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Optimal transfer of a *d*-level quantum state over pseudo-distance-regular networks

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Abstract

In the previous work (Jafarizadeh and Sufiani 2008 *Phys. Rev.* A **77** 022315), by using some techniques such as stratification and spectral distribution associated with the graphs, perfect state transfer (PST) of a qubit (spin $1/2$ particle) over distance-regular spin networks was discussed. In this paper, optimal transfer of an arbitrary *d*-level quantum state (qudit) over antipodes of more general networks called pseudo-distance-regular networks, is investigated. In other words, by using the same spectral analysis techniques and algebraic structures of pseudo-distance-regular graphs, we give an explicit analytical formula for suitable coupling constants in the specific Hamiltonians so that the state of a particular qudit initially encoded on one site will optimally evolve into the opposite site without any dynamical control, i.e., we show how to analytically derive the parameters of the system so that optimal state transfer can be achieved. Also, for the specific form of Hamiltonians that we consider, necessary conditions in order for PST to be achieved are given. Finally, for these Hamiltonians, PST and optimal imperfect ST over some important examples of pseudo-distance regular networks are discussed.

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1. Introduction

The transfer of quantum information, encoded in a quantum state, from one part of a physical unit, e.g., a qubit, to another part is a crucial ingredient for many quantum information processing protocols [2]. There are various physical systems that can serve as quantum channels, one of them being a quantum spin system. Quantum communication over short distances through a spin chain, in which adjacent qubits are coupled by equal strength has been studied in detail, and an expression for the fidelity of quantum state transfer has been obtained [3, 4]. Similarly, in [5], near perfect state transfer was achieved for uniform couplings providing that a spatially varying magnetic field was introduced. After the work of Bose [3], in which the potentialities of the so-called spin chains have been shown, several strategies were proposed to increase the transmission fidelity [6] and even to achieve, under appropriate conditions, perfect state transfer [7–12]. All of these proposals refer to ideal spin chains in which only nearest-neighbor couplings are present. In [7, 8], the d-dimensional hypercube with 2^d vertices has been projected to a linear chain with $d + 1$ sites so that, by considering fixed but different couplings between the qubits assigned to the sites, the perfect state transfer (PST) can be achieved over arbitrarily long distances in the chain. In [1], the so called distance-regular graphs have been considered as spin networks (in the sense that with each vertex of a distance-regular graph a qubit or a spin $1/2$ particle was associated) and PST over them has been investigated, where a procedure for finding suitable coupling constants in some particular spin Hamiltonians has been given so that perfect transfer of a quantum state between antipodes of the networks can be achieved. One of the aims of this paper is to extend this proposal to systems of particles with arbitrary number of levels (particles with arbitrary spin), the so-called qudits. These systems can be appeared in condensed matter and solid state physics such as the fermionic $SU(N)$ Hubbard model [13–15]. In [16], state transfer over spin chains of arbitrary spin has been discussed so that an arbitrary unknown qudit be transferred through a chain with rather good fidelity by the natural dynamics of the chain. In this work, we focus on the situation in which state transfer is optimal, i.e., the fidelity is maximum. Furthermore, we consider more general graphs called pseudo-distance-regular graphs or QD-type graphs [17–19] (distance-regular graphs are special kinds of pseudo-distance-regular ones) as underlying networks and give an analytical formula for optimal coupling constants in the specific Hamiltonians of the systems so that optimal transfer (transfer with maximum fidelity) of an arbitrary d-level quantum state over these networks can be achieved. To reach this aim, we use techniques such as stratification [17, 18, 20–24] and spectral distribution associated with the networks. Then we consider particular hamiltonians with nonlinear terms and give a method for finding an optimal set of coupling constants so that optimal state transfer between the first node of the networks and the opposite one can be achieved. Moreover, we give necessary conditions in order for PST (maximum fidelity attains 1) to be achieved, where it is shown that the pseudo-distance-regular networks with certain symmetry in their QD (Quantum Decomposition) parameters allow PST. More clearly, the networks for which the QD parameters α_i and ω_i satisfy the conditions $\alpha_i = \alpha_{D-i}$ and $\omega_{i+1} = \omega_{D-i}$ for $i = 0, 1, \ldots, D$ (D denotes the diameter of the networks) allow PST, i.e., for these type of networks the optimal fidelity attains its maximum value 1. Because of the fact that in distance regular networks (special case of pseudo-distance-regular networks) the stratification of the networks is reference independent, all of these networks for which the last stratum contains only one vertex have this type of symmetry and so allow PST, as in the previous work [1] has been considered. As examples, we will consider optimal state transfer and PST over some important pseudo-distance-regular networks such as the Tchebichef networks and G_n networks.

The organization of the paper is as follows: in section 2, we review some preliminary facts about graphs and their stratifications, pseudo-distance-regular graphs and spectral distribution associated with them. Section 3 is devoted to optimal transfer of a qudit over antipodes of pseudo-distance-regular networks, where an analytical formula for an optimal set of coupling constants in specific spin Hamiltonians, is given. In section 4, we consider optimal state transfer and PST over some important pseudo-distance-regular networks. The paper is ended with a brief conclusion and two appendices.

2. Preliminaries

In this section we recall some preliminaries related to graphs, their stratifications and the notion of pseudo-distance-regularity (as a generalization of distance regularity) of graphs.

2.1. Graphs and their stratifications

A graph is a pair $\Gamma = (V, E)$, where V is a non-empty set called the vertex set and E is a subset of $\{(\alpha, \beta) : \alpha, \beta \in V, \alpha \neq \beta\}$ called the edge set of the graph. The two vertices $\alpha, \beta \in V$ are called adjacent if $(\alpha, \beta) \in E$, and in that case we write $\alpha \sim \beta$. For a graph $\Gamma = (V, E)$, the adjacency matrix A is defined as

$$(A)_{\alpha,\beta} = \begin{cases} 1 & \text{if} \quad \alpha \sim \beta \\ 0 & \text{otherwise.} \end{cases} \tag{2.1}$$

The degree or valency of a vertex $\beta \in V$ is defined by

$$\kappa(\beta) = |\{\gamma \in V : \gamma \sim \beta\}|, \tag{2.2}$$

where $|\cdot|$ denotes the cardinality. The graph is called regular if the degree of all of the vertices be the same. A finite sequence $\beta_0, \beta_1, \ldots, \beta_n \in V$ is called a walk of length n if $\beta_{i-1} \sim \beta_i$ for all $i = 1, 2, \ldots, n$. Let $l^2(V)$ denote the Hilbert space of C-valued square-summable functions on V. With each $\beta \in V$ we associate a vector $|\beta\rangle$ such that the βth entry of it is 1 and all of the other entries of it are zero. Then, $\{|\beta\rangle : \beta \in V\}$ becomes a complete orthonormal basis of $l^2(V)$, so that the action of the adjacency matrix on $l^2(V)$ can be considered as

$$A|\beta\rangle = \sum_{\alpha \sim \beta} |\alpha\rangle. \tag{2.3}$$

We now we recall the notion of stratification for a given graph Γ. To this end, let $\partial(\beta, \gamma)$ be the length of the shortest walk connecting β and γ for $\beta \neq \gamma$. Now we fix a vertex $\alpha \in V$ as an origin of the graph, called the reference vertex. Then the graph Γ is stratified into a disjoint union of strata (with respect to the reference vertex α) as

$$V = \bigcup_{i=0}^{\infty} \Gamma_i(\alpha), \qquad \Gamma_i(\alpha) := \{\beta \in V : \partial(\beta, \alpha) = i\} \tag{2.4}$$

