycle $1, n, 2, n-1, 3, n-2, \dots, \frac{n+1}{2}+1, \frac{n+1}{2}, 1$. If $A \geq M_n$, then G_n is a subgraph of G. Since G_n is Hamiltonian, the graph G is also Hamiltonian.

If $A \not\geq M_n$, then there exist $i_0 > j_0$ such that $i_0 + j_0 \leq n+2$ and $A(i,j) = 0$ for all i, j with $i \geq i_0$ and $j \geq j_0$. This tells that neighbor of i is a subset of $\{1, 2, \dots, j_0 - 1\}$. Taking vertices $\{1, 2, \ldots, j_0-1\}$ off from G, each of the vertices $\{i_0, i_0+1, \ldots, n\}$ becomes isolated. The graph $G-\{1, 2, \ldots, j_0-1\}$ contains at least $|\{i_0, i_0+1, \ldots, n\}|+1$ components, which are isolated vertices $i_0, i_0+1, \ldots, n$ and a component contains vertex j_0. Since

$$|\{1, 2, \ldots, j_0-1\}| = j_0 - 1 \text{ and } |\{i_0, i_0+1, \ldots, n\}| = n - i_0 + 1,$$

the toughness $\tau(G)$ of G satisfies

$$\tau(G) \leq \frac{|\{1, 2, \ldots, j_0-1\}|}{c(G - \{1, 2, \ldots, j_0-1\})} \leq \frac{j_0 - 1}{n - i_0 + 2} \leq \frac{j_0 - 1}{j_0} < 1.$$

Since G is not 1-tough, G is not Hamiltonian.

■

The following proposition tells that the "non-Hamiltonian" property is preserved by a Kelmans transformation.

Proposition 6.31. *If G contains two vertices a, b which are in a k-cycle C of G^a_b then a and b are in a k-cycle C' of G. In particular, if G is non-Hamiltonian then G^a_b is non-Hamiltonian.*

Proof. Let $u, v \in N_C(a)$ be distinct. If $u, v \in N_G(a)$, then choose $C' = C$ and the proof is finished. Suppose $u \notin N_G(a)$ and $v \in N_G(a)$. By the definition of Kelmans transformation, we have $u \neq b$, $u \in N_G(b)$, and $u \notin N_C(b)$. We give C a direction from a to u and back to a. Let $x \in N_C(b)$ be the vertex before b in this direction. Note that $x \in N_C(a)$. Let C' be the cycle in G starting from a, following x, along the reversed direction of C to u, then to b, and following the direction of C back to a. Then C' is a k-cycle of G which contains b and a. The case $u \in N_G(a)$ and $v \notin N_G(a)$ is similar. Suppose for the last case $u \notin N_G(a)$ and $v \notin N_G(a)$. The above argument shows that $u, v \in N_G(b)$ and for the vertices $x, y \in N_C(b)$ along the direction of C, we have $x, y \in N_G(a)$. Let C' be the cycle in G starting from a, following x, along the reversed direction of C to u, then to b, following v, along the reversed direction of C to y and then back to a. Then C' is a k-cycle of G which contains b and a. ■

By Proposition 6.31, the Hamiltonicity of $(G_1\square G_2)_b^a$ is related to the Hamiltonicity of $G_1\square G_2$. However, $(G_1\square G_2)_b^a$ is not a Cartesian product graph in general. It is more interesting to consider graphs like $G_1\square(G_2)_b^a$. Contents about $G_1\square(G_2)_b^a$ will be discussed in Section 6.3.2.

6.3.2 Cartesian product of a path with a Kelmans transformation graph

We have used the perfect matchings and path factors of a graph to construct Hamiltonian cycles in Theorem 6.11. The following two lemmas consider the existence of perfect matchings and path factors of Kelmans transformation graphs.

