April 2019

Quantum Walks on Graphs: Group State Transfer

Luke Candler Brown
Worcester Polytechnic Institute

Continuous-Time Quantum Walks: Group State Transfer in Graphs

Relaxing the Conditions Imposed by Perfect State Transfer

Luke Brown
Advised by William J. Martin

A Major Qualifying Project, Presented to the Faculty of Worcester Polytechnic Institute in Partial Fulfillment of the Requirements for the Degree in Bachelor of Sciences by

---

Luke Brown
Advised and Approved by

Dr. William J. Martin

WPI

Contents

1. Introduction and Background 2
1.1. Graphs and Some Physics 3
1.2. More Graph Theory and Linear Algebra 4
1.3. Perfect State Transfer: A Survey 11
2. Group State Transfer 17
2.1. Fundamentals 17
2.2. Graph Symmetries 24
2.3. Graph Products 29
3. Examples 31
4. Further Research and Conclusions 35
References 36

GROUP STATE TRANSFER IN GRAPHS

Abstract. Quantum walks on graphs are known to be the fundamental process of quantum computing. Understanding quantum walks is then fundamental to the study and development of quantum computing algorithms. Graphs that exhibit perfect state transfer (PST), by which a quantum walk beginning at one vertex is guaranteed to end at another after a nonzero displacement in time, are of great interest to researchers in the field of quantum computing. The conditions imposed by PST are strong, and many of the graphs that are known to exhibit PST are highly symmetric, which provides motivation to relax the restrictions imposed by perfect state transfer. This project introduces the property of group state transfer (GST), by which quantum walks are guaranteed to transfer states between nontrivial vertex sets. We define GST, examine its implications for finite simple graphs, and provide examples of graphs that exhibit GST.

1. Introduction and Background

In 1981, Richard P. Feynman delivered a talk at the California Institute of Technology entitled *Simulating Physics with Computers* [9]. In his talk, Feynman discussed the notion of a universal computer, which is capable of simulating any physical system. Feynman demonstrated that any problem that may be solved by a universal computer may also be solved by a quantum computer, and that there are results which may be produced by a universal quantum computer that no classical probabilistic computer can solve [9]. In conclusion, he hypothesized that quantum computers, then merely theoretical, were the best candidates for universal computation. He stipulated, however, that the universal quantum computer should only require a number of components proportional to the spacetime volume of the physical system that it simulates.

A quantum walk is the quantum mechanical analog of a classical random walk. While the exact location of the walker is known throughout a classical random walk, a quantum walk is defined by the Schrödinger dynamics of a particle moving amongst the vertices of a graph [4]. Consequently, quantum walks have served as the quantum computing analog of random walks in the development of computer algorithms. In his 2006 paper, *Universal Computation by Quantum Walk*, Andrew M. Childs demonstrates that quantum walks on graphs, far from an obscure corner of quantum information theory, constitute the fundamental process of universal quantum computation [4]. That is, any problem that may be solved by a quantum computer may be solved by a quantum walk process. To understand quantum walks, then, is fundamental to the development of quantum computing algorithms [4].

Of great pertinence to the development of quantum computing algorithms is a property known as perfect state transfer (PST) that we will discuss in the following background section. A graph is said to have perfect state transfer between two vertices u and v if the quantum walk that begins at vertex u is guaranteed to end at vertex v after some nonzero displacement in time. This is a strong condition to impose, however, as we will show. Furthermore, many of the graphs that are known to have perfect state transfer are highly symmetric and grow exponentially in their number of vertices, violating Feynman's stipulation. This paper is concerned with relaxing the conditions imposed by perfect state transfer through the exploration of group state transfer, which requires that quantum walks transfer between nontrivial vertex sets, rather than individual vertices. We begin by introducing and discussing basic concepts from linear algebra and graph theory that are used in the theory of quantum walks. Next, we formally introduce group state transfer and explore its implications. Finally, we provide examples of graphs that exhibit perfect state transfer.

1.1. **Graphs and Some Physics.** A graph G is an ordered pair (V, E) of vertices V and edges E. Each edge $(u, v) \in E$ is, in turn, an ordered pair of vertices of G. For any pair of vertices $u, v \in V$ we say that u is adjacent to v in G, denoted $u \sim_G v$, if $(u, v) \in E$ or $(v, u) \in E$. If u is a vertex of graph G, then we define the neighborhood of u as

$$N(u) = \{v \in V : u \sim_G v\}.$$

When the graph is understood, then we simply denote that u is adjacent to v by $u \sim v$, and for simplicity's sake, if the graph $G = (V, E)$ has n vertices then we adopt that $V = \{1, \cdots, n\}$. Given a finite graph G, we may define the adjacency matrix A of G as follows.

Definition 1.1. Let $G = (V, E) = (\{1, \cdots, n\}, E)$ be a finite graph. The adjacency matrix of G is the matrix A that satisfies the following. For any $i, j = 1, \cdots, n$, $A_{i,j} = 1$ if $i \sim j$ and $A_{i,j} = 0$ otherwise.

We introduce some basic graph terminology and concepts.

Definition 1.2. Let $G = (V, E)$ be a graph. Then given any vertex $v \in V$, the degree of v is defined as

$$\deg v = |\{u \in V : v \sim_G u\}|.$$

Notation 1.3. Let $G = (V, E)$ be a graph.

(1) The vertex set V of G is sometimes denoted $V(G)$;
(2) the edge set E of G is sometimes denoted $E(G)$.

In this paper, we are only interested in simple undirected graphs.

Definitions 1.4. Let $G = (V, E)$ be a graph. Graph G is simple if the following are satisfied.

(1) The edges of graph G are unweighted;
(2) for any vertex $u \in V$, u is not adjacent to u;
(3) for any pair of adjacent vertices $u, v \in V$, there is exactly one edge joining u with v.

Graph G is undirected if, for any pair of vertices $u, v \in V$, $u \sim_G v$ if and only if $v \sim_G u$.

Remark 1.5. Let A be the adjacency matrix of a simple undirected graph G.

(1) Matrix A has entries in $\{0, 1\}$ and therefore satisfies $A \circ A = A$;
(2) Matrix A is square;
(3) Matrix A has zeros along the diagonal;
(4) Matrix A is symmetric. Matrix A is therefore orthogonally diagonalizable with real eigenvalues.

A continuous-time quantum walk is defined by the time evolution of a quantum mechanical system defined on a graph. We will briefly consider the physics behind quantum walks. Let $G = (V, E)$ be a graph on n vertices, and consider the n-level quantum mechanical system $\mathbb{C}^n$ prepared in state ψ, and equipped with the Hamiltonian $\mathcal{H} = -\hbar A$, where $\hbar$ is Planck's constant and A is the adjacency matrix of G. In this case, there is a standard basis vector e_u associated with each vertex $u \in V$.

Notation 1.6. Those who are familiar with quantum mechanics will recall the bra-ket notation, by which ket $|\psi\rangle$ is used to express a column vector of complex numbers describing the state of a quantum mechanical system, and bra $\langle\psi|$ is the complex conjugate transpose of $|\psi\rangle$. In this notation, inner products are easily expressed as $\langle\phi|\psi\rangle$. We will not use this notation, and throughout this paper, ψ will simply be used to describe a column vector in $\mathbb{C}^n$, with the inner product of ϕ and ψ expressed as $\bar{\phi}^T\psi$.

Those who are familiar with quantum mechanics will also note that, if $\theta_1, \cdots, \theta_k$ are the eigenvalues of the adjacency matrix A, if we are to measure the energy of this system at any given time, the possible outcomes are

$$-\hbar\theta_1, \cdots, -\hbar\theta_k.$$

A quantum walk on G is given by the time evolution of the quantum mechanical system we have defined on G, prepared in state $\psi(0)$, according to the Schrödinger equation,

$$i\hbar\frac{\partial\psi}{\partial t} = \mathcal{H}\psi,$$

where the Hamiltonian is given by $\mathcal{H} = -\hbar A$. Observe that this equation is solved by taking the exponential of the Hamiltonian operator.

$$\psi(t) = e^{-i\mathcal{H}t/\hbar}\psi(0) = e^{iAt}\psi(0).$$

In our discussion of quantum walks, we will express the unitary transition operator as

$$U_G(t) = e^{iAt},$$

where $G = (V, E)$ is the graph upon which the system has been defined. Suppose that this quantum-mechanical system is prepared in the state $\psi(0) = e_u$ for some vertex $u \in V$. As the system evolves, the resulting process is the quantum-mechanical analog of the classical random walk: the Schrödinger dynamics of a particle that is allowed to move from vertex to vertex in the graph [4].

As we have mentioned, quantum walks have been shown to be universal in quantum computing, in that any process that might be performed by a quantum computer may be performed by a quantum walk [4]. One phenomenon in particular, however, is of great interest to researchers in quantum algorithms.

Definition 1.7. Let $G = (V, E)$ be a graph with unitary transition operator $U_G(t)$. For vertices $u, v \in V$, graph G has (u, v)-perfect state transfer (PST) at time $t \in \mathbb{R}$ if, for some $\alpha \in \mathbb{C}$,

$$U_G(t)e_u = \alpha e_v.$$

1.2. **More Graph Theory and Linear Algebra.** If G is a graph with adjacency matrix A and unitary transition operator $U_G(t) = e^{iAt}$, then it is natural to discuss the various ways of calculating $U_G(t)$, and so we begin with a discussion of the exponential of a matrix. We motivate the matrix exponential by the following problem. Let $\psi(t)$ be a time-dependent vector in $\mathbb{C}^n$ such that each component of ψ is a differentiable function and $\psi(0) = \psi_0$, and let A be an $n \times n$ matrix that satisfies

$$\frac{d}{dt}\psi(t) = A\psi(t).$$

This differential equation is solved by the vector of continuous functions [15]

$$\psi(t) = e^{At}\psi_0,$$

where e^{At} is the exponential of the $n \times n$ matrix At.

Lemma 1.8. *[15] Let X be an $n \times n$ matrix with entries in $\mathbb{C}$. Then*

$$e^X = \sum_{k=0}^{\infty} \frac{X^k}{k!}.$$

Lemma 1.9. *[15] Let X and Y be $n \times n$ matrixes with entries in $\mathbb{C}$. Then,*

$$e^X e^Y = e^{X+Y}.$$

Definition 1.10. Let X be an $n \times n$ matrix with entries in $\mathbb{C}$. Then v is an eigenvector of X with corresponding eigenvalue θ if v is the nonzero vector satisfying

$$Xv = \theta v.$$

The following property is important to note.

Proposition 1.11. *[15] Let X be an $n \times n$ matrix with eigenvalues $\theta_1, \cdots, \theta_k$.*
(1) The eigenvalues of e^X are $e^{\theta_1}, \cdots, e^{\theta_k}$;
(2) if v is a θ-eigenvector of X, then v is an e^θ-eigenvalue of e^X.

Given the matrix X, we discuss three avenues for calculating e^X: the Jordan canonical form of X, the power series definition of e^X, and the singular value decomposition of X.

Definition 1.12. Given an eigenvalue $\lambda \in \mathbb{C}$ and a natural number $n \in \{1, 2, 3, \cdots\}$, the Jordan block $J_n(\lambda)$ is the $n \times n$ matrix given by [13]

$$J_n(\lambda) = \begin{pmatrix} \lambda & 1 & 0 & \cdots & 0 \\ 0 & \lambda & 1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & \lambda & 1 \\ 0 & 0 & \cdots & \cdots & \lambda \end{pmatrix}$$

Definition 1.13. Let X be an $n \times n$ complex matrix with eigenvalues $\theta_1, \cdots, \theta_k$, and corresponding multiplicities $m_1, \cdots, m_k$. The Jordan canonical form of X is the matrix $J[X]$ that is similar to X and satisfies [13]

$$J[X] = J_{m_1}(\theta_1) \oplus \cdots \oplus J_{m_k}(\theta_k) = \begin{pmatrix} J_{m_1}(\theta_1) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & J_{m_k}(\theta_k) \end{pmatrix}.$$

The matrix X is similar to its Jordan canonical form (namely, the Jordan canonical form $J[X]$ is X expressed in its Jordan basis), and so, for an $n \times n$ matrix P,

$$X = P^{-1}J[X]P.$$

Observe that

$$e^X = \sum_{k=0}^{\infty} \frac{(P^{-1}J[x]P)^k}{k!} = \sum_{k=0}^{\infty} \frac{P^{-1}J[X]^k P}{k!} = P^{-1}e^{J[X]}P.$$

Observe also that

$$e^{J[X]} = e^{J_{m_1}(\theta_1)} \oplus \cdots \oplus e^{J_{m_k}(\theta_k)} = \begin{pmatrix} e^{J_{m_1}(\theta_1)} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & e^{J_{m_k}(\theta_k)} \end{pmatrix}.$$

If X is diagonalizable, then

$$e^X = P^{-1} \begin{pmatrix} e^{\theta_1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & e^{\theta_m} \end{pmatrix} P.$$

If G is a finite, simple, undirected graph, then the adjacency matrix A of G is orthogonally diagonalizable, and so iAt is orthogonally diagonalizable for any time $t \in \mathbb{R}$. Suppose that $\theta_1, \cdots, \theta_k \in \mathbb{R}$ are the eigenvalues of A, and that the matrix P satisfies

$$A = P^T \begin{pmatrix} \theta_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \theta_k \end{pmatrix} P.$$

Then,

$$U_G(t) = P^T \begin{pmatrix} e^{i\theta_1 t} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & e^{i\theta_k t} \end{pmatrix} P.$$

For the next avenue of calculating $U_G(t)$, we consider a specific example.

