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APPLICATIONS OF GRAPH SPECTRA IN QUANTUM PHYSICS

Abstract. Graph spectra are closely related to many applications in quantum physics: a network of quantum particles with fixed couplings can be modelled by an underlying graph, with the Hamiltonian of such system approximated by the adjacency matrix of that graph, and the energy levels and states represented by the eigenvalues and eigenvectors of the adjacency matrix. From that viewpoint, quite a few quantum physics problems can be posed in terms of the spectral properties of the graph. In this chapter we survey one particular problem which received a lot of attention recently: the existence of *perfect state transfer* in the network of spin-1/2 particles.

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Contents

1. Introduction

Graph spectra have had a long history of applications in statistical physics, through dimer problem, and in chemistry, through Hückel's theory [31]. Here we survey another, more recent application of graph spectra in sciences, this time in quantum physics, through the problem of establishing perfect transfer of qubit states in the network of spin-1/2 particles. Most of the results we review here were published with last six years.

After necessary initial review in Section 2 of quantum mechanical terms and notions, assembled by a non-physicist for other non-physicists, the notion of perfect state transfer is defined in Section 3. These two sections are the only ones dealing with physical aspects of perfect state transfer, the rest of the survey being devoted to mathematical results. It turns out that it is not easy to find graphs admitting perfect state transfer between a pair of its vertices: in Section 4 it is shown that any automorphism of a graph fixing one vertex must fix the other vertex as well, and that the angles of both vertices have to coincide. Among paths, only those of lengths 2 and 3 admit perfect state transfer, while it does not exist in any longer path (Section 5). Regular, integral graphs turn out to be presently richest source of graphs with perfect state transfer: some particular examples are exhibited in Section 6, while the classes of cubelike and integral circulant graphs are treated in Sections 8 and 9. From known graphs with perfect state transfer it is possible

to construct new graphs admitting perfect state transfer: the Cartesian product of graphs is best suited in this respect (Section 7), while a few more specialized constructions are given in Section 10. In Section 11 we review a concept of routing of quantum states, which further builds upon the concept of perfect state transfer and may present the source of new, interesting mathematical problems. Concluding remarks are given in Section 12.

We review here perfect state transfer in uniformly coupled spin networks (simple graphs) only. Another aspect of perfect state transfer that we do not consider here is its physical implementation. There is a large body of physics literature on this topic, and most of it is listed in references, so that the interested researcher may find the list of references as a useful start point.

2. Basics of quantum mechanics

Bra-ket notation. Bra-ket notation was introduced in 1939 by Paul Dirac, and is also known as Dirac notation [92]. It is used to denote abstract vectors and linear functionals in mathematics, and it is a standard notation for describing quantum states in the theory of quantum mechanics. It is called bra-ket because the inner product of two states (vectors) is denoted by a bracket, $\langle x|y\rangle$, consisting of a left part *bra*, $\langle x|$, and a right part *ket*, $|y\rangle$. The bra $\langle x|$ represents a row vector x^T, while the ket $|y\rangle$ represents a column vector y. Thus, $\langle x|y\rangle$ is same as $x^T y$. If $A\colon H \to H$ is a linear operator, applying A to the ket $|y\rangle$ gives a new ket $A|y\rangle$. Thus, $\langle x|A|y\rangle$ is same as $x^T Ay$.

Classical and quantum description of mechanics A physical system is generally described by three basic ingredients: states; observables; and dynamics (or law of time evolution) or, more generally, a group of physical symmetries. A classical description can be given in a fairly direct way by a phase space model of mechanics: states are points in a symplectic phase space, observables are real-valued functions on it, time evolution is given by a one-parameter group of symplectic transformations of the phase space, and physical symmetries are realized by symplectic transformations [93].

In a quantum description, each physical system is associated with a (topologically) separable complex Hilbert space $\mathcal{H}$ with inner product $\langle x|y\rangle$. Rays (one-dimensional subspaces) in $\mathcal{H}$ are associated with states of the system. In other words, physical states can be identified with equivalence classes of unit vectors in $\mathcal{H}$, where two vectors represent the same state if they differ only by a phase factor. Physical observables are represented by densely-defined self-adjoint operators on $\mathcal{H}$. The expected value of the observable A for the system in state represented by the unit vector $|\psi\rangle \in \mathcal{H}$ is $\langle\psi|A|\psi\rangle$. The possible values of the observable A in any state must belong to the spectrum of A, and in the special case A has only discrete spectrum, the possible outcomes of measuring A are its eigenvalues.

Schrödinger equation and Hamiltonian The time evolution of the state is given by a differentiable function from $\mathbf{R}$, representing instants of time, to the Hilbert space of system states. The *Schrödinger equation* [91] says that, if $|\psi(t)\rangle$

denotes the state of the system at any one time t, then

$$H|\psi(t)\rangle = i\hbar\frac{d}{dt}|\psi(t)\rangle,$$

where H is a densely-defined self-adjoint operator, called the system Hamiltonian, i is the imaginary unit, and $\hbar$ is reduced Planck's constant. As an observable, H corresponds to the total energy of the system.

The Hamiltonian generates the time evolution of quantum states. Given the state at some initial time ($t = 0$), we can integrate Schrödinger equation to obtain the state at any subsequent time. In particular, if H is independent of time, then

$$|\psi(t)\rangle = e^{-\frac{itH}{\hbar}}|\psi(0)\rangle.$$

As everything in quantum setting is quantized in terms of $\hbar$, it is usual to assume $\hbar = 1$ so that times and energies can be treated as dimensionless. The operators

$$U(t) = e^{-itH} = \sum_{n\geqslant 0}\frac{i^n t^n H^n}{n!}$$

form a one-parameter unitary group $U(t)\colon \mathcal{H} \to \mathcal{H}$, which realize physical symmetries of the closed quantum system.

Spin Experiments show that most subatomic particles have a permanent, built-in angular momentum, which is not due to their motion through space. This quantity is called the *spin* [91], and it has no correspondence at all in conventional physics. The spin σ comes in units of $\hbar/2$ and it belongs to the discrete set of values: $\sigma \in \{-S\hbar, -(S-1)\hbar, \dots, +(S-1)\hbar, +S\hbar\}$, where S is the *spin quantum number* of a particle. All elementary particles of a given kind have the same spin quantum number S. One distinguishes *bosons* ($S = 0, 1, 2, \dots$) and *fermions* ($S = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$). Quanta of light are bosons with $S = 1$ and electrons are fermions with $S = 1/2$.

Qubit The unit of quantum information—the quantum analogue of the classical bit—is a quantum bit, or *qubit* [1, 95]. Contrary to a classical bit, the qubit is described by state of a spin-$\frac{1}{2}$ particle (although any two-level quantum system, such as quantum dot, may be used to describe qubit). The qubit has two basis states in which its spin can be measured: $|0\rangle$ corresponding to spin $-\frac{1}{2}$, and $|1\rangle$ corresponding to spin $+\frac{1}{2}$. A pure qubit state is a linear combination of $|0\rangle$ and $|1\rangle$,

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle,$$

where $\alpha, \beta \in \mathbf{C}$ are probability amplitudes. When we measure this qubit in the standard basis, the probability of outcome $|0\rangle$ is $|\alpha|^2$ and the probability of outcome $|1\rangle$ is $|\beta|^2$ (thus, $|\alpha|^2 + |\beta|^2 = 1$). Note, however, that when we measure the state of the qubit we alter the values of α and β: for instance, if the state $|0\rangle$ is measured, α is changed to 1 (up to phase) and β is changed to 0.

Geometrically, the state space of a single qubit can be represented by the Bloch sphere. This is a two-dimensional space which has an underlying geometry of the surface of a sphere, meaning that the single qubit register space has two local degrees of freedom. Represented on such a sphere, a classical bit could only be on

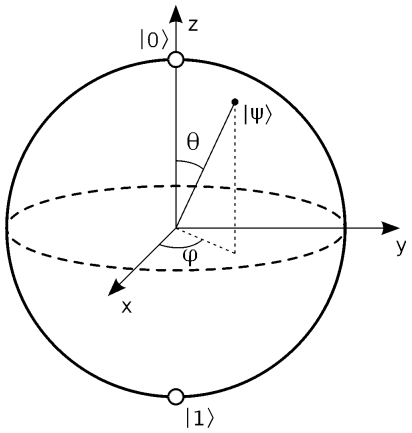

FIGURE 1. Bloch sphere.

the z-axis at the top or bottom of the sphere, in the locations where $|0\rangle$ and $|1\rangle$ are. The rest of the surface is inaccessible to a classical bit.

