

# Perfect state transfer in quantum walks on graphs

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We provide a brief survey of perfect state transfer in quantum walks on finite graphs. The ability to transfer a quantum state from one part of a quantum computer to another is a key ingredient of scalable architectures. Transfer through structures that do not require locally varying dynamic control simplifies the design and hence reduces the opportunities for errors to arise. Continuous time walks quantum walks on highly structured graphs exhibit perfect state transfer for the complete graph of size 2, the path of length 3, and the cycle of size 4. From these, larger graphs can be constructed, and the use of edge weights widens this set considerably. Discrete-time quantum walks have more flexibility through exploiting the coin degrees of freedom, but with the disadvantage that local control of the coin is required if the degree of the vertices varies. The closely related property of periodicity (exact return to the starting state) is also mentioned.

**Keywords:** quantum walks, quantum computation, quantum transport

## I. INTRODUCTION

Quantum walks on finite graphs provide useful simple models for quantum transport phenomena, and have been applied to spin chains for communication links in quantum computing [1], and exciton transfer in photosynthetic molecules [2, 3]. Transport problems are also known as hitting problems in computer science. Start and end points are specified, and the task is to efficiently travel between them. Hitting between the opposite corners of a hypercube [4, 5], and between the roots of two randomly joined binary trees [6], provided the first exponential computational speed up for algorithms based on quantum walks.

We distinguish three cases, provided by the examples just mentioned: perfect state transfer, highly desirable for quantum communications links; transfer with high fidelity, providing efficient energy or charge transfer for photosynthesis; and hitting probabilities that are at least not exponentially small, so that normal amplification techniques produce an efficient algorithm. One way to achieve approximate state transfer with high fidelity is to add a small amount of decoherence to the otherwise perfectly quantum dynamics. The recent results in the context of photosynthetic molecules all require this to match experimental data. Decoherence effects in quantum walks were reviewed by Kendon [7], while algorithmic use of quantum walks, including the hitting time algorithms, were reviewed by Ambainis [8].

In this paper we focus on the case of perfect state transfer. Recent reviews from the perspective of spin chain engineering have been provided by Bose [9] and Kay [10]. The problem is to find an arrangement of  $n$  interacting qubits in a network which allows perfect transfer of any quantum state over various distances. The network is typically described by a graph where the vertices represent the location of the qubits and the edges represent the pairwise coupling of the qubits. The graph has two special vertices labeled  $a$  and  $b$  which represent the input (source) and output (target) qubits, respectively. In most cases of interest, it is required that perfect state transfer be achieved without dynamic control over the interactions between the qubits. These are the so-called permanently coupled (unmodulated) spin networks. Our approach treats only quantum walk dynamics in the abstract environment of undirected graphs. We also discuss the closely related property of periodicity – exactly returning to the starting point at regular intervals – since perfect state transfer is often obtained from half a cycle of such periodic dynamics.

We begin by providing a summary of the basic graph theory used in this review, followed by a description of continuous- and discrete-time quantum walks on finite graphs. The extra degrees of freedom in the discrete-time quantum walk provided by the coin allow more instances of perfect state transfer to be achieved. Consequently, the problem has been studied in more detail in the continuous-time quantum walk, and we focus on the efforts to characterize the graphs on which perfect state transfer is possible. The continuous-time quantum walk is also more widely applicable as a model for physical and biological systems.

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## II. BASIC GRAPH THEORY

For any logical statement  $\mathcal{S}$ , we use the notation  $\llbracket \mathcal{S} \rrbracket$  to mean 1 if  $\mathcal{S}$  is true and 0 otherwise (see Graham *et al.* [11]). Let  $\mathbb{Z}_n$  denote the additive group of integers  $\{0, \dots, n-1\}$  modulo  $n$ . For a matrix  $A$ , we denote  $A^k$  as the  $k$ -th column of  $A$  and  $A_j$  as the  $j$ -th row of  $A$ . As is standard, we use  $I_n$  and  $J_n$  to denote the  $n \times n$  identity and all-one matrices, respectively; we drop the subscript  $n$  whenever the context is clear. We use  $X, Y, Z$  to denote the Pauli matrices.

The graphs  $G = (V, E)$  which we will study are finite, mostly simple, undirected, regular, and connected. The adjacency matrix  $A_G$  of a graph  $G$  is defined as

$$A_G[u, v] = \llbracket (u, v) \in E \rrbracket = \begin{cases} 1 & \text{if } (u, v) \in E \\ 0 & \text{otherwise} \end{cases} \quad (1)$$

We call a graph  $k$ -regular if each of its vertex has  $k$  adjacent neighbors. In most cases,  $G$  is also vertex-transitive, that is, for any  $a, b \in V$ , there is an automorphism  $\pi$  which maps  $a$  to  $b$ , that is,  $\pi(a) = b$ . A graph is called *integral* if its adjacency matrix has only integer eigenvalues. We use the standard notation  $K_n$  for the complete graph on  $n$  vertices,  $C_n$  for the cycle on  $n$  vertices, and  $P_n$  for the path on  $n$  vertices. Also, we use  $K_{m,n}$  to denote the complete bipartite graph with partitions of sizes  $m$  and  $n$ , respectively.

The complement  $\overline{G}$  of a graph  $G$  is defined on the same set of vertices but with the edge set  $\overline{E} = \{(x, y) : (x, y) \notin E\}$ . The Cartesian product  $G \oplus H$  of graphs  $G$  and  $H$  is a graph whose adjacency matrix is

$$A_{G \oplus H} = I \otimes A_H + A_G \otimes I \quad (2)$$

(see page 617 of Lovász [12]). The *join*  $G + H$  of graphs  $G$  and  $H$  is defined to satisfy  $\overline{G+H} = \overline{G} \cup \overline{H}$ ; that is, we connect all vertices of  $G$  with all vertices of  $H$  (see Schwenk and Wilson [13]). Equivalently, the adjacency matrix of  $G + H$  is given by

$$A_{G+H} = \begin{pmatrix} A_G & J \\ J & A_H \end{pmatrix}, \quad (3)$$

with the appropriate dimensions on the all-one  $J$  matrices.

The  $n$ -dimensional hypercube (or  $n$ -cube for short)  $Q_n$  is defined recursively as

$$Q_1 = K_2, \quad Q_n = K_2 \oplus Q_{n-1} = \begin{pmatrix} Q_{n-1} & I \\ I & Q_{n-1} \end{pmatrix}, \quad \text{for } n \geq 2 \quad (4)$$

with the appropriate dimensions on the identity  $I$  matrices. Similarly, the *Hamming* graph  $H(q, n)$  is defined as  $K_q^{\oplus n}$ , which may be viewed as a  $q$ -ary  $n$ -cube.

A *cone* on a graph  $G$  is the graph  $K_1 + G$ . Similarly, a (dis-)connected *double cone* on a graph  $G$  is the graph  $\overline{K_2} + G$ ,  $K_2 + G$ , respectively. When  $G$  is a complete graph, the connected double-cone is simply another complete graph whereas the disconnected double-cone is a complete graph with a missing edge (see [2, 14]).

A graph  $G$  is called a *circulant* if its adjacency matrix  $A_G$  is a circulant matrix. Recall that a circulant matrix  $A$  is completely specified by its first row, say  $[a_0, a_1, \dots, a_{n-1}]$ , and is defined as  $A[j, k] = a_{k-j \pmod{n}}$ , where  $j, k \in \mathbb{Z}_n$ ; or

$$A = \begin{pmatrix} a_0 & a_1 & \dots & a_{n-1} \\ a_{n-1} & a_0 & \dots & a_{n-2} \\ \vdots & \vdots & \dots & \vdots \\ a_1 & a_2 & \dots & a_0 \end{pmatrix} \quad (5)$$

Note that  $a_0 = 0$ , for simple graphs, and  $a_j = a_{n-j}$ , for undirected graphs. The best known families of circulant graphs include the complete graphs  $K_n$  and cycles  $C_n$ .