Example 1.14. Let $G = K_2$, the path on two vertices, and let $U(t) = U_G(t)$. The adjacency matrix A of K_2 is given by

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

Observe that $A^2 = I$, the identity matrix. As a result,

$$U(t) = e^{iAt} = \sum_{k=0}^{\infty} \frac{(iAt)^k}{k!} = I \sum_{k=0}^{\infty} \frac{(-1)^k t^{2k}}{(2k)!} + iA \sum_{k=0}^{\infty} \frac{(-1)^k t^{2k+1}}{(2k+1)!}.$$

Recall the Taylor series for the trigonometric functions $\sin t$ and $\cos t$.

$$\sin t = \sum_{k=0}^{\infty} \frac{t^k}{k!} \left(\frac{d^k}{dt^k} \sin t \right) \Big|_{t=0} = \sum_{k=0}^{\infty} \frac{(-1)^k t^{2k+1}}{(2k+1)!},$$

$$\cos t = \sum_{k=0}^{\infty} \frac{t^k}{k!} \left(\frac{d^k}{dt^k} \cos t \right) \Big|_{t=0} = \sum_{k=0}^{\infty} \frac{(-1)^k t^{2k}}{(2k)!}.$$

The Taylor series are then easily recognized.

$$U(t) = \cos tI + i \sin tA.$$

In this example, we find that the power series definition of $U(\tau)$ split into two recognized power series.

Definition 1.15. Let X be an $n \times n$ matrix. The minimal polynomial $m_X(z)$ of X is the monic polynomial of minimal degree $k \in \mathbb{N}$ such that

$$m_X(X) = 0.$$

Lemma 1.16. *Let A be the adjacency matrix of a simple, undirected graph G. If A has minimal polynomial $m_A(z)$ with degree k, then for some power series $f_1(t), \cdots, f_k(t)$ in t,*

$$U_G(t) = f_1(t)I + \cdots + f_k(t)A^{k-1}.$$

As we will see from the examples provided in this paper, the power series $f_1(t), \cdots, f_k(t)$ are sometimes easily recognizable, making this approach a convenient way to formulate the unitary transition operator $U_G(t)$.

Finally, we consider the spectral decomposition of a matrix. Let X be an $n \times n$ matrix, diagonalizable over $\mathbb{R}$, with eigenvalues $\theta_1, \cdots, \theta_k$. Let $E_{\theta_1}, \cdots, E_{\theta_k}$ denote the orthogonal projections onto the eigenspaces $V_{\theta_1}, \cdots, V_{\theta_k}$. In other words, for each j between 1 and k, E_{θ_j} is the orthogonal projection onto the eigenspace

$$V_{\theta_j} = \{v \in \mathbb{C}^n : Xv = \theta_j v\}.$$

We may decompose X as the following sum, referred to as the spectral decomposition of X [13].

$$X = \theta_1 E_{\theta_1} + \cdots + \theta_k E_{\theta_k}.$$

Recall that if A is the adjacency matrix of a simple, undirected graph, then A is a real symmetric matrix and therefore orthogonally diagonalizable. When we consider the spectral decomposition of a graph G, then we consider the spectral decomposition of the adjacency matrix A of G.

Proposition 1.17. *Let X be an $n \times n$ matrix, and let $p_d(z)$ be a degree-d polynomial. Then, if*

$$X = \sum_{j=1}^{k} \theta_j E_{\theta_j}$$

is the spectral decomposition of X, then

$$p_d(X) = \sum_{j=1}^{k} p_d(\theta_j) E_{\theta_j}.$$

Proof. For any exponent $h \in \mathbb{N}$, observe that because the projections $E_{\theta_1}, \cdots, E_{\theta_k}$ are orthogonal,

$$X^h = \left(\sum_{j=1}^{k} \theta_j E_{\theta_j} \right)^h = \sum_{j=1}^{k} \theta_j^h E_{\theta_j}.$$

As a result, if

$$p_d(z) = a_0 + a_1 z + a_2 z^2 + a_3 z^3 + \cdots + a_d z^d,$$

then

$$p_d(X) = a_0 I + a_1 X + a_2 X^2 + a_3 X^3 + \cdots + a_d X^d,$$

$$p_d(X) = a_0 I + a_1 \left(\sum_{j=1}^{k} \theta_j E_{\theta_j} \right) + a_2 \left(\sum_{j=1}^{k} \theta_j^2 E_{\theta_j} \right) + a_3 \left(\sum_{j=1}^{k} \theta_j^3 E_{\theta_j} \right) + \cdots + a_d \left(\sum_{j=1}^{k} \theta_j^d E_{\theta_j} \right),$$

$$p_d(X) = \sum_{j=1}^{k} \sum_{i=0}^{d} a_i \theta_j^i E_{\theta_j}$$

$$p_d(X) = \sum_{j=1}^{k} p_d(\theta_j) E_{\theta_j}.$$

■

Lemma 1.18. *Let X be an $n \times n$ matrix with spectral decomposition*

$$X = \sum_{j=1}^{k} \theta_j E_{\theta_j}$$

and let $p(z)$ be a power series that converges at θ_j for each $j = 1, \cdots, k$. Then,

$$p(X) = \sum_{j=1}^{k} p(\theta_j) E_{\theta_j}.$$

Proof. The power series $p(z)$ may be written as

$$p(z) = \sum_{j=0}^{\infty} \alpha_j z^j.$$

Consider the degree-d polynomial

$$p_d(z) = \sum_{j=0}^{d} \alpha_j z_j$$

and observe that $p(z) = \lim_{d \to \infty} p_d(z)$ for each $z \in \mathbb{R}$ at which $p(z)$ converges. By Proposition 1.17,

$$p_d(X) = \sum_{j=0}^{k} p_d(\theta_j) E_{\theta_j},$$

and so

$$p(X) = \lim_{d \to \infty} p_d(X) = \sum_{j=0}^{k} \lim_{d \to \infty} p_d(\theta_j) E_{\theta_j} = \sum_{j=1}^{k} p(\theta_j) E_{\theta_j}.$$

■

Let G be a simple, undirected graph with adjacency matrix A, and let $U(\tau) = U_G(\tau)$ be the unitary transition operator of G. If A has spectral decomposition

$$A = \theta_1 E_{\theta_1} + \cdots + \theta_k E_{\theta_k},$$

then

$$U(\tau) = e^{i\theta_1 \tau} E_{\theta_1} + \cdots + e^{i\theta_k \tau} E_{\theta_k}.$$

It is extremely useful to consider the spectral decomposition of the adjacency matrix in our consideration of quantum walks. Central to this consideration, however, is the task of determining the eigenvectors and eigenvalues of a graph, i.e., of the adjacency matrix. We consider this task in the following example. First, however, we must state a fact concerning eigenvectors of graphs.

Lemma 1.19. *Let $G = (V, E)$ be a graph on n vertices with adjacency matrix A, and let A have θ-eigenvector v. For any number $j \in \{1, \cdots, n\}$ let $v(j)$ be the jth component of v. For any vertex $u \in V$,*

$$\sum_{w \sim u} v(w) = \theta v(u).$$

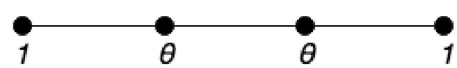
Example 1.20. Consider the path on four vertices P_4.

Suppose that v is a θ-eigenvector of P_4. Suppose that $v(1) = 0$. Then by Lemma 1.19,

$$v(1) = \theta v(2) = 0,$$

and, by extension, $v(3) = v(4) = 0$. We see that either $\theta = 0$ is an eigenvalue of P_4, or P_4 has no eigenvector for which $v(1) = 0$ or $v(4) = 0$ by Definition 1.10. We now enumerate four linearly independent eigenvectors v of P_4 for which $v(1) \neq 0$ and $v(4) \neq 0$, demonstrating that 0 is not an eigenvalue of P_4.

Let v be an eigenvector of P_4 such that $v(1) = v(4) = 1$. Then, by Lemma 1.19, the two interior vertices must take value θ.



When we apply the eigenvector equation of Lemma 1.19 to the two interior vertices, we obtain that

$$v(1) + v(3) = \theta v(2), \qquad 1 + \theta = \theta^2.$$

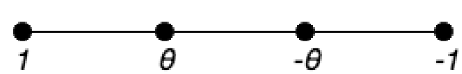
The quadratic formula yields two solutions to this equation.

$$\theta_1 = \phi = \frac{1 + \sqrt{5}}{2}, \qquad \theta_2 = \phi - \sqrt{5} = \frac{1 - \sqrt{5}}{2},$$

where $\phi = \frac{1+\sqrt{5}}{2}$ is the golden ratio. We have then obtained two (unnormalized) eigenvectors of P_4,

$$v_1 = (1, \phi, \phi, 1), \qquad v_2 = (1, \phi - \sqrt{5}, \phi - \sqrt{5}, 1).$$

Now, consider a new eigenvector v of P_4 for which $v(1) = 1$ and $v(4) = -1$ (that is, for which the first and the last components have opposite signs). Then, by Lemma 1.19, $v(2) = \theta$ and $v(3) = -\theta$.



Again, applying the eigenvector equation to either of the interior vertices of P_4 yields the quadratic equation

$$1-\theta=\theta^2$$

with solutions

$$\theta_3=\sqrt{5}-\phi=\frac{-1+\sqrt{5}}{2}, \qquad \theta_4=-\phi=\frac{-1-\sqrt{5}}{2},$$

which provide us with two more unnormalized eigenvectors of P_4,

$$v_3=(1,\sqrt{5}-\phi,\phi-\sqrt{5},-1), \qquad v_4=(1,-\phi,\phi,-1).$$

Note that v_1, v_2, v_3, and v_4 are four linearly independent vectors (they have distinct eigenvalues), and so we are done. We have found four spanning eigenvectors of P_4. To calculate the spectral decomposition of P_4 (i.e., the spectral decomposition of the adjacency matrix A of P_4), we use these eigenvectors to obtain orthogonal projection matrices $E_{\theta_1},\cdots,E_{\theta_4}$. For each $j=1,2,3,4$, let w_j be the normalized version of v_j.

$$w_j=\frac{v_j}{\|v_j\|}.$$

We then construct the idempotents.

$$E_\phi=w_1^Tw_1, \qquad E_{\phi-\sqrt{5}}=w_2^Tw_2, \qquad E_{\sqrt{5}-\phi}=w_3^Tw_3, \qquad E_{-\phi}=w_4^Tw_4.$$

The unitary transition operator is then obtained.

$$U_{P_4}(t)=e^{i\phi t}E_\phi+e^{i(\phi-\sqrt{5})t}E_{\phi-\sqrt{5}}+e^{i(\sqrt{5}-\phi)t}E_{\sqrt{5}-\phi}+e^{-i\phi t}E_{-\phi}.$$

Definition 1.21. Let $G_1=(V_1,E_1)$ and $G_2=(V_2,E_2)$ be graphs. The Cartesian product of G_1 and G_2 is the graph

$$H=G_1\square G_2=(V_1\times V_2,E')$$

that satisfies the following. If $(u,v),(u',v')\in V_1\times V_2$ then $(u,v)\sim_H(u',v')$ if and only if $u=u'$ and $v\sim_{G_2}v'$, or $u\sim_{G_1}u'$ and $v=v'$.

