State transfer on mixed graphs

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Abstract

Mixed graphs, which generalize both undirected and directed graphs, provide a natural framework for investigating a broader class of quantum transport phenomena, including perfect state transfer (PST) and multiple state transfer (MST). The Hermitian adjacency matrix, incorporating both symmetric and asymmetric edge structures, establishes a unified spectral framework that reveals quantum phenomena absent in undirected graphs. In this paper, we study PST and MST on mixed graphs using the Hermitian adjacency matrix, extending results from undirected graphs and focusing on phenomena such as periodicity, one-way PST, two-way PST, and MST. Additionally, we present novel results that contribute to a deeper understanding of quantum state transfer in mixed graphs.

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1 Introduction

In the past two decades, quantum information technology has developed rapidly. In 2003, Bose [5] first introduced the concept of perfect state transfer (PST for short) for spin chains, referring to the phenomenon where quantum information is preserved without loss.

Algebraic graph theory has proven to be an effective tool for studying quantum information by providing a structured framework to model quantum systems, related concepts can be found in [19]. For example, quantum state transfer in spin networks can be effectively analyzed using adjacency matrices, which reveal insights into state transfer efficiency. Graphs also enable the study of spectral properties that underlie quantum coherence and entanglement, highlighting their importance in this field.

In 2004-2005, Christandl et al. [8, 9] were the first to study PST using graph theory, with an initial focus on undirected graphs. In 2012, Godsil [15] showed that only a finite number of graphs exhibit PST, indicating that PST is a rare occurrence. For this reason, Godsil, Kirkland, Severini, and Smith [17] proposed the concept of pretty good state transfer. Godsil [13–15] also provided several characterizations of graphs that admit PST. For more results about PST, we refer the reader to [11].

For undirected graphs, Kay [24] proved that PST occurs only between two non-disjoint pairs of vertices. Unlike undirected graphs, some oriented graphs have been found to exhibit PST between multiple vertices. For this reason, Cameron, Fehrenbach, Granger, Hennigh, Shrestha, and Tamon [6] first explored PST in oriented graphs using Hermitian adjacency matrix, discovering that only K_2 and K_3 have universal state transfer (PST occurs between all vertices). Connelly, Grammel, Kraut, Serazo, and Tamon [10] extended the study of universal state transfer. Later, Godsil and Lato [18] introduced the concept of multiple state transfer (PST occurs between multiple vertices), abbreviated as MST, for oriented graphs, as a natural generalization of universal state transfer. In 2013, Bašić [2] provided a comprehensive characterization of integral circulant graphs admitting PST. Inspired by this work, Song and Lin presented thorough characterizations of integral oriented circulant graphs [27] and integral mixed circulant graphs [28] admitting PST and MST.

It is well known that periodicity is closely related to PST in graphs. For undirected graphs, Godsil [14] proved that PST can only occur at half of the minimum period, a fact closely related to the spectral symmetry of the adjacency matrix. In particular, PST is known to be time-symmetric: if PST occurs from vertex u to vertex v at time t, then it also occurs from v to u at the same time. This property originates from the notion of time-reversal symmetry in quantum physics [20]. Furthermore, due to its strong dependence on symmetry, PST tends to occur only in highly regular graph families, such as cubelike graphs [4, 7], Cayley graphs [1, 29], and strongly regular graphs [16].

However, for oriented graphs, the Hermitian adjacency matrix is skew-symmetric, destroying the symmetry present in undirected graphs. Consequently, the symmetry of PST is also broken. This asymmetry introduces new phenomena, such as the time of PST first occurs does not equal to the half of the minimum period. This effect, known as time-reversal symmetry breaking in quantum physics [20, 30], has significant implications for quantum state transfer, leading to new phenomena such as one-way PST and MST.

In this paper, we focus on mixed graphs and investigate the relationship between the time of the first PST, MST, and periodicity, as well as the direction of PST. By exploring these relationships, we aim to deepen the understanding of quantum state transfer in mixed graphs, which may have significant implications for enhancing the efficiency and control of quantum communication protocols.

The paper is organized as follows:

- In Section 2, we introduce fundamental concepts related to PST, MST, periodicity, and other relevant notions.
- In Section 3, we define and discuss one-way PST and two-way PST.
- In Section 4, we explore the relationship between periodicity and the time of the first PST, and explore MST on mixed graphs.
- In Section 5, we propose several results related to coherent algebras.
- In Section 6, we select proper minimal polynomials to obtain spectral decomposition through Lagrange interpolation.
- In Section 7, we present results concerning PST on mixed graphs with few distinct eigenvalues.

2 Perfect state transfer

A **mixed graph** $\Gamma = (V, E, A)$ consists of a set of vertices V, a set of undirected edges E, and a set of directed edges (or arcs) A. Specifically, Γ is **undirected** (resp. **oriented**) if it contains only undirected (resp. directed) edges. The **Hermitian adjacency matrix** of Γ, introduced by Liu and Li [25] and independently by Guo and Mohar [21], is defined as $H_\Gamma = (h_{uv})_{u,v\in V}$, where

$$h_{uv} = \begin{cases} 1, & \text{if } \{u, v\} \in E, \\ \mathrm{i}, & \text{if } (u, v) \in A, \\ -\mathrm{i}, & \text{if } (v, u) \in A, \\ 0, & \text{otherwise.} \end{cases}$$

Here $\mathrm{i} = \sqrt{-1}$. Clearly, H_Γ is a Hermitian matrix. In particular, if Γ is undirected (resp. oriented), then $H_\Gamma = A_\Gamma$ (resp. $H_\Gamma = \mathrm{i}\, S_\Gamma$), where A_Γ (resp. S_Γ) is the **adjacency matrix** (resp. **skew adjacency matrix**) of Γ. The eigenvalues of H_Γ are also referred to as the **eigenvalues** of Γ.

Let $\Gamma = (V, E, A)$ be a mixed graph with the Hermitian adjacency matrix H_Γ. We define the **transition matrix** of H_Γ by

$$U(t) = \exp(-\mathrm{i}\, t H_\Gamma),$$

where $\mathrm{i} = \sqrt{-1}$ and t is a real number. Note that $U(t)$ is a unitary matrix, with the following properties:

$$\begin{aligned} &\textbf{P1:}\ U(-t) = U(t)^{-1} = U(t)^*, \\ &\textbf{P2:}\ U(t+t') = U(t)U(t'), \end{aligned} \tag{1}$$

where $\cdot^*$ denotes the conjugate transpose.

For any vertex $v \in V$, let $\mathbf{e}_v$ be the vector defined on V such that $\mathbf{e}_v(u) = 1$ if $u = v$ and $\mathbf{e}_v(u) = 0$ otherwise. We say that Γ has **perfect state transfer** (PST for short) from start vertex u to end vertex v if there exists a time $t \in \mathbb{R}$ and a complex unimodular scalar γ such that

$$U(t)\mathbf{e}_u = \gamma \mathbf{e}_v.$$

Here, γ is a complex number of modulus 1, and it remains closed under multiplication and division. In particular, if

$$U(t')\mathbf{e}_u = \gamma \mathbf{e}_u,$$

we say that Γ is **periodic** at vertex u with period t'. Moreover, Γ is said to be periodic if there exists a time t such that $U(t)$ is diagonal.

For a subset $S \subseteq V$, we say that Γ has **multiple state transfer** (MST for short) on S if PST occurs between each pair of vertices in S. Note that the time when PST occurs between each pair of vertices in S is not necessarily the same. Let k be the number of vertices in S. Then we say that Γ has k-vertex MST if S is the largest subset of V on which MST occurs. In particular, Γ is said to be **universal state transfer** (UST for short) if it has MST on V.

For two vertices u and v in a mixed graph the definition of PST implies that $U(t)_{v,u} = \gamma$ if PST occurs from u to v at time t. Since $U(t)$ is a unitary matrix, all elements in the v-th row and u-th column, except for $U(t)_{v,u}$, must be zero. Hence, $U(t)$ has the following form:

$$U(t) = \begin{array}{cc} \begin{pmatrix} & 0 & \\ & \vdots & \\ & 0 & \\ 0 \cdots 0 & \gamma & 0 \cdots 0 \\ & 0 & \\ & \vdots & \\ & 0 & \end{pmatrix} & v \\ \begin{array}{ccc} & u & \end{array} & \end{array}.$$

Therefore, we have the following lemma.

Lemma 1. *If there exists a time t such that* PST *occurs from u to v, then at time t, all elements in the v-th row and the u-th column of $U(t)$ are zero, except for $U(t)_{v,u}$. In particular, we have $U_{u,u}(t) = U_{v,v}(t) = 0$ and the following form of the matrix $U(t)$:*

$$U(t) = \begin{array}{cc} \begin{pmatrix} & \vdots & & \vdots & \\ \cdots & 0 & \cdots & \gamma & \cdots \\ & \vdots & & \vdots & \\ \cdots & * & \cdots & 0 & \cdots \\ & \vdots & & \vdots & \end{pmatrix} & \begin{array}{c} \\ v \\ \\ u \\ \\ \end{array} \\ \begin{array}{ccccc} & v & & u & \end{array} & \end{array} .$$

It follows from Lemma 1 that a necessary condition for PST between the vertices u and v is the existence of a time t for which $U_{u,u}(t) = U_{v,v}(t) = 0$.