Unitary transformations that can be performed on pure qubit states correspond to rotations of the Bloch sphere. These rotations can be represented as combinations of rotations about the x-axis (σ_x), the y-axis (σ_y), or the z-axis (σ_z). For spin-$\frac{1}{2}$ particles, these basic rotations are represented by three Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Each Pauli matrix is an observable describing the spin of a particle in the three spatial directions.

Quantum computing A quantum computer is a computation device that makes direct use of quantum mechanical properties, such as superposition and entanglement, to represent data and perform operations on them [94]. Although quantum computing is still in its infancy, experiments have been carried out in which quantum computational operations were executed on a very small number of qubits. If large-scale quantum computers can be built, they will be able to solve certain problems much faster than any current classical computers (for example Shor's algorithm for prime factorization). Quantum computer do not allow the computations of functions that are not theoretically computable by classical computers, i.e., they do not alter the Church-Turing thesis. The gain is only in efficiency.

Quantum computers only run probabilistic algorithms. A quantum computer is said to *solve* a problem if, for every instance, its answer will be right with high probability. In classical randomized computation, the system evolves according to the application of stochastic matrices, which preserve that the probabilities add up to one (i.e., preserve the l_1 norm). In quantum computation, allowed operations are unitary transformations, which are effectively rotations. They preserve that

the sum of the squares add up to one, the Euclidean or l_2 norm). Consequently, since rotations can be undone by rotating backward, quantum computations are reversible.

When algorithm terminates, the result needs to be read off from a memory register. In a classical computer, which has a memory made up of bits, we sample from the probability distribution on the n-bit register to obtain one definite n-bit string. The memory register in a quantum computer is made up of n qubits, such that the state of each qubit is encoded with the state of the corresponding spin-$\frac{1}{2}$ particle. We read the quantum register by measuring qubit states, which is equivalent to collapsing the quantum state down to a classical distribution (with the coefficients in the classical state being the squared magnitudes of the coefficients for the quantum state) followed by sampling from that distribution. Note that n qubits can be in an arbitrary quantum superposition of up to 2^n different states simultaneously—this is a true advantage over classical computer which can only be in *one* of these 2^n states at any one time.

3. Perfect transfer of quantum states

An important task in quantum-information processing is the transfer of quantum states from one location (u) to another location (v). In general, photons are excellent flying qubits as they can be transmitted coherently over very large distances [38, 61], and optical systems, often employed in quantum communication and cryptography applications, transfer quantum states from u to v directly via photons [11, 12]. Thus, one possibility to transfer the quantum state is that it is imprinted onto a photon which is then used as the flying qubit over an optical fiber. However, it is very difficult to realize such transfer in solid-state quantum systems, as it requires perfect interface betwen photons and the main hardware of the quantum computer, and may not be worth it for short-distance communication (e.g., between two quantum processors).

Another way to accomplish quantum state transfer at short distance is by multiple applications of controlled swap operations along the communication line. However, every external manipulation inevitably induces noise in the system. It is therefore desirable to minimize the amount of external control on the system, to the point that it is not needed at all during the transfer. In such case, a *quantum wire*, the most fundamental unit of any quantum processing device, is made out of many interacting components [14, 28]. There are various physical systems that can serve as quantum wires, one of them being a quantum spin system. It is generally defined as a network of interacting qubits, whose dynamics is governed by a suitable Hamiltonian, e.g., the Heisenberg or XY Hamiltonian.

A quantum spin system is obtained by attaching a spin-$\frac{1}{2}$ particle to each vertex of a connected, finite graph $G = (V, E)$. To each vertex $i \in V$, one can associate a Hilbert space $\mathcal{H}_i \cong \mathbf{C}^2$, so that the Hilbert space associated with G is given by

$$\mathcal{H}_G = \bigotimes_{i \in V} \mathcal{H}_i \cong (\mathbf{C}^2)^{\otimes n},$$

where $n = |V|$ is the number of vertices in G. The dynamics of the system is governed by the XY Hamiltonian

$$H_G = \frac{1}{2} \sum_{(i,j)\in E(G)} J_{ij}[\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y],$$

where the symbols σ_i^x, σ_i^y and σ_i^z denote the Pauli matrices acting on the Hilbert space $\mathcal{H}_i$, and J_{ij} is the coupling strength between the vertices i and j of G. The couplings J_{ij} represent the weights of the edges of G, so that its adjacency matrix A_G is given by

$$A_{ij}(G) = \begin{cases} J_{ij}, & \text{if } (i,j) \in E \\ 0, & \text{if } (i,j) \notin E \end{cases}$$

Note that $J_{ij} = J_{ji}$ since H_G is Hermitian.

The total z component of the spin, given by

$$\sigma_{\text{tot}}^z = \sum_{i\in V} \sigma_i^z,$$

is conserved, i.e., $[\sigma_{\text{tot}}^z, H_G] = 0$. The Hilbert space $\mathcal{H}_G$ is then decomposed into invariant subspaces, each of which is a distinct eigenspace of the operator σ_{tot}^z.

For the purpose of quantum state transfer, it suffices to restrict our attention to the single excitation subspace $\mathcal{S}_G$, which is the n-dimensional eigenspace of σ_{tot}^z, corresponding to the eigenvalue $1 - \frac{n}{2}$. The quantum states initially in $\mathcal{S}_G$ will remain there under time evolution. A basis state in $\mathcal{S}_G$ corresponds to a configuration of spins in which all the spins except one are $|0\rangle$ and one spin is $|1\rangle$. Such a basis state can hence be denoted by the ket $|j\rangle$, where $j \in V$ is the vertex at which the spin is $|1\rangle_j$. Thus, $\{|j\rangle \colon j \in V\}$ denotes a complete set of orthonormal basis vectors spanning $\mathcal{S}_G$. When restricted to the subspace $\mathcal{S}_G$, H_G is represented, in this basis, by an $n \times n$ matrix which is *identical* to the adjacency matrix A_G. As known, the spectrum of the adjacency matrix of a graph is, by definition, the spectrum of the graph. In this way we see that the theory of graph spectra is relevant for the problems that we consider, i.e. in quantum computing. Some basic information on the theory of graph spectra can be found in the introductory chapter of this book, while further information may be found in the textbook [33].

The quantum spin system on G has the role of a (noiseless) quantum channel [28]. The process of transmitting a quantum state from u to v proceeds in four steps:

(1) Initialization of the spin system to the state $|\overline{0}\rangle := |0_u 0 \dots 0 0_v\rangle$. This is a zero-energy eigenstate of H_G.

(2) Creation of the quantum state $|\psi\rangle_u \in \mathcal{H}_u$ at vertex u to be transmitted. Let $|\psi\rangle_u = \alpha|0\rangle_u + \beta|1\rangle_u$ with $\alpha, \beta \in \mathbf{C}$ and $|\alpha|^2 + |\beta|^2 = 1$.

(3) Time evolution of the system for an interval of time, say t_0.

(4) Recovery of the state at vertex v.

The state of the entire spin system after step (2) is given by

$$|\Psi(0)\rangle = |\psi_u 0 \dots 0 0_v\rangle = \alpha|0_u 0 \dots 0 0_v\rangle + \beta|1_u 0 \dots 0 0_v\rangle = \alpha|\bar{0}\rangle + \beta|u\rangle.$$

Since the $|\overline{0}\rangle$ component of the state $|\Psi(0)\rangle$, as the zero-energy eigenstate of H_G, is invariant under the evolution, it suffices to focus on the evolution of the $|u\rangle$

component, i.e., to the choice $\alpha = 0$ and $\beta = 1$ above. This state evolves in time t to

$$|\Psi(t)\rangle = e^{-iA_G t}|u\rangle = \sum_{j=1}^{n} \beta_j(t)|j\rangle$$

with complex coefficients $\beta_j(t)$, where $1 = \sum_{j=1}^{n} |\beta_j(t)|^2$. At time t, the spin $|1\rangle_v$ may be measured at vertex v with probability $|\beta_v(t)|^2$, where

$$\beta_v(t) = \langle v|e^{-iA_G t}|u\rangle.$$

Thus, we say that G has *perfect state transfer* from u to v in time t if

$$|\langle v|e^{-iA_G t}|u\rangle| = 1.$$

In such case, $\langle j|e^{-iA_G t}|u\rangle = 0$ for all $j \neq v$. The effect of the modulus above is that the quantum state after transfer is not exactly equal $|v\rangle$, but rather $e^{i\phi}|v\rangle$. However, the phase factor $e^{i\phi}$ is not a problem, because ϕ will be a known quantity for G, and it can be corrected for with an appropriate phase gate.