Lemma 1.22. *If G and H are graphs with adjacency matrices A and B, respectively, and vertex sets of size n and m, respectively, then the adjacency matrix of $G\square H$ is given by*

$$A\otimes I_m+I_n\otimes B.$$

Proof. Let G and H be graphs with vertex sets $V(G)$ and $V(H)$, respectively, so that $|V(G)|=n$ and $|V(H)|=m$. Suppose that A is the adjacency matrix of G and B is the adjacency matrix of H. Let

$$(a,a'),(b,b')\in V(G\square H)=V(G)\times V(H).$$

By construction,

$$[A\otimes I_m+I_n\otimes B]_{(a,b),(a',b')}=1$$

if and only if $[A\otimes I_m]_{(a,b),(a',b')}=1$ or $[I_n\otimes B]_{(a,b),(a',b')}=1$.

If $[A\otimes I_m]_{(a,b),(a',b')}=1$, then $[A]_{a,a'}=1$ and $b=b'$.

If $[I_n\otimes B]_{(a,b),(a',b')}=1$, then $a=a'$ and $[B]_{b,b'}=1$. That is,

$$[A\otimes I_m+I_n\otimes B]_{(a,b),(a',b')}=1$$

if and only if $a=a'$ and $b\sim_H b'$ or $a\sim_G a'$ and $b=b'$. We have proven the lemma. ∎

As a result, we obtain the following lemma, also given by Godsil [7].

Lemma 1.23. *[7] Let G and H be graphs. Then,*

$$U_{G\square H}(t) = U_G(t) \otimes U_H(t).$$

Proof. Suppose that A is the adjacency matrix of G, and that B is the adjacency matrix of H. Suppose that G and H have n and m vertices, respectively. Then

$$U_{G\square H}(t) = e^{i(A\otimes I_m + I_n\otimes B)t} = e^{iA\otimes I_m\tau} e^{iI_n\otimes B\tau},$$

$$U_{G\square H}(t) = \left(e^{iAt} \otimes I_m\right)\left(I_n \otimes e^{iBt}\right) = e^{iAt} \otimes e^{iBt} = U_G(t) \otimes U_H(t).$$

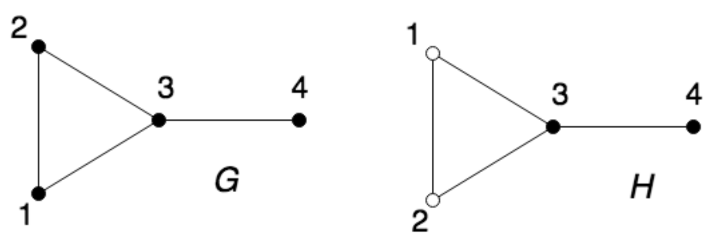
■

We now briefly discuss isomorphic graphs before returning to perfect state transfer. Let $G = (V, E)$ and $H = (V', E')$ be graphs with a bijection $\phi : V \to V'$ defined between their vertex sets such that, for any vertices $u, v \in V$, $\phi(u) \sim_H \phi(v)$ if and only if $u \sim_G v$. In this case, G and H are said to be isomorphic graphs, and ϕ is said to be an isomorphism.

Proposition 1.24. *[3] Let G and H be graphs with adjacency matrices A and B, respectively. G and H are isomorphic graphs if and only if there exists a permutation matrix P such that*

$$P^T AP = B.$$

We defer proof of this property until we use it in the next section of the paper. It can be seen from the property above that, if two graphs G and H are isomorphic, then they are the same up to a relabeling of their vertices, such as in the example below where the same vertex set is used for both graphs.



These graphs are isomorphic with isomorphism $\psi = P_{(1,2)}$, the permutation that swaps vertices 1 and 2 while leaving the others fixed. Clearly, in general, if G and H are isomorphic graphs with isomorphism ϕ, then for any vertex $v \in V(G)$, $\deg v = \deg \phi(v)$.

1.3. **Perfect State Transfer: A Survey.** The phenomenon of perfect state transfer is of great interest to those who design quantum computing algorithms. In the following, we state an important implication of PST and provide a survey of examples of graphs that are known to have perfect state transfer. In particular, we discuss the paths and the cubelike graphs.

Definition 1.25. [7] Let $G = (V, E)$ be a graph with adjacency matrix A, and suppose that the spectral decomposition of A contains idempotents

$$E_{\theta_1}, \cdots, E_{\theta_k}.$$

Let $u, v \in V$. Vertices u and v are cospectral if

$$\left(E_{\theta_j}\right)_{u,u} = \left(E_{\theta_j}\right)_{v,v}$$

for each $j = 1, \cdots, k$.

Definition 1.26. [7] Let $G = (V, E)$ be a graph with adjacency matrix A, and suppose that the spectral decomposition of A contains idempotents

$$E_{\theta_1}, \cdots, E_{\theta_k}.$$

Let $u, v \in V$. Vertices u and v are parallel if

$$E_{\theta_j} e_u \parallel E_{\theta_j} e_v$$

for each $j = 1, \cdots, k$.

Definition 1.27. [7] Let $G = (V, E)$ be a graph with $u, v \in V$. Vertices u and v are strongly cospectral if they are both cospectral and parallel.

The following is an important result due to Godsil [7].

Theorem 1.28. *[7] Let $G = (V, E)$ be a graph with $u, v \in V$. If G has (u, v)-PST at some time τ, then u and v are strongly cospectral.*

This property, along with the brief enumeration of examples to follow, demonstrate that graphs that exhibit perfect state transfer are rare.

Proposition 1.29. *[7] The path on two vertices, P_2, has perfect state transfer.*

Proof. This can be seen from calculation. If A is the adjacency matrix of P_2, then

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

Observe that

$$A^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad A^3 = A,$$

and let $U(t) = U_{P_2}(t)$. As a result,

$$U(t) = e^{iAt} = \sum_{k=0}^{\infty} \frac{(iAt)^k}{k!} = \cos(t) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + i \sin(t) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

If e_1 and e_2 are the standard basis vectors, then

$$U\left(\frac{\pi}{2}\right) e_1 = i e_2, \qquad U\left(\frac{\pi}{2}\right) e_2 = i e_1.$$

This shows that P_2 exhibits PST from each vertex to the other at time $\frac{\pi}{2}$. ∎

Proposition 1.30. *[7] The path on three vertices, P_3, has perfect state transfer.*

Proof. This, too, is easily obtained from calculation. If A is the adjacency matrix of P_3 with vertex set $V = \{1, 2, 3\}$, then A has minimal polynomial

$$m_A(z) = z^3 - 2z.$$

Thus, the following unitary transition operator is obtained. Observe, from the minimal polynomial given above, that

$$A^{2k} = 2^{k-1}\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix}, \qquad A^{2k+1} = 2^k A$$

for any $k = 1, 2, 3, \cdots$. Using

$$B = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix}, \qquad U(\tau) = U_{P_3}(\tau),$$

$$U(\tau) = \sum_{k=0}^{\infty} \frac{(-1)^k 2^{k-1} \tau^{2k}}{(2k)!} B + i \sum_{k=0}^{\infty} \frac{(-1)^k 2^k \tau^{2k+1}}{(2k+1)!} A + I_3 - \frac{1}{2} B,$$

where we have adjusted for the $k = 0$ term given by

$$\frac{(iA\tau)^0}{0!} = I_3.$$

Now,

$$U(\tau) = \frac{1}{2}\cos\left(\sqrt{2}\tau\right) B + \frac{i}{2}\sin\left(\sqrt{2}\tau\right) A + \frac{1}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix}.$$

Perfect state transfer at time $\tau = \frac{\pi}{\sqrt{2}}$ can clearly be seen from the matrix,

$$U_{P_3}\left(\frac{\pi}{\sqrt{2}}\right) = \begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix}.$$

At time $\tau = \frac{\pi}{\sqrt{2}}$ P_3 has $(1, 3)$-PST, $(2, 2)$-PST, and $(3, 1)$-PST. ∎

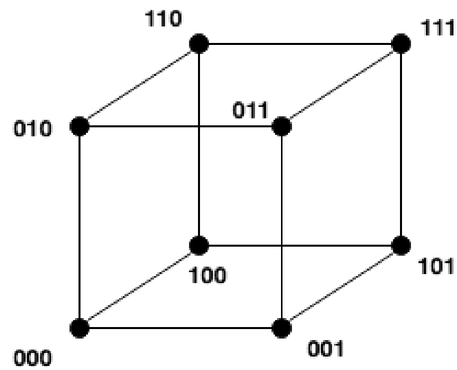
We have seen that the paths on two and three vertices have perfect state transfer. However, interestingly, these are exceptions.

Proposition 1.31. *[12] Let P_k be the unweighted path on k vertices. If $k > 3$, then P_k does not have perfect state transfer between any pair of vertices.*

It is interesting that among a family of graphs that are homeomorphic to one another, i.e., the paths, some graphs have PST and some do not. Indeed, the fact that a graph as simple as the path on four vertices does not have perfect state transfer is an illustration of the strength of the conditions imposed by PST. We continue by identifying examples of PST in another notable family of graphs: the cubelike graphs.

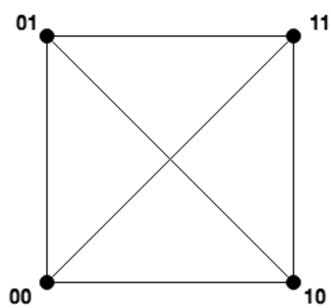
Definition 1.32. Let $G = (V, E) = (\mathbb{Z}_2^d, E)$ be a graph, and let $C \subseteq \mathbb{Z}_2^d$. Suppose that, for any binary words $u, v \in \mathbb{Z}_2^d$, $u \sim v$ if and only if $u + v \in C$. Then, G is the cubelike graph on $\mathbb{Z}_2^d$ with connecting set C.

The following are some examples of cubelike graphs. Consider, for instance, the cubelike graph on vertex set $\mathbb{Z}_2^3$ with connecting set $C = \{100, 010, 001\}$. For any two vertices $u, v \in \mathbb{Z}_2^3$, $u \sim_G v$ if and only if u and v differ in exactly one coordinate position.



Clearly the 3-cube $Q_3 = K_2 \Box K_2 \Box K_2$ is cubelike. We then consider another example.

Let G be the cubelike graph on $\mathbb{Z}_2^2$ with connecting set $C = \{01, 10, 11\} = \mathbb{Z}_2^2 \setminus \{00\}$. Then, for any $u, v \in \mathbb{Z}_2^2$, $u \sim_G v$ if and only if $u \neq v$. The result is K_4.



In general, the cubelike graph on $\mathbb{Z}_2^d$ with connecting set $C = \mathbb{Z}_2^d \setminus \{0\}$ is the complete graph K_{2^d}.

Observe that any binary word $w \in \mathbb{Z}_2^d$ induces a permutation F_w on $\mathbb{Z}_2^d$ given by

$$F_w(u) = u + w.$$

For any $w \in \mathbb{Z}_2^d$, let P_w be the matrix representation of F_w in the standard basis. Observe that, for any $w \in \mathbb{Z}_2^d$, the following are true [8].

(1) $P_w^2 = I$;
(2) if $w \neq 0$, $\operatorname{tr} P_w = 0$;
(3) if J is the all-ones matrix and $C \neq \mathbb{Z}_2^d$, $\sum_{w \in C} P_w = J$;
(4) for any $u \in \mathbb{Z}_2^d$, $P_{w+u} = P_w P_u$.

The following lemma is true by construction.

Lemma 1.33. *[8] If G is the cubelike graph on $\mathbb{Z}_2^d$ with connecting set C, then the adjacency matrix of G is given by*

$$A = \sum_{w \in C} P_w.$$

Let $\sigma = \sum_{w \in C} w$ so that

$$P_\sigma = \prod_{w \in C} P_w.$$

Lemma 1.34. *As a result of Lemma 1.33, cubelike graph G has the unitary transition matrix*

$$U_G(t) = \prod_{w \in C} e^{iP_w t}.$$

Theorem 1.35. *[8] Let G be the cubelike graph on $\mathbb{Z}_2^d$ with connecting set C, and let*

$$\sigma = \sum_{w \in C} w.$$

If $\sigma \neq 0$ then G has $(u, u+\sigma)$-PST at time $\frac{\pi}{2}$ for every $u \in \mathbb{Z}_2^d$. If $\sigma = 0$ then G has (u, u)-PST at time $\frac{\pi}{2}$ for each $u \in \mathbb{Z}_2^d$.