3 One-way PST and two-way PST

For mixed graphs, the Hermitian adjacency matrix is not necessarily symmetric. Consequently, quantum state transfer in mixed graphs becomes directional, giving rise to new phenomena such as one-way PST and two-way PST. We define these phenomena as follows.

For two vertices u and v in a mixed graph, let t and t' be the times when PST occurs from u to v and from v to u, respectively. We define that type of PST between vertices u and v as **two-way** if $t = t'$, and **one-way** otherwise. In fact, two-way PST occurs when two one-way PSTs take place simultaneously in opposite directions between the two vertices. A few examples of PST types are shown in Fig. 1.

$$u \longrightarrow v \qquad\qquad u \longleftarrow v \qquad\qquad u \longleftrightarrow v$$

$$U(t) = \begin{array}{cc} \begin{pmatrix} & \vdots & & \vdots & \\ \cdots & 0 & \cdots & \gamma & \cdots \\ & \vdots & & \vdots & \\ \cdots & * & \cdots & 0 & \cdots \\ & \vdots & & \vdots & \end{pmatrix} & \begin{array}{c} \\ v \\ \\ u \\ \\ \end{array} \\ \begin{array}{ccccc} & v & & u & \end{array} & \end{array} \quad U(t) = \begin{array}{cc} \begin{pmatrix} & \vdots & & \vdots & \\ \cdots & 0 & \cdots & * & \cdots \\ & \vdots & & \vdots & \\ \cdots & \gamma & \cdots & 0 & \cdots \\ & \vdots & & \vdots & \end{pmatrix} & \begin{array}{c} \\ v \\ \\ u \\ \\ \end{array} \\ \begin{array}{ccccc} & v & & u & \end{array} & \end{array} \quad U(t) = \begin{array}{cc} \begin{pmatrix} & \vdots & & \vdots & \\ \cdots & 0 & \cdots & \gamma & \cdots \\ & \vdots & & \vdots & \\ \cdots & \gamma & \cdots & 0 & \cdots \\ & \vdots & & \vdots & \end{pmatrix} & \begin{array}{c} \\ v \\ \\ u \\ \\ \end{array} \\ \begin{array}{ccccc} & v & & u & \end{array} & \end{array}$$

Fig. 1: Type of PST between vertices u and v.[1]

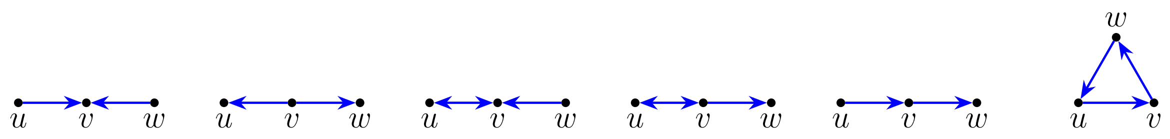
For undirected graphs, Kay [24] showed that if PST occurs between two vertices, it must be two-way. In contrast, mixed graphs can exhibit both two-way and one-way PST between two vertices. Notably, one-way PST between two vertices is a unique characteristic of mixed graphs having directed edges.

[1]Each arrow in Fig. 1 represents only the direction of transfer. The same convention applies to Fig. 2 and Fig. 3.

Lemma 1 implies a one-to-one correspondence in PST, meaning that at the time when PST occurs, a vertex cannot transfer to multiple vertices, nor can multiple vertices transfer to one vertex. Therefore, we can deduce the following lemma.

Lemma 2. *Let u and v be two vertices on a mixed graph. If there exists a time t such that* PST *occurs from u to v, then u and v can each serve as a start vertex and an end vertex only once.*

In Fig. 2, we show the cases of one-way PST between three vertices at the same time. It is evident that the pairs of vertices admitting two-way PST must be non-intersecting. For one-way PST between two or more vertices at the same time, PST is always one-way, and based on the direction of transfer, it forms either a directed path or a directed cycle, as shown in cases (e) and (f) in Fig. 2.



(a) No. (b) No. (c) No. (d) No. (e) Yes. (f) Yes.

Fig. 2: The cases of PST between three vertices at the same time.

However, if PST is allowed to occur at different times, all the cases illustrated in Fig. 2 would become possible. We now proceed to examine these cases.

Lemma 3. *Let u, v, w be three vertices on a mixed graph. If there exists one-way* PST *from u to v at time t_1, and one-way* PST *from v to w at time t_2, then there exists one-way* PST *from u to w at time $t_1 + t_2$.*

Proof. If there exists one-way PST from u to v at time t_1 and from v to w at time t_2, by definition of PST, this can be expressed as

$$U(t_1)\mathbf{e}_u = \gamma_1 \mathbf{e}_v,$$
$$U(t_2)\mathbf{e}_v = \gamma_2 \mathbf{e}_w.$$

Combining the above equations, we have

$$U(t_1 + t_2)\mathbf{e}_u = \gamma_1\gamma_2 \mathbf{e}_w.$$

Therefore, there exists one-way PST from u to w at time $t_1 + t_2$. □

From Lemma 3, we can easily extend to several cases, as shown in Fig. 3. Considering the direction of transfer, if one-way PST forms a directed path of length $k-1$, then Lemma 3 can be generalized to the following lemma.

Lemma 4. *Let $v_1, v_2, \ldots, v_k$ be k vertices on a mixed graph. If there exists one-way* PST *from v_i to v_{i+1} at time t_i for $i \in \{1, \ldots, k-1\}$, then there exists one-way* PST *from v_1 to v_k at time $t_1 + t_2 + \cdots + t_{k-1}$.*

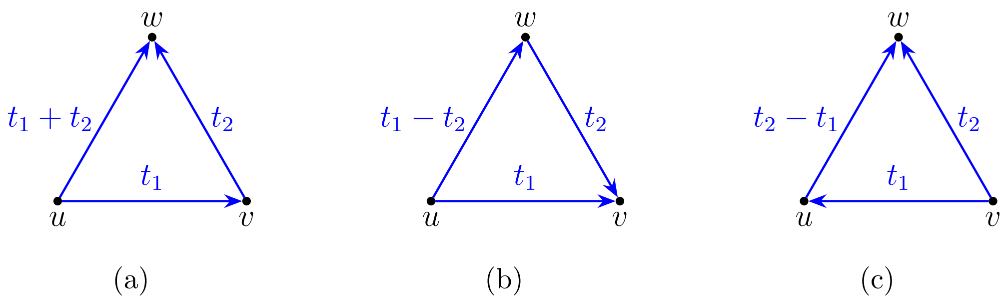


Fig. 3: The cases of PST between three vertices at different time.

Considering the direction of transfer, if one-way PST forms a cycle of length k, then we can easily deduce the following lemma.

Lemma 5. *Let $v_1, v_2, \dots, v_k$ be k vertices in a mixed graph. If there exists one-way* PST *from v_i to v_{i+1} (the indices are taken modulo k) at time t_i for $i \in \{1, \dots, k\}$, then these k vertices are periodic with a common period.*

Proof. According to Lemma 4, we have

$$U(t_1 + t_2 + \cdots + t_{k-1})\mathbf{e}_{v_1} = \gamma_1\gamma_2\cdots\gamma_{k-1}\mathbf{e}_{v_k}.$$

Since there exists one-way PST from v_k to v_1 at time t_k, by definition of PST, this can be expressed as

$$U(t_k)\mathbf{e}_{v_k} = \gamma_k\mathbf{e}_{v_1}.$$

Combining the above equations, we have

$$U(t_1 + t_2 + \cdots + t_k)\mathbf{e}_{v_1} = \gamma_1\gamma_2\cdots\gamma_k\mathbf{e}_{v_1}.$$

Therefore, the period of v_1 is $T = \sum_{i=1}^{k} t_i$. Similarly, all the other vertices have the same period. ☐

4 Periodicity and MST

In this section, we further investigate periodicity and MST. First, we consider periodicity in mixed graphs.

Let Γ be a mixed graph with the Hermitian adjacency matrix H_Γ. If mixed graphs contain no directed edges, then it is equivalent to an undirected graph. Therefore, PST in undirected graphs can be viewed as a special case of PST in mixed graphs. Consequently, many results established for undirected graphs can be extended to the case of mixed graphs.

In the case of undirected graphs, it is known that if PST occurs between two vertices at time t, then both vertices are periodic with a period dividing $2t$, as shown by Godsil [14, Lemma 1.1]. This result can be generalized to mixed graphs.