Note that $\Gamma_i(\alpha) = \emptyset$ may occur for some $i \geqslant 1$. In that case we have $\Gamma_i(\alpha) = \Gamma_{i+1}(\alpha) = \cdots = \emptyset$. With each stratum $\Gamma_i(\alpha)$ we associate a unit vector in $l^2(V)$ defined by

$$|\phi_i\rangle = \frac{1}{\sqrt{\kappa_i}} \sum_{\beta \in \Gamma_i(\alpha)} |\beta\rangle, \tag{2.5}$$

where $\kappa_i = |\Gamma_i(\alpha)|$ is called the ith valency of the graph ($\kappa_i := |\{\gamma : \partial(\alpha, \gamma) = i\}| = |\Gamma_i(\alpha)|$).

2.2. Pseudo-distance-regular graphs

Given a vertex $\alpha \in V$ of a graph Γ, consider stratification (2.4) with respect to α such that $\Gamma_i(\alpha) = \emptyset$ for $i > D$. Then we say that Γ is pseudo-distance-regular [19] around vertex α whenever for any $\beta \in \Gamma_k(\alpha)$ and $0 \leqslant k \leqslant D$ the numbers

$$c_k(\beta) := \frac{1}{\kappa(\beta)} \sum_{\gamma \in \Gamma_1(\beta) \cap \Gamma_{k-1}(\alpha)} \kappa(\gamma), \qquad a_k(\beta) := \frac{1}{\kappa(\beta)} \sum_{\gamma \in \Gamma_1(\beta) \cap \Gamma_k(\alpha)} \kappa(\gamma),$$
$$b_k(\beta) := \frac{1}{\kappa(\beta)} \sum_{\gamma \in \Gamma_1(\beta) \cap \Gamma_{k+1}(\alpha)} \kappa(\gamma) \tag{2.6}$$

do not depend on the considered vertex $\beta \in \Gamma_k(\alpha)$, but only on the value of k. In such a case we denote them by c_k, a_k and b_k, respectively.

In general, as the above definition suggests, the pseudo-distance-regular graphs need not be regular. If a pseudo-distance-regular graph be regular ($\kappa(\beta) = \kappa \equiv \kappa_1$ for all $\beta \in V$), the numbers c_k, a_k and b_k read as

$$c_k = |\Gamma_1(\beta) \cap \Gamma_{k-1}(\alpha)|, \qquad a_k = |\Gamma_1(\beta) \cap \Gamma_k(\alpha)|, \qquad b_k = |\Gamma_1(\beta) \cap \Gamma_{k+1}(\alpha)|, \tag{2.7}$$

where we tacitly understand that $\Gamma_{-1}(\alpha) = \emptyset$.

The notion of pseudo-distance regularity has a close relation with the concept of QD-type graphs introduced by Obata [17] for which we have

$$A|\phi_l\rangle = \sqrt{\omega_{l+1}}|\phi_{l+1}\rangle + \alpha_l|\phi_l\rangle + \sqrt{\omega_l}|\phi_{l-1}\rangle, \qquad l \geqslant 0, \tag{2.8}$$

where the parameters $\omega_{l+1} = \frac{\kappa_{l+1}}{\kappa_l}c_{l+1}^2$ and $\alpha_l = a_l$, for $l \geqslant 0$ are called QD parameters.

One should notice that the vectors $|\phi_i\rangle, i = 0, 1, \ldots, D-1$ form an orthonormal basis for the so-called Krylov subspace $K_D(|\phi_0\rangle, A)$ defined as

$$K_D(|\phi_0\rangle, A) = \mathrm{span}\{|\phi_0\rangle, A|\phi_0\rangle, \ldots, A^{D-1}|\phi_0\rangle\}. \tag{2.9}$$

Then it can be shown that [25], the orthonormal basis $|\phi_i\rangle$ are written as

$$|\phi_i\rangle = P_i(A)|\phi_0\rangle, \tag{2.10}$$

where $P_i(A) = d_0 + d_1 A + \cdots + d_i A^i$ is a polynomial of degree i in indeterminate A (for more details see for example [20, 25]).

It may be noted that the pseudo-distance-regularity is a generalization of the notion of distance-regularity which is defined as follows:

Definition (distance-regular graphs)**.** *A pseudo-distance-regular graph* $\Gamma = (V, E)$ *is called distance-regular with diameter* D *if for all* $k \in \{0, 1, \ldots, D\}$, *and* $\alpha, \beta \in V$ *with* $\beta \in \Gamma_k(\alpha)$, *the numbers* $c_k(\beta)$, $a_k(\beta)$ *and* $b_k(\beta)$ *defined in (2.6) depend only on* k *but do not depend on the choice of* α *and* β.

It should also be noted that the stratification of distance-regular graphs will be independent of the choice of the reference vertex (the vertex with respect to which stratification is done).

2.3. Spectral distribution of the graphs

It is well known that, for any pair $(A, |\phi_0\rangle)$ of a matrix A and a vector $|\phi_0\rangle$, one can assign a measure μ as follows:

$$\mu(x) = \langle\phi_0|E(x)|\phi_0\rangle, \tag{2.11}$$

where $E(x) = \sum_i \left|u_i^{(x)}\right\rangle\left\langle u_i^{(x)}\right|$ is the operator of projection onto the eigenspace of A corresponding to the eigenvalue x. Then for any polynomial $P(A)$ of A one can write

$$P(A) = \int P(x)E(x)\,\mathrm{d}x, \tag{2.12}$$

where for a discrete spectrum the above integrals are replaced by summation. The immediate consequence of the above relations is

$$\langle\phi_0|P(A)|\phi_0\rangle = \int_R P(x)\mu(x)\,\mathrm{d}x, \tag{2.13}$$

Then, using equation (2.10) and orthogonality of the unit vectors $|\phi_i\rangle, i = 0, 1, \ldots, D$ given in equation (2.5), we have

$$\delta_{ij} = \langle\phi_i|\phi_j\rangle = \int_R P_i(x)P_j(x)\mu(x)\,\mathrm{d}x, \tag{2.14}$$

The above relation implies an isomorphism from the Hilbert space of the stratification (the space spanned by $|\phi_i\rangle, i = 0, 1, \ldots, D$) onto the closed linear span of the orthogonal polynomials with respect to the measure μ.