Proof. This proof is due to Godsil and Cheung [8]. By Lemma 1.34, cubelike graph G has the unitary transition matrix

$$U_G\Big(t\Big) = \prod_{w \in C} e^{iP_w t}.$$

For any $w \in C$, $P_w^2 = I$ and so for any $t \in \mathbb{R}$

$$e^{iP_w t} = \sum_{k=0}^{\infty} \frac{(iP_w t)^k}{k!} = \cos tI + i \sin tP_w,$$

giving

$$U_G(t) = \prod_{w \in C} \Big(\cos tI + i \sin tP_w\Big).$$

As a result,

$$U_G\left(\frac{\pi}{2}\right) = \prod_{w \in C} (iP_w) = i^{|C|} P_\sigma.$$

If $\sigma = 0$, then $U_G(\frac{\pi}{2})$ is diagonal, so that for every standard basis vector e_j,

$$U_G\left(\frac{\pi}{2}\right) e_j = \alpha e_j$$

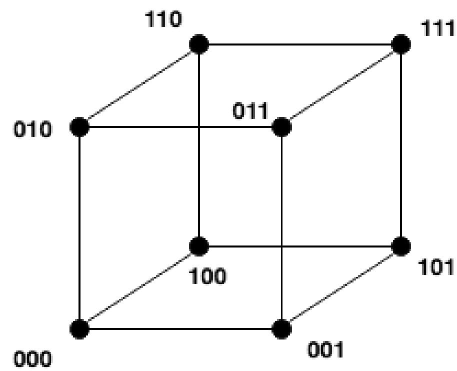
for some $\alpha \in \mathbb{C}$ with $|\alpha| = 1$. If $\sigma \neq 0$ then, for any standard basis vector e_w corresponding to the vertex $w \in \mathbb{Z}_2^d$,

$$U_G\left(\frac{\pi}{2}\right) e_w = \alpha e_{w+\sigma}$$

for some $\alpha \in \mathbb{C}$ with $|\alpha| = 1$. For any $w \in \mathbb{Z}_2^d$ graph G has $(w, w+\sigma)$-PST at time $\tau = \frac{\pi}{2}$. ■

We illustrate with an example.

Example 1.36. Let G be the cubelike graph on $\mathbb{Z}_2^3$ with connecting set $C = \{100, 010, 001\}$ (observe that this is the 3-cube, $Q_3 = K_2 \square K_2 \square K_2$).



To apply the proposition, we merely calculate $\sigma = 100 + 010 + 001 = 111 \neq 0$. By the proposition, the 3-cube has perfect state transfer at time $\frac{\pi}{2}$ between pairs of antipodal vertices. This can easily be checked by calculating the value of $U_G(\frac{\pi}{2})$ directly. The cube G has eigenvalues $(-3, -1, 1, 3)$ with multiplicities 1, 2, 2 and 1 respectively. For each eigenvalue θ let E_θ denote the θ-idempotent, i.e., the orthogonal projection onto the θ-eigenspace.

$$U_G\left(\frac{\pi}{2}\right) = e^{-3i\frac{\pi}{2}}E_{-3} + e^{-i\frac{\pi}{2}}E_{-1} + e^{i\frac{\pi}{2}}E_1 + e^{3i\frac{\pi}{2}}E_3 = -i\begin{pmatrix} 0 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 0 \end{pmatrix}.$$

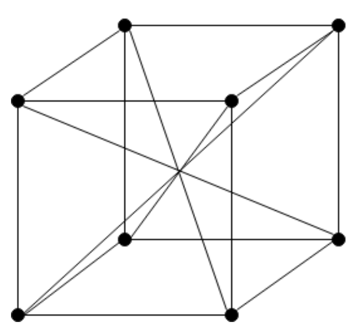
This calculation corresponds perfectly to our expectation that

$$U_G\left(\frac{\pi}{2}\right) = i^{|C|}P_{111} = -i\begin{pmatrix} 0 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 0 \end{pmatrix}.$$

Consider, however, the graph G' that is obtained by adding an element to the connecting set C of G.

$$G' = (\mathbb{Z}_2^3, E), \qquad C' = \{100, 010, 001, 111\}.$$

A new cubelike graph is obtained, shown below.



Note that, for this graph, $\sigma = 100 + 010 + 001 + 111 = 000$. Thus, this graph is periodic at each vertex with period $\frac{\pi}{2}$.

Observe that, while the cubelike graphs constitute an infinite family of graphs that are either periodic or have perfect state transfer, they are highly symmetric. Furthermore, because the vertex set of a cubelike graph must be $\mathbb{Z}_2^d$ for some d, the number of vertices required grows exponentially with the distance between u and v if the graph has (u, v)-PST. The paths, which grow linearly in the number of vertices with the distance between endpoints u and v, do not exhibit perfect state transfer beyond the path of length three, demonstrating that PST is a strong condition to impose. In the next section, we seek to relax the conditions imposed by perfect state transfer.

2. Group State Transfer

2.1. **Fundamentals.** We consider continuous-time quantum walks as the time evolution of the n-level quantum-mechanical system defined by simple finite graph $G = (V, E)$ on n vertices, prepared in the initial state ψ. The previous section demonstrated the rarity of perfect state transfer through an enumeration of PST examples within certain families of graphs, and by stating the implication of strong cospectrality. This section, in contrast, is motivated by the desire to obtain a more relaxed phenomenon of quantum information transfer that generalizes PST, but for which we may generate examples more easily. To that end, we introduce group state transfer, or GST, in which state transfer occurs between two subsets of vertices S and T.

Definition 2.1. Let G be a graph and let $S, T \subseteq V(G)$ so that $S \neq V(G)$. We say that G has (S, T)-group state transfer, or GST, at time $\tau \in \mathbb{R}$ if, for all $\psi \in \mathbb{C}^{|G|}$ such that $\operatorname{Supp} \psi \subseteq S$, $\phi = U_G(\tau)\psi$ satisfies $\operatorname{Supp} \phi \subseteq T$.

We sometimes consider a specific instance of group state transfer known as fractional revival.

Definition 2.2. Let $G = (V, E)$ be a graph with $S \subseteq V$. Graph G has fractional revival on S at time τ if G has (S, S)-GST at time τ.

Given this formal notion of group state transfer, we adopt the following conventions. If G is a graph with vertex set $V = \{1, \cdots, n\}$, then let e_j be the j^{th} standard basis vector, for $j = 1, \cdots, n$. If $S \subseteq V$ is a set of vertices of the graph G then define

$$\langle S \rangle = \operatorname{Span}_{\mathbb{C}}\{e_u : u \in S\}.$$

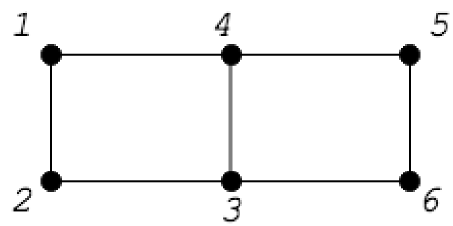
In other words, $\langle S \rangle$ denotes the subspace of all ψ satisfying $\operatorname{Supp} \psi \subseteq S$. If graph G has (S, T)-GST at τ, then we order the vertices V of G so that

$$S = \{1, \cdots, j_S\}, \qquad T = \{j_T, \cdots, j_T + |T| - 1\}$$

where $j_S = |S|$. The following are then satisfied.

$$\{j_T, \cdots, j_S\} = S \cap T, \qquad \{j_T + |T|, \cdots, n\} = V \cap S^C \cap T^C.$$

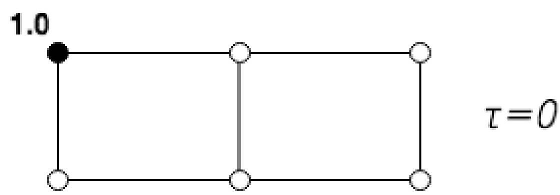
Example 2.3. We motivate the concept of group state transfer with an example. Consider the 6-level quantum mechanical system defined on the following graph.

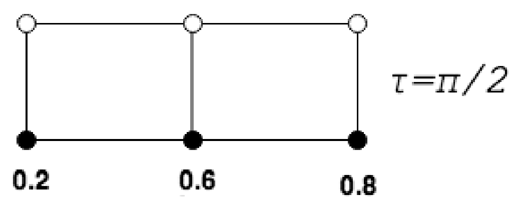


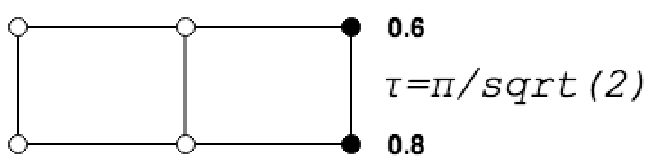
In the following figures, we depict the time evolution of this quantum system, prepared in the state, $\psi = e_1$. The following figures represent the state of the system at time $\tau = \frac{\pi}{2}$ and $\tau = \frac{\pi}{\sqrt{2}}$. At each vertex of G in the following figures, the value of

$$P_j(\tau) = \left| e_j^T U_G(\tau) \psi \right|^2$$

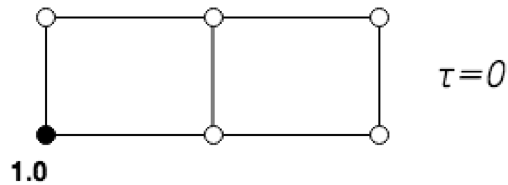
is represented. If $P_j(\tau) = 0$, then the jth vertex is depicted as an empty circle (no fill). Otherwise, it is represented as a filled circle with an approximation of $P_j(\tau)$.

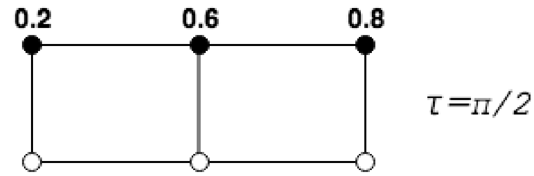


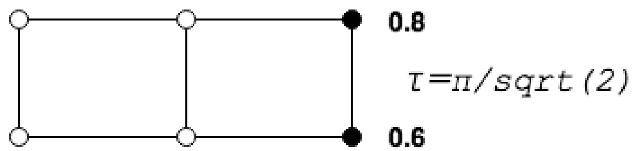




In the following figures, again, we depict the time evolution of the quantum system. This time, however, the quantum system has been prepared in the state, $\psi(0) = e_2$.







We see several instances of group state transfer in this example. This graph has $(\{1\},\{2,3,6\})$-GST, as well as $(\{2\},\{1,4,5\})$-GST at $\frac{\pi}{2}$. We now show that this graph has $(\{1,2\},\{5,6\})$-GST at $\frac{\pi}{\sqrt{2}}$. Let ψ satisfy $\psi \subseteq \operatorname{Supp}(\{1,2\})$. Then,

$$\psi = c_1e_1 + c_2e_2.$$

Thus, by the results shown above, for some $\alpha_1, \alpha_2 \in \mathbb{C}$,

$$U_G\left(\frac{\pi}{\sqrt{2}}\right)\psi = c_1\left(\alpha_1e_5 + \alpha_2e_6\right) + c_2\left(\alpha_2e_5 + \alpha_1e_6\right) = (c_1\alpha_1 + c_2\alpha_2)e_5 + (c_1\alpha_2 + c_2\alpha_1)e_6.$$

Clearly, $\operatorname{Supp} U_G\left(\frac{\pi}{\sqrt{2}}\right)\psi \subseteq \{5,6\}$. This shows that $P_2 \square P_3$ exhibits group state transfer.

It is natural to observe that perfect state transfer is a special case of group state transfer, in which the origin and target sets both have cardinality one. We then make an initial observation.

Proposition 2.4. *Graph G has $(\{u\},\{v\})$-GST at time τ if and only if G has (u,v)-PST at τ.*

Proposition 2.5. *If Graph G has (u_j,v_j)-PST at time τ for sets of vertices $\{u_1,\cdots,u_k\}$ and $\{v_1,\cdots,v_k\}$, then G has $(\{u_1,\cdots,u_k\},\{v_1,\cdots,v_k\})$-GST at τ.*

Proof. Suppose that graph G has (u_j,v_j)-PST at τ for sets of vertices $\{u_1,\cdots,u_k\}$ and $\{v_1,\cdots,v_k\}$. Then, if ψ satisfies

$$\operatorname{Supp}\psi \subseteq \{u_1,\cdots,u_k\},$$

Then

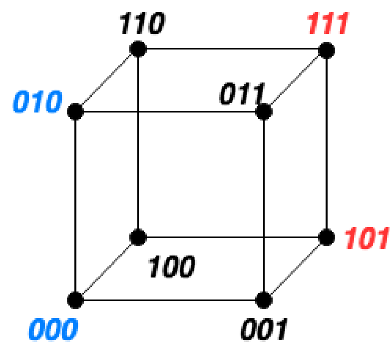
$$\psi \in \langle \{u_1, \cdots, u_k\} \rangle, \qquad \psi = c_1 e_{u_1} + \cdots + c_k e_{u_k}.$$

Now,

$$U_G(\tau)\psi = c_1\alpha_1 e_{v_1} + \cdots + c_k \alpha_k e_{v_k},$$

where $\alpha_1, \cdots, \alpha_k \in \mathbb{C}$ satisfy $|\alpha_1| = \cdots = |\alpha_k| = 1$. Thus, if $\operatorname{Supp}\psi \subseteq \{u_1, \cdots, u_k\}$, then $\operatorname{Supp} U_G(\tau)\psi \subseteq \{v_1, \cdots, v_k\}$, proving that GST is exhibited at τ. ∎

Example 2.6. Consider the 3-cube $Q_3 = K_2 \square K_2 \square K_2$, i.e., the cubelike graph on $\mathbb{Z}_2^3$ with connecting set $\{100, 010, 001\}$. By Theorem 1.35, Q_3 has (among other instances) $(000, 111)$-PST and $(010, 101)$-PST at time $\frac{\pi}{2}$ as shown in the diagram below.