Lemma 6. *Let Γ be a mixed graph with two vertices u and v, and suppose that Γ is periodic at v with the minimum period T. If* PST *occurs from u to v at time t, then* PST *also occurs from v to u at time $kT - t$ for any $k \in \mathbb{N}$.*

Proof. Assume there exists PST from u to v at time t. Based on the definition of PST, we obtain $U(t)\mathbf{e}_u = \gamma \mathbf{e}_v$. It can be transformed into

$$U(-t)\mathbf{e}_v = \frac{1}{\gamma}\mathbf{e}_u.$$

By property **P2** (1) and periodicity of v, we have

$$U(kT - t)\mathbf{e}_v = U(kT)U(-t)\mathbf{e}_v = U(-t)\mathbf{e}_v.$$

Combining the above equations, we have

$$U(kT - t)\mathbf{e}_v = \frac{1}{\gamma}\mathbf{e}_u.$$

This implies that there exists PST from v to u at time $kT - t$. □

Lemma 7. *Let Γ be a mixed graph with two vertices u and v, and suppose that Γ is periodic at both u and v with the minimum period T. If* PST *occurs between vertices u and v, then one-way* PST *occurs only twice: from u to v and from v to u within one period, and the sum of the two times is equal to T.*

We extend the result presented by Godsil in [14, Lemma 3.1] to mixed graphs.

Lemma 8. *Let Γ be a mixed graph with two vertices u and v, and suppose that Γ is periodic at both u and v with the minimum period T. If* PST *first occurs between vertices u and v at time t, then $t \leqslant T/2$.*

Proof. Suppose PST first occurs between vertices u to v at time t. By Lemma 6, Γ has PST between vertices u and v at time t and $T - t$. If $t > T/2$, it follows that

$$T - t < T - \frac{T}{2} = \frac{T}{2},$$

which leads to a contradiction. □

Next, we investigate MST in mixed graphs focusing on the vertex subset on which MST occurs.

Let Γ be a mixed graph with a vertex subset $S = \{v_1, v_2, \ldots, v_k\}$. First, we study the periodicity of vertices in S. If there exists MST between the vertices in S, then by definition of MST, any two vertices in S admit one-way PST. Hence, these one-way PSTs induce a directed cycle on S of length k, where each arrow represents the direction of state transfer (possibly at different times). According to Lemma 5, we can deduce the following lemma.

Lemma 9. *Let* Γ *be a mixed graph with a vertex subset* S*. If* Γ *has* MST *between the vertices in* S*, then any vertex in* S *is periodic with the same period.*

From Lemma 9, we observe that the necessary condition for MST is that every vertex in S must have the same period. Hence, we assume that each vertex in S is periodic with the minimum period T. Let $U(t)[S]$ denote the submatrix of $U(t)$ corresponding to the vertex subset $S = \{v_1, v_2, \ldots, v_k\}$. For simplicity, we define $|A| := (|a_{ij}|)_{n\times n}$ for any complex matrix $A = (a_{ij}) \in \mathbb{C}^{n\times n}$, where $|A|$ denotes the entrywise modulus of A. Consequently, we have

$$|U(T)[S]| = I. \tag{2}$$

Second, we study the similarity of vertices in S. Let Γ be a mixed graph with the Hermitian adjacency matrix H. Suppose there exists PST from u to v. Since the powers of H and $U(t)$ commute, the definition of PST implies that

$$U(t)H^k\mathbf{e}_u = \gamma H^k\mathbf{e}_v,$$

for all $k \in \mathbb{N}$. Taking the norm of both sides gives

$$\|H^k\mathbf{e}_u\|^2 = \|H^k\mathbf{e}_v\|^2,$$

which indicates that the weighted sum of the neighbours (and hence the degree) of u equals to that of v. Therefore, u and v are similar.

Now suppose that there exists MST between the vertices in $S = \{v_1, v_2, \ldots, v_k\}$. By the definition of MST and Lemma 2, we can deduce the following lemma.

Lemma 10. *Let* Γ *be a mixed graph and let* $S = \{v_1, \ldots, v_k\}$*. Suppose* MST *occurs between the vertices in* S*. If one-way* PST*s first occurs at time* t*, then* $|U(t)[S]|$ *acts cyclically on* S*.*

Proof. Suppose MST occurs between the vertices in S. Then any two vertices in S admit one-way PST, it follows that all vertices in S are similar and have the same degree. By Lemma 2, each vertex appears exactly once as a start vertex and exactly once as an end vertex. It follows that these one-way PSTs form a cycle of length k at the same time.

To sum up, if one-way PSTs first occurs at time t, then the submatrix $U(t)[S]$ must have exactly one nonzero entry γ of modulus one in each row and each column, though these entries need not be identical. Therefore, $|U(t)[S]|$ acts cyclically on S. $\square$

According to above lemma, let

$$|U(t)[S]| = C_k \quad \text{or} \quad |U(t)[S]| = C_k^\top,$$

where C_k is the $k \times k$ circulant matrix defined by

$$C_k = \begin{array}{c} \\ v_1 \\ v_2 \\ \vdots \\ v_{k-1} \\ v_k \end{array}\!\!\begin{array}{c} \begin{array}{ccccc} v_1 & v_2 & v_3 & \cdots & v_k \end{array} \\ \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \end{pmatrix}_{k\times k} \end{array},$$

and where $*^\top$ denotes the transpose of matrix $*$.

Without loss of generality, let t be the first time at which PST occurs. Then the following holds:

$$|U(t)[S]| = C_k.$$

According to Lemma 3, for time kt we have

$$|U(kt)[S]| = (C_k)^k = I. \tag{3}$$

Let T denote the minimum period of vertex subset S. By Eq. (2) and Eq. (3), we have $T = kt$. It follows that t must be a rational multiple of T. Based on this analysis, we derive the following theorem.

Theorem 11. *Let Γ be a mixed graph with vertex subset $S = \{v_1, v_2, \ldots, v_k\}$ and the minimum period T. If Γ has k-vertex* MST *between the vertices in S, then the following statements hold:*

(i) *The set of times at which* PST *occurs within one period is*

$$\left\{\frac{T}{k}, \frac{2T}{k}, \ldots, \frac{(k-1)T}{k}\right\};$$

(ii) $|U(jT/k)[S]| = (C_k)^j$ *or* $|U(jT/k)[S]| = (C_k^\top)^j$, *for* $j \in \{1, 2, \ldots k-1\}$.

Note that two-way PST only occurs at time $T/2$, otherwise one-way PST, and MST only occurs at a rational multiple of the period.

Theorem 12. *Let Γ be a mixed graph with the minimum period T. Suppose* PST *first occurs at time $t = kT$ with $k \in \mathbb{R} \cap (0, 1)$. Then we have the following cases:*

(i) *If $k = 1/2$, then* PST *occurs between two vertices and two-way.*

(ii) *If $k \neq 1/2$, then there exists one-way* PST *between two vertices or* MST *between multiple vertices. Specifically, if $k \in \mathbb{R} \setminus \mathbb{Q}$, then* PST *occurs between two vertices and one-way.*

Proof. **Case (i)** When $t = T/2$, let a and b be two vertices. We have

$$U(T/2)\mathbf{e}_a = \gamma_1 \mathbf{e}_b \quad \text{and} \quad U(T/2)\mathbf{e}_b = \gamma_2 \mathbf{e}_a,$$

it follows that there exists two-way PST between vertices a and b at time $T/2$. Suppose that there exists a time $t < T/2$ such that two-way PST occurs between vertices a and b on Γ, it follows that

$$U(t)\mathbf{e}_a = \gamma_1 \mathbf{e}_b \quad \text{and} \quad U(t)\mathbf{e}_b = \gamma_1 \mathbf{e}_a.$$

Then we have

$$U(2t)\mathbf{e}_a = U(t)U(t)\mathbf{e}_a = \gamma_1 U(t)\mathbf{e}_b = \gamma_1\gamma_2 \mathbf{e}_a.$$

Therefore, $2t < T$ is a period of Γ, which leads to a contradiction.

Case (ii) The conclusion obviously holds. □

From Lemma 10, we can easily obtain the following lemma.

Lemma 13. *Let* Γ *be a mixed graph with vertex subset* S*. Suppose* MST *occurs between the vertices in* S*, and let* u *and* v *be vertices in* S*. Then there exists a one-way* PST *from* u *to* v *at time* t *if and only if* $U(t)_{v,u} = \gamma$ *and* $U(t)_{u,v} = 0$*, where* $|\gamma| = 1$*, i.e.* $U(t)$ *has the following form:*

$$U(t) = \begin{array}{cc} \begin{pmatrix} & \vdots & & \vdots & \\ \cdots & 0 & \cdots & \gamma & \cdots \\ & \vdots & & \vdots & \\ \cdots & 0 & \cdots & 0 & \cdots \\ & \vdots & & \vdots & \end{pmatrix} & \begin{array}{c} \\ v \\ \\ u \\ \\ \end{array} \\ \begin{array}{ccccc} \quad & v & \quad\quad & u & \quad \end{array} & \end{array}.$$

According to **Toeplitz decomposition** [2] [23, Theorem 4.1.2], any matrix A can be uniquely decomposed as $A = H + S$, where H is a Hermitian matrix and S is a skew-Hermitian matrix. For convenience, define $U(t) = V(t) + W(t)$, where

$$V(t) = \frac{U(t) + U(t)^*}{2}$$

and

$$W(t) = \frac{U(t) - U(t)^*}{2}.$$

If $U(t)_{v,u} = \gamma$ and $U(t)_{u,v} = 0$, by Lemma 13, then it follows that

$$|V(t)_{v,u}| = |W(t)_{v,u}| = \frac{1}{2}.$$

We obtain a necessary condition for the existence of MST as follows.