Now, substituting (2.10) into (2.8) and rescaling P_k as $Q_k = \sqrt{\omega_1 \ldots \omega_k} P_k$, the spectral distribution μ will be characterized by the property of orthonormal polynomials $\{Q_k\}$ defined recurrently by

$$Q_0(x) = 1, \qquad Q_1(x) = x - \alpha_0,$$
$$x Q_k(x) = Q_{k+1}(x) + \alpha_k Q_k(x) + \omega_k Q_{k-1}(x), \qquad k = 1, 2, \ldots, D. \tag{2.15}$$

In fact, as has been discussed in [1], the spectral distribution μ can be obtained via the Stieltjes function [26, 27] defined as

$$G_\mu(x) = \frac{Q_D^{(1)}(x)}{Q_{D+1}(x)} = \sum_{l=0}^{D} \frac{\gamma_l}{x - x_l}, \tag{2.16}$$

where the polynomials $\{Q_k^{(1)}\}$ are defined recurrently as

$$Q_0^{(1)}(x) = 1, \qquad Q_1^{(1)}(x) = x - \alpha_1,$$
$$x Q_k^{(1)}(x) = Q_{k+1}^{(1)}(x) + \alpha_{k+1} Q_k^{(1)}(x) + \omega_{k+1} Q_{k-1}^{(1)}(x), \qquad k \geqslant 1, \tag{2.17}$$

x_l's are the simple roots of the polynomial $Q_{D+1}(x)$ and the coefficients γ_l appearing in (2.16) are calculated as

$$\gamma_l := \lim_{x \to x_l} [(x - x_l) G_\mu(x)]. \tag{2.18}$$

Then the spectral distribution can be determined in terms of $x_l, l = 0, 1, \ldots, D$ and the Gauss quadrature constants $\gamma_l, l = 0, 1, \ldots, D$ as

$$\mu(x) = \sum_{l=0}^{D} \gamma_l \delta(x - x_l) \tag{2.19}$$

(for more details see [1, 18, 26, 28, 29]).

According to the above arguments, we have an algorithm for uniquely determining the spectral distribution $\mu(x)$ associated with the networks. It is sufficient to know the QD parameters α_i and ω_i corresponding to the networks; then, the polynomials $Q_D^{(1)}(x)$ and $Q_{D+1}(x)$ are obtained via recursion relations (2.15) and (2.17) so that the Stieltjes function $G_\mu(x)$ is obtained via (2.16). Finally, using equation (2.18) and the fact that x_l's are roots of $Q_{D+1}(x)$, the spectral distribution $\mu(x)$ is uniquely determined via (2.19).

3. Optimal state transfer of a qudit over antipodes of pseudo-distance-regular networks

3.1. State Transfer in d-dimensional Quantum Systems

A d-dimensional quantum system associated with a simple, connected, finite graph $G = (V, E)$ is defined by attaching a d-level particle to each vertex of the graph so that one can associate a Hilbert space $\mathcal{H}_i \simeq \mathcal{C}^d$ with each vertex $i \in V$. The Hilbert space associated with G is then given by

$$\mathcal{H}_G = \otimes_{i\in V} \mathcal{H}_i = (\mathcal{C}^d)^{\otimes N}, \tag{3.1}$$

where $N := |V|$ denotes the total number of vertices (sites) in G.

Then the quantum state transfer protocol involves two steps: initialization and evolution. First, a quantum state

$$|\psi\rangle_A = a_0|0\rangle_A + \sum_{\nu=1}^{d-1} a_\nu|\nu\rangle_A \in \mathcal{H}_A$$

(with $a_\nu \in \mathcal{C}$ and $\sum_{\nu=0}^{d-1}|a_\nu|^2 = 1$) to be transmitted is created. The state of the entire spin system after this step is given by

$$|\psi(t=0)\rangle = |\psi_A\rangle \otimes |0\ldots 00_B\rangle = a_0|0_A\rangle \otimes |0\ldots 00_B\rangle \\ + a_1|1_A\rangle \otimes |0\ldots 00_B\rangle + \cdots + a_{d-1}|(d-1)_A\rangle \otimes |0\ldots 00_B\rangle. \tag{3.2}$$

Then, the network couplings are switched on and the whole system is allowed to evolve under $U(t) = \mathrm{e}^{-\mathrm{i}Ht}$ for a fixed time interval, say t_0.

Now, assume that the Hamiltonian H has a specific form so that $H|0_A\rangle \otimes |0\ldots 00_B\rangle = 0$ and also a state with k excited sites is mapped to another state with excitation at the same number (k) of sites (such as the Hamiltonian given by equation (3.9)). Then, the final state at time t_0 takes the following form:

$$|\psi(t_0)\rangle = a_0|0_A 0\ldots 00_B\rangle + \sum_{\nu=1}^{d-1} a_\nu \left\{\sum_{k=1}^{N} f_{kA}^{(\nu)}(t_0)|0\ldots \underbrace{\nu}_{k\text{th}} 0\ldots 0\rangle\right\}, \tag{3.3}$$

where $f_{kA}^{(\nu)}(t_0) := \langle 0\ldots 0 \underbrace{\nu}_{k\text{th}} 0\ldots 0|\,\mathrm{e}^{-\mathrm{i}Ht_0}|\nu_A 0\ldots 0\rangle$ for $k = 1, 2, \ldots, N$; $\nu = 1, \ldots, d-1$.

In order to perfectly transfer the state $|\psi_A\rangle$ to the site B (in order to achieve PST), the following conditions must be fulfilled

$$\left|f_{AB}^{(\nu)}(t_0)\right| = 1 \qquad \text{for} \quad \nu = 1, 2, \ldots, d-1 \qquad \text{and some} \quad 0 < t_0 < \infty \tag{3.4}$$

which can be interpreted as the signature of perfect communication (or PST) between A and B in time t_0. The effect of the modulus in (3.4) is that state (3.3) will be

$$|\psi(t_0)\rangle = a_0|0_A 0\ldots 0_B\rangle + \sum_{\nu=1}^{d-1} \mathrm{e}^{\mathrm{i}\phi_\nu} a_\nu |0_A 0\ldots 0\rangle \otimes |\nu\rangle_B,$$

so the state at B, after transmission, will no longer be $|\psi\rangle_A$, but will be of the form

$$a_0|0\rangle + \sum_{\nu=1}^{d-1} \mathrm{e}^{\mathrm{i}\phi_\nu} a_\nu |\nu\rangle_B. \tag{3.5}$$

The phase factors $\mathrm{e}^{\mathrm{i}\phi_\nu}$ for $\nu = 1, 2, \ldots, d-1$ are independent of $a_0, \ldots, a_{d-1}$ and will thus be known quantities for the graph, which one can correct with appropriate phase gates.