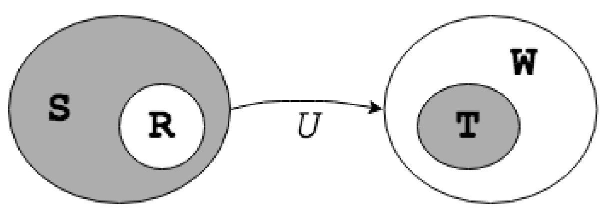
By Proposition 2.5, Q_3 then has group state transfer between the blue and red vertices shown above at time $\frac{\pi}{2}$. That is, Q_3 has $(\{000, 010\}, \{101, 111\})$-GST at time $\frac{\pi}{2}$.

To further explore the properties of group state transfer, we consider some basic properties.

Proposition 2.7. *If graph G has (S, T)-GST at time τ, then the following are true.*

(1) If $T \subseteq W$, then G has (S, W)-GST at τ;
(2) If $R \subseteq S$, then G has (R, T)-GST at τ.

Proof. The unitary matrix $U_G(\tau)$ maps $\langle S \rangle$ to $\langle T \rangle$ injectively.



Because $T \subseteq W$, $U_G(\tau)$ also maps $\langle S \rangle$ to $\langle W \rangle$, that is,

$$\{U_G(\tau)\psi : \psi \in \langle S \rangle\} \subseteq \langle T \rangle \subseteq \langle W \rangle.$$

Because $R \subseteq S$, $U_G(\tau)$ also maps $\langle R \rangle$ to $\langle T \rangle$. ∎

The following proposition constitutes what may be considered a property of entropy, that is, that quantum information may not be mapped into a space of lower dimension.We have discussed the possibility that a graph G may have group state transfer between two vertex sets of equal magnitude. It is plain that a graph G may have group state transfer from S to T, for which $|T| \geq |S|$. Take, for example, a quantum system defined on graph G, that has been prepared in the state

$$\psi = \alpha e_u,$$

where u is a vertex of G. Plainly,

$$U_G(\tau)\psi \in \langle V(G)\rangle.$$

Any graph then has group state transfer from any single vertex to the entire vertex set. By the same reasoning, any graph $G = (V, E)$ has group state transfer from any nontrivial subset of V to all of V. In the following, we prove that it is not possible for any graph to have group state transfer from a larger to a smaller vertex set.

Proposition 2.8. *If graph G has (S,T)-GST at τ, then $|S| \leq |T|$.*

Proof. Suppose that G is a graph with (S,T)-GST at time τ and that $U(\tau) = U_G(\tau)$. Let

$$\operatorname{Im} U(\tau)|_S = \{U(\tau)\psi : \psi \in \langle S\rangle\}$$

and observe that $\operatorname{Im} U(\tau)|_S \subseteq \langle T\rangle$. Because $U(\tau)$ is injective,

$$\dim \operatorname{Im} U(\tau)|_S = |S| \leq \dim\langle T\rangle = |T|.$$

■

I offer an alternate proof of this property that demonstrates the block-matrix form of the unitary transition operator, $U_G(\tau)$. We will find this useful in the consideration of group state transfer. From the definition of GST, it is clear that, if G has (S,T)-GST at τ, then, under the conventional ordering, $U_G(\tau)$ has the following form, where 0 is the all-zeros matrix block, and a star denotes a matrix block which may or may not be zero. Recall that, under the conventional ordering, $V(G) = \{1, 2, \cdots, j_T, \cdots, j_S, \cdots, j_T + |T| - 1, j_T + |T|, \cdots, n\}$, with $S = \{1, \cdots, j_S\}$ and $T = \{j_T, \cdots, j_T + |T| - 1\}$.

$$U_G(\tau) = \begin{pmatrix} 0 & 0 & * & * \\ * & * & * & * \\ * & * & * & * \\ 0 & 0 & * & * \end{pmatrix}$$

Because $U_G(\tau)$ is symmetric, we know more about the location of zero blocks in the block-matrix form of $U_G(\tau)$.

$$U_G(\tau) = \begin{pmatrix} 0 & 0 & * & 0 \\ 0 & * & * & 0 \\ * & * & * & * \\ 0 & 0 & * & * \end{pmatrix}.$$

Accordingly, by symmetry, we express $U_G(\tau)$ in the following block-matrix form, where $P_{i,j}^T = P_{j,i}$ for each i and j.

$$U_G(\tau) = \begin{pmatrix} 0 & 0 & P_{1,3} & 0 \\ 0 & P_{2,2} & P_{2,3} & 0 \\ P_{3,1} & P_{3,2} & P_{3,3} & P_{3,4} \\ 0 & 0 & P_{4,3} & P_{4,4} \end{pmatrix}.$$

The alternate proof of the proposition follows.

Proof. Suppose that graph G has (S,T)-GST at τ. Consider the vertices of G under the conventional ordering, and partition the vertices of G in the following manner where $\sqcup$ denotes the disjoint union.

$$V(G) = \Big(S \setminus I\Big) \sqcup I \sqcup \Big(T \setminus S\Big) \sqcup \Big(V(G) \cap S^C \cap T^C\Big),$$

Where $I = S \cap T$. Now, consider $U_G(\tau)$ in the block structure endowed by the partition described above. In the block matrix below, $P_{i,j}^T = P_{j,i}$ for each i and j.

$$U_G(\tau) = \begin{pmatrix} 0 & 0 & P_{1,3} & 0 \\ 0 & P_{2,2} & P_{2,3} & 0 \\ P_{3,1} & P_{3,2} & P_{3,3} & P_{3,4} \\ 0 & 0 & P_{4,3} & P_{4,4} \end{pmatrix}.$$

Because $U_G(\tau)$ is unitary, each column of $U_G(\tau)$ is a unit vector. As a result,

$$|S| = \|P_{1,3}\|_{\mathcal{F}}^2 + \|P_{2,2}\|_{\mathcal{F}}^2 + \|P_{2,3}\|_{\mathcal{F}}^2,$$

$$|T| = \|P_{1,3}\|_{\mathcal{F}}^2 + \|P_{2,2}\|_{\mathcal{F}}^2 + 2\,\|P_{2,3}\|_{\mathcal{F}}^2 + \|P_{3,3}\|_{\mathcal{F}}^2 + \|P_{4,3}\|_{\mathcal{F}}^2.$$

Thus,

$$|T| - |S| = \|P_{2,3}\|_{\mathcal{F}}^2 + \|P_{3,3}\|_{\mathcal{F}}^2 + \|P_{4,3}\|_{\mathcal{F}}^2 \geq 0.$$

∎

We use the block-matrix form of the unitary transition matrix $U_G(\tau)$ to prove the following theorem.

Theorem 2.9. *Assume that graph G has (S,T)-GST at time τ and $|S| = |T|$. Then the following are true, where $I = S \cap T$.*

(1) G has (T,S)-GST at time τ;
(2) G has $(S \setminus I, T \setminus I)$-GST at τ;
(3) G has $(T \setminus I, S \setminus I)$-GST at τ;

Proof. If graph G has (S,T)-GST at τ, then under the conventional ordering,

$$U_G(\tau) = \begin{pmatrix} 0 & 0 & P_{1,3} & 0 \\ 0 & P_{2,2} & P_{2,3} & 0 \\ P_{3,1} & P_{3,2} & P_{3,3} & P_{3,4} \\ 0 & 0 & P_{4,3} & P_{4,4} \end{pmatrix}.$$

Recall that

$$|T| - |S| = \|P_{2,3}\|_{\mathcal{F}}^2 + \|P_{3,3}\|_{\mathcal{F}}^2 + \|P_{4,3}\|_{\mathcal{F}}^2 \geq 0.$$

As a result, if $|S| = |T|$,

$$\|P_{2,3}\|_{\mathcal{F}}^2 = \|P_{3,3}\|_{\mathcal{F}}^2 = \|P_{4,3}\|_{\mathcal{F}}^2 = 0,$$

and so, using the fact that $U_G(\tau)$ is symmetric,

$$U_G(\tau) = \begin{pmatrix} 0 & 0 & P_{1,3} & 0 \\ 0 & P_{2,2} & 0 & 0 \\ P_{3,1} & 0 & 0 & 0 \\ 0 & 0 & 0 & P_{4,4} \end{pmatrix}.$$

We see, from this matrix, all three instances of GST described in the statement of the proposition. ■

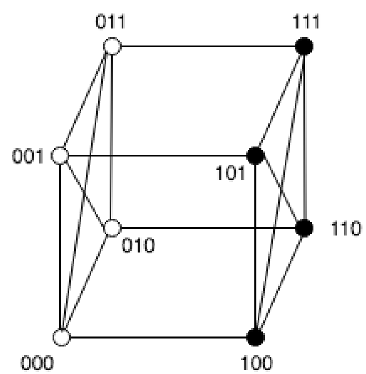
Corollary 2.10. *If G is a graph with (S,T)-GST at time τ such that $|S| = |T|$, then there exists a pair of vertex sets S' and T' of G that satisfy the following.*

(1) Graph G has (S',T')-GST at time τ;
(2) sets S' and T' have the same cardinality, i.e., $|S'| = |T'|$,
(3) sets S' and T' are disjoint, i.e., $S' \cap T' = \emptyset$.

Example 2.11. For the purposes of this example, we return to the cubelike graphs. Let G be the cubelike graph on $\mathbb{Z}_2^3$ with connecting set $C = \{100, 010, 001, 011\}$. Let vertex sets S and T be given as follows.

$$S = \{0\alpha\beta : \alpha, \beta \in \mathbb{Z}_2\}, \qquad T = \{1\alpha\beta : \alpha, \beta \in \mathbb{Z}_2\}.$$

In the following diagram, the elements of S are denoted using empty circles (not filled in), while the elements of T are denoted using filled circles.



Observe that it is also the case that $G = K_4 \square K_2$, and so, if $A(K_4)$ is the adjacency matrix of K_4 and $A(G)$ is the adjacency matrix of G,

$$A(G) = A(K_4) \otimes I_2 + I_4 \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} A(K_4) & I_4 \\ I_4 & A(K_4) \end{pmatrix}.$$

Observe that

$$\sigma = \sum_{u \in C} u = 100 \neq 000.$$

Applying theorem 1.35, for each vertex $u \in \mathbb{Z}_2^3$, G has $(u, 100 + u)$-PST at time $\frac{\pi}{2}$. As a result, clearly, G has (S,T)-GST at time $\frac{\pi}{2}$. In this case, $|S| = |T|$, and so G also has (T,S)-GST at time $\frac{\pi}{2}$. What about a case where $S \cap T \neq \emptyset$?

Rather than taking S and T to be given as above, suppose that

$$S = \{000, 010, 001, 011, 101\}, \qquad T = \{100, 110, 101, 111, 001\}, \qquad S \cap T = \{001, 101\}.$$

We use this example to numerically demonstrate the consequences of this proposition.

Claim 2.12. Graph G has (S,T)-GST at time $\frac{\pi}{2}$.

Proof. By Theorem 1.35, we know that G has $(u, 100+u)$-PST at time $\frac{\pi}{2}$ for each vertex $u \in \mathbb{Z}_2^3$. Let $\psi \in \langle S \rangle$. Then,

$$\psi = \sum_{u \in S} c_u e_u.$$

For every binary word $u \in S$, $100 + u \in T$. Thus,

$$U_G\left(\frac{\pi}{2}\right)\psi = \sum_{v \in T} d_v e_v.$$

■

Similarly, because $100 + v \in S$ for every binary word $v \in T$, G has (T, S)-GST at time $\frac{\pi}{2}$.

Claim 2.13. Let $I = S \cap T = \{001, 101\}$. Graph G has $(S \setminus I, T \setminus I)$-GST at time $\frac{\pi}{2}$.