The *communication distance* of a graph G is the maximum distance between vertices u and v of G for which perfect state transfer is possible. For a fixed number of qubits, the basic question is to find quantum spin systems which maximize the communication distance.

The time evolution of states in $\mathcal{S}_G$ under the action of the Hamiltonian H_G may also be interpreted as a *continuous-time quantum walk* on G, first considered by Farhi and Gutmann in 1998 [35] (see also [25]). The quantum walks are interesting in their own right due to their property of universal quantum computation [26].

Let λ_k and $|\mu_k\rangle$ be the eigenvalues and the unit eigenvectors of A_G, for $k = 1, \ldots, n$. Recall that, if f is a complex function defined on the eigenvalues of A, then

$$f(A_G) = \sum_{i=1}^{n} f(\lambda_i)|\mu_i\rangle\langle\mu_i|.$$

In particular,

$$e^{-iA_G t} = \sum_{i} e^{-i\lambda_i t}|\mu_i\rangle\langle\mu_i|,$$

and

$$\langle v|e^{-iA_G t}|u\rangle = \langle v|\left\{\sum_{k=1}^{n} e^{-i\lambda_k t}|\mu_k\rangle\langle\mu_k|\right\}|u\rangle.$$

One can use this formula to check that paths with two and three vertices have perfect state transfer between their end-vertices:

(a) For path $P_2 = (\{1,2\}, \{\{1,2\}\})$ we have

$$\langle 1|e^{-iA_{P_2} t}|2\rangle = -i\sin t \quad \text{and} \quad |\langle 1|e^{-iA_{P_2}\frac{\pi}{2}}|2\rangle| = 1.$$

(b) For path $P_3 = (\{1,2,3\}, \{\{1,2\},\{2,3\}\})$ we have

$$\langle 1|e^{-iA_{P_3} t}|3\rangle = -\sin^2(t/\sqrt{2}) \quad \text{and} \quad |\langle 1|e^{-iA_{P_3}\frac{\pi}{\sqrt{2}}}|3\rangle| = 1.$$

4. Consequences of perfect state transfer on relations between vertices

Let G be a graph of the quantum spin system with unit couplings and adjacency matrix A. Godsil [40] has recently derived few important lemmas on the relationship between vertices among which perfect state transfer occurs. Let $\mathrm{Aut}(G)_v$ denotes the group of automorphisms of G that fix its vertex v.

Lemma 4.1. [40] *If G admits perfect state transfer from u to v, then* $\mathrm{Aut}(G)_u = \mathrm{Aut}(G)_v$.

Proof. We identify the automorphisms of G with the permutation matrices that commute with A. Since e^{-iAt} is a polynomial in A, any permutation matrix from $\mathrm{Aut}(G)$ commutes with e^{-iAt}. If the automorphism associated with P fixes u, then $P|u\rangle = |u\rangle$. If perfect state transfer takes place at time τ and $H = e^{-iA\tau}$, then there is $\gamma \in \mathbf{C}$ such that $|\gamma| = 1$ and $H|u\rangle = \gamma|v\rangle$. So

$$\gamma P|v\rangle = PH|u\rangle = HP|u\rangle = H|u\rangle = \gamma|v\rangle$$

and thus v is fixed by P as well. Thus, $\mathrm{Aut}(G)_u \subseteq \mathrm{Aut}(G)_v$. The argument is same when we replace u and v, hence $\mathrm{Aut}(G)_v \subseteq \mathrm{Aut}(G)_u$ as well. □

Vertices u and v of G are *cospectral* if $\phi(G-u,t) = \phi(G-v,t)$, where $\phi(G,t) = \prod_{k=1}^{n}(t-\lambda_k)$ is the characteristic polynomial of G. Alternatively, u and v are cospectral if they have the same angles [32].

Lemma 4.2. [40] *If G admits perfect state transfer from u to v, then u and v are cospectral.*

Proof. By Cramer's rule,

$$((tI-A)^{-1})_{u,u} = \frac{\phi(G-u,t)}{\phi(G,t)}$$

and so using the spectral decomposition we find that

$$\frac{\phi(G-u,t)}{\phi(G,t)} = \sum_{k=1}^{n} \frac{\langle \mu_k|u\rangle^2}{t-\lambda_k}.$$

Let $\theta_1, \ldots, \theta_r$ be all distinct values among $\lambda_1, \ldots, \lambda_n$, and let $\mu_{j_i}, \mu_{j_i+1}, \ldots, \mu_{j_{i+1}-1}$ be the eigenvectors corresponding to θ_i, $1 \leqslant i \leqslant r$. The orthogonal projection onto the eigenspace corresponding to θ_i is given by

$$E_i = \sum_{k=j_i}^{j_{i+1}-1} |\mu_k\rangle\langle\mu_k|.$$

Assume we have perfect state transfer from u to v at time τ and set $H = e^{-iA\tau}$. Then there is $\gamma \in \mathbf{C}$ such that $|\gamma| = 1$ and $H|u\rangle = \gamma|v\rangle$. Since H is a polynomial in A, it commutes with each projection E_i and therefore

$$\gamma E_i|v\rangle = E_i H|u\rangle = HE_i|u\rangle.$$

As H is unitary, this implies that $E_i|v\rangle$ and $E_i|u\rangle$ have the same length, i.e.,

$$\sum_{k=j_i}^{j_{i+1}-1} \langle \mu_k|v\rangle^2 = \sum_{k=j_i}^{j_{i+1}-1} \langle \mu_k|u\rangle^2.$$

From this we conclude that $G-u$ and $G-v$ have the same characteristic polynomial. Thus u and v are cospectral. □

5. Eigenvalue ratio condition and periodic graphs

We say that G is *periodic relative to the vertex* u if there is a time t such that

$$|\langle u|e^{-iAt}|u\rangle| = 1.$$

We say that G is *periodic* if there is a time t such that e^{-iAt} is diagonal, i.e., if G is periodic relative to each of its vertices at the same time.

Theorem 5.1. [27, 39] *If G has perfect state transfer from u to v at time t_0, then G is periodic relative to u and v at time $2t_0$.*

Proof. With G initialized in the state $|u\rangle$, after time t_0 we have the state

$$e^{-iAt_0}|u\rangle = e^{i\phi}|v\rangle.$$

Since A is a symmetric matrix, it also holds that

$$e^{-iAt_0}|v\rangle = e^{i\phi}|u\rangle.$$

Thus, after another period of time t_0 we have the state

$$e^{-iA2t_0}|u\rangle = e^{-iAt_0}e^{i\phi}|v\rangle = e^{i2\phi}|u\rangle,$$

and the graph is periodic with period $2t_0$. □

The above proof also shows that if there is perfect state transfer between u and v at time t_0, then perfect state transfer also occurs for all times t of the form

$$t = (2k+1)t_0, \qquad \text{where } k \in \mathbf{Z}.$$

Theorem 5.2. [27, 39] *Let G has eigenvalues λ_j with corresponding eigenvectors $|x_j\rangle$, $j = 1, \ldots, n$. If G is periodic relative to the vertex u, then for each quadruple λ_k, λ_l, λ_r, λ_s of eigenvalues of G, such that $\langle x_k|u\rangle$, $\langle x_l|u\rangle$, $\langle x_r|u\rangle$, $\langle x_s|u\rangle \neq 0$ and $\lambda_r \neq \lambda_s$,*

$$\frac{\lambda_k - \lambda_l}{\lambda_r - \lambda_s} \in \mathbf{Q}. \tag{5.1}$$

The condition (5.1) is called the *eigenvalue ratio condition*.

Proof. Let $|u\rangle = \sum_j a_j|x_j\rangle$ and examine the state of a periodic graph with period $2t_0$:

$$e^{-iA_G 2t_0}|u\rangle = \sum_j a_j e^{-i\lambda_j 2t_0}|x_j\rangle = e^{i2\phi}\sum_j a_j|x_j\rangle = e^{i2\phi}|u\rangle.$$

Since the eigenvectors $|x_j\rangle$ are linearly independent, we have that for each j with $a_j = \langle x_j|u\rangle \neq 0$

$$2\lambda_j t_0 + 2\phi = 2m_j\pi \quad \text{for some } m_j \in \mathbf{Z}.$$

Thus,

$$\frac{\lambda_k - \lambda_l}{\lambda_r - \lambda_s} = \frac{m_k - m_l}{m_r - m_s} \in \mathbf{Q}.$$

□

Note that the condition $\langle x_k|u\rangle$, $\langle x_l|u\rangle$, $\langle x_r|u\rangle$, $\langle x_s|u\rangle \neq 0$ in the above theorem does not appear in [27].