Alternatively, a circulant graph  $G = (V, E)$  can be specified by a subset  $S \subseteq \mathbb{Z}_n$ , where  $(j, k) \in E$  if  $k - j \in S$ . Thus,  $S$  defines the set of *edge distances* between adjacent vertices. In this case, we write  $G = \text{Circ}(n, S)$ . We assume that  $S$  is closed under taking inverses: if  $d \in S$ , then  $-d \in S$ . For a divisor  $d$  of  $n$ , let  $G_n(d) = \{k : \gcd(n, k) = d, 1 \leq k < n\}$ . It was proved by So [16] that a circulant  $\text{Circ}(n, S)$  is integral if and only if  $S = \bigcup_{d \in D} G_n(d)$ , for some subset  $D$  of  $D_n$ , where  $D_n = \{d : d|n, 1 \leq d < n\}$  is the set of divisors of  $n$ . That is, a circulant is integral if its edge distances are elements of  $G_n(d)$ ,  $d \in D$ , for some subset  $D \subseteq D_n$ . We denote this family of integral circulants as  $\text{ICG}_n(D)$  (following the notation used by Bašić *et al.* [17]).

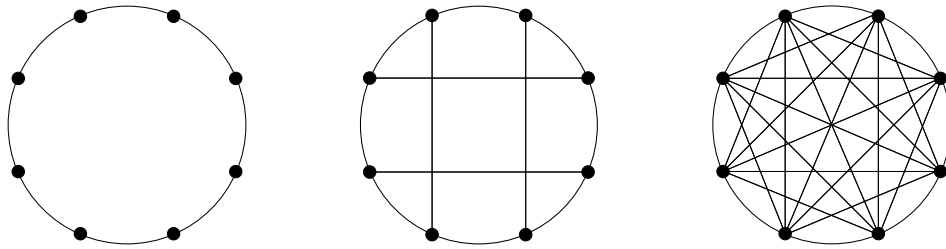


FIG. 1: Examples of circulants of order 8. From left to right: (i) the cycle  $C_8$ . (ii) the 3-dimensional cube  $Q_3$ . (iii) the complete graph  $K_8$ ; (see Angeles-Canul *et al.* [15] for a similar but distinct illustration).

All circulant graphs  $G$  on  $n$  vertices are diagonalizable by the  $n \times n$  Fourier matrix  $F_n$  whose columns  $|F_n^k\rangle$  are defined as  $\langle j|F_n^k\rangle = \omega_n^{jk}/\sqrt{n}$ , where  $\omega_n = \exp(2\pi i/n)$ . In fact, we have  $FAF^\dagger = \sqrt{n} \cdot \text{diag}(FA_0)$ , for any circulant  $A$ , where  $A^0 = A|0\rangle$  is the first column of  $A$ . This shows that the eigenvalues of  $A$  are simply given by

$$\lambda_j = \sum_{k=0}^{n-1} a_{n-k} \omega_n^{jk}. \quad (6)$$

A generalized notion of circulant graphs may be defined using group theory (see Diaconis [18]). Let  $\mathcal{G}$  be a finite group of order  $n$  and  $f : \mathcal{G} \rightarrow \mathbb{C}$  be a complex-valued function over  $\mathcal{G}$ . A  $\mathcal{G}$ -circulant matrix defined by  $f$  is a  $n \times n$  matrix whose rows and columns are indexed by elements of  $\mathcal{G}$ . The  $\mathcal{G}$ -circulant matrix  $\text{Circ}(\mathcal{G}, f)$  defined by  $f$  is given by  $\text{Circ}(\mathcal{G}, f)_{a,b} = f(b \cdot a^{-1})$ , for  $a, b \in \mathcal{G}$ . Our standard circulant matrices (and graphs) defined above are simply the class of  $\mathbb{Z}_n$ -circulants. The generalized  $n$ -cubes considered by Adamczak *et al.* [19] and Bernasconi *et al.* [20] are simply  $\mathbb{Z}_2^n$ -circulants. One may also view the Cayley graph of the symmetric group  $S_n$ , studied in Gerhardt and Watrous [21], as a  $S_n$ -circulant.

For more background on algebraic graph theory, we refer the reader to the monograph by Biggs [22] and to the survey article by Schwenk and Wilson [13].

### III. QUANTUM WALKS ON FINITE GRAPHS

Just as for classical random walks, quantum walks can be defined for both discrete time steps and continuous time evolution. The basic properties of quantum walks have been covered in depth elsewhere (see Kempe [23] for a useful review), here we provide brief definitions to establish notation and properties relevant to this work.

#### A. Continuous-time quantum walk

A *continuous-time quantum walk* on a graph  $G = (V, E)$  is defined using the Schrödinger equation with the real symmetric adjacency matrix  $A_G$  as the Hamiltonian. If  $|\psi(t)\rangle \in \mathbb{C}^{|V|}$  is a time-dependent amplitude vector on the vertices of  $G$ , then the evolution of the quantum walk is given by

$$|\psi(t)\rangle = e^{-itA_G} |\psi(0)\rangle, \quad (7)$$

where  $|\psi(0)\rangle$  is the initial amplitude vector. We usually assume that  $|\psi(0)\rangle$  is a unit vector, with  $\langle x|\psi(0)\rangle = \mathbb{1}[x = a]$ , for some start vertex  $a \in V(G)$ . The amplitude of the quantum walk on vertex  $a$  at time  $t$  is given by  $\psi_a(t) = \langle a|\psi(t)\rangle$ , while the probability of vertex  $a$  at time  $t$  is  $p_a(t) = |\langle a|\psi(t)\rangle|^2$ .

We say  $G$  has *perfect state transfer* from vertex  $a$  to vertex  $b$  at time  $t$  if

$$|\langle b|e^{-itA_G}|a\rangle| = 1, \quad (8)$$

where  $|a\rangle, |b\rangle$  denote the unit vectors corresponding to the vertices  $a$  and  $b$ , respectively. The graph  $G$  has perfect state transfer if there exist vertices  $a$  and  $b$  in  $G$  and a time  $t \in \mathbb{R}^+$  so that Equation (8) holds. We say that  $G$  has *universal perfect state transfer* if (8) occurs between all distinct pairs of vertices  $a$  and  $b$  of  $G$ . We call a graph  $G$  *periodic* if for any state  $|\psi\rangle$ , there is a time  $t$  so that  $|\langle \psi|e^{-itA_G}|\psi\rangle| = 1$ .

## B. Discrete-time quantum walks

In correspondence with discrete-time classical random walks, a *discrete-time quantum walk* has a quantum coin that is “tossed” each time step to determine which direction to move in. The coin is a quantum system of size  $d_{\max}$ , the largest degree of any vertex in the graph. The full quantum system is thus a combination of the position and the coin, we write the basis states as  $|x, c\rangle$  where the first label is the vertex and the second the coin. A general state of a discrete-time quantum walk at time  $t$  can thus be written

$$|\psi(t)\rangle = \sum_{x,c} \alpha_{x,c}(t) |x, c\rangle, \quad (9)$$

where  $\alpha_{x,c}(t) \in \mathbb{C}$ .

The coin is “tossed” by applying a unitary operator, usually designed to ensure that only available paths can be chosen, i.e., based on the degree  $d \leq d_{\max}$  at each vertex. A common choice is the unitary based on the Grover diffusion operator, which has elements  $C_{ij}^{(G)} = 2/d - \delta_{ij}$ . For example, the  $d = 3$  case is

$$\mathbf{C}_3^{(G)} = \frac{1}{3} \begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix}. \quad (10)$$

Except in the  $d = 4$  case, the Grover coin operator is biased, since the incoming direction (corresponding to the diagonal entry) is treated differently from the outgoing directions. However, it is symmetric under interchange of any outgoing coin directions, and is in fact the symmetric unitary operator furthest from the identity [24]. The  $d = 4$  Grover coin operator is unbiased, since all the entries are  $\pm\frac{1}{2}$ ,

$$\mathbf{C}_4^{(G)} = \frac{1}{2} \begin{pmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{pmatrix}. \quad (11)$$

The DFT (discrete Fourier transform) coin operator is unbiased for all  $d$ , but asymmetric in that you cannot interchange the labels on the directions without changing the coin operator: each direction acquires its own phase shift. For  $d = 3$ , it looks like

$$\mathbf{C}_3^{(D)} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 \\ 1 & \omega_3 & \omega_3^2 \\ 1 & \omega_3^2 & \omega_3 \end{pmatrix}, \quad (12)$$

where  $\omega_3 = e^{2i\pi/3}$  and  $\omega_3^2 = e^{-2i\pi/3}$  are the complex cube roots of unity.