Lemma 6.32. *If G has no perfect matching, then G_b^a has no perfect matching for any distinct $a, b \in V(G)$.*

Proof. Let M be a perfect matching of G_b^a. If $ab \in M$, then the edges of M are all belong to $E(G)$. Hence M is also a perfect matching of G.

If $ab \notin M$ and $bx, ay \in M$. Then $bx, ax \in E(G)$ by the definition of the Kelmans transformation. If $ay \in E(G)$, then M is a perfect matching of G. If $ay \notin E(G)$, then $by \in M$ by the definition of the Kelmans transformation, so $M\backslash\{bx, ay\} \cup \{by, ax\}$ is a perfect matching of G. ■

Lemma 6.33. *If G has no path factor, then G_b^a has no path factor for any distinct $a, b \in V(G)$.*

Proof. Let M be a path factor of G_b^a. If M is a subgraph of G, then there is nothing to prove. If not, then there exists $x \in N_M(a)\backslash N_G(a)$. The definition of Kelmans transformation implies that $x \in N_G(b)$. Let

$$M' = M \cup \{bx : x \in N_M(b)\backslash N_G(b)\}\backslash\{ax : x \in N_M(a)\backslash N_G(a)\}.$$

Then $\deg_{M'}(b) = \deg_M(b) + |N_M(a) \backslash N_G(a)|$, $\deg_{M'}(a) = \deg_M(a) - |N_M(a) \backslash N_G(a)|$ and $\deg_{M'}(w) = \deg_M(w)$ for all $w \neq a, b$.

Note that $N_{M'}(b) \subseteq N_G(a)$. If $\deg_{M'}(b) > 2$, then pick $\deg_{M'}(b) - 2$ vertices $y \in N_{M'}(b)$, delete edges by from M' and add edges ay to obtain a spanning subgraph M'' of G with each vertex of degree 1 or 2. If each component of M'' is a path, then M'' is a path factor of G. If M'' contain cycles, delete an arbitrary edge from each of the cycles, we get a path factor. ■

Corollary 6.34. *Let H be a connected bipartite graph. Let n be an even integer and $n \geq 4\Delta(H) - 2$. If there exist $a, b \in V(H)$ such that $P_n \square H_b^a$ is Hamiltonian, then $P_n \square H$ is Hamiltonian.*

Proof. If there exist $a, b \in V(H)$ such that $P_n \square H_b^a$ is Hamiltonian, then by Corollary 6.25, H_b^a has a path factor. By Lemma 6.33, H contains a path factor. Therefore, $P_n \square H$ is Hamiltonian by Corollary 6.25. ■

7 Concluding remarks

In this dissertation, we generalize the concept of Kelmans transformation to nonnegative matrices. With minor constraints, we show that the largest real eigenvalue of a nonnegative matrix will not decrease after a Kelmans transformation.

The general version of the Kelmans transformation is applicable on matrices related to mixed graphs. We extend the relation $G \le G_b^a$ into a partial order on the set $\mathcal{G}(n,m)$ of the isomorphism classes of mixed graphs of order n and size m; then characterize the maximal/minimal elements in some of the subposets and weak subposets of $(\mathcal{G}(n,m), \le)$.

We also apply the general version of the Kelmans transformation on the researches of the spectral theory of A_α-matrices, which combines the spectral theories of adjacency matrix and signless Laplacian matrix. For an application, we show that for $\alpha \in [0,1]$ and a mixed tree T of order n and size m, the A_α-spectral radius $\rho_\alpha(T)$ satisfies

$$\rho_\alpha(T) \le \frac{1}{2}\left(\alpha n + \sqrt{\alpha^2 n^2 - 4\alpha^2(n-1) + 4(1-\alpha)^2(m-n+1)}\right).$$

The methods we introduce is also applicable on other mixed graphs. To find the extremal values of the A_α-spectral radius of mixed graphs is a direction of future works.