Lemma 14. *Let* Γ *be a mixed graph with vertex subset* S*. Suppose* MST *occurs between the vertices in* S*, and let* u *and* v *be vertices in* S*. If there exists a one-way* PST *from* u *to* v *at time* t*, then*

$$|V(t)_{v,u}| = |W(t)_{v,u}| = \frac{1}{2}.$$

By Theorem 11 and Lemma 14, we easily obtain the following lemma.

Lemma 15. *Let* Γ *be a mixed graph with* k*-vertex subset* S*. Suppose* MST *occurs between the vertices in* S*, and let* u *and* v *be vertices in* S*. If one-way* PST *first occurs at time* t*, then*

$$|V(t)[S]| = |W(t)[S]| = \frac{C_k + C_k^\top}{2}.$$

[2] This decomposition is also referred to as **Cartesian decomposition**, a term used in earlier works such as Halmos [22].

5 Coherent algebras

In this section, we will extend some of the results presented by Godsil in [13]. First, we will introduce some concepts. A **coherent algebra** W is an algebra of matrices over the real or complex field that satisfies the following conditions:

(i) W is closed with respect to the Hermitian adjoint, which is defined by $A^* = (a_{i,j})^* = (\overline{a_{j,i}})$ for $A = (a_{i,j}) \in W$;

(ii) $I \in W$, where I is the identity matrix;

(iii) $J \in W$, where J is the all-one matrix;

(iv) W is closed with respect to Schur-Hadamard multiplication $\circ$, where $A \circ B = (a_{i,j} b_{i,j})$ for $A = (a_{i,j}), B = (b_{i,j}), A, B \in W$.

Each coherent algebra W has a unique basis of 01-matrices $\{A_1, \ldots, A_r\}$ such that:

(i) $\sum_{i=1}^{r} A_i = J$;

(ii) For all $1 \leqslant i \leqslant r$, there exists j, $1 \leqslant j \leqslant r$, such that $A_i^\top = A_j$, where $A_i^\top$ is the matrix transposed to A_i;

(iii) $A_i A_j = \sum_{k=1}^{r} p_{i,j}^k A_k$.

Godsil [13] proved that if PST occurs in a graph contained within a coherent algebra, then there exists a time t such that $U(t)$ is a scalar multiple of a permutation matrix of order two with a zero diagonal. Consequently, the number of vertices in the graph must be even.

In this section, we extend this result by introducing the concept of a "mixed graph in a coherent algebra." Specifically, we define a graph Γ as a mixed graph in a coherent algebra if $A(\Gamma)$ can be expressed as an algebraic sum of distinct elements of the 01-basis.

Let P denote the set of permutation matrices of size $n \times n$. It follows that P is contained in the set W, and any graph whose automorphism group acts transitively on its vertices can be classified within a coherent algebra.

Theorem 16. *Let Γ be a mixed graph in a coherent algebra with vertices u and v and minimum period T. If* PST *first occurs from u to v at time T/k for some positive integer k, then $|P| \neq I, |P^2| \neq I, \ldots, |P^{k-1}| \neq I$, $|P^k| = I$, where P is a permutation matrix.*

Proof. Let H be the Hermitian adjacency matrix of Γ. Since $U(t)$ is a polynomial in H, it follows that $U(t)$ lies in the algebra generated by H for all $t \in \mathbb{R}$. In particular, if $|U(t)_{u,v}| = 1$ for some pair of vertices u and v, then by the definition of PST, we must have

$$|U(t)| = P.$$

Using property **P2** (1), we have

$$U(kt) = U(t)^k,$$

for any $k \in \mathbb{N}^+$. Let $T = kt$ and obtain

$$|U(T)| = |U(t)^k| = |P^k|.$$

If it further holds that $|U(T)| = I$, then it follows that

$$|P^k| = I,$$

where $k \in \mathbb{N}^+$. $\square$

According to Theorem 16, we can easily deduce the following corollary.

Corollary 17. *Let Γ be a mixed graph in a coherent algebra with vertices u and v and minimum period T. If* PST *first occurs from u to v at time T/k for some positive integer k, then the number of vertices of Γ is a multiple of k.*

6 Spectral decomposition and minimal polynomials

Let H be a Hermitian matrix. Let $\lambda_1, \ldots, \lambda_s$ denote all the distinct eigenvalues of H. By **spectral decomposition** [12, Theorem 5.1], we have

$$H = \sum_{j=1}^{s} \lambda_j E_{\lambda_j},$$

where E_{λ_j} is the eigenprojector corresponding to λ_j. Note that

- $\sum_{j=1}^{s} E_{\lambda_j} = I$,
- $E_{\lambda_j}^2 = E_{\lambda_j}$,
- $E_{\lambda_j} E_{\lambda_k} = \mathbf{0}$, for $j \neq k$,

where I and $\mathbf{0}$ are the identity matrix and the zero matrix, respectively. According to spectral decomposition, we have

$$U_H(t) = \exp(-\mathrm{i}\, tH) = \sum_{j=1}^{s} \exp(-\mathrm{i}\, t\lambda_j) E_{\lambda_j}. \tag{4}$$

Suppose that Hermitian matrix H can be diagonalized. The **minimal polynomial** of H is given by

$$m_H(x) = \prod_{j=1}^{s} (x - \lambda_j),$$

where λ_j represents the distinct eigenvalues of H. In this case, Ben Taher and Rachidi [3, Corollary 2] gave formulas for polynomial decomposition of the matrix exponential $\exp(tH)$ using **Lagrange's interpolation**. We modify $\exp(tH)$ to $\exp(-\mathrm{i}\, tH)$ and rephrase the description as follows.

Lemma 18. *Let H be the Hermitian matrix with the minimal polynomial*

$$m_H(x) = \prod_{j=1}^{s} (x - \lambda_j) .$$

Then we have

$$U_H(t) = \sum_{j=1}^{s} \exp(-\mathrm{i}\, t\lambda_j) \prod_{d=1,d\neq j}^{s} \frac{H - \lambda_d I}{\lambda_j - \lambda_d}.$$

Based on Lemma 18 and Eq. (4), we have

$$E_{\lambda_j} = \prod_{d=1,d\neq j}^{s} \frac{H - \lambda_d I}{\lambda_j - \lambda_d}.$$

Now, we give two formulas in the polynomial decomposition of $\exp(-\mathrm{i}\, tH)$ for some special cases based on some minimal polynomial.

First, we assume that the Hermitian matrix H does not have eigenvalue 0 and its eigenvalues are symmetric about 0. Then the minimal polynomial is

$$m_H(x) = \prod_{j=1}^{s} \left(x^2 - \lambda_j\right) .$$

According to spectral decomposition and Lemma 18, we can obtain the following lemma.

Lemma 19. *Let H be the Hermitian matrix with the minimal polynomial*

$$m_H(x) = \prod_{j=1}^{s} \left(x^2 - \lambda_j\right) .$$

Then we have

$$U_H(t) = \sum_{j=1}^{s} \left(\cos(t\sqrt{\lambda_j})I - \frac{\mathrm{i}\sin(t\sqrt{\lambda_j})}{\sqrt{\lambda_j}} H \right) F_j,$$

where

$$F_j = \prod_{d=1,d\neq j}^{s} \frac{H^2 - \lambda_d I}{\lambda_j - \lambda_d}.$$

Proof. According to Lemma 18 and Eq. (4), we have

$$\begin{aligned} U_H(t) &= \exp(-\mathrm{i}\, tH) \\ &= \sum_{j=1}^{s} \left(\exp(-\mathrm{i}\, t\sqrt{\lambda_j}) E_{\lambda_j} + \exp(-\mathrm{i}\, t(-\sqrt{\lambda_j})) E_{-\lambda_j} \right) \\ &= \sum_{j=1}^{s} \left(\exp(-\mathrm{i}\, t\sqrt{\lambda_j}) \frac{H - (-\sqrt{\lambda_j})I}{\sqrt{\lambda_j} - (-\sqrt{\lambda_j})} F_j + \exp(\mathrm{i}\, t\sqrt{\lambda_j}) \frac{H - \sqrt{\lambda_j} I}{-\sqrt{\lambda_j} - \sqrt{\lambda_j}} F_j \right) \end{aligned}$$

$$
\begin{aligned}
&= \sum_{j=1}^{s} \left(\frac{(H+\sqrt{\lambda_j} I)\exp(-\mathrm{i}\, t\sqrt{\lambda_j})}{2\sqrt{\lambda_j}} - \frac{(H-\sqrt{\lambda_j} I)\exp(\mathrm{i}\, t\sqrt{\lambda_j})}{2\sqrt{\lambda_j}} \right) F_j \\
&= \sum_{j=1}^{s} \left(\cos(t\sqrt{\lambda_j}) I - \frac{\mathrm{i}\sin(t\sqrt{\lambda_j})}{\sqrt{\lambda_j}} H \right) F_j. \qquad \square
\end{aligned}
$$

Second, we assume that the Hermitian matrix H has eigenvalue 0 and its eigenvalues are symmetric about 0. Then the minimal polynomial is

$$
m_H(x) = \prod_{j=1}^{s} x \left(x^2 - \lambda_j \right).
$$

Similar to the above lemma, we have the following lemma.