A conditional shift operator is then used to move the quantum walker to adjacent vertices. This requires a (classical) mapping between coin states and the ends of the edges to be specified [25, 26].

$$\zeta : \mathbb{Z}_{|V|} \times \mathbb{Z}_d \rightarrow \mathbb{Z}_{|V|} \times \mathbb{Z}_d : (x, c) \mapsto \zeta(x, c) = (y, k), \quad (13)$$

where  $(x, c)$  and  $(y, k)$  label each end of edge  $(x, y)$ . The shift then acts as

$$S|x, c\rangle = |y, k\rangle, \quad (14)$$

which updates the position of the walker and the coin state according to the mapping  $\zeta$  in eq. (13). In other words, the shift operator moves the walker and coin to the vertex  $u$  along edge  $(x, y)$ . We note that, by our stipulation that  $c$  and  $k$  label opposite ends of  $(x, y)$ , it follows that  $S = S^{-1}$ , and is thus unitary as required for quantum evolution.

The sequence of a coin toss and a conditional swap is a transition over the unit time step, which we denote by unitary  $T = SC$ . A walk of  $t$  steps is thus produced by applying  $T$  repeatedly  $t$  times,  $|\psi(t)\rangle = T^t|\psi(0)\rangle$ . We can now define the same useful quantities as for the continuous-time walk. For a walk starting at vertex  $a$ , we generally have the freedom to specify the coin states,

$$|\psi(0)\rangle = \sum_c \alpha_{a,c}(0) |a, c\rangle. \quad (15)$$

The probability of vertex  $a$  is  $p_a(t) = \sum_c |\langle a, c | \psi(t) \rangle|^2$ , i.e., we combine all the coin states at the chosen vertex. The equivalent condition for perfect state transfer is

$$\sum_{c, c_0} |\langle b, c | T^t | a, c_0 \rangle| = 1 \quad (16)$$

where  $c$  are the coin states at vertex  $b$  and  $c_0$  are the chosen initial coin states on vertex  $a$ . In other words, we don't care about the coin states, only that the walker started at vertex  $a$  and arrives at vertex  $b$ .

#### IV. SIMPLE GRAPHS

We start by describing the known results for perfect state transfer using a continuous-time quantum walk on simple graphs, those without self-loops or multiple edges between the same pair of vertices. From the small graphs on which perfect state transfer is achieved, larger graphs which still support perfect state transfer can be constructed.

##### A. Small graphs

It is elementary to verify that  $K_2$ ,  $P_3$  and  $Q_2 = C_4$  all have perfect state transfer between their antipodal vertices. These small graphs exhibit interesting limiting cases as well since it can also be shown (using elementary means) that  $K_3$ ,  $P_4$ , and  $K_4$  do not have perfect state transfer.

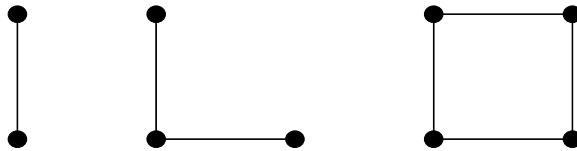


FIG. 2: Small perfect state transfer graphs. From left to right: (a)  $K_2$ ; (b)  $P_3$ ; (c)  $C_4$ .

On  $K_2$ , the continuous-time quantum walk has a time-dependent amplitude vector given by

$$|\psi(t)\rangle = e^{-itA}|0\rangle = \begin{pmatrix} \cos(t) \\ -i \sin(t) \end{pmatrix} \quad (17)$$

which implies  $P(t) = (\cos^2(t) \ \sin^2(t))^T$ . This exhibits perfect state transfer at times  $t = (2\mathbb{Z} + 1)\pi/2$ .

The adjacency matrix of  $P_3$  (a path on three vertices) is given by

$$A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad (18)$$

The eigenvalues of  $A$  are  $\lambda_0 = 0$  and  $\lambda_{\pm} = \pm\sqrt{2}$  with eigenvectors  $|v_0\rangle = \frac{1}{2}(-1 \ 0 \ 1)^T$ , and  $|v_{\pm}\rangle = \frac{1}{2}(1 \ \pm\sqrt{2} \ 1)^T$ . Thus, a continuous-time quantum walk on  $P_3$  has a time-dependent amplitude vector given by

$$|\psi(t)\rangle = e^{-itA}|0\rangle = \frac{-1}{\sqrt{2}}|v_0\rangle + \frac{1}{2} \sum_{\pm} e^{\mp it\sqrt{2}} |v_{\pm}\rangle = \frac{1}{2} \begin{pmatrix} (1 + \cos(\sqrt{2}t)) \\ -i\sqrt{2} \sin(\sqrt{2}t) \\ \cos(\sqrt{2}t) - 1 \end{pmatrix} \quad (19)$$

Thus, the instantaneous probability distribution at time  $t$  is:

$$p_0(t) = (1 - 2\Gamma)^2, \quad p_1(t) = 4\Gamma(1 - \Gamma\Delta^2), \quad p_2(t) = (2\Gamma)^2, \quad (20)$$

where  $\Gamma = \sin^2(t/\sqrt{2})/2$ . Combining the first and third expressions, we get  $\sqrt{p_2(t)} = 1 - \sqrt{p_0(t)}$ , which shows that  $t$  can be chosen so that any probability distribution on the three vertices is reached. This implies that  $P_3$  has (end-to-end) perfect state transfer.

The argument for  $C_4$  is similar to  $K_2$  by viewing it as a hypercube (treated in detail in section IV C).

## B. Cliques and joins

It is easy to show that  $K_n$ , for  $n \geq 3$ , does not have perfect state transfer. But, Bose *et al.* [14] found an interesting way to create perfect state transfer in  $K_n$  between a pair of vertices  $a$  and  $b$ : simply remove the edge between  $a$  and  $b$ . This result was stated in the XYZ (Laplacian) interaction model. For the XY (adjacency) model, this observation was generalized using graph joins in Angeles-Canul *et al.* [15, 27]. Note that  $\overline{K_n}$ , for  $n \geq 3$ , is simply the graph join of  $K_2$  and  $K_{n-2}$ . More specifically, Bose *et al.* [14] studied the graph join of  $\overline{K_2}$  and  $\overline{K_{n-2}}$ . A natural question which arises here is what properties of a regular graph  $G$  do we need so that the joins  $\{K_2, \overline{K_2}\} + G$  has perfect state transfer. This was studied in [15] where precise conditions on  $G$  were given so that the join graph has perfect state transfer. For a prime  $p$ , we denote  $S_p(n)$  to be the largest non-negative integer  $j$  so that  $p^j$  divides  $n$ .

**Theorem 1** (Angeles-Canul *et al.* [15]) *Let  $G$  be a  $k$ -regular graph on  $n$  vertices.*

1. *Let  $\Delta = \sqrt{k^2 + 8n}$ . Then,  $\overline{K_2} + G$  has perfect state transfer between the two (non-adjacent) vertices of  $\overline{K_2}$  if  $\Delta$  is an integer and  $k, \Delta \equiv 0 \pmod{4}$  with  $S_2(k) \neq S_2(\Delta)$ ,*
2. *Let  $\kappa = k - 1$  and  $\Delta = \sqrt{\kappa^2 + 8n}$ . Then,  $K_2 + G$  has perfect state transfer between the two (adjacent) vertices of  $K_2$  if  $\Delta$  is an integer and  $\kappa, \Delta \equiv 0 \pmod{8}$ .*

Using  $k \equiv 0 \pmod{4}$ ,  $n = k + 2$ ,  $\Delta = k + 4$  satisfy the conditions of Theorem 1, and thus the graph  $\mathcal{G} = \overline{K_2} + G$  has perfect state transfer. In this case,  $\mathcal{G}$  can be represented by a type of circulant graph called a *hyperoctahedral*, or *cocktail-party*, graph (see Biggs [22] and Figure 3). These graphs are formed by removing  $n/2 + 1$  disjoint edges from  $K_{n+2}$ . This class of graphs, also known as *cross polytope* graphs, was studied earlier by Tsomokos *et al.* [3].