Periodicity of a graph at each of its vertices may be characterized by its spectrum alone.

Lemma 5.1. [39] *Let the eigenvalues of G be $\lambda_1, \ldots, \lambda_n$. Then G is periodic if and only if the ratio of any two non-zero eigenvalues is rational.*

Theorem 5.3. [39] *A graph G is periodic if and only if either:*

(a) *The eigenvalues of G are integers, or*
(b) *The eigenvalues of G are rational multiples of $\sqrt{\Delta}$, for some square-free integer Δ. In this case, G is bipartite.*

The graphs whose eigenvalues are all integers are called *integral graphs*. They have been a sort of a mathematical curiosity for a number of years: cubic integral graphs have been, for example, characterized 25 years ago in [21], and independently in [78]. A number of other results on integral graphs with bounded maximum degree and on integral trees are surveyed in [7, 89]. For application of integral graphs in multiprocessor systems, see the chapter "Multiprocessor interconnection networks" in this book.

The graphs whose eigenvalues are all rational multiples of $\sqrt{\Delta}$ have not been explicitly studied before. They are, perhaps, most easily found among semiregular graphs.

We have shown that perfect state transfer exists in paths with two and three vertices. We will now show, following [27], that there is no perfect state transfer in path P_n for $n \geqslant 4$. Suppose contrary, that there exists perfect state transfer between u and v in P_n for some $n \geqslant 4$. We will show that there is a set of eigenvalues λ_k, λ_l, λ_r, λ_s of P_n that violates the eigenvalue ratio condition.

The eigenvalues of P_n are given by $\lambda_i = 2\cos\frac{\pi i}{n+1}$ for $i = 1, \ldots, n$, and the eigenvectors are given by [28]

$$x_i = \sqrt{\frac{2}{n+1}} \sum_{j=1}^{n} \sin\frac{\pi ij}{n+1} |j\rangle.$$

Choosing $k = 2$, $l - 1$, $r = 1$ and s, we see that the eigenvalue ratio condition requires that

$$\frac{\cos\frac{2\pi}{n+1}}{\cos\frac{\pi}{n+1}} \in \mathbf{Q}. \tag{5.2}$$

Further, $\langle x_1|u\rangle$, $\langle x_n|u\rangle \neq 0$ for all u, and $\langle x_2|u\rangle$, $\langle x_{n-1}|u\rangle \neq 0$ unless n is odd and u is the center of P_n (however, in such case, v has to satisfy $\langle x_2|v\rangle$, $\langle x_{n-1}|v\rangle \neq 0$). Assume that

$$\frac{\cos\frac{2\pi}{n+1}}{\cos\frac{\pi}{n+1}} = \frac{p}{q}, \quad \text{for } p, q \in \mathbf{Z}.$$

Using the trigonometric identity

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

we can write

$$\Big(\cos\frac{\pi}{n+1}\Big)^2 - \frac{p}{2q}\cos\frac{\pi}{n+1} - \frac{1}{2} = 0$$

which is a monic polynomial in $\cos\frac{\pi}{n+1}$ with rational coefficients. Thus, $\cos\frac{\pi}{n+1}$ has to be an algebraic integer with degree $\leqslant 2$.

On the other hand, Lehmer proved (see, for example, [70]) that if $n > 1$ and $\gcd(k, n+1) = 1$, then $\cos\frac{\pi k}{n+1}$ is an algebraic integer of degree $\phi(2(n+1))/2$, where ϕ is the Euler phi function. For $n \geqslant 3$ it can be shown [74] that

$$\phi(n) \geqslant \frac{n}{e^{\gamma}\log\log n + 3/\log\log n}$$

holds, with $\gamma \approx 0.5772$ Euler's constant. Using this bound, and inspecting values not covered by it, we can see that $\phi(2(n+1))/2 \geqslant 3$ for $n \geqslant 6$. Thus, $\cos\frac{\pi}{n+1}$ is an algebraic number of degree $\geqslant 3$, and so $\cos\frac{2\pi}{n+1}/\cos\frac{\pi}{n+1}$ has to be irrational, violating the eigenvalue ratio condition (5.2). Hence, perfect state transfer is impossible in paths with $n \geqslant 6$. The cases $n = 4$ and $n = 5$ are easily proved by direct evaluation.

6. Some regular graphs with perfect state transfer

Integral graphs represent a class of graphs that naturally satisfies eigenvalue ratio condition. There are only thirteen connected cubic integral graphs [21, 78], so the next theorem follows easily:

Theorem 6.1. [79] *The 3-dimensional cube is the only periodic, connected cubic graph with perfect state transfer between two different vertices.*

4-regular integral graphs are not fully characterized, except those that do not have ± 3 as an eigenvalue [82]. However, all 4-regular integral graphs with up to 24 vertices are known [83]. Among them, there is a triplet of cospectral graphs on 16 vertices with perfect state transfer, one of which is a 4-dimensional cube (Fig. 2).

Regular graphs with perfect state transfer are not necessarily periodic. An example of such graph was found by Matthew Russell [75], who showed that the complement of the union of four cycles C_3, C_4, C_4 and C_5 has perfect state transfer at time $\pi/2$ between antipodal vertices in both C_4s, but it is not periodic at time π relative to vertices belonging to C_3 and C_5. At time 2π it is periodic relative to vertices belonging to C_3, but still not periodic relative to vertices in C_5.

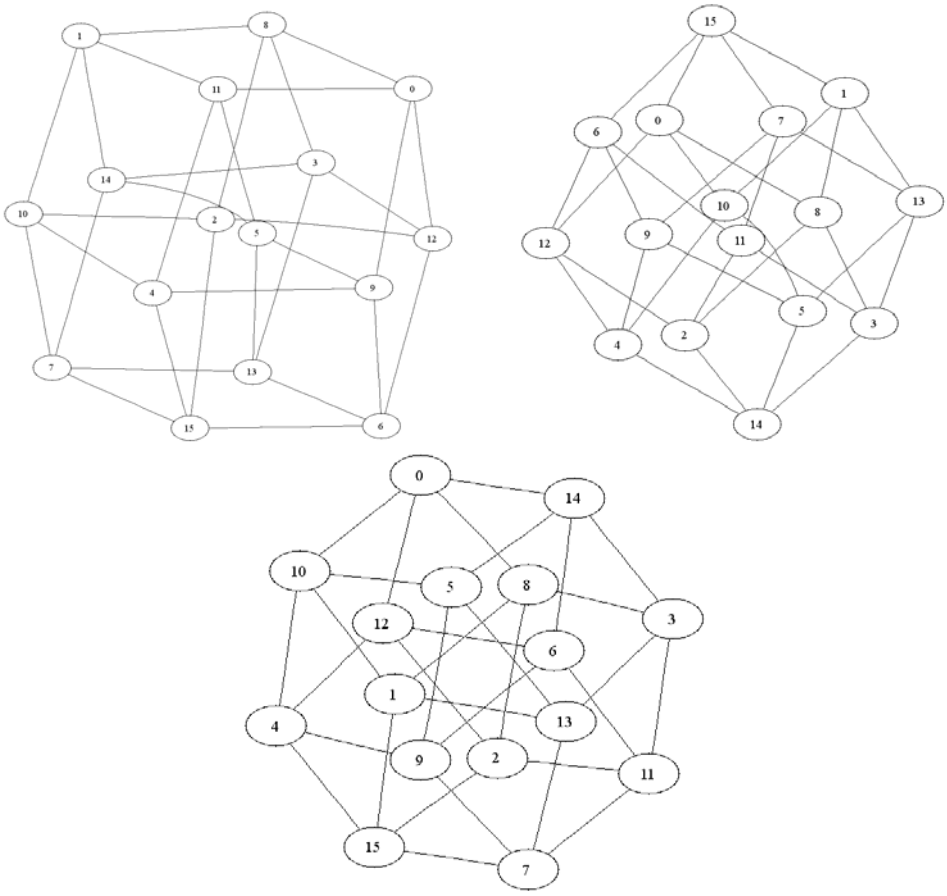

FIGURE 2. 4-regular integral graphs on 16 vertices with perfect state transfer.