We also give new sufficient conditions of the Hamiltonicity of graphs. We prove that except some specific graphs, if the A_α-spectral radius of a graph is large enough, then the graph is Hamiltonian. However, the bounds we give in Proposition 6.6 and Proposition 6.9 are still improvable. For example, the following proposition gives a sufficient condition of Hamiltonicity using the minimum degree and the spectral radius of a graph.

Proposition 7.1 ([32]). *Let $k \ge 2$, $n \ge k^3 + k + 4$, and let G be a graph of order n, with minimum degree $\delta(G) \ge k$. If*

$$\rho(G) \ge n - k - 1,$$

then G is Hamiltonian unless $G = K_1 \vee (K_{n-k-1} \cup K_k)$ or $G = K_k \vee (K_{n-2k} \cup \overline{K_k})$.

Here we provide a problem to conclude this dissertation.

Problem 7.2. Does there exist a bound $f(\delta(G), \alpha)$ such that a graph G of order n with

$$\rho(G) \geq n - f(\delta(G), \alpha)$$

is Hamiltonian unless G belongs to some certain graph classes?

References

[1] J. Akiyama, D. Avis, H. Era, On a $\{1,2\}$-factor of a graph, *TRU Math.* 16 (1980) 97–102.

[2] F. Atik, P. Panigrahi, On the distance and distance signless Laplacian eigenvalues of graphs and the smallest Gerŝgorin disc, *Electron. J. Linear Algebra*, 34 (2018) 191–-204.

[3] D. Bauer, H.H. Broersma, H.H. Veldman, Not every 2-tough graph is Hamiltonian, *Discrete Appl. Math.* 99 (2000) 317–321.

[4] Z.R. Bogdanowicz, Undirected simple connected graphs with minimum number of spanning trees, *Discrete Math.* 309 (2009) 3074–3082.

[5] J.A. Bondy, Variations on the Hamiltonian theme, *Canad. Math. Bull.* 15 (1972) 57–62.

[6] A.E. Brouwer, W.H. Haemers, *Spectra of graphs*, Springer, 2012.

[7] J.I. Brown, C.J. Colbourn, and J. S. Devitt, Network transformations and bounding network reliability, *Networks* 23(1) (1993) 1–17.

[8] Y.-J. Cheng, C.-A. Liu, C.-W. Weng, Counterexamples of the Bhattacharya-Friedland-Peled conjecture, arXiv:2112.01124 [math.CO].

[9] Y.-J. Cheng, C.-W. Weng, A matrix realization of spectral bounds of the spectral radius of a nonnegative matrix, arXiv:1711.03274.

[10] V. Chvátal, On Hamiltonian's ideals, *J. Combin. Theory Ser. B* 12 (1972) 163–168.

[11] V. Chvátal, Tough graphs and hamiltonian circuits, *Discrete Math.* 5 (1973) 215–228.

[12] V. Chvátal, P.L. Hammer, Aggregation of inequalities in integer programming, *Ann. Discret. Math.* 1 (1977) 145–162.

[13] P. Csikvári, On a conjecture of V. Nikiforov, *Discrete Math.* 309 (2009) 4522–4526.

[14] R. Čada, E. Flandrin, H. Li, Hamiltonicity and pancyclicity of cartesian products of graphs, *Discrete Math.* 309 (2009) 6337–6343.

[15] K. Das, Maximizing the sum of squares of the degrees of a graph, *Discrte Math.* 285 (2004) 57–66.

[16] V. Dimakopoulos, L. Palios, A.S. Poulakidas, On the Hamiltonicity of the Cartesian product, *Inform. Process. Lett.* 96 (2005) 49–53.

[17] G. Dirac, Some theorems on abstract graphs, *Proc. Lond. Math. Soc.* 2 (1952) 69–81.

[18] M. Fiedler, V. Nikiforov, Spectral radius and Hamiltonicity of graphs, *Linear Algebra Appl.* 432 (2010) 2170–2173.

[19] H.A. Ganie, M. Baghipur, on the generalized adjacency spectral radius of digraphs, *Linear Multilinear Algebra.* DOI: 10.1080/03081087.2020.1844614.