The model we will consider is a pseudo-distance-regular network consisting of N sites labeled by $\{1, 2, \ldots, N\}$ and diameter D. In [1], we introduced the PST of a qubit in terms of the $SU(2)$ generators. Let us now consider a state with d levels. First, we prepare the generators for $SU(d)$ systems and thereby introduce the Hamiltonians for a qudit system. The generators of $SU(d)$ group may be conveniently constructed by the elementary matrices of d dimension, $\{e_{pq}|p, q \in \{0, 1, \ldots, d-1\}\}$. The elementary matrices are given by

$$(e_{pq})_{ij} = \delta_{ip}\delta_{jq}, \qquad 0 \leqslant i, \quad j \leqslant d-1; \\ e_p := e_{pp}. \tag{3.6}$$

which are matrices with one matrix element equal to unity and all others equal to zero. These matrices satisfy the commutation relation

$$[e_{pq}, e_{rs}] = \delta_{sp}e_{rq} - \delta_{qr}e_{ps}.$$

There are $d(d-1)$ traceless matrices

$$\lambda^{+}_{pq} = e_{pq} + e_{qp},$$
$$\lambda^{-}_{pq} = \frac{1}{i}(e_{pq} - e_{qp}); \qquad 0 \leqslant p < q \leqslant d-1, \tag{3.7}$$

which are the off-diagonal generators of the $SU(d)$ group. The $d-1$ additional traceless matrices

$$H_m = \sqrt{\frac{2}{(m+1)(m+2)}}\left\{\sum_{k=0}^{m} e_k - (m+1)e_{m+1}\right\}; \qquad m = 0, 1, \ldots, d-2 \tag{3.8}$$

are the diagonal generators so that we obtain a total of d^2-1 generators. $SU(2)$ generators are, for instance, given as $\sigma_x = \lambda^{+}_{01} = e_{01} + e_{10}$, $\sigma_y = \lambda^{-}_{10} = -i(e_{01} - e_{10})$ and $\sigma_z = H_0 = e_0 - e_1$.

We now assume that at time $t = 0$, the qudit in the first (input) site of the network is prepared in the state $|\psi_{in}\rangle$. We wish to transfer the state to the *N*th (output) site of the network with unit efficiency after a well-defined period of time. As regards the above argument, we choose the standard basis $\{|i\rangle, i = 0, 1, \ldots, d-1\}$ for an individual qudit and assume that initially all particles are in the state $|0\rangle$; i.e., the network is in the state $|\underline{0}\rangle = |0_A 00\ldots 00_B\rangle$. We then consider the dynamics of the system to be governed by the quantum-mechanical Hamiltonian

$$H_G = \sum_{m=0}^{D} J_m P_m \left(\frac{1}{2}\sum_{i\sim j} \vec{\lambda}_i \cdot \vec{\lambda}_j + \sum_{i=1}^{N} \kappa(i) e^{(i)}_{\alpha} - |E|\left(\frac{d-1}{d}\right) I_{d^N}\right), \tag{3.9}$$

where, $e^{(i)}_{\alpha}$ is the projection operator $I \otimes \ldots \otimes I \otimes \underbrace{e_{\alpha}}_{i} \otimes I \ldots I$ with $e_{\alpha} \equiv e_{\alpha,\alpha} = |\alpha\rangle\langle\alpha|$ defined as in (3.6), $|E|$ is the number of the edges of the graph, $\vec{\lambda}_i$ is a d^2-1 dimensional vector with generators of $SU(d)$ as its components acting on the one-site Hilbert space $\mathcal{H}_i$, J_m is the coupling strength between the reference site 1 and all of the sites belonging to the *m*th stratum with respect to 1, and P_m's are polynomials given in (2.10) which are obtained using three term recursion relations (2.15) and the fact that $P_m = \frac{1}{\sqrt{\omega_1\omega_2\ldots\omega_m}} Q_m$. As is seen from equation (3.9), the terms of the hamiltonian for $m \geqslant 1$ are nonlinear functions of $\sum_{i\sim j} \vec{\lambda}_i \cdot \vec{\lambda}_j$.

In the following we note that the term $H_{ij} := \vec{\lambda}_i \cdot \vec{\lambda}_j$ in hamiltonian (3.9), restricted to the one particle subspace (the subspace of the full Hilbert space spanned by the states with only one site excited), is related to the adjacency matrix of the corresponding graph. To do so, we write H_{ij} as follows:

$$H_{ij} = \sum_{0\leqslant p<q\leqslant d-1} \left(\lambda^{+(i)}_{pq} \otimes \lambda^{+(j)}_{pq} + \lambda^{-(i)}_{pq} \otimes \lambda^{-(j)}_{pq}\right) + \sum_{m=0}^{d-2} H^{(i)}_m \otimes H^{(j)}_m. \tag{3.10}$$

Before we proceed, one should note that we have

$$e^{(i)}_{pq} \otimes e^{(j)}_{rs} = E^{(i,j)}_{(p-1)d+r,(q-1)d+s}, \tag{3.11}$$

where the upper indices (i) and (j) denote the sites which e_{pq} and e_{rs} act on respectively, whereas $E^{(i,j)}_{pq}$ are elementary matrices that act on the d^2 dimensional Hilbert space $\mathcal{H}^{(i)} \otimes \mathcal{H}^{(j)}$. Then, from the fact that

$$\lambda^{+(i)}_{pq} \otimes \lambda^{+(j)}_{pq} + \lambda^{-(i)}_{pq} \otimes \lambda^{-(j)}_{pq} = 2\left(e^{(i)}_{pq} \otimes e^{(j)}_{qp} + e^{(i)}_{qp} \otimes e^{(j)}_{pq}\right),$$

and using the notation

$$(m,n) \equiv m + (n-1)d,$$

one can obtain

$$\sum_{0\leqslant p<q\leqslant d-1}\left(\lambda_{pq}^{+(i)}\otimes\lambda_{pq}^{+(j)}+\lambda_{pq}^{-(i)}\otimes\lambda_{pq}^{-(j)}\right)=2\sum_{0\leqslant p<q\leqslant d-1}\left[E^{(i,j)}_{(q,p),(p,q)}+E^{(i,j)}_{(p,q),(q,p)}\right]. \quad (3.12)$$

We now evaluate the term $\sum_{m=0}^{d-2} H_m^{(i)}\otimes H_m^{(j)}$ in (3.10) in terms of the elementary matrices $E_{pq}^{(i,j)}$ as follows: First, we note that

$$H_m^{(i)}\otimes H_m^{(j)}=\frac{2}{(m+1)(m+2)}\left\{\sum_{p=0}^{m}\sum_{p'=0}^{m}E^{(i,j)}_{(p',p)}\right. \\ \left.-(m+1)\sum_{p=0}^{m}\left[E^{(i,j)}_{(m+1,p)}+E^{(i,j)}_{(p,m+1)}\right]+(m+1)^2E^{(i,j)}_{(m+1,m+1)}\right\}. \quad (3.13)$$

equation (3.13) can be rewritten as follows:

$$H_m^{(i)}\otimes H_m^{(j)}=\left\{\frac{2}{(m+1)(m+2)}\sum_{p=0}^{m}E^{(i,j)}_{(p,p)}+\frac{2(m+1)}{m+2}E^{(i,j)}_{(m+1,m+1)}\right\} \\ +\left\{\frac{2}{(m+1)(m+2)}\sum_{p,p'=0;\,p\neq p'}^{m}E^{(i,j)}_{(p',p)}-\frac{2}{m+2}\sum_{p=0}^{m}\left[E^{(i,j)}_{(m+1,p)}+E^{(i,j)}_{(p,m+1)}\right]\right\}. \quad (3.14)$$

Then one can show that

$$\sum_{m=0}^{d-2}H_m^{(i)}\otimes H_m^{(j)}=2\sum_{p=0}^{d-1}E^{(i,j)}_{(p,p)}-\frac{2}{d}I, \quad (3.15)$$

for proof see appendix A.