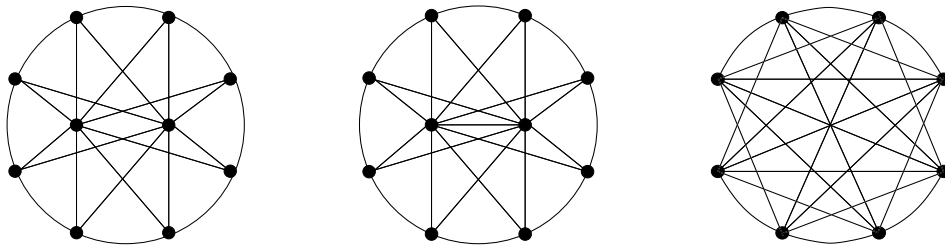


FIG. 3: Double Cones. From left to right: (a)  $\overline{K_2} + C_8$ ; (b)  $K_2 + C_8$ ; (c) Cocktail Party graph; (see Angeles-Canul *et al.* [15] for a similar but distinct illustration).

Godsil [28] (Section 10, question (b)) asked if there is a construction for an infinite family of non-periodic graphs with the perfect state transfer property. We describe a construction of such a family using Theorem 1.

**Corollary 2** (Angeles-Canul *et al.* [15]) *For  $\ell \geq 2$ ,  $\overline{K_2} + (C_{2(2\ell-1)} \oplus C_{2\ell+1})$  is a non-periodic graph which has perfect state transfer.*

*Proof* Let  $G = C_{2(2\ell-1)} \oplus C_{2\ell+1}$ , for  $\ell \geq 2$ . Note that  $G$  is a  $k$ -regular graph with  $k = 4$  and  $n = 2(4\ell^2 - 1)$  vertices. Using the notation of Theorem 1, we have  $\Delta = \sqrt{k^2 + 8n} = 8\ell$ . The eigenvalues of  $G$  are given by the sum of the eigenvalues of the two cycles:

$$\lambda(G) = \lambda(C_{2(2\ell-1)}) + \lambda(C_{2\ell+1}). \quad (21)$$

Recall that the eigenvalues of an  $n$ -cycle are given by  $2 \cos(2\pi k/n)$ , for  $k = 0, \dots, n-1$ . So, each cycle has 2 (its degree) as its largest eigenvalue. Thus, the sums of the cycle eigenvalues contain both integers and irrational numbers. For  $n = 5$  and  $n \geq 7$ , at least some of these values are irrational. This is because the only rational values of  $\cos((a/b)\pi)$ , for  $a, b \in \mathbb{Z}$ , are  $\{0, \pm 1/2, \pm 1\}$  (see Corollary 3.12 in Niven [29]). Note that  $2(2\ell - 1) \geq 5$  and  $2\ell + 1 \geq 5$  hold for  $\ell \geq 2$ , and that both expressions cannot equal 6.

The eigenvalues of  $\mathcal{G} = \overline{K_2} + G$  will then be all of the eigenvalues of  $G$  (except for 4), 0, and  $\lambda_{\pm} = \frac{1}{2}(4 \pm 8\ell) = 2 \pm 4\ell$  (by the proof of Theorem 1). This means that  $\mathcal{G}$  has a mixture of integral and irrational eigenvalues. By Lemma 4.1 in Godsil [28], this implies that the graph  $\mathcal{G}$  is non-periodic. Since  $\Delta = 8\ell$  is an integer and  $S_2(k) \neq S_2(\Delta)$ , Theorem 1 shows that  $\mathcal{G}$  has perfect state transfer.  $\square$



Taking  $\ell = 2$  in Corollary 2, we get  $\mathcal{G} = \overline{K}_2 + C_5 \oplus C_6$ . Again by Lemma 4.1 in Godsil [28],  $\mathcal{G}$  is non-periodic since its eigenvalues contain both integers and irrational numbers. By Corollary 2, we know it has perfect state transfer although it violates the *eigenvalue ratio* condition (see Saxena *et al.* [30] and Godsil [28])

$$\frac{\lambda_k - \lambda_\ell}{\lambda_r - \lambda_s} \in \mathbb{Q}, \quad (22)$$

for  $\lambda_r \neq \lambda_s$ . This is in contrast to Theorem 2.1 of Godsil [28] and to the mirror-symmetric networks of in Christandl *et al.* [31] (see Section III). The double-cone construction in Corollary 2 is mirror-symmetric with respect to the two vertices of  $\overline{K}_2$ .

### C. Hypercubes

In contrast to  $K_2$ , the 4-cycle  $C_4$  is not a limiting case. Christandl *et al.* [32] showed that the  $n$ -cube  $Q_n$  has perfect state transfer, for any  $n$ . This includes  $K_2 = Q_1$ , and  $C_4 = Q_2$ , the two-dimensional binary hypercube. This property of the  $n$ -cube also follows from the proof of a uniform mixing theorem due to Moore and Russell [24]. The Moore-Russell theorem essentially shows that  $Q_n$  behaves like  $n$  highly synchronized but independent copies of  $K_2$ . In fact, for regular graphs  $G$  and  $H$ , the adjacency matrix of  $G \oplus H$  is a sum of commuting terms  $I \otimes H$  and  $G \otimes I$ . Thus,

$$|\psi_{G \oplus H}(t)\rangle = e^{-it(G \oplus H)}|g_0, h_0\rangle \quad (23)$$

$$= e^{-it(I \otimes H)} e^{-it(G \otimes I)}(|g_0\rangle \otimes |h_0\rangle) \quad (24)$$

$$= (e^{-itG}|g_0\rangle) \otimes (e^{-itH}|h_0\rangle) \quad (25)$$

$$= |\psi_G(t)\rangle \otimes |\psi_H(t)\rangle, \quad (26)$$

where we have used  $\exp(I \otimes A) = I \otimes \exp(A)$ . This implies that  $G \oplus H$  is uniform mixing at time  $t^*$  if and only if both  $G$  and  $H$  are uniform mixing at time  $t^*$ . We can recursively apply the above observation to  $n$  copies of  $K_2$  and obtain the seminal theorem of Moore and Russell. Perfect state transfer between the all-zero and the all-one vertices, also follows immediately from this.

**Theorem 3** (Moore and Russell [24]) *For any  $n \geq 0$ , we have  $|\psi_{Q_n}(t)\rangle = |\psi_{K_2}(t)\rangle^{\otimes n}$ . Moreover,  $|\psi_{Q_n}(t)\rangle|0\rangle^{\otimes n} = \cos^n(t)$ , which implies that at  $t^* = (2\mathbb{Z} + 1)\pi/4$ , we have uniform mixing.*

Generalizing this observation further, Bernasconi *et al.* [20] completely characterized the  $\mathbb{Z}_2^n$ -circulant graphs (see Diaconis [18]) by proving that they all have antipodal perfect state transfer at times that are multiples of  $\pi/2$ . The proof utilizes Fourier analysis over the Abelian group  $\mathbb{Z}_2^n$ .

### D. Closure graph operators

It is natural to study operators which can preserve perfect state transfer on graphs. Two most natural ones are the Cartesian product  $G \oplus H$  and the join  $G + H$  of graphs  $G$  and  $H$ . The following theorem is a natural generalization of an observation made by Christandl *et al.* [32] on  $K_2^{\oplus n}$  and  $P_3^{\oplus n}$  and of Theorem 3. It is a closure theorem for the Cartesian product and join operators on graphs.