Lemma 20. *Let H be the Hermitian matrix with the minimal polynomial*

$$
m_H(x) = x \prod_{j=1}^{s} \left(x^2 - \lambda_j \right).
$$

Then we have

$$
U_H(t) = \sum_{j=1}^{s} \frac{\cos(t\sqrt{\lambda_j}) H^2 - \mathrm{i}\sqrt{\lambda_j}\sin(t\sqrt{\lambda_j}) H}{\lambda_j} F_j + \prod_{j=1}^{s} \frac{H^2 - \lambda_j I}{(-1)^s \lambda_j},
$$

where

$$
F_j = \prod_{d=1, d\neq j}^{s} \frac{H^2 - \lambda_d I}{\lambda_j - \lambda_d}.
$$

Proof. According to Lemma 18 and Eq. (4), we have

$$
\begin{aligned}
U_H(t) &= \exp(-\mathrm{i}\, tH) \\
&= \sum_{j=1}^{s} \left(\exp(-\mathrm{i}\, t\sqrt{\lambda_j}) E_{\lambda_j} + \exp(-\mathrm{i}\, t(-\sqrt{\lambda_j})) E_{-\lambda_j} \right) + \exp(-\mathrm{i}\, t0) E_0 \\
&= \sum_{j=1}^{s} \Bigg(\exp(-\mathrm{i}\, t\sqrt{\lambda_j}) \frac{(H - (-\sqrt{\lambda_j}) I)}{(\sqrt{\lambda_j} - (-\sqrt{\lambda_j}))} \frac{(H - 0I)}{(\sqrt{\lambda_j} - 0)} F_j \\
&\qquad + \exp(\mathrm{i}\, t\sqrt{\lambda_j}) \frac{(H - \sqrt{\lambda_j} I)}{(-\sqrt{\lambda_j} - \sqrt{\lambda_j})} \frac{(H - 0I)}{(-\sqrt{\lambda_j} - 0)} F_j \Bigg) \\
&\qquad + \prod_{j=1}^{s} \frac{\left(H - \sqrt{\lambda_j} I\right)\left(H - (-\sqrt{\lambda_j} I)\right)}{\left(0 - \sqrt{\lambda_j}\right)\left(0 - (-\sqrt{\lambda_j})\right)} \\
&= \sum_{j=1}^{s} \left(\frac{H(H+\sqrt{\lambda_j} I)\exp(-\mathrm{i}\, t\sqrt{\lambda_j}) + H(H-\sqrt{\lambda_j} I)\exp(\mathrm{i}\, t\sqrt{\lambda_j})}{2\lambda_j} \right) F_j
\end{aligned}
$$

$$
\begin{aligned}
&\quad + \prod_{j=1}^{s} \frac{H^2 - \lambda_j I}{(-1)^s \lambda_j} \\
&= \sum_{j=1}^{s} \frac{\cos(t\sqrt{\lambda_j})H^2 - \mathrm{i}\sqrt{\lambda_j}\sin(t\sqrt{\lambda_j})H}{\lambda_j} F_j + \prod_{j=1}^{s} \frac{H^2 - \lambda_j I}{(-1)^s \lambda_j}. \qquad \square
\end{aligned}
$$

It is clear that F_j can be expressed as a matrix polynomial in H^2. Since H is a Hermitian matrix, it follows that H^2 is symmetric, and thus F_j is also symmetric. Suppose that there exists one-way (or two-way) PST between vertices u and v. By Lemma 19 and Lemma 20, if the adjacency relation between vertices u and v is symmetric (or asymmetric), then the PST is two-way (or one-way). However, this does not always hold. For example, oriented path P_2 and complete graph K_3 for which there exists a directed edge. However, we believe these are just special examples. Therefore, this leads to the following question:

Problem 21. Are there only finitely many graphs with two-way (or one-way) PST between vertices u and v with a directed (or an undirected) edge between u and v?

Based on Lemma 19 and Lemma 20, and assuming the above questions hold, the following conjecture is proposed.

Conjecture 22. Let Γ be a mixed graph with the Hermitian adjacency matrix H, and the minimal polynomial is $m_H(x) = \prod_{j=1}^{s} (x^2 - \lambda_j)$ or $m_H(x) = x\prod_{j=1}^{s} (x^2 - \lambda_j)$. Suppose that there exists PST between vertices u and v. Then the following holds, except for finitely many exceptional graphs:

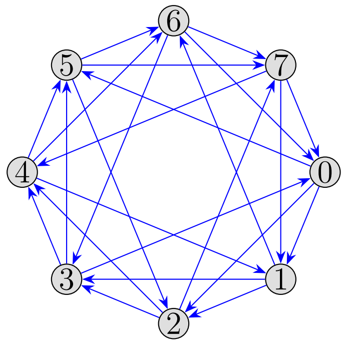
(i) PST is one-way if and only if there exists an oriented edge between vertices u and v.

(ii) PST is two-way if and only if no adjacent edge or there exists an undirected edge between vertices u and v.

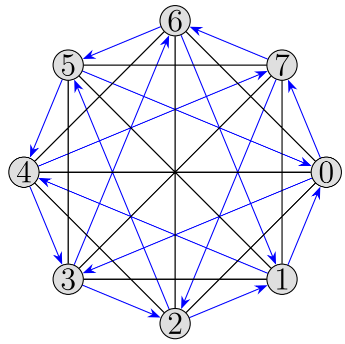
For undirected graphs, Kay [24] proved that PST occurs only between two non-disjoint pairs of vertices, that is, two vertices are not adjacent. However, mixed graphs are different; there exist cases where two vertices are adjacent. Recently, Song and Lin [28] characterized some mixed graphs with PST and MST. From this we can find infinite examples where PST occurs and two vertices are adjacent.

Example 23. Two-way PST occurs between non-adjacent vertices:
For each $k \in \{0, 1, \ldots, 7\}$, in the integral oriented circulant graph $G(8, \{1, 2, 5\})$, there exists two-way PST between vertices k and $(k + 4) \bmod 8$, and one-way PST between vertices k and $(k+2) \bmod 8$. Furthermore, MST occurs between vertices k, $(k+2) \bmod 8$, $(k + 4) \bmod 8$, and $(k + 6) \bmod 8$. See subfigure (a) of Fig. 4.

Example 24. Two-way PST occurs between adjacent vertices:
For each $k \in \{0, 1, \ldots, 7\}$, in the integral mixed circulant graph $G(8, \{2, 3, 4, 6, 7\})$, there exists two-way PST between vertices k and $(k + 4) \bmod 8$. See subfigure (b) of Fig. 4.



(a) Integral oriented circulant graphs $G(8, \{1, 2, 5\})$



(b) Integral mixed circulant graphs $G(8, \{2, 3, 4, 6, 7\})$

Fig. 4: Examples of one-way PST and two-way PST

7 Mixed graphs with few distinct eigenvalues

According to Lemma 18, Lemma 19 and Lemma 20, a greater number of distinct eigenvalues generally leads to increased complexity of the transition matrix $U(t)$. Hence, it is natural to investigate the structure of mixed graphs whose Hermitian adjacency matrices have relatively few distinct eigenvalues.

7.1 Two distinct eigenvalues

Let Γ be a mixed graph with the Hermitian adjacency matrix H_Γ. In this subsection, suppose H_Γ has exactly two distinct eigenvalues, denoted by λ_1 and λ_2 with $\lambda_1 > \lambda_2$. Then the minimal polynomial of H_Γ is

$$m_{H_\Gamma}(x) = (x - \lambda_1)(x - \lambda_2).$$

In this case, the transition matrix $U(t)$ can be expressed as

$$\begin{aligned} U(t) &= \exp(-\mathrm{i}\, t H_\Gamma) \\ &= \exp(-\mathrm{i}\, t\lambda_1)\frac{H_\Gamma - \lambda_2 I}{\lambda_1 - \lambda_2} + \exp(-\mathrm{i}\, t\lambda_2)\frac{H_\Gamma - \lambda_1 I}{\lambda_2 - \lambda_1} \\ &= \frac{\exp(-\mathrm{i}\, t\lambda_1) - \exp(-\mathrm{i}\, t\lambda_2)}{\lambda_1 - \lambda_2} H_\Gamma + \frac{\lambda_1 \exp(-\mathrm{i}\, t\lambda_2) - \lambda_2 \exp(-\mathrm{i}\, t\lambda_1)}{\lambda_1 - \lambda_2} I. \end{aligned}$$

If Γ has PST between vertices a and b at time t, then the following conditions must hold:

$$\frac{\lambda_1 \exp(-\mathrm{i}\, t\lambda_2) - \lambda_2 \exp(-\mathrm{i}\, t\lambda_1)}{\lambda_1 - \lambda_2} = 0 \tag{5}$$

and

$$\left| \frac{\exp(-\mathrm{i}\, t\lambda_1) - \exp(-\mathrm{i}\, t\lambda_2)}{\lambda_1 - \lambda_2} (H_\Gamma)_{a,b} \right| = 1. \tag{6}$$

From Eq. (5), it follows that

$$\exp(-\mathrm{i}\, t(\lambda_1 - \lambda_2)) = \frac{\lambda_1}{\lambda_2} \in \mathbb{R}\,.$$

This implies, $\lambda_1 = -\lambda_2$, and thus $t = \frac{k\pi}{2\lambda_1}$ for $k \in 2\,\mathbb{N}+1$. Substituting into Eq. (6), we further obtain $\lambda_1 = 1$, $\lambda_2 = -1$, and the transition matrix $U(t)$ simplifies to

$$U(t) = -\mathrm{i}\, H_\Gamma \sin(t) + I\cos(t).$$

Therefore, we have the following theorem.