This proof follows from Theorem 2.9. Similarly, it is easy to see that G has $(T \setminus I, S \setminus I)$-GST at time $\frac{\pi}{2}$.

2.2. **Graph Symmetries.** It is natural to question the relationship between group state transfer and graph automorphisms. We then continue with a brief discussion of graph automorphisms and their relationship to quantum walks.

Definition 2.14. Let $G = (V, E)$ be a graph, and let σ be a permutation on V. Permutation σ is an automorphism of G if, for any $u, v \in V$, $u \sim v$ if and only if $\sigma(u) \sim \sigma(v)$.

Given any graph G, the automorphisms of G form a group, denoted $\operatorname{Aut} G$, under composition.

Definition 2.15. Let $G = (V, E)$ be a graph with automorphism group $\operatorname{Aut} G$. Then, for any vertex $u \in V$, the orbit of u is given by

$$\mathcal{O}(u) = \{\sigma(u) : \sigma \in \operatorname{Aut} G\}.$$

Definition 2.16. Let $G = (V, E)$ be a graph. Then, for any vertex $u \in V$, the stabilizer of u is given by

$$\operatorname{Stab} u = \{\sigma \in \operatorname{Aut} G : \sigma(u) = u\}.$$

These two concepts are combined in the following well-known result, known as the Orbit-Stabilizer Theorem.

Theorem 2.17. *[14] Let $G = (V, E)$ be a graph. Then, for any vertex $u \in V$,*

$$|\mathcal{O}(u)||\operatorname{Stab} u| = |\operatorname{Aut} G|.$$

We may generalize the notions defined above to sets of multiple vertices.

Definition 2.18. Let $G = (V, E)$ be a graph with $W \subseteq V$. The orbit of W is the set of vertex sets

$$\mathcal{O}(W) = \{\sigma(W) : \sigma \in \operatorname{Aut} G\}.$$

Definition 2.19. Let $G = (V, E)$ be a graph with $W \subseteq V$. The set-wise stabilizer of W is given by

$$\operatorname{Stab} W = \{\sigma \in \operatorname{Aut} G : \sigma(W) = W\}.$$

Naturally, these set-level definitions of orbits and stabilizers lead to a set-wise Orbit-Stabilizer Theorem.

Theorem 2.20. *Let $G = (V, E)$ be a graph. Then, for any vertex set $W \subseteq V$,*

$$|\mathcal{O}(W)||\operatorname{Stab} W| = |\operatorname{Aut} G|.$$

Lemma 2.21. *Let G and H be graphs on the same vertex set with adjacency matrices A and B, respectively. Then G and H are isomorphic if and only if there exists a permutation matrix P satisfying $P^T AP = B$.*

Proof. Suppose that G and H are isomorphic graphs on the vertex set, $V(G) = V(H) = V$. Then, there exists a bijection,

$$\phi : V \to V,$$

so that $u \sim_G v$ if and only if $\phi(u) \sim_H \phi(v)$. Bijection ϕ is then a permutation on V. Let $\mathcal{B}$ be the standard basis and let $P = [\phi]_{\mathcal{B}}$, that is, let P be the permutation matrix representation of ϕ in the standard basis. Then, $(P^T AP)_{u,v} = 1$ if $\phi^{-1}(u) \sim_G \phi^{-1}(v)$, and $(P^T AP)_{u,v} = 0$ otherwise. That is, $(P^T AP)_{u,v} = 1$ if $u \sim_H v$, and $(P^T AP)_{u,v} = 0$ otherwise. Thus,

$$P^T AP = B.$$

The converse may also be proven similarly. ■

Corollary 2.22. *Let G be a graph with adjacency matrix A, and let σ be an automorphism of G. If P_σ is the permutation matrix representation of σ, then $P_\sigma A = AP_\sigma$.*

Proof. If σ is an automorphism of graph $G = (V, E)$, then σ is an isomorphism from G to G. By the previous lemma and using the fact that $P_\sigma^{-1} = P_\sigma^T$,

$$P_\sigma^T AP_\sigma = A, \qquad AP_\sigma = P_\sigma A.$$

■

We proceed with a few definitions pertinent to graph automorphisms and quantum walks.

Definition 2.23. Let G be a graph with adjacency matrix A. The commutant algebra $\mathcal{C}$ of A (also known as the centralizer algebra) is given as follows.

$$\mathcal{C}(A) = \{B \in \mathcal{M}_n(\mathbb{C}) : AB = BA\}$$

where $\mathcal{M}_n(\mathbb{C})$ is the set of all $n \times n$ matrices over the complex numbers.

Definition 2.24. Let G be a graph with adjacency matrix, A. Then the adjacency algebra of G, denoted

$$\langle I, A, A^2, A^3, \cdots \rangle,$$

is the set of all polynomials in A with complex coefficients.

We know that the automorphisms of a graph $G = (V, E)$ are exactly the permutations on V that commute with the adjacency matrix A. That is, if $|V| = n$ and we identify S_n as the group of $n \times n$ permutation matrices,

$$\operatorname{Aut} G = S_n \cap \mathcal{C}(A).$$

As a result, $\operatorname{Aut} G \subseteq \mathcal{C}(A)$. Let $p \in \langle I, A, A^2, A^3, \cdots \rangle$. Then

$$p = c_1 I + \cdots + c_k A^{k-1}, \qquad Ap = c_1 A + \cdots = c_k A^k = pA.$$

Thus, $\langle I, A, A^2, A^3, \cdots \rangle \subseteq \mathcal{C}(A)$. However, generally,

$$\mathcal{C}(A) \neq \langle I, A, A^2, A^3, \cdots \rangle.$$

If G is a graph with adjacency matrix A, and $\sigma \in \operatorname{Aut} G$, then

$$P_\sigma U_G(\tau) = P_\sigma \left(I + iA\tau - \frac{A^2\tau^2}{2} - \frac{iA^3\tau^3}{6} + \cdots \right) = \left(I + iA\tau - \frac{A^2\tau^2}{2} - \frac{iA^3\tau^3}{6} + \cdots \right) P_\sigma = U_G(\tau)P_\sigma.$$

We now consider the following result concerning perfect state transfer.

Proposition 2.25. *Let G be a graph with (u,v)-PST at time τ, and suppose that σ is a permutation in the automorphism group of G. Then, G has $(\sigma(u), \sigma(v))$-PST at time τ.*

Proof. Let P_σ be the matrix representation of permutation, σ. Then,

$$U_G(\tau)e_{\sigma(u)} = U_G(\tau)P_\sigma e_u = P_\sigma U_G(\tau)e_u = P_\sigma \alpha e_v = \alpha e_{\sigma(v)},$$

For some $\alpha \in \mathbb{C}$. ■

We make the following observation.

Remark 2.26. Let G be a graph with adjacency matrix A and unitary transition operator $U(\tau)$. Then,

$$\mathcal{C}(A) \subseteq \mathcal{C}(U(\tau)).$$

Proposition 2.27. *Suppose that G is a graph with (u,v)-PST at τ, and suppose $\sigma \in \operatorname{Aut} G$. Then the w^{th} entry of $U_G(\tau)e_{\sigma u}$ is $\alpha\delta_{w,\alpha v}$ where α is a complex number of modulus 1 and δ is the Kronecker delta.*

Proof.

$$e_w^T U_G(\tau)e_{\sigma u} = e_w^T U_G(\tau)P_\sigma e_u = e_w^T P_\sigma U_G(\tau)e_u = \alpha e_w^T P_\sigma e_v = \alpha e_w^T e_{\sigma v} = \alpha\delta_{w,\sigma v}.$$

■

Proposition 2.28. *Suppose that graph $G = (V,E)$ has $(\{v\}, V(G)\backslash\{j\})$-GST at τ. Let $\mathcal{O}(u)$ be the orbit containing u under the action of $\operatorname{Aut} G$. Suppose that $v \in \mathcal{O}(u)$. If $\sigma \in \operatorname{Aut} G$ satisfies $\sigma : u \mapsto v$, then G has $(\{u\}, V(G) \setminus \{\sigma^{-1}j\})$-GST at τ.*

Proof. Under the conventional ordering, let P_σ denote the permutation matrix representation of $\sigma \in \operatorname{Aut} G$ and let $U(\tau) = U_G(\tau)$. Because $P_\sigma \in \mathcal{C}(U(\tau))$,

$$P_\sigma U(\tau)e_u = U(\tau)e_v.$$

Observe

$$e_j^T P_\sigma U(\tau)e_u = \left(P_\sigma^{-1} e_j \right)^T U(\tau)e_u = e_{\sigma^{-1}(j)}^T U(\tau)e_u.$$

At the same time,

$$e_j^T P_\sigma U(\tau)e_u = e_j^T U(\tau)e_v = 0$$

by our hypothesis that G has $(\{v\}, V(G) \setminus \{j\})$-GST at time τ. As a result,

$$e_{\sigma^{-1}(j)}^T U(\tau)e_u = 0.$$

Let ψ satisfy $\operatorname{Supp}\psi = \{u\}$, so that $\psi = ce_u$ for some nonzero $c \in \mathbb{C}$.

$$e_{\sigma^{-1}(j)}^T U(\tau)\psi = ce_{\sigma^{-1}(j)}^T U(\tau)e_u = 0.$$

We see then that G has $(\{u\}, V(G) \setminus \{\sigma^{-1}j\})$-GST at time τ. ■

In general, however, the following may also be said.

Theorem 2.29. *Suppose that graph $G = (V, E)$ has (S, T)-GST at time τ and let $\sigma \in \operatorname{Aut} G$. Then, G has $(\sigma(S), \sigma(T))$-GST at time τ.*

Proof. Let $\psi \in \langle \sigma(S) \rangle$ and let $U(\tau) = U_G(\tau)$. Then,

$$U(\tau)\psi = U(\tau)P_\sigma \phi$$

for some $\phi \in \langle S \rangle$ where P_σ is the permutation matrix representation of σ. Let $\phi' = U(\tau)\phi$ and observe that $\phi' \in \langle T \rangle$ because G exhibits (S, T)-GST.

$$U(\tau)\psi = U(\tau)P_\sigma \phi = P_\sigma U(\tau)\phi = P_\sigma \phi' \in \langle \sigma(T) \rangle.$$

Because $\operatorname{Supp} U(\tau)\psi \subseteq \langle \sigma(T) \rangle$, we have proven that G exhibits $(\sigma(S), \sigma(T))$-GST at time τ. ■

Proposition 2.30. *If G has (u, v)-PST at τ, then G has $(\mathcal{O}(u), \mathcal{O}(v))$-GST at τ. G also has $(\mathcal{O}(v), \mathcal{O}(u))$-GST at τ, where $\mathcal{O}(u)$ and $\mathcal{O}(v)$ denote the orbit under any subgroup H of* $\operatorname{Aut} G$.

Proof. For any vertex $u' \in \mathcal{O}(u)$, there exists a group element $\sigma \in \operatorname{Aut} G$ such that $\sigma : u \mapsto u'$. Thus, by Godsil [7], graph G has (u', v')-PST at τ, where $v' = \sigma(v)$. As a result, for each $u' \in \mathcal{O}(u)$, there exists vertex $v' \in \mathcal{O}(v)$ such that G has (u', v')-PST at τ. The fact that G exhibits $(\mathcal{O}(u), \mathcal{O}(v))$-GST at time τ follows from Proposition 2.5. We recall that if G has (u, v)-PST at time τ then G also has (v, u)-PST at time τ and, by the same reasoning, we obtain that G has $(\mathcal{O}(v), \mathcal{O}(u))$-GST at time τ. ■

An important consequence is that u and v must satisfy $|\mathcal{O}(u)| = |\mathcal{O}(v)|$ if G has (u, v)-PST.

Example 2.31. For this example, we turn again to the cubelike graphs. Let G be a cubelike graph with connecting set C and suppose that $\sigma \neq 0$ where

$$\sigma := \sum_{u \in C} u.$$

Then, for any vertex $u \in \mathbb{Z}_2^d$, G has $(\mathcal{O}(u), \mathcal{O}(\sigma + u))$-GST at time $\tau = \frac{\pi}{2}$. Similarly, if $\sigma = 0$, then, for any vertex $u \in \mathbb{Z}_2^d$, G has fractional revival on $\mathcal{O}(u)$ at time $\tau = \frac{\pi}{2}$.