One can also find examples of nonintegral periodic graphs with perfect state transfer. Besides already known P_3, such graph is the bipartite complement of the union of $2k$ copies of P_3, $k \geqslant 1$, which has perfect state transfer between end vertices of the same copy of P_3 at time $\pi/\sqrt{2}$. It has even number of vertices and distinct eigenvalues $\pm(2k-1)\sqrt{2}, \pm\sqrt{2}$ and 0, thus answering a problem (a) from Section 10 in the first version of Godsil' paper [39].

7. Cartesian product of graphs

Perfect state transfer is impossible in paths of length larger than two. Clearly it is desirable to find a graph that allows perfect state transfer over larger distances, and with that goal in mind, we examine the d-fold Cartesian product of the path P_3, which we denote by $P_3^{\otimes d}$.

The Cartesian product of two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ is a graph $G_1 + G_2$ whose vertex set is set $V_1 \times V_2$ and two of its vertices (u_1, u_2) and (v_1, v_2) are adjacent if and only if one of the following holds: (i) $u_1 = v_1$ and $\{u_2, v_2\} \in E_2$, or (ii) $u_2 = v_2$ and $\{u_1, v_1\} \in E_1$. Let A_{G_1} and A_{G_2} be the adjacency matrices of G_1 and G_2, and let $\{\lambda_i(G_1)\colon 1 \leqslant i \leqslant |V_1|\}$ and $\{\lambda_j(G_2)\colon 1 \leqslant j \leqslant |V_2|\}$ denote the sets of eigenvalues of G_1 and G_2, respectively. The adjacency matrix of $G_1 + G_2$ is given by

$$A_{G_1+G_2} = A_{G_1} \otimes I_{G_2} + I_{G_1} \otimes A_{G_2},$$

where $\otimes$ denotes the Kronecker product of matrices. The eigenvalues of $G_1 + G_2$ are then precisely the numbers $\lambda_i(G_1) + \lambda_j(G_2)$. For the Hamiltonian of $G_1 + G_2$ we have

$$\begin{aligned} e^{-iA_{G_1+G_2}t} &= e^{-i(A_{G_1}\otimes I_{G_2} + I_{G_1}\otimes A_{G_2})t} \\ &= e^{-i(A_{G_1}\otimes I_{G_2})t} e^{-i(I_{G_1}\otimes A_{G_2})t} \\ &= (e^{-iA_{G_1}t} \otimes I_{G_2})(I_{G_1} \otimes e^{-iA_{G_2}t}) \\ &= e^{-iA_{G_1}t} \otimes e^{-iA_{G_2}t}. \end{aligned}$$

Cartesian product of graphs is thus well related to perfect state transfer.

Theorem 7.1. [5] *For $j = 1, \ldots, m$, the graph G_j has perfect state transfer from a_j to b_j at time t^* if and only if $\mathcal{G} = G_1 + \cdots + G_m$ has perfect state transfer from $(a_1, \ldots, a_m)$ to $(b_1, \ldots, b_m)$ at time t^*.*

Proof. We prove the claim for $m = 2$. From above,

$$\langle b_1, b_2|e^{-iA_{G_1+G_2}t}|a_1, a_2\rangle = \langle b_1|e^{-iA_{G_1}t}|a_1\rangle\langle b_2|e^{-iA_{G_2}t}|a_2\rangle.$$

This shows that G_1+G_2 has perfect state transfer from (a_1, a_2) to (b_1, b_2) at time t^* if and only if G_1 has perfect state transfer from a_1 to b_1 at time t^* and G_2 has perfect state transfer from a_2 to b_2 at time t^*. The general claim now follows by induction. □

Let $A = (1, 1, \ldots, 1)$ and $B = (3, 3, \ldots, 3)$ denote the antipodal points of $P_3^{\otimes d}$. If we select time $t^* = \pi/\sqrt{2}$, we get perfect state transfer from 1 to 3 in each copy of P_3. Thus, we achieve perfect state transfer between A and B in $P_3^{\otimes d}$ at time t^* (as well as between any vertex and its mirror, such as $(1, 1, 1, 2, 3) \mapsto (3, 3, 3, 2, 1)$). The communication distance provided by $P_3^{\otimes d}$ is equal to $2d = 2\log_3 n$, where $n = 3^d$ is the number of vertices of $P_3^{\otimes d}$.

Perfect state transfer can also be achieved between the antipodal vertices of the hypercube Q_d in time $t^* = \pi/2$ for arbitrary d. This is because $Q_d = P_2^{\otimes d}$ and perfect transfer occurs across P_2 in this time. In this case, the communication distance is somewhat smaller and equal to $\log_2 n$.

The Cartesian product is a special case of non-complete extended p-sum (NEPS) of graphs. Let $\mathcal{B} \subseteq \{0, 1\}^n \setminus \{(0, \ldots, 0\}$ such that there exists $\beta \in \mathcal{B}$ with $\beta_i = 1$ for each $i = 1, \ldots, n$. The NEPS$(G_1, \ldots, G_n; \mathcal{B})$ is the graph with the vertex set $V(G_1) \times \cdots \times V(G_n)$, in which two vertices $(u_1, \ldots, u_n)$ and $(v_1, \ldots, v_n)$ are

adjacent if there exists $\beta \in \mathcal{B}$ such that for each $i = 1, \ldots, n$, $u_i = v_i$ if $\beta_i = 0$ and $\{u_i, v_i\} \in E(G_i)$ if $\beta_i = 1$.

The simplest case, NEPS of P_2s, has been studied in [13] under the name of *cubelike graphs*.

8. Cubelike graphs

Let $\mathbf{Z}_2^n$ be the additive abelian group $(\mathbf{Z}_2)^{\times n}$. Each element of $\mathbf{Z}_2^n$ is represented as a binary vector of length n. Let Ω be an arbitrary subset of $\mathbf{Z}_2^n \setminus \{0\}$. If w and v are two binary vectors of the same length, then $w \oplus v$ denotes the vector obtained by elementwise addition modulo 2. The Cayley graph $X(\mathbf{Z}_2^n, \Omega)$, having the binary vectors of length n as its vertices, with two vertices w and v adjacent if and only if $w \oplus v \in \Omega$, is called *cubelike graph* [13]. Note that the cubelike graph $X(\mathbf{Z}_2^n, \Omega)$ is actually the same as $\mathrm{NEPS}(P_2, \ldots, P_2; \Omega)$.

The above definition of a cubelike graph embraces every possible set $\Omega \neq \{0\}$. When Ω is the standard generating set of $\mathbf{Z}_2^n$, the graph $X(\mathbf{Z}_2^n, \Omega)$ is isomorphic to the hypercube Q_n.

Theorem 8.1. [13] *Let $X(\mathbf{Z}_2^n, \Omega)$ be a cubelike graph and let $a, b \in \mathbf{Z}_2^n$. For $t = \pi$, perfect state transfer exists between a and b if and only if $a = b$. For $t = \pi/2$, perfect state transfer exists between a and b if and only if $a \oplus b = u$ and $u = \bigoplus_{w \in \Omega} w \neq 0$.*

As a simple consequence, there are various ways to *route* information between any two nodes of a network whose vertices correspond to the elements of $\mathbf{Z}_2^n$. Let $\Omega = \{w_1, \ldots, w_r\}$ be a generating set of $\mathbf{Z}_2^n$. Let $\bigoplus_{w_i \in \Omega} w_i = w \neq 0$. Let us define $C = \{w, w_1, \ldots, w_r\}$ and $C_i = C \setminus \{w_i\}$. Since the sum of the elements of C_i is nonzero, the Cayley graph $X(\mathbf{Z}_2^n, C_i)$ has perfect state transfer between a and b such that $a \oplus b = w_i$ at time $\pi/2$. The simplest case arises when we choose r and take the vectors $w_1, \ldots, w_r$ to be the standard basis of $\mathbf{Z}_2^n$. Then $X(\mathbf{Z}_2^n, C_i)$ is the *folded d-cube* and by using a suitable sequence of the graphs $X(\mathbf{Z}_2^n, C_i)$, we can arrange perfect state transfer from the zero vector to any desired element of $\mathbf{Z}_2^n$.

For example, consider the case $\Omega = \{w_1, w_2, w_3\}$ with $w_1 = (100)$, $w_2 = (010)$ and $w_3 = (001)$. Then $w = (111)$. The graph $X(\mathbf{Z}_2^3, C)$ is illustrated in Fig. 3-left. Since $w_1 = w_2 \oplus w_3 \oplus w$, there is perfect state transfer between 000 and $w_1 = 100$ at time $\pi/2$, given that $000 \oplus 100 = 100$ (see Fig. 3-right). Also, there is perfect state transfer for the pairs $\{010, 110\}$, $\{001, 101\}$ and $\{011, 111\}$. Note that $X(\mathbf{Z}_2^3, C_1)$ is isomorphic to the 3-dimensional hypercube.