Theorem 25. *The only mixed graphs with exactly two distinct eigenvalues that admit* PST *are K_2, or its signed and oriented graphs.*

7.2 Three distinct eigenvalues

Let Γ be a mixed graph with the Hermitian adjacency matrix H_Γ. In this subsection, suppose that H_Γ has exactly three distinct eigenvalues: 0, $\sqrt{\lambda}$, and $-\sqrt{\lambda}$, for some $\lambda > 0$. Then the minimal polynomial of H_Γ is

$$m_\Gamma(x) = x(x^2 - \lambda).$$

By Lemma 20, the transition matrix $U(t)$ can be written as

$$U(t) = \exp(-\mathrm{i}\, tH_\Gamma) = I - \frac{\mathrm{i}\sin(t\sqrt{\lambda})}{\sqrt{\lambda}} H_\Gamma + \frac{\cos(t\sqrt{\lambda}) - 1}{\lambda} H_\Gamma^2. \tag{7}$$

Using Toeplitz decomposition, we have

$$V(t) = \frac{U(t) + U(t)^*}{2} = I + \frac{\cos(t\sqrt{\lambda}) - 1}{\lambda} H_\Gamma^2 \tag{8}$$

and

$$W(t) = \frac{U(t) - U(t)^*}{2} = -\frac{\mathrm{i}\sin(t\sqrt{\lambda})}{\sqrt{\lambda}} H_\Gamma. \tag{9}$$

It is evident from Eq. (7) that

$$U\left(\frac{2\pi}{\sqrt{\lambda}}\right) = I,$$

which implies that the graph Γ is periodic with the minimum period $T = 2\pi/\sqrt{\lambda}$.

Throughout this section, we fix $T = 2\pi/\sqrt{\lambda}$.

If PST occurs between vertices u and v at time t, by Lemma 1, then the diagonal entries satisfy

$$U(t)_{u,u} = U(t)_{v,v} = 0.$$

Since the time of PST occurs is symmetric about $T/2$, without loss of generality, it suffices to determine whether PST occurs within the interval $(0, T/2]$.

Next, we determine the times $t \in (0, T/2]$ in which PST may occur.

Assume that

$$(H_\Gamma^2)_{u,u} = (H_\Gamma^2)_{v,v} = d > 0.$$

From Eq. (7), we have

$$U(t)_{u,u} = U(t)_{v,v} = 1 + \frac{\cos(t\sqrt{\lambda}) - 1}{\lambda} d.$$

For $U(t)_{u,u} = U(t)_{v,v} = 0$, we obtain

$$\cos(t\sqrt{\lambda}) = 1 - \frac{\lambda}{d}. \tag{10}$$

Let λ and d be positive real numbers. Assume that the equation Eq. (10) has no real roots. Then, we have

$$1 - \frac{\lambda}{d} \notin [-1, 1],$$

which implies $\lambda > 2d$, and hence no PST occurs between the vertices u and v in Γ.

Theorem 26. *Let Γ be a mixed graph with exactly three distinct eigenvalues 0, $\sqrt{\lambda}$, and $-\sqrt{\lambda}$. If $(H_\Gamma^2)_{u,u} = (H_\Gamma^2)_{v,v} = d > 0$ and $\lambda > 2d$, then no* PST *occurs between the vertices u and v.*

Assume that the equation Eq. (10) has real roots. Then $0 < \lambda \leqslant 2d$. We define

$$\alpha = \frac{\arccos(1 - \lambda/d)}{2\pi}.$$

Solving Eq. (10) gives

$$t = \alpha T = \frac{2\pi\alpha}{\sqrt{\lambda}}. \tag{11}$$

Substituting Eq. (11) into Eq. (10), we have

$$\cos(2\pi\alpha) = \cos(t\sqrt{\lambda}) = 1 - \frac{\lambda}{d}. \tag{12}$$

Theorem 27 (**[26, Niven's Theorem]**)**.** *Suppose that both θ and $\cos(\pi\theta)$ are rational numbers. Then*

$$\cos(\pi\theta) \in \left\{0, \pm 1, \pm\frac{1}{2}\right\}.$$

By Theorem 27 and Eq. (12), we have α is rational only if $\cos(2\pi\alpha) \in \{0, \pm 1, \pm 1/2\}$; otherwise, α is irrational.

Next, we explore the conditions of PST occurs when the transfer time t is a rational or irrational multiple of period.

Table 1: The existence of PST and associated $\cos(2\pi\alpha)$ values

Cases	α	$\cos(2\pi\alpha)$	$t\sqrt{\lambda}$	λ	The existence of PST	First time t of PST
1	0	1	0	0	No	–
2	1/6	1/2	$\pi/3$	$d/2$	No	–
3	1/4	0	$\pi/2$	d	No	–
4	1/2	−1	π	$2d$	Yes	$T/2$
5	1/3	−1/2	$2\pi/3$	$3d/2$	Yes	$T/3$

7.2.1 Rational multiple of period

We first consider the case where the transfer time t is a rational multiple of the period T, that is, $t = \alpha T$ for some $\alpha \in \mathbb{Q}$. In this case $\cos(2\pi\alpha)$ can only take values in the set $\{0, \pm 1, \pm 1/2\}$. The possible cases are summarized in the following table.

Suppose that the first transfer time t of PST is a rational multiple of the period T, i.e.,

$$t = \alpha T.$$

Based on Table 1, we have the following result.

Theorem 28. *Let $\alpha \in \mathbb{Q}$. If $\alpha \in \{0, 1/6, 1/4\}$, then no* PST *occurs in* Γ.

Proof. We analyze the three cases separately:

Case 1: When $\alpha = 0$. This implies $\lambda = 0$. This contradicts that $\lambda > 0$, and hence no PST occurs.

Case 2: When $\alpha = 1/6$, it follows that $t = T/6$. Substituting this into Eq. (8) and Eq. (9), we obtain

$$V\left(\frac{T}{6}\right) = I - \frac{H_\Gamma^2}{2\lambda}, \qquad W\left(\frac{T}{6}\right) = -\frac{\mathrm{i}\sqrt{3}H_\Gamma}{2\sqrt{\lambda}}.$$

Then, by Lemma 14, we have

$$\left|V\left(\frac{T}{6}\right)_{v,u}\right| = \left|W\left(\frac{T}{6}\right)_{v,u}\right| = \frac{1}{2}.$$

It follows that

$$|(H_\Gamma)_{v,u}| = 1 \quad \text{and} \quad \frac{\sqrt{3}}{2\sqrt{\lambda}} = \frac{1}{2},$$

which implies $\lambda = 3$.

Then, by Lemma 4 and definition and MST, if one-way PST occurs at $t = T/6$, it must also occur at $t = T/2$. Now substituting $t = T/2$ and $\lambda = 3$ into Eq. (7), we obtain

$$U\left(\frac{T}{2}\right) = I - \frac{2H_\Gamma^2}{3}.$$

To admit one-way PST, some off-diagonal entry of $U(T/2)$ must be equal to ± 1. However, since the off-diagonal entries of H_Γ^2 are integers, the off-diagonal entries of $U(T/2)$ are of the form $-2k/3$ for some integer k, which cannot equal ± 1.

This contradiction implies that no PST occurs at time $T/2$. By Lemma 4, it follows that no PST occurs at time $T/6$ either. Therefore, this case does not hold.

Case 3: When $\alpha = 1/4$, it follows that $t = T/4$. Substituting into Eq. (8) and Eq. (9), we have

$$V\left(\frac{T}{4}\right) = I - \frac{H_\Gamma^2}{\lambda}, \qquad W\left(\frac{T}{4}\right) = -\frac{\mathrm{i}\, H_\Gamma}{\sqrt{\lambda}}.$$

Then, by Lemma 14, we have

$$\left| V\left(\frac{T}{4}\right)_{v,u} \right| = \left| W\left(\frac{T}{4}\right)_{v,u} \right| = \frac{1}{2}.$$

It follows that

$$|(H_\Gamma)_{v,u}| = 1 \quad \text{and} \quad \frac{1}{\sqrt{\lambda}} = \frac{1}{2},$$

which implies $\lambda = 4$.