[20] H. Guo, B. Zhou, On the α-spectral radius of graphs, *Appl. Anal. Discrete Math.* 14 (2020) 431–458.

[21] J. Harant, P.J. Owens, Non-Hamiltonian $\frac{5}{4}$-tough maximal planar graphs, *Discrete Math.* 147 (1995) 301–305.

[22] X. Huang, H. Lin, J. Xue, The Nordhaus-Gaddum type inequalities of A_α-matrix. *Appl. Math. Comput.* 365 (2020) 124716.

[23] A. Kabela, T. Kaiser, 10-tough chordal graphs are hamiltonian, *J. Combin. Theory Ser. B* 122 (2017) 417–427.

[24] N. Kahl, Graph vulnerability parameters, compression, and threshold graphs. *Discrete Appl. Math.* 292 (2021) 108–116.

[25] L. Kao, C.-W. Weng, A note on the largest real eigenvalue of a nonnegative matrix, *Appl. Math. Sci.* 15(12) (2021) 553–557.

[26] L. Kao, C.-W. Weng, The relation between Hamiltonian and 1-tough properties of the Cartesian product graphs, *Graphs Combin.* 37(3) (2021) 933–943.

[27] A.K. Kelmans, On graphs with randomly deleted edges, *Acta Math. Hungar* 37 (1981) 77–88.

[28] E. Lenes, E. Mallea-Zepeda, J. Rodríguez, New bounds for the α-indices of graphs, *Mathematics* 8(10) (2020) 1668.

[29] B. Li, B, Ning, Spectral analogues of Erdős' and Moon-Moser's theorems on Hamiltonian cycles, *Linear Multilinear Algebra.* 64 (2016) 1152–1169.

[30] D. Li, Y. Chen, J. Meng, A_α-spectral radius of trees and unicyclic graphs with given degree sequence, *Appl. Math. Comput.* 363 (2019) 124622.

[31] J. Liu, X. Wu, J. Chen, B. Liu, The A_α-spectral radius characterization of some digraphs, *Linear Algebra Appl.* 563 (2019) 63–74.

[32] V. Nikiforov, Spectral radius and Hamiltonicity of graphs with large minimum degree, *Czechoslovak Math. J.* 66 (2016) 925–940.

[33] V. Nikiforov, Merging the A- and Q-spectral theories, *Appl. Anal. Discrete Math.* 11 (1) (2017) 81–107.

[34] L. Kao, Hamiltonian properties of Cartesian product graphs, Master Thesis, National Chaio Tung University, (2016) $<$ https://hdl.handle.net/11296/q89fq7 $>$.

[35] V. Nikiforov, G. Pastén, O. Rojo, R.L. Soto, On the A_α-specra of trees, *Linear Algebra Appl.* 520 (2017) 286–306.

[36] O. Ore, Note on Hamiltonian circuits, *Amer. Math. Monthly* 67 (1960) 55.

[37] J. Petersen, Die Theorie der regulären graphs, *Acta Math.* 15 (1891) 193–220.

[38] O. Rojo, The maximal α-index of trees with k pendent vertices and its computation, *eletronic J. Linear algebra.* 36 (2020) 38–48.

[39] M. Rosenfeld, D. Barnette, Hamiltonian circuits in certain prisms, *Discrete Math.* 5 (1973) 389–-394.

[40] W. Xi, W, So, L. Wang, On the A_α spectral radius of digraphs with given parameters, *Linear Multilinear Algebra.* DOI: 10.1080/03081087.2020.1793879.

[41] L. You, M. Yang, W. So, W. Xi, On the spectrum of an equitable quotient matrix and its application, *Linear Algebra Appl.* 577 (2019) 21–40.

[42] G.D. Yu, Y.Z. Fan, Spectral conditions for a graph to be Hamiltonian-connected, *Appl. Mech. Mater.* 336 (2013) 2329–2334.