A special case has been left open in the above theorem: when $\bigoplus_{w \in \Omega_f} w = 0$. Although it was suggested in [13] that cubelike graphs with this property do not allow perfect state transfer, examples of such graphs on 32 vertices were recently found in [29]. Let M be the matrix with the elements of Ω as its columns. Its row space is a binary code, with $\mathrm{supp}(x)$ and $\mathrm{wt}(x)$ denoting the support and the Hamming weight of x (i.e., the set of positions and the number of 1s in binary string x).

Theorem 8.2. [29] *Let $X(\mathbf{Z}_2^n, \Omega)$ be a cubelike graph with matrix M and suppose u is its vertex distinct from 0. Then the following are equivalent:*

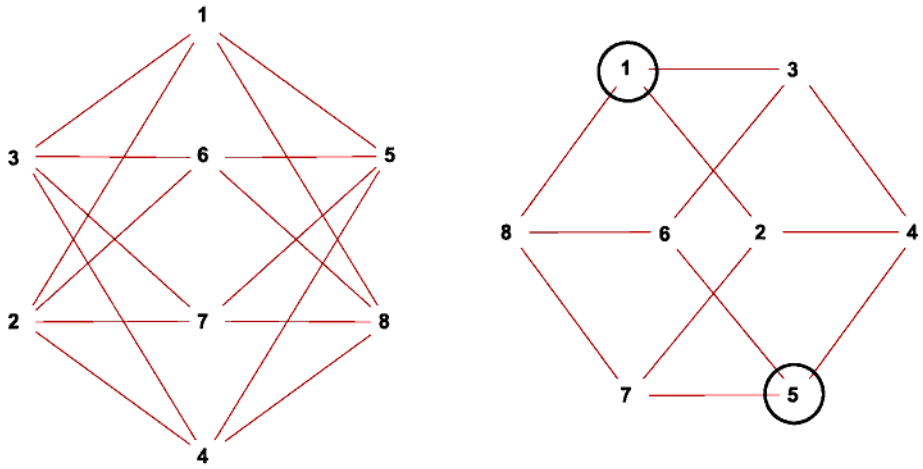

FIGURE 3. Left: The graph $X(\mathbf{Z}_2^3, C)$, where $C = \{100, 010, 001, 111\}$. This graph is isomorphic to the complete bipartite graph $K_{4,4}$. Right: The graph $X(\mathbf{Z}_2^3, C_1)$, where $C_1 = \{010, 001, 111\}$. This graph is isomorphic to the hypercube of dimension 3.

(a) *There is perfect state transfer from* 0 *to* u *at time* $\pi/2\Delta$.
(b) *All words in* Ω *have weight divisible by* Δ *and* $\Delta^{-1}\mathrm{wt}(a^T M)$ *and* $a^T u$ *have the same parity for all vectors* $a \in \mathbf{Z}_2^n$.
(c) Δ *divides* $|\mathrm{supp}(u) \cap \mathrm{supp}(v)|$ *for any two code words* u *and* v.

9. Integral circulant graphs

Circulant graphs are an important class of interconnection networks used in parallel and distributed computing [48]. They are another class of graphs extensively studied for the existence of perfect state transfer. For $n \in \mathbf{N}$ and $S \subseteq \{1, \ldots, n-1\}$, the *circulant graph* $G(n, S)$ is the graph with n vertices, labelled with integers modulo n, such that each vertex i is adjacent to $|S|$ other vertices $i + s \pmod n$ for each $s \in S$. The set S is called the *symbol* of $G(n, S)$. As we consider undirected graphs, we assume that $s \in S \Leftrightarrow n - s \in S$, so that the vertex i is adjacent to both $i \pm s \pmod n$ for each $s \in S$. The adjacency matrix A of the circulant graph $G(n, S)$ is diagonalizable by the Fourier matrix F whose columns $|F_k\rangle$ are defined as $\langle j|F_k\rangle = \omega_n^{jk}/\sqrt{n}$, where $\omega_n = e^{2\pi i/n}$ [5]. In fact, we have $FAF^\dagger = \sqrt{n}\mathrm{diag}(FA_0)$, for any circulant matrix A, where A_0 is the first column of A. This shows that the eigenvalues of A are given by

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

So [81] has characterized the integral circulant graphs. Let

$$G_n(d) = \{k\colon \gcd(n,k) = d,\ 1 \leqslant k < n\}$$

be a set of all integers less than n having the same greatest common divisor d with n. In particular, $|G_n(d)| = \phi(n/d)$, where

$$\phi(m) = |\{s\colon \gcd(m,s) = 1,\ 1 \leqslant s < m\}$$

denotes the Euler phi-function. Let D_n be a set of positive divisors d of n, with $d \leqslant n/2$.

Theorem 9.1. [81] *A circulant graph $G(n,S)$ is integral if and only if*

$$S = \bigcup_{d\in D} G_n(d)$$

for some set of divisors $D \subseteq D_n$.

Actually, integral circulants were characterized long before by Bridges and Mena in 1979 [16], they also extended their result to Cayley graphs of abelian groups in 1982 [17].

For a set of divisors $D = \{d_1,\dots,d_k\} \subseteq D_n$, we shortly denote by $\mathrm{ICG}_n(D)$ an integral circulant graph $G\big(n, \bigcup_{i=1}^{k} G_n(d_i)\big)$. $\mathrm{ICG}_n(D)$ is connected if and only $\gcd(n,d_1,\dots,d_k) = 1$ [81].

It was shown in [10] that perfect state transfer is possible in $\mathrm{ICG}_n(D)$ for even n only, in which case perfect state transfer exists between antipodal vertices a and $a + n/2$, for each a.

The integral circulants with $D = \{1\}$ are also called the *unitary Cayley graphs.*

Theorem 9.2. [10] *The only unitary Cayley graphs* $\mathrm{ICG}_n(\{1\})$ *with perfect state transfer are P_2 and $C_4 \cong P_2^{\otimes 2}$.*

The cocktail-party graph, which is a complete graph K_n minus a perfect matching, has perfect state transfer between antipodal vertices at distance two [86]. It is another example of an integral circulant graph with $S = \{1,\dots,n-1\} \setminus \{n/2\}$.

Among other integral circulant graphs (non-unitary and non-cocktail-party), the smallest graphs with perfect state transfer are $\mathrm{ICG}_8(\{1,2\})$ and $\mathrm{ICG}_8(\{1,4\})$, shown in Fig. 4. They represent two infinite families of integral circulants with perfect state transfer.

Theorem 9.3. [8] *For n divisible by 8, the integral circulant graphs* $\mathrm{ICG}_n(\{1,n/2\})$ *and* $\mathrm{ICG}_n(\{1,n/4\})$ *have perfect state transfer between antipodal vertices.*

Further examples of integral circulants with perfect state transfer have been found in [5], using the concept of circulant join. For a n-vertex graph G and a $n \times n$ $(0,1)$-matrix C, the *circulant join* $G \bigtriangledown_C G$ is a graph with adjacency matrix

$$A_{G\bigtriangledown_C G} = \begin{bmatrix} A_G & C \\ C & A_G \end{bmatrix}.$$

This operation generalizes the usual join $G \bigtriangledown G = G \bigtriangledown_J G$ and $K_2 + G = G \bigtriangledown_I G$. If u is a vertex of G, then we denote by (u,s), $s \in \{0,1\}$, the vertex u in the s-th copy of G in $G \bigtriangledown_C G$.

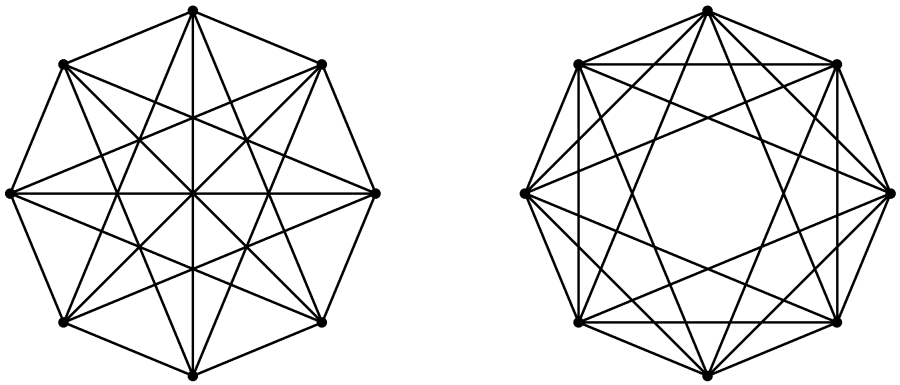

FIGURE 4. The integral circulant graphs $\mathrm{ICG}_8(\{1,2\})$ and $\mathrm{ICG}_8(\{1,4\})$.