Definition 2.32. Let $G = (V, E)$ be a graph with unitary transition operator $U(t)$. Then, for any vertex set $S \subseteq V$, define

$$F(S, t) = \operatorname{Supp} \operatorname{Im} U(\tau)|_S.$$

Proposition 2.33. *Let $G = (V, E)$ be a graph so that $S \subseteq V$. Then*

$$\operatorname{Stab} S \subseteq \operatorname{Stab} F(S, t).$$

Proof. Let $u \in F(S, t)$. If $w = U(-t)e_u$ then

$$\operatorname{Supp} w \subseteq S.$$

Let $\sigma \in \operatorname{Stab} S$. Then

$$P_\sigma e_u = P_\sigma U(t) w = U(t) P_\sigma w \in \langle F(S, t) \rangle$$

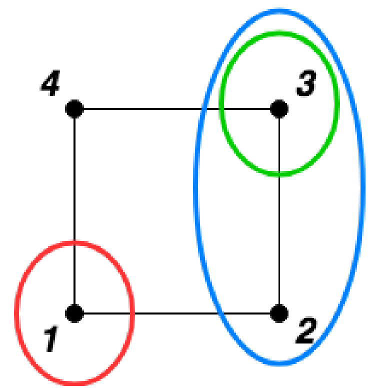
because $P_\sigma w \in \langle S \rangle$. Thus, clearly, $\sigma \in \operatorname{Stab} F(S, t)$. ■

Remark 2.34. In the above proposition, graph G has $(S, F(S,t))$-GST at time τ. However, if graph G has (S,T)-GST at τ then, in general, it is not true that

$$\operatorname{Stab} S \subseteq \operatorname{Stab} T.$$

This is demonstrated by the following example.

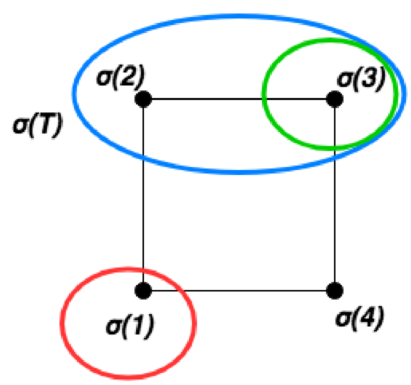
Example 2.35. Let $G = C_4$ be the 4-cycle with vertices $\{1,2,3,4\}$ as shown below. Let $S = \{1\}$, $T = \{2,3\}$, and $W = \{3\}$. In the figure below, S is shown in red, T in blue, and W in green.



Observe that G is also the cubelike graph on $\mathbb{Z}_2^2$ with connecting set $C = \{10, 01\}$. From Theorem 1.35, with $F(S,t)$ given as in Proposition 2.33, $F(S,t) = W$. It is also clearly the case that

$$\operatorname{Stab} S \subseteq \operatorname{Stab} W.$$

Let σ be the reflection that exchanges 2 and 4. Even though G has (S,T)-GST at $\frac{\pi}{2}$, it is clearly not the case that $\sigma \in \operatorname{Stab} T$.



Corollary 2.36. *If $G = (V,E)$ is a graph with $S \subset V$ satisfying $|S| = |F(S,t)|$ for some time t, then* $\operatorname{Stab} S = \operatorname{Stab} F(S,t)$.

This follows from Proposition 2.33 and Theorem 2.9.

Corollary 2.37. *If $G = (V, E)$ is a graph with $S \subseteq V$, then*

$$|\mathcal{O}(F(S,t))| \leq |\mathcal{O}(S)|$$

where $\mathcal{O}(S)$ is the orbit of S under the action of any subgroup H of $\operatorname{Aut} G$.

This follows from Theorem 2.20 and from the fact that $\operatorname{Stab} S \subseteq \operatorname{Stab} F(S,t)$.

2.3. **Graph Products.** Suppose that G_1 and G_2 are graphs, and $P(.,.)$ is some graph product (e.g., cartesian product, strong product, et cetera) and that $H = P(G_1, G_2)$. We now consider the following question. If G_1 or G_2 has group state transfer, then under what circumstances does H have group state transfer, and between what vertex sets? We begin by considering the cartesian graph product.

We adopt the following convention. If $V(G_1) = \{1, 2, \cdots, n_1\}$ and $V(G_2) = \{1, 2, \cdots, n_2\}$ then we number the vertices $V(G_1) \times V(G_2) = V(P(G_1, G_2)) = V(G_1 \square G_2)$ $\{1, \cdots, n\}$ so that $n = n_1 n_2$. The vertices $\{(i, j) : 1 \leq j \leq n_2\}$ will be numbered from $n_2(i-1)+1$ to $n_2 i$.

Proposition 2.38. *Let G_1 and G_2 be graphs that satisfy the following.*

(1) Graph G_1 has (S, T)-GST at τ.
(2) Graph G_2 has (X, Y)-GST at τ.

Then, $G_1 \square G_2$ has $(S \times X, T \times Y)$-GST at τ, where $\square$ denotes the Cartesian graph product.

Proof. Let $U_1(\tau) = U_{G_1}(\tau)$ and $U_2(\tau) = U_{G_2}(\tau)$.

Suppose that graph G_1 has (S, T)-GST at τ, and graph G_2 has (X, Y)-GST at τ. If

$$\psi = \sum_{u \in S} c_u e_u$$

then

$$U_1(\tau)\psi = \sum_{v \in T} d_v e_v.$$

Similarly, if

$$\psi = \sum_{u \in X} a_u e_u$$

then

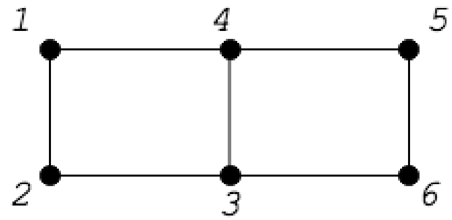
$$U_2(\tau)\psi = \sum_{v \in Y} b_v e_v.$$

Thus, if $s \in S$, $x \in X$, and $\phi = e_s \otimes e_x$, then

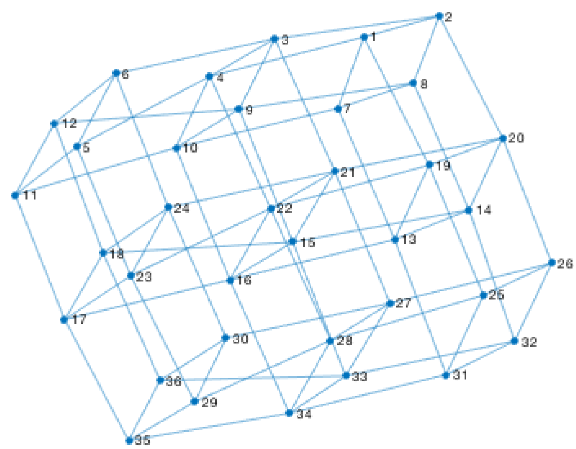
$$\Big(U_1(\tau) \otimes U_2(\tau)\Big)(e_s \otimes e_x) = \Big(U_1(\tau) e_s\Big) \otimes \Big(U_2(\tau) e_x\Big) = \psi_T \otimes \psi_Y$$

for some $\psi_T \in \langle T \rangle$ and $\psi_Y \in \langle Y \rangle$. Thus, $U_{G_1 \square G_2}(\tau)\phi \in \langle T \times Y \rangle$. The result then follows by applying linearity. ■

Example 2.39. As an example, we return to the graph, $G = P_3 \square P_2$.



Consider, instead, $H = G\square G$. Recall that the vertex set of H is $V(G) \times V(G)$ and that, for each $(u,v),(u',v') \in V(H)$, $(u,v) \sim_H (u',v')$ if and only if $u = u'$ and $v \sim_G v'$, or $u \sim_G u'$ and $v = v'$. In this case, by the above proposition, G has $(\{1,2\}\times\{1,2\},\{5,6\}\times\{5,6\})$-GST at time $\frac{\pi}{\sqrt{2}}$. This constitutes an instance of GST between two vertex sets of size four in the following product graph.



Perhaps it is not altogether surprising that we should obtain group state transfer in H, which is a product of copies of P_3 and P_2, both of which have perfect state transfer. It is interesting, however, that by considering a larger product graph, we have obtained GST between two vertex sets of relatively small cardinality, that is, between sets of size 4 in a graph with 36 vertices.

Proposition 2.40. *Let G and H be graphs, so that G has (S,T)-GST at τ and H has vertex set V. Then $G\square H$ has $(S\times V, T\times V)$-GST at τ.*

Proof. If G has (S,T)-GST at τ then, under the conventional ordering, $U_G(\tau)$ has the block structure

$$\begin{pmatrix} 0 & 0 & P_{1,3} & 0 \\ 0 & P_{2,2} & P_{2,3} & 0 \\ P_{3,1} & P_{3,2} & P_{3,3} & P_{3,4} \\ 0 & 0 & P_{4,3} & P_{4,4} \end{pmatrix}.$$

Recall Lemma 1.23. $U_{G\Box H}(\tau)$ has the following block structure.

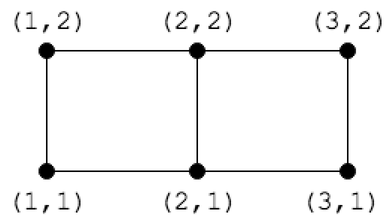
$$\begin{pmatrix} 0 & 0 & P_{1,3} & 0 \\ 0 & P_{2,2} & P_{2,3} & 0 \\ P_{3,1} & P_{3,2} & P_{3,3} & P_{3,4} \\ 0 & 0 & P_{4,3} & P_{4,4} \end{pmatrix} \otimes U_H(\tau) = \begin{pmatrix} 0 & 0 & P_{1,3}\otimes U_H(\tau) & 0 \\ 0 & P_{2,2}\otimes U_H(\tau) & P_{2,3}\otimes U_H(\tau) & 0 \\ P_{3,1}\otimes U_H(\tau) & P_{3,2}\otimes U_H(\tau) & P_{3,3}\otimes U_H(\tau) & P_{3,4}\otimes U_H(\tau) \\ 0 & 0 & P_{4,3}\otimes U_H(\tau) & P_{4,4}\otimes U_H(\tau) \end{pmatrix}.$$

■

Similarly, the following may be demonstrated.

(1) If G and H are graphs such that G has vertex set V and H has (S,T)-GST at τ, then $G\Box H$ has $(V\times S, V\times T)$-GST at τ.
(2) If G is a graph with (S_1,T_1)-GST at τ and H is a graph with (S_2,T_2)-GST at τ, then $G\Box H$ has $(S_1\times S_2, T_1\times T_2)$-GST at τ.

Example 2.41. We return again to the example that we have already considered: the graph $G = P_3\Box P_2$.



For the purposes of this example, let $\{1,2,3\}$ be the vertex set of P_3, and let $\{1,2\}$ be the vertex set of P_2. We see that P_3 has $(1,3)$-PST at time $\frac{\pi}{\sqrt{2}}$, and that P_2 has $(1,2)$-PST at time $\frac{\pi}{2}$. Thus, from the above corollaries, we can say the following.

(1) The product graph, $P_3\Box P_2$, has $(\{1,2,3\}\times\{1\}, \{1,2,3\}\times\{2\})$-GST at $\frac{\pi}{2}$.
(2) The product graph, $P_3\Box P_2$, has $(\{1\}\times\{1,2\}, \{3\}\times\{1,2\})$-GST at $\frac{\pi}{\sqrt{2}}$.

The instances listed above exhibit group state transfer between vertex sets of equal size. As a result,

(1) Graph $P_3\Box P_2$, has $(\{1,2,3\}\times\{2\}, \{1,2,3\}\times\{1\})$-GST at $\frac{\pi}{2}$, and
(2) Graph $P_3\Box P_2$, has $(\{3\}\times\{1,2\}, \{1\}\times\{1,2\})$-GST at $\frac{\pi}{\sqrt{2}}$.

Furthermore, it is known that P_3 has periodicity on vertex 2 at time $\frac{\pi}{\sqrt{2}}$. As a result, it is known that $P_3\Box P_2$ has fractional revival on $\{2\}\times\{1,2\}$ at time $\frac{\pi}{\sqrt{2}}$.

3. Examples

We have seen that the paths on two and three vertices have perfect state transfer, as well as the cubelike graphs. We then consider further examples of group state transfer, to which we may apply the properties and observations of the previous section.

We first consider the bipartite graphs. Our strategy now is to exploit the underlying structure of a graph to obtain GST. Given matrix B with entries in $\{0,1\}$, the following is the adjacency matrix of a bipartite graph.

$$A = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}.$$

From Godsil [7] we obtain the following under power expansion.

$$U(t) = \begin{pmatrix} \cos\left(t\sqrt{BB^T}\right) & i\sin\left(t\sqrt{BB^T}\right)B \\ i\sin\left(t\sqrt{B^TB}\right)B^T & \cos\left(t\sqrt{B^TB}\right) \end{pmatrix} = \begin{pmatrix} C_1(t) & iK(t) \\ iK^T(t) & C_2(t) \end{pmatrix}.$$

We enumerate three particular cases of GST on a bipartite graph G with adjacency matrix A, that has an S-T bipartition.