**Theorem 4** (Angeles-Canul *et al.* [15]) *We have the following results:*

1. The graphs  $G_j$ , where  $1 \leq j \leq m$ , have perfect state transfer from  $a_j$  to  $b_j$  at time  $t^*$  if and only if  $\mathcal{G} = \bigoplus_{j=1}^m G_j$  has perfect state transfer from  $(a_1, \dots, a_m)$  to  $(b_1, \dots, b_m)$  at time  $t^*$ .
2. Let  $G$  be an  $n$ -vertex regular graph with perfect state transfer between vertex  $a$  and  $b$ . For  $m \geq 1$ , the  $m$ -fold self-join  $G^{+m}$  has perfect state transfer between vertices  $a$  and  $b$  (in the same copy of  $G$ ) provided  $\Delta = 0$ , where

$$\Delta = (mn)^{-1} \left( (m-1)(e^{itn} - 1) + e^{-it(m-1)n} - 1 \right) \langle 1_n | e^{-itA_G} | a \rangle. \quad (27)$$

where  $A_G$  is the adjacency matrix of  $G$  and  $|1_n\rangle$  is the all-one column vector of length  $n$ .

The proof of the above theorem relied in showing that  $\langle 0, b | e^{-itA_{\hat{G}}} | 0, a \rangle = \langle b | e^{-itA_G} | a \rangle + \Delta$ , where  $\hat{G} = G^{(+m)}$ , the  $m$ -fold self-join of  $G$ . Since the expression  $\langle 1_n | e^{-itA_G} | a \rangle$  is related to a uniform mixing requirement on  $G$ , this connects a perfect state transfer property to a non-uniform mixing property.

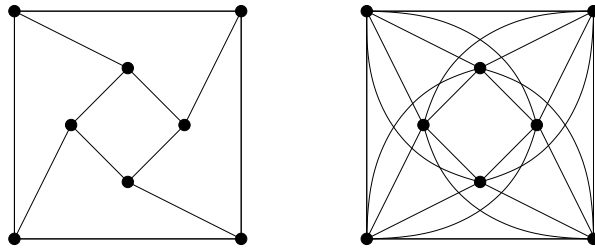


FIG. 4: Standard circulant joins on  $C_4$ . From left to right: (a) Cartesian bunkbed  $C_4 +_I C_4$ ; (b) Self-join  $C_4 +_J C_4$ ; (see Angeles-Canul *et al.* [15] for a similar but distinct illustration).

## V. PERIODICITY IN INTEGRAL CIRCULANTS

Saxena *et al.* [30] initiated the study of periodic quantum dynamics on circulant graphs. This is akin to a recurrent behavior of classical random walks on graphs. To achieve periodic behavior, they proved that the integrality of the graph spectrum is a necessary and sufficient condition. Perfect state transfer is a property which implies periodicity. Note that if the quantum walk achieves a perfect state transfer from  $a$  to  $b$  at time  $t^*$ , then it is periodic for  $a$  in time  $2t^*$ . Bašić *et al.* [17, 33] proved the following powerful results on perfect state transfer in integral circulants.

**Theorem 5** (Bašić *et al.* [17, 33]) *The following results hold:*

1. Integral circulants with odd order have no perfect state transfer.
2. The only integral circulants in  $\text{ICG}_n(\{1\})$  with perfect state transfer are  $K_2$  and  $C_4$ .
3. The integral circulants  $\text{ICG}_n(\{1, n/4\})$  and  $\text{ICG}_n(\{1, n/2\})$ , for  $n$  divisible by 8, have perfect state transfer.

In this class of integral circulants, we have an example of graphs with perfect state transfer between non-antipodal vertices. This answers a question posed by Godsil [28], since prior to this, most examples exhibit perfect state transfer only between antipodal vertices.

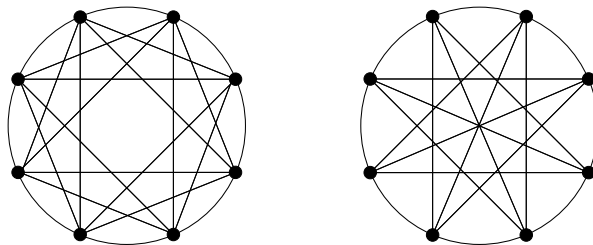


FIG. 5: Integral circulants with perfect state transfer. From left to right: (a)  $\text{ICG}_8(\{1, 2\})$ ; (b)  $\text{ICG}_8(\{1, 4\})$ . Perfect state transfer occurs from  $x$  to  $x + 4$  at time  $\pi/2$  in both graphs (see [33]); (see Angeles-Canul *et al.* [15] for a similar but distinct illustration).

Angeles-Canul *et al.* [15] described new constructions of perfect state transfer integral circulants. This is achieved by using a new graph operator which preserves perfect state transfer as well as the circulant property of the graph inputs. For a  $n$ -vertex graph  $G$  and a  $n \times n$  Boolean matrix  $C$ , define the *circulant join*  $\mathcal{G} = G +_C G$  as a graph whose adjacency matrix is

$$A_{\mathcal{G}} = \begin{pmatrix} A_G & C \\ C^T & A_G \end{pmatrix}. \quad (28)$$

That is, we take two copies of  $G$  and connect vertices from the corresponding copies using the matrix  $C$ . Here, we do not require that  $C$  be the adjacency matrix of a graph. This operation interpolates between the standard join  $G + G$



and the bunkbed (hypercube) operator  $K_2 \oplus G$ . The Cartesian product  $K_2 \oplus G$  is recovered by taking  $C = I$ , and the standard join  $G + G$  (where all edges between vertices from the distinct copies of  $G$  are present) by taking  $C = J$  (the all-one matrix).

The next theorem shows that if  $G$  has perfect state transfer at time  $t^*$ , then so does  $G +_c G$  at time  $t^*$  provided  $\cos(t^* \sqrt{C^T C}) = \pm I$ . Moreover,  $G +_c G$  is a circulant graph whenever  $C$  is a palindrome circulant; that is, the sequence which defines  $C$  is a palindrome. This yields a construction of new families of circulants with perfect state transfer, namely,  $\text{ICG}_n(\{2, n/2^b\} \cup Q)$ ,  $b \in \{1, 2\}$ , where  $n$  is divisible by 16 and  $Q$  is a subset of the odd divisors of  $n$ . For these constructions where there are two copies of a graph  $G$  involved, if  $u$  is a vertex of  $G$ , then we denote  $(u, 0)$  as vertex  $u$  in the first copy of  $G$  and  $(u, 1)$  as vertex  $u$  in the second copy of  $G$ .

**Theorem 6** (Angeles-Canul *et al.* [15]) *Let  $C$  be a  $n \times n$  circulant matrix. If  $G$  is a  $n$ -vertex circulant graph with perfect state transfer from  $a$  to  $b$  at time  $t^*$ , then the circulant join  $G +_c G$  has perfect state transfer from vertex  $(a, 0)$  to vertex  $(b, s)$ ,  $s \in \{0, 1\}$ , at time  $t^*$  provided that*

$$\left[ \cos(t^* \sqrt{B}) \right]^{1-s} \left[ \sin(t^* \sqrt{B}) B^{-1/2} C^T \right]^s = \pm I \quad (29)$$

where  $B = C^T C$ , and  $B^{-1}$  exists whenever  $s = 1$ . Moreover,  $G +_c G$  is a circulant graph if  $C$  is a palindrome circulant matrix, where  $c_j = c_{n-1-j}$ , for  $j = 0, \dots, n-1$ .

For  $n = 2^u$ , where  $u \geq 3$ , the only Boolean circulant matrices  $C$  that yield a circulant graph  $G +_c G$ , for an  $n$ -vertex  $G$ , are the trivial matrices, namely,  $C \in \{I_n, J_n, O_n\}$ , where  $O_n$  is the  $n \times n$  all-zero matrix. The next theorem shows that for  $n$  that is a multiple of 8, if  $n$  has a non-trivial odd divisor, then there exist integral circulant graphs  $\text{ICG}_{2n}(D)$ , for  $|D| \geq 3$ , with perfect state transfer which are obtained from non-trivial circulant joins. This generalizes the integral circulants found by Bašić *et al.* [17, 33].