Theorem 9.4. [5] *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 $G \bigtriangledown_C G$ has perfect state transfer from vertex $(a,0)$ to vertex (b,s), $s \in \{0,1\}$, at time t^* provided that*

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

where $B = C^TC$ and B^{-1} exists whenever $s = 1$. Also, $G \bigtriangledown_C G$ is a circulant graph if C is a palindrome circulant matrix, where $c_j = c_{n-1-j}$, for $j = 0, 1, \ldots, n-1$.

Corollary 9.1. [5] *If G is a n-vertex circulant graph that has perfect state transfer from a to b at time t^*, then so does the circulant graph $G \bigtriangledown G$ provided $nt^* \in 2\pi\mathbf{Z}$.*

Theorem 9.5. [5] *Let $n = 2^u m$, where $u \geqslant 3$ and $m \geqslant 3$ is an odd number. Suppose that $G = \mathrm{ICG}_n(D)$, for $D = \{1, n/4\}$ or $D = \{1, n/2\}$. For any subset $Q \subset D_m \cup \{m\}$, there is an $(0,1)$-circulant matrix $C \notin \{I_n, J_n, O_n\}$ so that*

$$G \bigtriangledown_C G = \mathrm{ICG}_{2n}(2D \cup Q)$$

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

Corollary 9.2. [5] *For $n = 2^u$, for $u \geqslant 3$, the integral circulants $\mathrm{ICG}_{2n}(\{1,2,n/2\})$ and $\mathrm{ICG}_{2n}(\{1,2,n\})$ have perfect state transfer from 0 to n at time $t^* = \pi/2$.*

Still, the integral circulants with perfect state transfer exhibit very small communication distance, as their diameter is of order $O(\ln\ln n)$ [84], inferior to the communication distance $2\log_3 n$ found in a P_3-cube [27].

Besides few examples of perfect state transfer above, one can actually find more results in the literature on the nonexistence of perfect state transfer in integral circulants:

Theorem 9.6. *An integral circulant graph $\mathrm{ICG}_n(D)$ does not have perfect state transfer if any of the following conditions hold:*

(i) *n is odd* [76];
(ii) *n/d is odd for every $d \in D$* [10];
(iii) *n is an even square-free integer* [8];
(iv) *$n = 2p^2$ for a prime number p* [9].
(v) *n is not square-free, $D \neq \{1, n/2\}$, there exists an* isolated divisor *$d_0 \in D$ such that $\gcd(d_0, d) = 1$ for every $d \in D \setminus \{d_0\}$ and n/d_0 is square-free* [9];
(vi) *$n \in 4\mathbf{N} + 2$ and n/d is not square-free for each divisor $d \in D$* [9];

10. Other graph compositions

Angeles-Canul et al. [5] and Ge et al. [37] have considered a number of graph compositions which yield graphs with perfect state transfer under suitable conditions. Here we review the results on perfect state transfer in direct product, generalized lexicographic product and join of graphs.

The *direct product* $G \times H$ is a graph defined on $V(G) \times V(H)$ where (g_1, h_1) is adjacent to (g_2, h_2) if $(g_1, g_2) \in E(G)$ and $(h_1, h_2) \in E_H$. The adjacency matrix of $G \times H$ is $A_G \otimes A_H$.

Theorem 10.1. [37] *Let G be a graph with perfect state transfer at time t_G so that*

$$t_G \operatorname{Spec}(G) \subset \mathbf{Z}\pi.$$

Then $G \times H$ has perfect state transfer if H is a circulant graph with odd eigenvalues.

Note that Q_{2n} has eigenvalues $\lambda_k = 2n - 2k$, for $k = 0, 1, \ldots, 2n$ and perfect state transfer time $t = \pi/2$. Also, $P_3^{\otimes n}$ has eigenvalues from $\lambda_k \in \mathbf{Z}\sqrt{2}$ and perfect state transfer time $t = \pi/\sqrt{2}$. In both cases, we have $t\lambda_k \in \mathbf{Z}\pi$ for all k. Thus, $Q_{2n} \times H$ and $P_3^{\otimes n} \times H$ have perfect state transfer for any circulant H with odd eigenvalues. For example, we may let $H = K_m$ be the complete graph of order m, for an even integer m.

The *generalized lexicographic product* $G_C[H]$ of graphs G and H, under the square $(0,1)$-matrix C indexed by vertices of H, is a graph on $V_G \times V_H$ where (g_1, h_1) is adjacent to (g_2, h_2) if and only if either $(g_1, g_2) \in E_G$ and $C(h_1, h_2) = 1$, or, $g_1 = g_2$ and $(h_1, h_2) \in E_H$. The adjacency matrix of $G_C[H]$ is $A_{G_C[H]} = A_G \otimes A_C + I_G \otimes A_H$. The standard lexicographic product $G[H]$ is obtained by setting $C = J_H$.

Theorem 10.2. [37] *Let G and H be perfect state transfer graphs with a common time t, with H being a circulant graph. Suppose that*

$$t|V_H| \operatorname{Spec}(G) \subset 2\pi\mathbf{Z}.$$

Then the lexicographic product $G_{J_H - I_H}[H]$ has perfect state transfer at time t.

Theorem 10.3. [37] *Let G be an arbitrary graph and let H be a regular graph with perfect state transfer at time t_H from h_1 to h_2, for $h_1, h_2 \in V_H$. Then $G[H]$ has perfect state transfer from (g, h_1) to (g, h_2) for any $g \in V_G$, if*

$$t_H|V_H| \operatorname{Spec}(G) \subset 2\pi\mathbf{Z}.$$

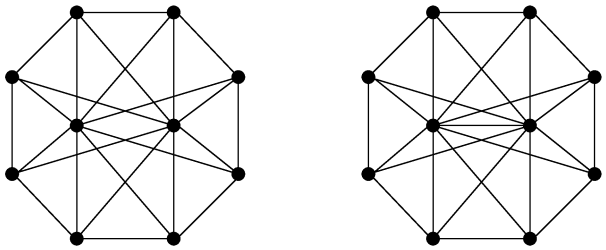

FIGURE 5. Double cones $\overline{K_2} \bigtriangledown C_8$ and $K_2 \bigtriangledown C_8$.

Corollary 10.1. [37] *Suppose H is a k_H-regular graph with perfect state transfer at time $t_H = \frac{\pi}{2} k_H$ and G is an integral graph. Then $G[H]$ has perfect state transfer provided $k_H |V_H| \operatorname{Spec}(G) \subset 4\mathbf{Z}$.*

The n-cube Q_n is a n-regular graph on 2^n vertices which has perfect state transfer at time $n\frac{\pi}{2}$. Thus, for any integral graph G, the composition graph $G[Q_n]$ has perfect state transfer if $n \geqslant 2$.

The *join* $G \bigtriangledown H$ is a graph defined on $V(G) \cup V(H)$ obtained by taking disjoint copies of G and H and by connecting all vertices of G to all vertices of H. The adjacency matrix of $G \bigtriangledown H$ is $\left[\begin{smallmatrix} A_G & J \\ J & A_H \end{smallmatrix}\right]$. The *cone* of a graph G is defined as $K_1 \bigtriangledown G$. The *double cone* of G is $\overline{K_2} \bigtriangledown G$, whereas the *connected double cone* is $K_2 \bigtriangledown G$.

Bose et al. [15] observed that, although K_n does not exhibit perfect state transfer, perfect state transfer is created between any two of its vertices by removing an edge between them. Note that this graph is the double cone $\overline{K_2} \bigtriangledown K_{n-2}$.

The existence of perfect state transfer in a join of two arbitrary regular graphs may be reduced to the existence of perfect state transfer in one of the graphs along with certain structure-independent constraints on the sizes and degrees of the graphs.

Theorem 10.4. [5] *Let G be a m-vertex k_G-regular graph and let H be an n-vertex k_H-regular graph. Let a and b be two vertices in G. Then*

$$\langle b|e^{-iA_{G\bigtriangledown H}t}|a\rangle = \langle b|e^{-iA_G t}|a\rangle + \frac{e^{-ik_G t}}{m}\Big\{e^{it\delta/2}\Big[\cos\Big(\frac{\Delta t}{2}\Big) - i\Big(\frac{\delta}{\Delta}\Big)\sin\Big(\frac{\Delta t}{2}\Big)\Big] - 1\Big\}$$

where $\delta = k_G - k_H$ and $\Delta = \sqrt{\delta^2 + 4mn}$.