(1) Graph G has (S,T)-GST at $t=\tau$ if $C_1(\tau)=0$;
(2) graph G has (T,S)-GST at $t=\tau$ if $C_2(\tau)=0$;
(3) graph G exhibits fractional revival on S and T at time τ.

Consider a matrix B with entries in $\{0,1\}$. We observe that BB^T and B^TB are symmetric, and therefore orthogonally diagonalizable. Thus,

$$BB^T = P^T \begin{pmatrix} \lambda_1^2 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_k^2 \end{pmatrix} P, \qquad \sqrt{BB^T} = P^T \begin{pmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_k \end{pmatrix} P.$$

Example 3.1. Consider the case where $\lambda_1, \cdots \lambda_k$, the eigenvalues of BB^T, are odd integers. Then, the bipartite graph given by

$$A = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}$$

has (S,T)-GST at time $\tau = \pi/2$.

Proof. Let the spectrum of BB^T be given by $n_1^2, \cdots, n_k^2$, where for each j, n_j is an odd integer. We know

$$\sqrt{BB^T} = P^T \begin{pmatrix} n_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & n_k \end{pmatrix} P.$$

Given a matrix, X, we can define a trigonometric function of X as a power series

$$\cos(X) = \sum_{j=0}^{\infty} (-1)^j \frac{X^{2j}}{(2j)!},$$

where $X^0 = I$, the identity matrix. Thus,

$$\cos\left(\frac{\pi}{2}\sqrt{BB^T}\right) = P^T \begin{pmatrix} \cos\left(\frac{\pi}{2}n_1\right) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \cos\left(\frac{\pi}{2}n_k\right) \end{pmatrix} P = \begin{pmatrix} 0 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0 \end{pmatrix} = C_1\left(\frac{\pi}{2}\right).$$

Because $C_1(\pi/2) = 0$, $G(A)$ has (S,T)-GST at $\tau = \pi/2$. ■

Proposition 3.2. *Let G be a bipartite graph with adjacency matrix*

$$A(G) = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix},$$

and let $\lambda_1, \cdots, \lambda_k$ be the eigenvalues of $\sqrt{BB^T}$. Suppose that B is $n \times m$, and that G has partition $\{S, T\}$ where S consists of vertices 1 through n, and T consists of vertices $n+1$ through $n+m$.

- *If $\lambda_1, \cdots, \lambda_k$ are odd integers, then G has (S,T)-GST at $\tau = \pi/2$;*
- *if $\lambda_1, \cdots, \lambda_k$ are even integers, then G exhibits fractional revival on S and T at time $\tau = \frac{\pi}{2}$.*

Remark 3.3. Plainly,

$$U_{P_2}(\tau) = \cos(\tau) I_2 + i\sin(\tau) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

and so P_2 has PST at $\tau = \pi/2$ from endpoint to endpoint. However, this does not carry over into GST at $\tau = \pi/2$ on $C_6 = P_2 \times K_3$. Here, we use the graph tensor product defined as follows. If $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are graphs, then

$$H = G_1 \times G_2 = (V_1 \times V_2, E')$$

is the graph for which, if $(u_1, v_1), (u_2, v_2) \in V_1 \times V_2$, $(u_1, v_1) \sim_H (u_2, v_2)$ if and only if $u_1 \sim_{G_1} u_2$ and $v_1 \sim_{G_2} v_2$. It is known that, if A is the adjacency matrix of G_1 and B is the adjacency matrix of G_2, then the adjacency matrix of $G_1 \times G_2$ is given by $A \otimes B$.

The complete graph K_3 has spectrum $(-1, -1, 2)$ and through power series expansion, we obtain that

$$U_{C_6}(\tau) = I_2 \otimes \cos(A(K_3)\tau) + i \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \sin(A(K_3)\tau).$$

Because the adjacency matrix $A(K_3)$ is orthogonally diagonalizable,

$$\cos(A(K_3)t) = P^T \begin{pmatrix} \cos(t) & 0 & 0 \\ 0 & \cos(t) & 0 \\ 0 & 0 & \cos(2t) \end{pmatrix} P$$

where P is an orthogonal matrix with rows the eigenvectors of $A(K_3)$. At $\tau = \pi/2$ we obtain that

$$\cos(A(K_3)\tau) = P^T \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} P = \frac{-1}{3} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}.$$

Similarly,

$$\sin(A(K_3)\tau) = P^T \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} P = \frac{-1}{3} \begin{pmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix}.$$

We have failed to force any components of $U_{C_6}(\frac{\pi}{2})$ to zero.

The finite grids, $P_j \square P_k$, constitute a family of the bipartite graphs which we will consider for cases of group state transfer. Let $H_{j,k}$ denote the j by k grid $P_j \square P_k$.

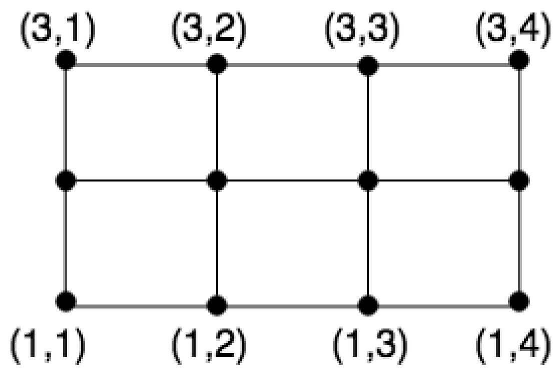
Remark 3.4. Let $U(\tau) = U_{H_{j,k}}(\tau)$ denote the unitary transition operator of the $j \times k$ grid $H_{j,k} = P_j \square P_k$. Let $U_j(\tau)$ denote the unitary transition operator of P_j and let $U_k(\tau)$ denote the unitary transition operator of P_k. Then

$$U(\tau) = U_j(\tau) \otimes U_k(\tau).$$

Remark 3.5. If path P_j has (S,T)-GST at time τ and path P_k has (S',T')-GST at time τ, then the grid $H_{j,k}$ has $(S \times S', T \times T')$-GST at time τ.

These remarks follow directly from the results proven in the previous section. We use the following examples to illustrate these properties of grids.

Example 3.6. Consider the 3×4 grid $H_{3,4} = P_3 \square P_4$. Denote the vertex set of P_3 by $\{1,2,3\}$ and the vertex set of P_4 by $\{1,2,3,4\}$.



By the previous remarks, if $U(\tau) = U_{H_{2,3}}(\tau)$, $U_3(\tau) = U_{P_3}(\tau)$, and $U_4(\tau) = U_{P_4}(\tau)$, then

$$U(\tau) = U_3(\tau) \otimes U_4(\tau).$$

Let $B = U_4(\frac{\pi}{\sqrt{2}})$.

$$U\left(\frac{\pi}{\sqrt{2}}\right) = \begin{pmatrix} 0 & 0 & -B \\ 0 & -B & 0 \\ -B & 0 & 0 \end{pmatrix}$$

is the expression of the unitary transition operator of $H_{3,4}$ in block matrix form, demonstrating the following.

(1) Grid $H_{3,4}$ has $(\{1\} \times \{1,2,3,4\}, \{3\} \times \{1,2,3,4\})$-GST at time $\frac{\pi}{\sqrt{2}}$;
(2) grid $H_{3,4}$ has $(\{3\} \times \{1,2,3,4\}, \{1\} \times \{1,2,3,4\})$-GST at time $\frac{\pi}{\sqrt{2}}$;
(3) grid $H_{3,4}$ has fractional revival on $\{2\} \times \{1,2,3,4\}$ at time $\frac{\pi}{\sqrt{2}}$.

We begin with the first observation. Let $z = (0,0,0,0)$ be the all-zeros column vector of length four. Then, if ψ satisfies $\operatorname{Supp}\psi \subseteq \{1\} \times \{1,2,3,4\}$ then

$$\psi = \begin{pmatrix} \phi \\ z \\ z \end{pmatrix}$$

for some vector ϕ.

$$U\left(\frac{\pi}{\sqrt{2}}\right)\psi = \begin{pmatrix} 0 & 0 & -B \\ 0 & -B & 0 \\ -B & 0 & 0 \end{pmatrix} \psi = \begin{pmatrix} z \\ z \\ -B\phi \end{pmatrix}.$$

As a result, $\operatorname{Supp} U(\frac{\pi}{\sqrt{2}})\psi \subseteq \{3\}\times\{1,2,3,4\}$, demonstrating that $H_{3,4}$ has $(\{1\}\times\{1,2,3,4\}, \{3\}\times\{1,2,3,4\})$-GST at time $\frac{\pi}{\sqrt{2}}$. Because these two vertex sets have equal cardinality, $H_{3,4}$ also has $(\{3\}\times\{1,2,3,4\}, \{1\}\times\{1,2,3,4\})$-GST at time $\frac{\pi}{\sqrt{2}}$. By the fact that

$$U\left(\frac{\pi}{\sqrt{2}}\right)\begin{pmatrix} z \\ \phi \\ z \end{pmatrix} = \begin{pmatrix} 0 & 0 & -B \\ 0 & -B & 0 \\ -B & 0 & 0 \end{pmatrix} \begin{pmatrix} z \\ \phi \\ z \end{pmatrix} = \begin{pmatrix} z \\ -H\phi \\ z \end{pmatrix},$$

fractional revival also easily follows.

4. Further Research and Conclusions

This paper has introduced the notion of group state transfer and has investigated examples of graphs that exhibit group state transfer. Future work will be needed, however, to expand the basis of examples of graphs that exhibit GST, and to explore the applicability of group state transfer to the development of quantum computing algorithms. The topological properties of graphs that exhibit group state transfer must also be examined; it is interesting that quantum walks do not behave consistently on different graphs that are homeomorphic to one another. The paths, for instance, are homeomorphic, but the unweighted paths on two and three vertices exhibit perfect state transfer, while P_k for $k > 3$ does not. In future work, we also intend to develop a notion of generalized strong cospectrality, which may have implications for cases of group state transfer.

In conclusion, we have shown that graphs may be obtained that exhibit GST, but not PST. Group state transfer, then, holds the potential to relax the strong conditions imposed by perfect state transfer, yielding families of examples that are not required to be highly symmetric. Future work will then be required to assess the usefulness of graphs that exhibit group state transfer to quantum computing.

References

[1] Alperin, J. L., Bell, and Rowan B. *Groups and Representations.* Springer, Graduate Texts in Mathematics. 1995.

[2] Bondy, Adrian. Murty, M. Ram. *Graph Theory.* Springer, Graduate Texts in Mathematics. 2008.

[3] Chartrand, Gary. Zhang, Ping. *A First Course in Graph Theory.* Dover, Boston. 2012.

[4] Childs, Andrew. *Universal Computation by Quantum Walk.* Physical Review Letters 102 (18). 2009.

[5] Coutinho, Gabriel, Chan, Ada, Tamon, Christino, Vinet, Luc, Zhan, Hanmeng. *Quantum Fractional Revival on Graphs.* arXiv:1801.09654v1 [quant-ph].

[6] Friedberg, Stephen H., Insel, Arnold J., and Spence, Lawrence E. *Linear Algebra.* 4th ed. Pearson. 2003.

[7] Godsil, Christopher, and Coutinho, Gabriel. *Graph Spectra and Continuous Quantum Walks.*

[8] Godsil, Christopher, and Cheung, Wang-Chi. *Perfect State Transfer in Cubelike Graphs.* Linear Algebra and its Applications, 435(10). Pages 2469-2474. 2011.

[9] Feynman, Richard. *Simulating Physics with Computers.* California Institute of Technology. 1981.

[10] Godsil, Christopher, and Royle, Gordon. *Algebraic Graph Theory.* Springer-Verlag, New York City. 2001.

[11] Kempton, Mark, Lippner, Gabor, and Yau, Shing-Tung. *Perfect State Transfer on Graphs with a Potential*

[12] Lippner, Gabor. Kempton, Mark. Yau, Shing-Tung. *Perfect State Transfer on Graphs with a Potential.* arXiv:1611.02093v2 [math.CO].

[13] Nair, M. Thamban. Singh, Arindama. *Linear Algebra.* ISBN 978-981-13-0925-0. Springer, Singapore. 2018.

[14] Roman, Stevan. *Fundamentals of Group Theory: An Advanced Approach.* Springer, New York City. 2010.

[15] Waltman, Paul. *A Second Course in Elementary Differential Equations.* Dover, Mineola, New York. 2004.