Therefore, using (3.12) and (3.15), H_{ij} in (3.10) is written as follows

$$H_{ij}=2\sum_{0\leqslant p<q\leqslant d-1}\left[E^{(i,j)}_{(q,p),(p,q)}+E^{(i,j)}_{(p,q),(q,p)}\right]+2\sum_{p=0}^{d-1}E^{(i,j)}_{(p,p)}-\frac{2}{d}I. \quad (3.16)$$

One should now note that the permutation matrix P_{ij} which permutes the ith and jth qudits, can be written in terms of the elementary basis E_{pq} as

$$P_{ij}=\sum_{p,q=0}^{d-1}E^{(i,j)}_{(p,q),(q,p)}=\sum_{p=0}^{d-1}E^{(i,j)}_{(p,p)}+\sum_{0\leqslant p<q\leqslant d-1}\left[E^{(i,j)}_{(p,q),(q,p)}+E^{(i,j)}_{(q,p),(p,q)}\right]. \quad (3.17)$$

Then equation (3.16) takes the following form:

$$H_{ij}=2P_{ij}\otimes I_{d^{N-2}}-\frac{2}{d}I_{d^N}, \quad (3.18)$$

where, I_{d^N} is a $d^N\times d^N$ identity matrix ($N:=|V|$ is the number of vertices or sites).

Now, we denote a state in which the ith site has been exited to the level ν by $|\nu_i\rangle\equiv|0\ldots\ldots0\underbrace{\nu}_{i}0\ldots0\rangle$. Since the permutation operators P_{ij} do not change the number and type of excited local states ($S^{(\nu)}$ for $\nu=1,2,\ldots,d-1$ are invariant subspaces of P_{ij}), the hamiltonian can be diagonalized in each subspace $S^{(\nu)}$ spanned by the vectors $|\nu_i\rangle$, $i=1,\ldots,N$, for $\nu=1,\ldots,d-1$.

We will refer to the states with only one site excited as one particle states and the subspace spanned by these vectors comprise the one-particle sector of the full Hilbert space. Then the whole one particle subspace S can be written as

$$S=S^{(1)}\oplus S^{(2)}\oplus\cdots\oplus S^{(d-1)}.$$

In other words, in d^N dimensional Hilbert space, we deal with $d-1$ one-particle subspaces (recall that, each of these subspaces has dimension *N*). In the case of state transfer of a qubit ($d=2$), we have only one one-particle subspace of dimension *N*.

Now let $|l^{(\nu)}\rangle \in S^{(\nu)}$ denote the vector state all components of which are 0 except for *l*, i.e., $|l^{(\nu)}\rangle = |00\ldots0\underbrace{\nu}_{l}0\ldots0\rangle$. Then we have

$$\sum_{i\sim j} P_{ij}|l^{(\nu)}\rangle = \left(\sum_{i\sim j,i,j\neq l} P_{ij} + \sum_{i\sim l} P_{il}\right)|l^{(\nu)}\rangle$$
$$= \sum_{i\sim l}|i^{(\nu)}\rangle + (|E| - \kappa(l))|l^{(\nu)}\rangle = \left\{A + |E|I - \sum_{i=1}^{N}\kappa(i)e_\nu^{(i)}\right\}|l^{(\nu)}\rangle$$

One can easily show that the operator $\sum_{i\sim j} P_{ij}$, restricted to the one particle subspace $S^{(\nu)}$, can be related to the adjacency matrix *A* as follows

$$\sum_{i\sim j} P_{ij} = A + |E|I_N - \sum_{i=1}^{N}\kappa(i)e_\nu^{(i)}, \tag{3.19}$$

For regular graphs, where we have $\kappa(i)\equiv\kappa$ for all $i = 1, 2, \ldots, N$, equation (3.19) reads as

$$\sum_{i\sim j} P_{ij} = A + \kappa\left(\frac{N-2}{2}\right)I_N, \tag{3.20}$$

in which we have substituted $|E| = \frac{N\kappa}{2}$.

Then, using (3.18) and (3.19), the hamiltonian in (3.9) restricted to each one-particle subspace $S^{(\nu)}$, for $\nu = 1, 2, \ldots, d-1$, can be written in terms of the adjacency matrix *A* as follows:

$$H_G = \sum_{m=0}^{D} J_m P_m\left(\sum_{i\sim j} P_{ij} - \frac{|E|}{d}I_N + \sum_{i=1}^{N}\kappa(i)e_\nu^{(i)} - |E|\left(\frac{d-1}{d}\right)I_{d^N}\right) = \sum_{m=0}^{D} J_m P_m(A). \tag{3.21}$$

For the purpose of the optimal transference of a qudit, we consider pseudo-distance-regular graphs with $\kappa_D = |\Gamma_D(\alpha)| = 1$, i.e., the last stratum of the graph contains only one site. Then, we try to obtain the coupling constants $J_l, l = 0, 1, \ldots, D$ in such a way that the amplitudes $\langle\phi_i^{(\nu)}|\,\mathrm{e}^{-\mathrm{i}Ht_0}|\phi_0^{(\nu)}\rangle$ for $i = 0, 1, \ldots, D-1$ be minimum and the amplitude $\langle\phi_D^{(\nu)}|\,\mathrm{e}^{-\mathrm{i}Ht_0}|\phi_0^{(\nu)}\rangle$ be maximum. Recall that we have

$$|\phi_0^{(\nu)}\rangle = |\nu0\ldots0\rangle, |\phi_i^{(\nu)}\rangle = P_i(A)|\phi_0^{(\nu)}\rangle; \qquad \nu = 1, 2, \ldots, d-1.$$