Then, by Lemma 4 and definition and MST, if one-way PST occurs at $t = T/4$, it must also occur at $t = T/2$. Now substituting $t = T/2$ and $\lambda = 4$ into Eq. (7), we obtain

$$U\left(\frac{T}{2}\right) = I - \frac{H_\Gamma^2}{2}.$$

By Table 1, let $d = \lambda = 4$. Then the diagonal entry of $U(T/2)$ is not equal to 0 at the vertices u and v. This implies that no PST occurs at time $T/2$. By Lemma 4, it follows that no PST occurs at time $T/4$ either. Therefore, this case does not hold. $\square$

Under the conditions given in cases 4 and 5 of Table 1, we next prove the necessary and sufficient conditions for the existence of two-way PST at time $T/2$ and 3-vertex MST.

For case 4 on Table 1. Let $S = \{u, v\}$ be a pair of vertices in mixed graph Γ. Then we have the following theorem.

Theorem 29. *Let $\alpha \in \mathbb{Q}$ and $H_\Gamma[S] = O$. If $\alpha = 1/2$, then the following two statements are equivalent:*

(i) Γ *has two-way* PST *between vertices u and v at time $T/2$;*

(ii) $H_\Gamma^2[S] = \frac{\lambda}{2}(I - C_2)$.

Proof. Let $\alpha = 1/2$. Then $t = T/2$. Substituting into Eq. (7), we have

$$U\left(\frac{T}{2}\right) = I - \frac{2H_\Gamma^2}{\lambda}. \tag{13}$$

(i) ⇒ (ii): Since $H_\Gamma[S] = O$, the vertices u and v are not adjacent. If Γ has two-way PST between vertices u and v at time $T/2$, then by the definition of PST,

$$\left| U\left(\frac{T}{2}\right)[S] \right| = C_2. \tag{14}$$

Substituting Eq. (14) into Eq. (13) and simplifying, we obtain

$$H_\Gamma^2[S] = \frac{\lambda}{2}\big(I \pm C_2\big).$$

Since $H_\Gamma[S]$ corresponds to the induced subgraph on S and its row sums are all zero, the row sums of $H_\Gamma^2[S]$ are also zero. Hence,

$$H_\Gamma^2[S] = \frac{\lambda}{2}\big(I - C_2\big).$$

(i) ⇐ (ii): By substituting the condition

$$H_\Gamma^2[S] = \frac{\lambda}{2}\big(I - C_2\big)$$

into Eq. (13), we directly obtain

$$\left| U\left(\frac{T}{2}\right)[S] \right| = C_2,$$

which implies that there exists two-way PST between vertices u and v at time $T/2$. □

Example 30. Consider the integral oriented circulant graph $\Gamma = G(4, \{1\})$. The Hermitian adjacency matrix H_Γ of Γ is given by

$$H_\Gamma = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ v_4 \end{array} \!\!\begin{array}{c} \begin{array}{cccc} v_1 & v_2 & v_3 & v_4 \end{array} \\ \begin{pmatrix} 0 & \mathrm{i} & 0 & -\mathrm{i} \\ -\mathrm{i} & 0 & \mathrm{i} & 0 \\ 0 & -\mathrm{i} & 0 & \mathrm{i} \\ \mathrm{i} & 0 & -\mathrm{i} & 0 \end{pmatrix} \end{array}, \quad H_\Gamma^2 = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ v_4 \end{array} \!\!\begin{array}{c} \begin{array}{cccc} v_1 & v_2 & v_3 & v_4 \end{array} \\ \begin{pmatrix} 2 & 0 & -2 & 0 \\ 0 & 2 & 0 & -2 \\ -2 & 0 & 2 & 0 \\ 0 & -2 & 0 & 2 \end{pmatrix} \end{array}.$$

The matrix H_Γ has three distinct eigenvalues: 0, 2, and -2. It follows that $\lambda = 4$, and the minimum period is $T = \pi$. Let $S = \{v_1, v_3\}$ be two vertices in Γ. Then we have

$$H_\Gamma[S] = O \quad \text{and} \quad H_\Gamma^2[S] = 2(I - C_2).$$

By Eq. (13), we compute

$$U\left(\frac{\pi}{2}\right)[S] = I - \frac{H_\Gamma^2[S]}{2} = C_2.$$

Therefore, Γ has two-way PST between vertices v_1 and v_3 at time $\pi/2$.

For case 5 on Table 1. Let $S = \{u, v, w\}$ be three vertices in mixed graph Γ. Then we have the following theorem.

Theorem 31. *Let $\alpha \in \mathbb{Q}$ and $H_\Gamma[S] = \pm\,\mathrm{i}(C_3 - C_3^\top)$. If $\alpha = 1/3$, then the following two statements are equivalent:*

(i) *Γ has 3-vertex* MST *between the vertices in $S = \{u, v, w\}$;*

(ii) $\lambda = 3$, $H_\Gamma^2[S] = 2I - (C_3 + C_3^\top)$.

Proof. Let $\alpha = 1/3$. Then $t = T/3$. Substituting into Eq. (7), Eq. (8) and Eq. (9), we have

$$U\left(\frac{T}{3}\right) = I - \frac{\mathrm{i}\sqrt{3}H_\Gamma}{2\sqrt{\lambda}} - \frac{3H_\Gamma^2}{2\lambda}. \tag{15}$$

$$V\left(\frac{T}{3}\right) = I - \frac{3H_\Gamma^2}{2\lambda}, \qquad W\left(\frac{T}{3}\right) = -\frac{\mathrm{i}\sqrt{3}H_\Gamma}{2\sqrt{\lambda}}. \tag{16}$$

(i) $\Rightarrow$ (ii): If Γ has 3-vertex MST between the vertices in $S = \{u, v, w\}$, which implies the first time of PST occurs $t = T/3$. Let

$$H_\Gamma[S] = \pm\,\mathrm{i}(C_3 - C_3^\top). \tag{17}$$

Substituting Eq. (17) into Eq. (16), and by Lemma 15, we have

$$\left|W\left(\frac{T}{3}\right)[S]\right| = \left|\left(-\frac{\mathrm{i}\sqrt{3}H_\Gamma}{2\sqrt{\lambda}}\right)[S]\right| = \frac{C_3 + C_3^\top}{2}.$$

By simplifying the calculation, we have

$$\lambda = 3.$$

Substituting this into Eq. (16), and by Lemma 15, we have

$$\left|V\left(\frac{T}{3}\right)[S]\right| = \left|\left(I - \frac{H_\Gamma^2}{2}\right)[S]\right| = \frac{C_3 + C_3^\top}{2}.$$

By simplifying the calculation, we have

$$H_\Gamma^2[S] = 2I \mp (C_3 + C_3^\top).$$

Since $H_\Gamma[S]$ corresponds to the induced subgraph on S and its row sums are all zero, the row sums of $H_\Gamma^2[S]$ are also zero. Hence,

$$H_\Gamma^2[S] = 2I - (C_3 + C_3^\top).$$

(i) $\Leftarrow$ (ii): By substituting the condition

$$\lambda = 3,\ H_\Gamma[S] = \pm\,\mathrm{i}(C_3 - C_3^\top),\ \text{and}\ H_\Gamma^2[S] = 2I - (C_3 + C_3^\top)$$

into Eq. (15), we directly obtain

$$\left| U\left(\frac{T}{3}\right)[S]\right| = C_3 \text{ or } C_3^\top,$$

which implies that there exists 3-vertex MST between the vertices in $S = \{u, v, w\}$. $\square$

Example 32. Consider the integral oriented circulant graph $\Gamma = G(3, \{1\})$. The Hermitian adjacency matrix H_Γ of Γ is given by

$$H_\Gamma = \begin{array}{c c} & \begin{array}{ccc} v_1 & v_2 & v_3 \end{array} \\ \begin{array}{c} v_1 \\ v_2 \\ v_3 \end{array} & \begin{pmatrix} 0 & \mathrm{i} & -\mathrm{i} \\ -\mathrm{i} & 0 & \mathrm{i} \\ \mathrm{i} & -\mathrm{i} & 0 \end{pmatrix} \end{array}, \quad H_\Gamma^2 = \begin{array}{c c} & \begin{array}{ccc} v_1 & v_2 & v_3 \end{array} \\ \begin{array}{c} v_1 \\ v_2 \\ v_3 \end{array} & \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix} \end{array}.$$

The matrix H_Γ has three distinct eigenvalues: 0, $\sqrt{3}$, and $-\sqrt{3}$. It follows that $\lambda = 3$, and the minimum period is $T = 2\pi/\sqrt{3}$. Let $S = \{v_1, v_2, v_3\}$ be three vertices in Γ. Then we have

$$H_\Gamma[S] = \mathrm{i}(C_3 - C_3^\top) \quad \text{and} \quad H_\Gamma^2[S] = 2I - (C_3 + C_3^\top).$$

By Eq. (15), we compute

$$U\left(\frac{2\pi}{3\sqrt{3}}\right)[S] = I - \frac{\mathrm{i}\, H_\Gamma[S]}{2} - \frac{H_\Gamma^2[S]}{2} = C_3.$$

Therefore, Γ has 3-vertex MST between the vertices in $S = \{v_1, v_2, v_3\}$, and PST first occurs at time $\frac{2\pi}{3\sqrt{3}}$.