**Theorem 7** (Angeles-Canul *et al.* [15]) *Let  $n = 2^u m$ , where  $u \geq 3$  and  $m \geq 3$  is an odd number. Suppose that  $G = \text{ICG}_n(D)$ , for  $D = \{1, n/4\}$  or  $D = \{1, n/2\}$ . For any subset  $Q \subset \overline{D}_m$ , there is a Boolean circulant matrix  $C \notin \{I_n, J_n, O_n\}$  so that*

$$G +_c G = \text{ICG}_{2n}(2D \cup Q) \quad (30)$$

has perfect state transfer from 0 to  $n/2$  in  $G$  at time  $t^* = \pi/2$ ,

Recently, Bašić and Petković [34] extended their work to integral circulants whose order are non-square-free.

## VI. PATHS AND WEIGHTS

Another limiting behavior was given by  $P_3$ . Christandl *et al.* [32] showed that  $P_n$  with  $n \geq 4$  has no perfect state transfer between the antipodal vertices (endpoints). But, Christandl *et al.* [31] then showed that a hypercubic weighting scheme applied to the edges of  $P_n$  yields antipodal perfect state transfer (see Figure 6). This is essentially a projection of the  $n$ -cube onto the path on  $n$  vertices. It is unclear if this weighting scheme for  $P_n$  is unique, but it underscores the (potential) positive role of edge weights to achieve perfect state transfer.

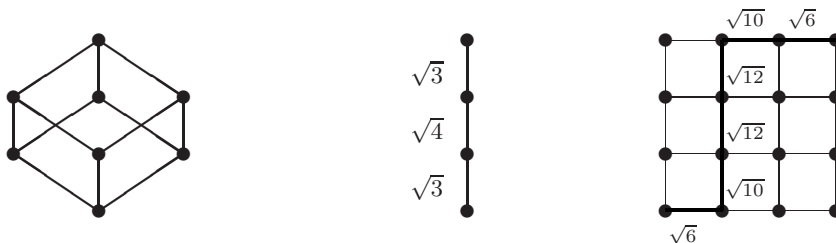


FIG. 6: Universal *near*-perfect state transfer on any weighted graph. (a)  $Q_n$  has vertex-to-vertex PST (Bernasconi *et al.* [20]) (b) Hypercubic-weighted  $P_n$  has antipodal PST (Christandl *et al.* [32]) (c) Hypercubic weighting of any path between source and target; (see Angeles-Canul *et al.* [27] for a similar but distinct illustration).

Here, we consider edge-weighted graphs  $\tilde{G} = (V, E, \omega)$ , where  $\omega : E \rightarrow \mathbb{R}$  is a map assigning weights to edges. In the simplest case, we start with an unweighted graph  $G = (V, E)$  and add self-loops with weight  $\alpha$  to all vertices and assign a weight of  $\beta$  to all edges; we denote such a graph by  $\tilde{G}(\alpha, \beta)$ . The adjacency matrix of  $\tilde{G}$  is  $\alpha I + \beta A_G$ .

On the role of weights for perfect state transfer, Casaccino *et al.* [2] made the following interesting observation. Although  $K_n$  does not have perfect state transfer (between any two vertices due to vertex transitivity), it has perfect state transfer between a pair of vertices if the two vertices are given self-loops with a certain weighting. We describe this idea by looking at an explicit example involving  $K_3$ .

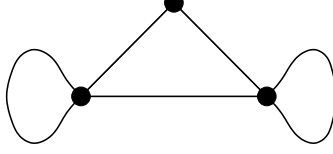


FIG. 7: Perfect state transfer on  $K_3$  with weights and self-loops; no perfect state transfer otherwise.

The eigenvalues of  $K_3$  are 2 (simple) and  $-1$  (with multiplicity two) with eigenvectors  $|F_k\rangle$ , where  $|F_k\rangle$  are the columns of the Fourier matrix, with  $\langle j|F_k\rangle = \omega_3^{jk}/\sqrt{3}$ , for  $j, k \in \{0, 1, 2\}$  (see Biggs [22]). The quantum walk on  $K_3$  yields

$$\langle 1|e^{-itK_3}|0\rangle = \langle 1|\left\{\sum_{k=0}^2 e^{-it\lambda_k}|F_k\rangle\langle F_k|\right\}|0\rangle = -\frac{2}{3}ie^{-it/2}\sin(3t/2). \quad (31)$$

So, it is clear that there is no perfect state transfer on  $K_3$ . We add self-loops on the first two vertices (say, vertex 0 and vertex 1) with weight  $\mu$  and a edge weight of  $\eta$  between them. The adjacency matrix of  $\tilde{K}_3$  is given by

$$\tilde{K}_3 = \begin{pmatrix} \mu & \eta & 1 \\ \eta & \mu & 1 \\ 1 & 1 & 0 \end{pmatrix} \quad (32)$$

with eigenvalues  $\lambda_0 = \mu - \eta$  and  $\lambda_{\pm} = 2\alpha_{\pm}$ , where  $\alpha_{\pm} = \frac{1}{4}(\delta \pm \Delta)$ ,  $\delta = \mu + \eta$  and  $\Delta = \sqrt{\delta^2 + 8}$ . The corresponding (unnormalized) orthogonal eigenvectors are  $|v_0\rangle = (1 \ -1 \ 0)^T$  and  $|v_{\pm}\rangle = (\alpha_{\pm} \ \alpha_{\pm} \ 1)^T$ . The perfect state transfer between the first two vertices are given by

$$\langle 1|e^{-it\tilde{K}_3}|0\rangle = \langle 1|e^{-it\tilde{K}_2}|0\rangle + \frac{1}{2}e^{-it\delta} \left\{ e^{it\delta/2} \left[ \cos\left(\frac{\Delta}{2}t\right) - i\frac{\delta}{\Delta}\sin\left(\frac{\Delta}{2}t\right) \right] - 1 \right\}, \quad (33)$$

where  $\tilde{K}_2$  is  $\tilde{K}_2(\mu, \eta)$ . This is reminiscent of Theorem 4. Since on  $K_2$  we have  $\langle 1|e^{-itK_2}|0\rangle = -i\sin(t)$ , the weighted  $\tilde{K}_2$  has perfect state transfer at time  $t^* = (2\mathbb{Z} + 1)\pi/2\eta$  (since  $\mu$  becomes an irrelevant phase factor and  $\eta$  translates into a time-scaling).

So, for perfect state transfer, it suffices to require  $\cos(\delta\pi/4\eta)\cos(\Delta\pi/4\eta) = 1$ . Equivalently, it suffices to have the following three conditions:

- $A = \delta/4\eta$  be an integer;
- $B = \Delta/4\eta$  be an integer; and
- $A \equiv B \pmod{2}$  or that  $A$  and  $B$  have the same parity.

From the first two conditions, we require that  $\delta/\Delta$  be a rational number  $p/q < 1$  with  $\gcd(p, q) = 1$ . After simplifications, we obtain  $\delta = p/\Gamma$  and  $\Delta = q/\Gamma$ , where  $\Gamma = \sqrt{(q^2 - p^2)/8}$ . So, choose  $\eta = 1/4\Gamma$  so that both  $\delta/4\eta$  and  $\Delta/4\eta$  are integers. That is, choose odd integers  $p$  and  $q$  satisfying  $\gcd(p, q) = 1$ ; this satisfies all three conditions above. Thus, there are infinitely many weights  $\mu$  and  $\eta$  (through choices of odd integers  $p$  and  $q$ ) which allow perfect state transfer on  $\tilde{K}_3$ .

The above analysis shows that edge weights are sufficient for perfect state transfer, complementing results of Casaccino *et al.* [2] for self-loop weights on  $K_n$ . This analysis is generalized to an arbitrary join of two regular graphs in the following theorem.