One can easily show that the amplitudes $\langle\phi_i^{(\nu)}|\,\mathrm{e}^{-\mathrm{i}Ht_0}|\phi_0^{(\nu)}\rangle$, for $i = 0, 1, \ldots, D$ are independent of the value of ν, i.e., it suffices to evaluate them for one choice of ν, say $\nu = 1$. Then, by choosing $\nu = 1$ and using the spectral analysis techniques, we can write

$$\langle\phi_i^{(1)}|\,\mathrm{e}^{-\mathrm{i}Ht_0}|\phi_0^{(1)}\rangle = \sum_{k=0}^{D}\gamma_k P_i(x_k)\,\mathrm{e}^{-\mathrm{i}t_0\sum_{m=0}^{D}J_m P_m(x_k)}, \qquad i = 0, 1, \ldots, D.$$

Denoting $\mathrm{e}^{-\mathrm{i}t_0\sum_{m=0}^{D}J_m P_m(x_k)}$ by η_k, the above constraints are rewritten as follows:

$$\langle\phi_i^{(1)}|\,\mathrm{e}^{-\mathrm{i}Ht_0}|\phi_0^{(1)}\rangle = \sum_{k=0}^{D} P_i(x_k)\eta_k\gamma_k, \qquad i = 0, 1, \ldots, D. \tag{3.22}$$

For the purpose of optimal state transfer we maximize the amplitude

$$\langle\phi_D^{(1)}|\,\mathrm{e}^{-\mathrm{i}Ht_0}|\phi_0^{(1)}\rangle = \sum_{k=0}^{D} P_D(x_k)\eta_k\gamma_k$$

with respect to the coupling constants $J_l, l = 0, 1, \ldots, D$, so that the probability $|\langle\phi_D|\,\mathrm{e}^{-\mathrm{i}Ht_0}$ $|\phi_0\rangle|^2$ attains its maximum value. To this end, we have

$$\max\left\{\left|\sum_{k=0}^{D} P_D(x_k)\eta_k\gamma_k\right|^2\right\} = \max\left\{\left|\sum_{k=0}^{D} |P_D(x_k)\gamma_k|\,\mathrm{e}^{\mathrm{i}\pi\epsilon_k}\eta_k\right|^2\right\} = \left(\sum_{k=0}^{D}|P_D(x_k)\gamma_k|\right)^2, \tag{3.23}$$

where we have used the fact that the sum of some complex numbers takes its maximum absolute value if all of numbers have the same phase (ϵ_k is 0 or 1 depending on the sign of $P_D(x_k)$). Result (3.23) implies that the optimal quantum state transfer on the pseudo-distance-regular graphs for which the last stratum has one vertex can be achieved with optimal fidelity

$$F_{\mathrm{opt.}} \equiv \max\langle\phi_D|\,\mathrm{e}^{-\mathrm{H}t_0}|\phi_0\rangle = \sum_{k=0}^{D}|P_D(x_k)\gamma_k|, \tag{3.24}$$

which is the same as the average of $P_D(x_k)$ for $k = 0, 1, \ldots, D$.

Now, we are going to give an explicit formula for the optimal coupling constants $J_m, m = 0, 1, \ldots, D$ for which the optimal state transfer can be achieved. To this end we recall that, as the above arguments indicate, the phase factors $\mathrm{e}^{\mathrm{i}\pi\epsilon_k}\eta_k$ in (3.23) must be equal for all $k = 0, 1, \ldots, D$, that is we must have

$$\mathrm{e}^{\mathrm{i}\pi\epsilon_k}\eta_k = \mathrm{e}^{-\mathrm{i}(2t_0\sum_{m=0}^{D} J_m P_m(x_k) - \pi\epsilon_k)} = \mathrm{e}^{\mathrm{i}\phi},$$

or equivalently

$$-2t_0\sum_{m=0}^{D} J_m P_m(x_k) = \phi + (2l_k - \epsilon_k)\pi. \tag{3.25}$$

From the orthogonality relation (2.14) and using (2.19), one can obtain

$$\delta_{ij} = \langle\phi_i|\phi_j\rangle = \sum_{l=0}^{D} P_i(x_l)\gamma_l P_j(x_l) \quad\to\quad \mathrm{P}W\mathrm{P}^t = I \quad\to\quad \mathrm{P}^{-1} = W\mathrm{P}^t, \tag{3.26}$$

where $\mathrm{P}_{ij} := P_i(x_j)$ and $W := \mathrm{diag}(\gamma_0, \gamma_1, \ldots, \gamma_D)$. Therefore, P is invertible and so result (3.25) can be rewritten as

$$(J_0, J_1, \ldots, J_D) = -\frac{1}{2t_0}[\phi + (2l_0 + \epsilon_0)\pi, \phi + (2l_1 + \epsilon_1)\pi, \ldots, \phi + (2l_D + \epsilon_D)\pi](W\mathrm{P}^t), \tag{3.27}$$

or

$$J_k = -\frac{1}{2t_0}\sum_{m=0}^{D}[\phi + (2l_m + \epsilon_m)\pi](W\mathrm{P}^t)_{mk}, \tag{3.28}$$

where l_k for $k = 0, 1, \ldots, D$ are integers which can be chosen arbitrarily. Result (3.28) gives an explicit formula for suitable coupling constants so that optimal state transfer between the first node ($|\phi_0\rangle$) and the opposite one ($|\phi_D\rangle$) can be achieved.

As result (3.24) indicates, if the conditions $P_D(x_k) = \pm 1$ for $k = 0, 1, \ldots, D$ be fulfilled, then the fidelity $F_{\mathrm{opt.}}$ attains its maximum value $\sum_{k=0}^{D}|P_D(x_k)\gamma_k| = \sum_{k=0}^{D}\gamma_k = 1$, i.e., the perfect state transfer takes place. In the appendix B, we use the Christoffel–Darboux identity [26] from the theory of orthoghonal polynomials to show that the condition $P_D(x_k) = \pm 1$ (the necessary condition for PST) is satisfied by the graphs for which the QD parameters are as follows:

$$\alpha_i = \alpha_{D-i}; \qquad \omega_{i+1} = \omega_{D-i}, \qquad i = 0, 1, \ldots, D. \tag{3.29}$$

That is, for the graphs with QD parameters as in (3.29), we have $P_D(x_k) = \pm 1$ and so the optimal fidelity $F_{\text{opt.}}$ is 1.

It should be noted that in the case of distance-regular networks for which the last stratum contains only one vertex, as has been considered in Ref [1], conditions (3.29) are satisfied. This is because of the fact that in distance regular networks stratification is independent of the choice of the reference vertex and so the QD parameters are symmetric in the sense that conditions (3.29) are fulfilled and hence these networks allow PST.

4. Examples

In this section we consider PST and optimal imperfect state transfer over some important pseudo-distance-regular networks.