7.2.2 Irrational multiple of period

We next consider the case where the transfer time t is an irrational multiple of the period T, that is, $t = \alpha T$ for some $\alpha \in \mathbb{R} \setminus \mathbb{Q}$. Let

$$\cos(2\pi\alpha) = 1 - \frac{\lambda}{d} \notin \left\{0, \pm 1, \pm\frac{1}{2}\right\}.$$

By Theorem 27, we have

$$\alpha = \frac{\arccos(1 - \lambda/d)}{2\pi} \in \mathbb{R} \setminus \mathbb{Q},$$

By the Pythagorean identity, we have

$$\sin(2\pi\alpha) = \frac{\sqrt{\lambda(2d - \lambda)}}{d},$$

with $0 < \lambda \leqslant 2d$. Substituting $t = \alpha T$ into Eq. (7), the transition matrix $U(t)$ can be written as

$$U(\alpha T) = \exp(-\mathrm{i}\,\alpha T H_\Gamma) = I - \mathrm{i}\,\frac{\sqrt{2d-\lambda}H_\Gamma}{d} - \frac{H_\Gamma^2}{d}. \tag{18}$$

Suppose that PST occurs between the vertices in $S = \{u, v\}$ at time $t = \alpha T$. By Theorem 12, since $\alpha \neq 1/2$, it follows that PST is one-way. Then, we can easily see that there exists directed edge between vertices u and v. Therefore,

$$H_\Gamma[S] = \pm\,\mathrm{i}\,E_2, \tag{19}$$

where E_2 denotes the 2×2 skew-symmetric matrix

$$E_2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

Let $H_\Gamma^2[S] = \beta J + (d-\beta)I$, where β denotes the number of common neighbors of u and v. Since u and v are connected by a directed edge, a direct calculation from Eq. (19) shows that $\beta = d-1$. Substituting this into $H_\Gamma^2[S]$, we obtain

$$H_\Gamma^2[S] = (d-1)J + I. \tag{20}$$

Substituting Eq. (19) and Eq. (20) into Eq. (18), and simplifying, we have

$$U(\alpha T)[S] = \pm\frac{\sqrt{2d-\lambda}}{d}E_2 + \frac{d-1}{d}(I-J). \tag{21}$$

Now, if one-way PST occurs at $t = \alpha T$, then there exists the modulus of the off-diagonal entry must be 1. That is

$$\left|\pm\frac{\sqrt{2d-\lambda}}{d} - \frac{d-1}{d}\right| = 1.$$

By simplifying the calculation, we have

$$\begin{cases} \sqrt{2d-\lambda} = 1, & \text{if the sign is negative,} \\ \lambda = 6d - 4d^2 - 1, & \text{if the sign is positive.} \end{cases}$$

Squaring both sides and simplifying, considering that $0 < \lambda \leqslant 2d$, we obtain

$$\begin{cases} \lambda = 2d-1, & \text{if the sign is negative,} \\ \lambda = d = 1, & \text{if the sign is positive.} \end{cases}$$

Suppose that the first transfer time t of PST is an irrational multiple of the period T, i.e.,

$$t = \alpha T.$$

We have the following result.

Theorem 33. *Let* $\alpha = \frac{\arccos(1-\lambda/d)}{2\pi} \in \mathbb{R}\setminus\mathbb{Q}$ *and* $H_\Gamma[S] = \pm\,\mathrm{i}\,E_2$ *and* $H_\Gamma^2[S] = (d-1)J + I$. *Then the following two statements are equivalent:*

(i) Γ *has one-way* PST *between the vertices in* $S = \{u, v\}$ *at time* $t = \alpha T$*;*

(ii) *If the sign of* $H_\Gamma[S]$ *is positive, then* $\lambda = d = 1$*; otherwise,* $\lambda = 2d - 1$.

Proof. **(i)** $\Rightarrow$ **(ii)**: According to the above discussion, this case holds.

(i) $\Leftarrow$ **(ii)**: When $\lambda = d = 1$, it is obviously true. Now we consider $\lambda = 2d - 1$. Substituting this into Eq. (21), we have

$$U(\alpha T)[S] = \frac{1}{d}(-E_2 + (d-1)(I - J)).$$

Therefore, each off-diagonal entry of $U(\alpha T)[S]$ is given by

$$\frac{1}{d}\left(\pm 1 - (d-1)\right) = \begin{cases} -1, & \text{if the sign of } E_2 \text{ is positive,} \\ \frac{2}{d} - 1, & \text{if the sign of } E_2 \text{ is negative.} \end{cases}$$

Therefore, Γ has one-way PST between the vertices in $S = \{u, v\}$ at time $t = \alpha T$. $\square$

Example 34. Consider the mixed graph Γ with the Hermitian adjacency matrix H_Γ is given by

$$H_\Gamma = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ v_4 \end{array} \begin{array}{c} \begin{array}{cccc} v_1 & v_2 & v_3 & v_4 \end{array} \\ \begin{pmatrix} 0 & \mathrm{i} & 1 & 1 \\ -\mathrm{i} & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix} \end{array}, \quad H_\Gamma^2 = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ v_4 \end{array} \begin{array}{c} \begin{array}{cccc} v_1 & v_2 & v_3 & v_4 \end{array} \\ \begin{pmatrix} 3 & 2 & \mathrm{i} & \mathrm{i} \\ 2 & 3 & -\mathrm{i} & -\mathrm{i} \\ -\mathrm{i} & \mathrm{i} & 2 & 2 \\ -\mathrm{i} & \mathrm{i} & 2 & 2 \end{pmatrix} \end{array}.$$

The matrix H_Γ has three distinct eigenvalues: 0, $\sqrt{5}$, and $-\sqrt{5}$. It follows that $\lambda = 5$, $d = 3$, and the minimum period is $T = 2\pi/\sqrt{5}$. Let $S = \{v_1, v_2\}$ be two vertices in Γ. Then, we have

$$H_\Gamma[S] = -\,\mathrm{i}\,E_2 \quad \text{and} \quad H_\Gamma^2[S] = 2J + I.$$

By Eq. (21), we compute

$$\begin{aligned} U\left(\frac{\arccos(-2/3)}{\sqrt{5}}\right)[S] &= \frac{1}{3}(-E_2 + 2(I - J)) \\ &= \frac{1}{3}\left(-\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} + 2\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}\right) \\ &= \begin{pmatrix} 0 & -\frac{1}{3} \\ -1 & 0 \end{pmatrix}. \end{aligned}$$

Therefore, Γ has one-way PST between the vertices in $S = \{v_1, v_2\}$ at time $\frac{\arccos(-2/3)}{\sqrt{5}}$.

8 Conclusion

In this paper, we studied perfect state transfer (PST) and multiple state transfer (MST) on mixed graphs using Hermitian adjacency matrix as the spectral framework. By extending known results from undirected and oriented graphs, we characterized one-way PST, two-way PST, and MST in mixed graphs, and examined their connections with graph periodicity. Our findings show that the presence of directed edges breaks the symmetry of the graph, leading to time-reversal asymmetry and giving rise to phenomena such as directional state transfer and non-symmetric transfer times.

We focused on mixed graphs with few distinct eigenvalues and identified conditions under which PST and MST can occur. In particular, we established necessary and sufficient conditions for PST when the transfer time is either a rational or an irrational multiple of the period. Moreover, we derived explicit expressions for the transition matrix via spectral decomposition, Lagrange interpolation, and minimal polynomials, illustrating the influence of eigenvalue structure on quantum transport behavior.

So far, we have observed four types of state transfer: one-way PST between two vertices, two-way PST between two vertices, MST between three vertices, and MST between four vertices. All known examples, except for the one-way PST between two vertices, occur at rational multiples of the minimum period. These results naturally lead to the following open questions:

Problem 35. Are all instances of one-way PST between two vertices associated with irrational multiples of the period? If not, provide a counterexample.

Problem 36. Is there a mixed graph that admits MST between more than four vertices?

At the end of this paper, we considered mixed graphs with two or three distinct eigenvalues, where the spectral structure allows for direct analysis. However, as the number of distinct eigenvalues increases, the structure of the transition matrix becomes more intricate, and the analysis of PST correspondingly more difficult. It would be an interesting direction for future research to extend the techniques developed in this paper to the study of PST on mixed graphs with more than three distinct eigenvalues, which may reveal deeper connections between spectral complexity and quantum dynamics.

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