This theorem may be applied to the double cones $\overline{K_2} \bigtriangledown G$ and $K_2 \bigtriangledown G$. For a prime p, let $S_p(n)$ denote the largest non-negative integer j so that $p^j | n$.

Corollary 10.2. [5] *For any k-regular graph G on n vertices, $\overline{K_2} \bigtriangledown G$ has perfect state transfer between the two non-adjacent vertices of $\overline{K_2}$ if $\Delta = \sqrt{k^2 + 8n}$ is an integer and $k, \Delta \equiv 0 \pmod 4$ with $S_2(k) \neq S_2(\Delta)$.*

This corollary may be used to answer a question of Godsil [39, Section 10, question (b)]: for $l \geqslant 2$, the double-cone graphs $\overline{K_2} \bigtriangledown (C_{2(2l-1)} + C_{2l+1})$ are nonperiodic and have perfect state transfer. They have mixture of integral and irrational eigenvalues, so they violate the eigenvalue ratio condition, and hence cannot be periodic.

Corollary 10.3. [5] *For any k-regular graph G on n vertices, $K_2 \bigtriangledown G$ has perfect state transfer between the two adjacent vertices of K_2 if $\Delta = \sqrt{(k-1)^2 + 8n}$ is an integer and $k - 1, \Delta \equiv 0 \pmod 8$.*

11. Perfect routing of quantum states

The transfer of quantum states was introduced as a protocol to simplify interaction between distant qubits in a quantum architecture that has locality restrictions, as in solid state systems [71]. The perfect transfer protocols are designed to transfer a quantum state which is input on a given site, onto a specific, corresponding output site. Although it is desirable to assume no interaction with the system, and just let its (fixed) Hamiltonian generate the state transfer, this assumption does not use a vital element of the state transfer protocol—it is implicitly assumed that one is able to introduce the quantum state onto the input node, and remove it from the output node, quickly in comparison to the Hamiltonian dynamics. This additional level of control enables several new features, as recently observed in [72].

We start by considering a one-dimensional system of $3N + 1$ qubits, as depicted in Fig. 6(a), in order to illustrate the basic idea of the construction. The fixed XY Hamiltonian takes the form

$$H = \frac{1}{2} \sum_{\{i,j\} \in E} J_{i,j} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y)$$

where E is the set of edges of the graph depicted in Fig. 6(a) and $J_{i,j} = 1$ unless $\{i, j\} = \{3k, 3k+1\}$ for some k, in which case $J_{i,j} = -1$. Same as in Section 3, the Hamiltonian is spin preserving,

$$\left[H, \sum_{i=1}^{3N+1} \sigma_i^z \right] = 0,$$

and we assume that all spins are initialised in the $|0\rangle$ state. By introducing the state to be transferred on a particular spin, the system is placed in a superposition of 0 and 1 excitations. The 0 excitation subspace is a single state, which is invariant under the Hamiltonian evolution, and we concentrate on the single excitation subspace. The basis states in this subspace are denoted by $|n\rangle = |0\rangle^{\otimes n-1} |1\rangle |0\rangle^{\otimes 3N+1-n}$.

The crucial observation is that, for example, $(|2\rangle + |3\rangle)/2$ is a 0 eigenstate for $(\sigma_2^x \sigma_4^x + \sigma_2^y \sigma_4^y) - (\sigma_3^x \sigma_4^x + \sigma_3^y \sigma_4^y)$, and similarly, $(|2\rangle - |3\rangle)/2$ is a 0 eigenstate for $(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y) + (\sigma_1^x \sigma_3^x + \sigma_1^y \sigma_3^y)$. This means that one can rewrite the basis states as $|\lambda_{3n+1}\rangle = |3n+1\rangle$, $|\lambda_{3n+2}\rangle = (|3n+2\rangle + |3n+3\rangle)/2$, and $|\lambda_{3n+3}\rangle = (|3n+2\rangle - |3n+3\rangle)/2$, leaving the Hamiltonian with a direct sum structure as depicted in Fig. 6(b). Each subsystem is now a uniformly coupled path of length 2 or 3, which achieves perfect transfer in time $\pi/\sqrt{2}$ or $\pi/2$, respectively.

Thus, starting with a state $|\lambda_{3n}\rangle$, after a time $\pi/2$, we obtain $|\lambda_{3n+2}\rangle$ from Hamiltonian dynamics. Now, observe that a fast application of the local rotations (but globally applied) $U = \prod_{i=1}^{N} \sigma_{3n}^z$ converts between states $|\lambda_{3n+2}\rangle$ and $|\lambda_{3n+3}\rangle$, i.e., it transfers the state from one subsystem to the next. Hence, starting from

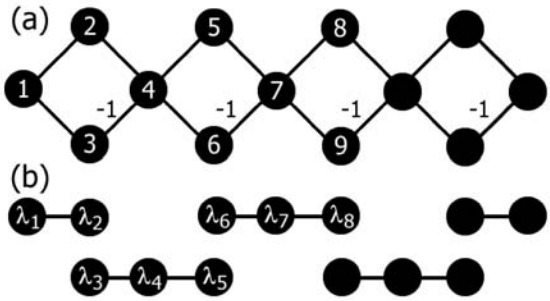

FIGURE 6. (a) A quasi-one-dimensional routing structure. The circles represent qubits, and the lines indicate a coupling between pairs of qubits of strength $+1$, unless -1 is indicated. (b) Under a basis transformation, a simple direct sum structure is apparent. In this case, all coupling strengths are equal to $\sqrt{2}$.

$|\lambda_{3n+2}\rangle$, we apply U every $\pi/2$ and after $|m-n|\pi/2$, we get the state $|\lambda_{3m+2}\rangle$. This achieves the long range transfer, and a few further details given in [71] are needed to show how to convert from the input state, either $|3n+1\rangle$ or $|3n+2\rangle$ to $|\lambda_{3n+2}\rangle$ and back to the output state, with the help of the local magnetic fields.

Thus, we can perfectly propagate a quantum state along the length of the system, between any two vertices in a time proportional to the distance between them. Since the subsystems in Fig. 6(b) are independent, we can actually have multiple excitations in the system provided they are each separated by at least one subsystem. Thus, multiple states can be transferred at once, enabling a transfer rate which is in excess of that achievable in perfect state transfer schemes. These results are easily generalized to two and more dimensions, yielding networks which can perfectly route quantum states from arbitrary vertices in a time linear in the distance to be covered.

Perfect routing of quantum states has also been studied in [30], where it is shown that multiple vertices can faithfully send entanglement through the oscillator hypercube network *at the same time*.

12. Conclusion

Due to the bound in the total length of this article, we have surveyed here the perfect state transfer in uniformly coupled spin networks (simple graphs) only. When one allows non-uniform couplings in the network, such as in the previous section on routing of quantum states, then it is possible, for example, to engineer the couplings such that an arbitrarily long path enables the perfect state transfer between its ends, leading to the notion of quantum wires [27].

Another aspect of perfect state transfer that we did not consider here is its physical implementation. There is a large body of physics literature on this topic, and most of it is listed in references below, so that the interested researcher may find it as a useful start point. The technique of perfect routing of quantum states [30,

71, 72] appears to be especially promising in bringing the quantum state transfer closer to its physical realization.

The problem of the maximum communication distance is very much untouched. The largest known communication distance of $2\log_3 n$ was achieved already for one of the very first perfect state transfer networks, the Cartesian product $P_3^{\otimes d}$ of three-vertex paths [28]. The integral circulants, due to their extremely small diameter $O(\log\log n)$, are unable to provide larger communication distances. The situation is similar with other constructions, which in some cases cannot perform better than to achieve perfect state transfer between vertices at a small constant distance (2 or 3). Thus, it is a main open problem to see whether a larger communication distance, for example, of order $O(\sqrt{n})$, may be achieved.

Among graph compositions, most elegant connection to the perfect state transfer is exhibited by the Cartesian product of graphs, which is a particular case of NEPS. Bernasconi et al. [13] have, with a single unresolved case, managed to characterize perfect state transfer in cubelike graphs, which itself is NEPS of P_2s. Thus, the next interesting question is to find out whether similar conditions will enable perfect state transfer in NEPS of P_3s.

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