4.1. An example of a pseudo-distance-regular network with PST

4.1.1. Tchebichef graphs of the second kind. By choosing Tchebichef polynomials of the second kind with scaling factor $1/2^k$ as orthogonal polynomials appearing in recurrence relation (2.15), i.e., $Q_n(x) = 2^{(k-1)n}U_n(x/2^k)$, one can obtain a class of finite and infinite QD graphs of Tchebichef type, with QD parameters $\omega_l = 2^{2(k-1)}, l = 1, 2, \ldots, D; \alpha_l = 0$, $l = 0, 1, \ldots, D$, such that the Stieltjes function can be obtained as [20, 21]

$$G_\mu(x) = \frac{1}{2^{k-1}} \frac{U_D\left(\frac{x}{2^k}\right)}{U_{D+1}\left(\frac{x}{2^k}\right)}.$$

Therefore, the corresponding spectral distributions can be written as

$$\mu(x) = \frac{2}{D+2} \sum_l (-1)^l \sin \frac{(l+1)\pi}{D+2} \sin \frac{(D+1)(l+1)\pi}{D+2} \delta \left(x - 2^k \cos \frac{(l+1)\pi}{D+2} \right).$$

Then x_l's (the roots of the Tchebishef polynomial $Q_{D+1}(x) = \sqrt{2^{D+1}} U_{D+1}(\frac{x}{2^k})$) and the coefficients γ_l are given by

$$\begin{aligned} x_l &= 2^k \cos \frac{(l+1)\pi}{D+2}, \\ \gamma_l &= \frac{2(-1)^l}{D+2} \sin \frac{(l+1)\pi}{D+2} \sin \frac{(D+1)(l+1)\pi}{D+2}, \qquad l = 0, 1, \ldots, D. \end{aligned} \tag{4.1}$$

Therefore, we have $\mathrm{P}_{ij} = U_i\left(\frac{x_j}{2^k}\right) = U_i\left(\cos \frac{\pi(j+1)}{D+2}\right)$ or equivalently

$$\mathrm{P} = \begin{pmatrix} 1 & 1 & \ldots & 1 \\ U_1\left(\cos \frac{\pi}{D+2}\right) & U_1\left(\cos \frac{2\pi}{D+2}\right) & \ldots & U_1\left(\cos \frac{(D+1)\pi}{D+2}\right) \\ \vdots & \vdots & \ldots & \vdots \\ U_D\left(\cos \frac{\pi}{D+2}\right) & U_D\left(\cos \frac{2\pi}{D+2}\right) & \ldots & U_D\left(\cos \frac{(D+1)\pi}{D+2}\right) \end{pmatrix}. \tag{4.2}$$

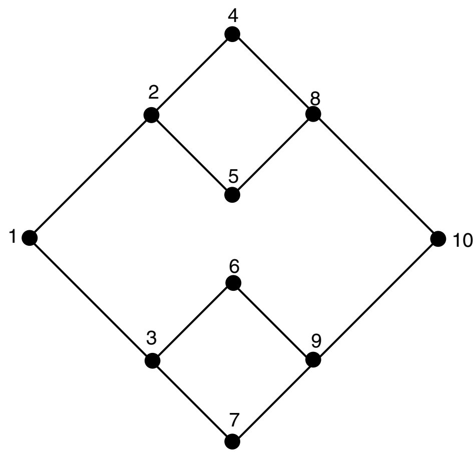

Figure 1. The network G_2.

Furthermore, as is seen from (4.2), the matrix P is a polynomial transformation [31]. By using result (3.28), we obtain

$$J_l = -\frac{1}{2t_0}\sum_{m=0}^{D}\frac{2(-1)^m}{D+2}\sin\frac{(m+1)\pi}{D+2}\sin\frac{(D+1)(m+1)\pi}{D+2} \times [\phi + (2l_m + \epsilon_m)\pi]U_l\left(\cos\frac{(m+1)\pi}{D+2}\right), \tag{4.3}$$

for $l = 0, 1, \ldots, D$.

4.1.2. The special case: the networks G_n. By choosing $k = \frac{3}{2}$ in the above example, we obtain a sequence of networks G_n. The networks G_n presented in [30] consist of two balanced binary trees of height n with the 2^n leaves of the left tree identified with the 2^n leaves of the right tree in the simple way shown in figure 1 (for $n = 2$). The number of vertices in G_n is $2^{n+1} + 2^n - 2$. For the purpose of PST over G_n, we prepare the initial state to be transferred at the left root of the graph and want to calculate the suitable strength coupling constants so that the probability of the presence of the initial state at the right root be equal to 1 for some finite time t_0. One can show that G_n is a pseudo-distance-regular graph with $D+1 = (2n+1)$ strata, where stratum j consists of 2^{j-1} vertices for $j = 1, 2, \ldots, n+1$ and $2^{(2n+1-j)}$ for $j = n+1, \ldots, 2n+1$. Then its QD parameters are

$$\alpha_i = 0, \qquad i = 0, 1, \ldots, 2n; \qquad \omega_i = 2, \qquad i = 1, 2, \ldots, 2n.$$

Now, as result (4.3) implies, in order for PST to be achieved, the coupling constants must be chosen as

$$J_l = -\frac{1}{2t_0}\sum_{m=0}^{2n}\frac{(-1)^m}{n+1}\sin\frac{(m+1)\pi}{2(n+1)}\sin\frac{(2n+1)(m+1)\pi}{2(n+1)} \times [\phi + (2l_m + \epsilon_m)\pi]U_l\left(\cos\frac{(m+1)\pi}{2(n+1)}\right), \tag{4.4}$$

for $l = 0, 1, \ldots, 2n$.

In the following, we consider the case $n = 2$ in detail. In this case, we have

$$x_0 = \sqrt{6}, \qquad x_1 = \sqrt{2}, \qquad x_2 = 0, \qquad x_3 = -\sqrt{2}, \qquad x_4 = -\sqrt{6};$$

$$\gamma_0 = \gamma_4 = \tfrac{1}{12}, \qquad \gamma_1 = \gamma_3 = \tfrac{1}{4}, \qquad \gamma_2 = \tfrac{1}{3}.$$

Then, we have

$$\mathrm{P} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ \sqrt{3} & 1 & 0 & -1 & -\sqrt{3} \\ 2 & 0 & -1 & 0 & 2 \\ \sqrt{3} & -1 & 0 & 1 & -\sqrt{3} \\ 1 & -1 & 1 & -1 & 1 \end{pmatrix} \to$$

$$\mathrm{P}^{-1} = W\mathrm{P}^t = \frac{1}{12}\begin{pmatrix} 1 & \sqrt{3} & 2 & \sqrt{3} & 1 \\ 3 & 3 & 0 & -3 & -3 \\ 4 & 0 & -4 & 0 & 4 \\ 3 & -3 & 0 & 3 & -3 \\ 1 & -\sqrt{3} & 2 & -\sqrt{3} & 1 \end{pmatrix}.$$

Now, using equation (4.3), one can obtain the following suitable coupling constants in order for PST between the most left and the most right nodes to be achieved:

$$J_0 = -\frac{\phi + 2\pi/3}{2t_0}, \qquad J_1 = J_3 = \frac{\pi}{4\sqrt{3}t_0}, \qquad J_2 = -\frac{\pi}{6t_0}, \qquad J_4 = \frac{2\pi}{3t_0}.$$