**Theorem 8** (Angeles-Canul *et al.* [27]) For  $j \in \{1, 2\}$ , let  $\tilde{G}_j(\mu_j, \eta_j)$  be a  $k_j$ -regular graph on  $n_j$  vertices, where each vertex has a self-loop with weight  $\mu_j$  and each edge has weight  $\eta_j$ . Also, for  $j \in \{1, 2\}$ , let  $\kappa_j = \mu_j + \eta_j k_j$ . Suppose that  $a$  and  $b$  are two vertices in  $\tilde{G}_1$ . Let  $\mathcal{G} = \tilde{G}_1(\mu_1, \eta_1) + \tilde{G}_2(\mu_2, \eta_2)$  be the join of the weighted graphs. Then,

$$\langle b | e^{-itA_{\mathcal{G}}} | a \rangle = \langle b | e^{-itA_{\tilde{G}_1}} | a \rangle + \frac{e^{-it\kappa_1}}{n_1} \left\{ e^{it\delta/2} \left[ \cos\left(\frac{\Delta t}{2}\right) - i \left(\frac{\delta}{\Delta}\right) \sin\left(\frac{\Delta t}{2}\right) \right] - 1 \right\} \quad (34)$$

where  $\delta = \kappa_1 - \kappa_2$  and  $\Delta = \sqrt{\delta^2 + 4n_1 n_2}$ .

As a corollary of Theorem 8, we can analyze perfect state transfer in a weighted double-cone on any regular graph. Here we consider weighting both components of the cone using a set of uniform weightings. The following corollary is a generalization of a similar result observed by Casaccino *et al.* [2].

**Corollary 9** (Angeles-Canul *et al.* [27]) For any  $k$ -regular graph  $G$  on  $n$  vertices and any  $b \in \{0, 1\}$ , there exist weights  $\mu, \eta \in \mathbb{R}^+$  so that the double-cone  $\tilde{K}_2^b(\mu, \eta) + G$  has perfect state transfer between the two vertices of  $\tilde{K}_2^b$ .

Given that weighting the source and target vertices is useful for perfect state transfer in the complete graph (or in a join with any regular graph), it is natural to ask if this scheme works also in other settings. Casaccino *et al.* [2] made the following interesting conjecture on the role of weighted self-loops on paths (their conjecture was supported by numerical experiments).

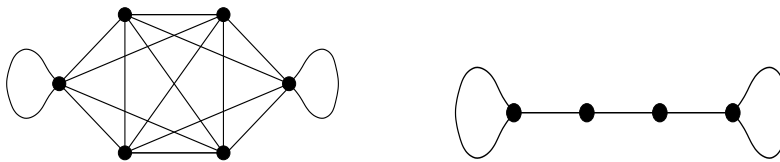


FIG. 8: (a) Complete graph minus an edge: perfect state transfer (between disconnected vertices) exists with weighted self-loops (b) Perfect state transfer conjecture on  $n$ -path with weighted self-loops. See Casaccino *et al.* [2].

**Conjecture 10** (Path teleportation) Let  $\tilde{P}_n(\alpha)$  be a path on  $n$  vertices where its two endpoint vertices are given self-loops with weight  $\alpha$ . For any  $n$ , there is a choice of  $\alpha$  so that  $\tilde{P}_n(\alpha)$  has antipodal perfect state transfer.

## VII. DISCRETE-TIME WALKS

The equivalent properties for discrete-time quantum walks are less well studied, in part because analytical methods are more involved due to the coin degrees of freedom and discrete nature of the dynamics. Results for the continuous-time walk rarely carry over to the discrete time walk for perfect state transfer, even the hypercube, which admits the same solution method [24], does not exhibit perfect state transfer for the discrete-time walk. Notable work has been done by Krovi and Brun [35] to characterize the opposite to perfect state transfer, the conditions under which hitting times become infinite, i.e., no transfer occurs at all. The continuous-time equivalent of this in disordered systems was first described by Anderson [36] and is by now well known. Their work emphasizes the importance of symmetry for obtaining nice properties such as perfect state transfer or fast mixing with quantum walks.

The scattering theory methods developed by Feldman and Hillery [37, 38] also provide a powerful analytical tools for analyzing discrete-time quantum walks on graphs. Two tails are attached to the starting and ending states, the quantum walk sent in on the incoming tail, and the time taken for it to emerge on the outgoing tail determined. They provide a method for combining graphs, but although the method is obviously highly suited to state transfer calculations, it has not been used for this purpose to date.

Perfect state transfer for discrete-time walks has been recently studied by Lovett *et al.* [39], where the goal was to provide a “wire” structure on which a discrete-time walk would propagate deterministically. This can be achieved on a path  $P_n$ , using either a Pauli  $X$  coin operator, or the identity (depending on how the edges are labeled). This is a somewhat trivial solution that does not allow the wire to be connected to vertices of greater degree without some reflection occurring.

Less trivially, on structures with vertices of even degree, perfect state transfer occurs when half the edges are joined with each neighbor, to form structures like that shown in figure 9. In contrast to most of the graphs studied for the

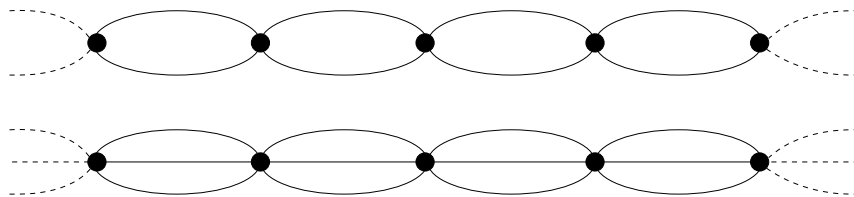
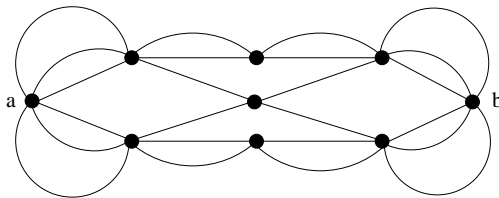


FIG. 9: Chains formed from vertices of degree 4 and degree 6.

continuous-time quantum walk, these are not simple graphs, the multiple edges between pairs of nodes are necessary to achieve perfect state transfer. The coin operator used at each vertex is the Grover coin operator. The chain can be terminated by vertices of half the degree, provided the initial coin state and coin operator are suitably chosen to distribute the amplitude equally over all vertices. It is easily seen that

$$C_d^{(G)} \begin{pmatrix} \alpha \\ \vdots \\ \alpha \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{2}{d} - 1 & \frac{2}{d} & \cdots & \frac{2}{d} \\ \frac{2}{d} & \frac{2}{d} - 1 & \cdots & \frac{2}{d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{2}{d} & \frac{2}{d} & \cdots & \frac{2}{d} - 1 \end{pmatrix} \begin{pmatrix} \alpha \\ \vdots \\ \alpha \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \alpha \\ \vdots \\ \alpha \end{pmatrix}. \quad (35)$$

It is now possible to join these wires together, e.g., four of the wires in the top example in fig. 9 can converge at a vertex of degree 8, provided two of the wires are “incoming” and two are “outgoing” in the propagation of the quantum walk. From this, it is possible to construct many graphs on which the discrete-time walk can exhibit perfect

FIG. 10: Graph with perfect state transfer between vertices  $a$  and  $b$ , formed by combining chain units to preserve equal amplitude on each edge.

state transfer, a simple example is given in fig. 10. The coin degree of freedom allows more possibilities than for the continuous-time walk. However, they have not been succinctly characterized, not even for this method using the Grover coin operator.

### VIII. PERIODICITY IN CYCLES

Perfect state transfer often occurs half way through a periodic cycle, as with the examples already give in section V for integral circulants with the continuous-time walk. The first explicit mention of periodic behaviour in discrete-time quantum walks was by Travaglione and Milburn [40], who noted that the discrete-time quantum walk is exactly periodic on  $C_4$ . Tregenna *et al.* [41] then found numerically that (for suitable choices of coin parameters)  $C_2$  has period 2,  $C_3$  period 12,  $C_4$  period 8,  $C_5$  period 60,  $C_6$  period 12,  $C_8$  period 24, and  $C_{10}$  period 60, see table I. It is known from these numerical results that, for half the period the even cycles up to  $C_{10}$  provide perfect state transfer between opposite pairs of vertices, and for cycles divisible by four, perfect instantaneous mixing at a quarter of the period.

Following Tregenna *et al.* [41], the condition for periodicity in cycles can be derived analytically. The discrete-time quantum walk on a cycle has been solved exactly [42], by transforming into the Fourier basis of the position  $x \in \mathbb{Z}_n$ .

TABLE I: Known periods in a walk on a cycle. Coin phase  $\delta = 0$  unless specified.

$n$	period	$\Omega$ bias in coin $\rho$
2	2	$\frac{1}{2}$
3	12	$\frac{1}{3}, \delta = \frac{\pi}{3}$
4	8	$\frac{1}{2}$
5	60	$\left(\frac{\sin(\pi/6)}{\sin(\pi/5)}\right)^2, \delta = \frac{3\pi}{5}$
6	12	$\frac{1}{3}$
8	24	$\frac{1}{2}$
10	60	$\left(\frac{\sin(\pi/6)}{\sin(\pi/5)}\right)^2 \simeq 0.7236$
16	<i>chaotic</i>	$\frac{1}{2}$

The finite state space of the particle gives rises to a discrete, finite momentum space defined by

$$|\tilde{\psi}_n(k, t)\rangle = \frac{1}{\sqrt{n}} \sum_{x=0}^n |\psi_n(x, t)\rangle e^{2\pi i k x / n}, \quad (36)$$

for  $k \in \{0, 1, \dots, n-1\}$ . In momentum space, the evolution operator becomes

$$\mathbf{C}_k^{(n)} = \begin{pmatrix} \sqrt{\rho} e^{2\pi i k / n} & \sqrt{1-\rho} e^{i(2\pi k / n + \theta)} \\ \sqrt{1-\rho} e^{i(-2\pi k / n + \phi)} & -\sqrt{\rho} e^{i(-2\pi k / n + \theta + \phi)} \end{pmatrix}. \quad (37)$$

A single step of the walk becomes

$$|\tilde{\psi}(k, t+1)\rangle = \mathbf{C}_k^{(n)} |\tilde{\psi}(k, t)\rangle, \quad (38)$$

and  $t$  steps

$$|\tilde{\psi}(k, t+1)\rangle = (\mathbf{C}_k^{(n)})^t |\tilde{\psi}(k, 0)\rangle. \quad (39)$$

The operator  $\mathbf{C}_k^{(n)}$  may be diagonalized, yielding eigenvalues

$$\lambda_k^\pm = \pm e^{i\delta} e^{\pm i\omega_k^{(n)}}, \quad (40)$$

where

$$\sin(\omega_k^{(n)}) = \sqrt{\rho} \sin(2\pi k / n - \delta), \quad (41)$$

and  $\delta = (\theta + \phi)/2$ . The possible solutions for  $\omega_k^{(n)}$  are bounded by  $\sin^{-1}(\sqrt{\rho})$ , e.g., for  $\rho = 1/2$ , there are two solutions for  $\omega_k^{(n)}$  one in each of the regions  $[\pi/4, 3\pi/4]$  and  $[-\pi/4, -3\pi/4]$ . The first solution corresponds to  $\lambda_k^+$  and the second to  $\lambda_k^-$ . Expressing  $\mathbf{C}_k^{(n)}$  in terms of its eigenvalues and eigenvectors,  $(\mathbf{C}_k^{(n)})^t = (\lambda_k^+)^t |\tilde{\xi}_k^+\rangle \langle \tilde{\xi}_k^+| + (\lambda_k^-)^t |\tilde{\xi}_k^-\rangle \langle \tilde{\xi}_k^-|$ , gives

$$|\tilde{\psi}(k, t)\rangle = (\lambda_k^+)^t |\tilde{\xi}_k^+\rangle \langle \tilde{\xi}_k^+ | \tilde{\psi}(k, 0)\rangle + (\lambda_k^-)^t |\tilde{\xi}_k^-\rangle \langle \tilde{\xi}_k^- | \tilde{\psi}(k, 0)\rangle \quad (42)$$

The condition that must be satisfied for exact periodicity  $\Omega$  is that the wavefunctions  $|\psi(k, t)\rangle$  and  $|\psi(k, t + \Omega)\rangle$  must be equal, giving

$$(\lambda_k^\pm)^\Omega = 1 \quad \forall k \in \{0, 1, \dots, n-1\}. \quad (43)$$

Using the expression for the eigenvalues this becomes,

$$\begin{aligned} (\delta + \omega_k) \Omega &= 2\pi j_+, \\ (\delta - \omega_k + \pi) \Omega &= 2\pi j_-, \end{aligned} \quad (44)$$

where  $j_{\pm}$  are integers. Substituting these into eq. (41) gives

$$\cos\left(\frac{\pi j}{\Omega}\right) = \sqrt{\rho} \cos\left(\frac{2\pi k}{n} - \frac{\pi m}{\Omega}\right) \quad \forall k, \quad (45)$$

where  $\rho$  is the bias in the coin operator,  $m$  is an integer specifying the relative phases in the coin operator through  $m\pi/\Omega - \pi/2 = \delta = (\theta + \phi)/2$ ,  $k$  is the integer Fourier variable, and  $j$  is an integer that can be different for each  $k$ , but must be odd or even to match whether  $m$  is odd or even. Clearly, the larger  $n$  is, the harder it is to find solutions for eq. (45) for all  $k$  at the same time (apart from the trivial solutions for  $\rho = 0$  or  $1$ ). Tregenna *et al.* [41] conjecture that there are only a finite number of such solutions and that they have found nearly all, if not all of them.

Tregenna *et al.* also briefly explored periodicity on two dimensional torii, where a section of a 2-dimensional grid is joined up at opposite edges (periodic boundary conditions). When a Hadamard coin operator is used for each pair of opposite directions, and a torus made from suitable small rectangles, periodicity is also obtained in the cases predictable from Table I. For a closed Möbius strip or Klein bottle, the twisted dimension is only periodic if the size is half that in Table I, because the twist causes the walk to traverse the cycle twice before returning to its initial state. The Grover coin operator shows the same periodicities as the Hadamard coin operator. However, a DFT coin operator only shows periodicity for a torus of dimensions  $4 \times 4$ , and not at all on the twisted surfaces. This is due to the asymmetry of the DFT coin operator compared to the Grover and Hadamard coin operators. During the double circuit of the twisted surface, the wavefunction interferes with a mirror image of itself, so periodicity will only be observed with coin operators that produce suitably mirror symmetric distributions.

## IX. SUMMARY AND OUTLOOK

A summary of known results on perfect state transfer (PST) on finite graphs for continuous-time quantum walks is given in table II.

TABLE II: Perfect state transfer with continuous-time quantum walk on several classes of graphs.

Graph family	PST
Complete graphs	No[14] (unless weighted[2, 27])
Paths (greater than 3)	No[32] (unless weighted[31, 43])
Hypercubic graphs	Yes[20]
Hamming graphs	Yes (if weighted[27])
Integral circulants	Partial[3, 15, 17, 33]

For the discrete-time quantum walk, the cycles  $C_2$ ,  $C_4$ ,  $C_6$ ,  $C_8$ , and  $C_{10}$ , and related torii that can be formed from them, are the only simple graphs for which perfect state transfer is known to be possible for the discrete-time quantum walk. When multiple edges are allowed, chains and derived structures exhibiting perfect state transfer can be constructed using the Grover coin and equal numbers of incoming and outgoing edges.

Nonetheless, useful structures for providing communications between components in a quantum computer are provided by the known cases. For the continuous-time quantum walk, the weighted paths are the most promising, if engineered coupling strengths can be achieved, with a variety of multi-path graphs to choose from if not. For the discrete-time quantum walk the chain also gives an unlimited length, if multiple edges can be engineered. For simple graphs, the path formed from cycles up to  $C_{10}$  can provide perfect transfer up to 5 steps.

Among the many interesting open questions related to perfect state transfer for continuous-time quantum walk on graphs we note in particular:

- a characterization of integral circulants with perfect state transfer;
- a characterization of periodic graphs (see Godsil [28]);
- a proof of a conjecture made by Casaccino *et al.* [2] on perfect state transfer for  $P_n$  using weighted self-loops.

For the discrete-time walk much more remains unexplored. A proof of the periodicity property for small cycles, and a complete characterization of the types of graphs obtained from the chains would provide insights to enable these results to be extended to further classes of graphs. For both continuous- and discrete-time quantum walks, the robustness of perfect state transfer under imperfect dynamics due to a noisy environment is of practical concern for all these methods, and deserves further study.



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