4.2. Examples of the pseudo-distance-regular networks with optimal imperfect state transfer

4.2.1. Tchebichef graphs of the first kind. By choosing Tchebichef polynomials of the first kind with scaling factor $\frac{1}{2\sqrt{2}}$ as orthogonal polynomials appearing in recurrence relation (2.15), i.e., $Q_n(x) = 2^{n/2+1}T_n(x/2\sqrt{2})$, one can obtain a class of finite and infinite QD graph of Tchebichef type, with QD parameters

$$\omega_1 = 4, \quad \omega_l = 2, \quad l = 2, 3, \ldots, D; \quad \alpha_l = 0, \quad l = 0, 1, 2, \ldots, D$$

(see figure 2 for $D = 5$) such that the Stieltjes function becomes

$$G_\mu(x) = \frac{1}{D+1}\frac{T'_{D+1}\left(\frac{x}{2\sqrt{2}}\right)}{T_{D+1}\left(\frac{x}{2\sqrt{2}}\right)},$$

where T_i's are the Tchebishef polynomials of the first kind. Then the polynomials $P_i(x)$ are given by

$$P_i(x) = \frac{1}{\sqrt{2^{-(i+1)/2}}}Q_i(x) = \sqrt{2}T_i\left(\frac{x}{2\sqrt{2}}\right), \tag{4.5}$$

and x_l's and the coefficients γ_l are given by

$$x_l = 2\sqrt{2}\cos\frac{(2l+1)\pi}{2(D+1)}; \qquad \gamma_l = \frac{1}{D+1}, \qquad l = 0, 1, \ldots, D, \tag{4.6}$$

so that the corresponding spectral distribution can be written as

$$\mu(x) = \frac{1}{D+1}\sum_l \delta(x - 2\sqrt{2}\cos\frac{(2l+1)\pi}{2(D+1)}), \qquad l = 0, 1, \ldots, D.$$

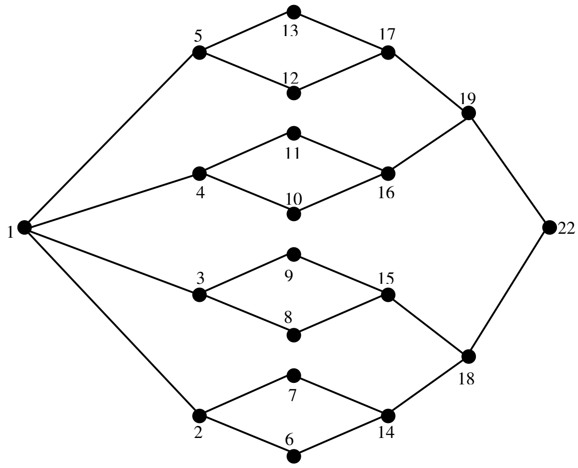

Figure 2. The Tchebichef graph of the first kind with $D = 5$.

From equations (4.5) and (4.6), we have

$$\mathrm{P}_{ij} = \sqrt{2}T_i\left(\cos\frac{(2j+1)\pi}{2(D+1)}\right).$$

Therefore, it is seen that in order to have $P_D(x_k) = \pm 1$ for $k = 0, 1, \ldots, D$, the equalities

$$P_D(x_k) = \sqrt{2}T_D\left(\cos\frac{(2k+1)\pi}{2(D+1)}\right) = \sqrt{2}\cos\frac{D(2k+1)\pi}{2(D+1)} = \pm 1, \qquad \text{for} \quad k = 0, 1, \ldots, D$$

or equivalently

$$\frac{D(2k+1)\pi}{2(D+1)} = (2l+1)\frac{\pi}{4} \quad \rightarrow \quad 2D(2k+1) = (D+1)(2l+1), \qquad \text{for} \quad k = 0, 1, \ldots, D$$

must be fulfilled. The above equalities can not be fulfilled for even D, hence PST can not be achieved for even D. For odd D, the equalities can or can not be satisfied which must be checked in each case. In the following we consider the case $D = 5$ in detail. In this case, we have

$$x_0 = -2, \quad x_1 = 2, \quad x_2 = \sqrt{3}-1, \quad x_3 = -1-\sqrt{3}, \quad x_4 = 1+\sqrt{3}, \quad x_5 = 1-\sqrt{3};$$

$$\gamma_l = \tfrac{1}{6}, \qquad l = 0, 1, \ldots, 5.$$

Then, we have

$$\mathrm{P} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & 1 & \frac{\sqrt{3}-1}{2} & -\frac{\sqrt{3}+1}{2} & \frac{\sqrt{3}+1}{2} & \frac{1-\sqrt{3}}{2} \\ \frac{\sqrt{6}}{2} & 0 & -\frac{\sqrt{6}}{2} & -\frac{\sqrt{6}}{2} & 0 & \frac{\sqrt{6}}{2} \\ 1 & -1 & -1 & 1 & 1 & -1 \\ -\sqrt{2} & -\sqrt{2} & \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \\ 1 & -1 & \frac{\sqrt{3}+1}{2} & \frac{-\sqrt{3}+1}{2} & \frac{\sqrt{3}-1}{2} & -\frac{\sqrt{3}+1}{2} \end{pmatrix}.$$

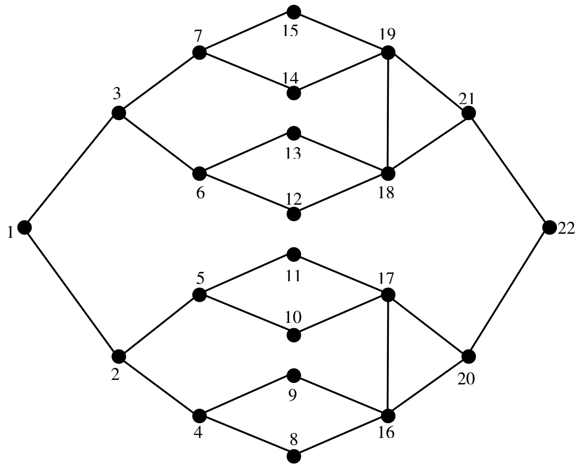

Figure 3. The asymmetric G_n network for $n = 3$.

Since conditions $P_5(x_k) = \pm 1$ for $k = 0, 1, \ldots, 5$ are not satisfied, PST cannot be achieved. By using result (3.28), one can obtain the following optimal coupling constants in order for optimal state transfer between the most left and the most right nodes to be achieved:

$$J_0 = -\frac{2\phi + \pi}{4t_0}, \quad J_1 = \frac{\pi(\sqrt{3} - 1)}{12t_0}, \quad J_2 = J_4 = 0, \quad J_3 = \frac{\pi}{12t_0}, \quad J_5 = \frac{\pi(\sqrt{3} + 1)}{12t_0}.$$

By choosing these coupling constants, we obtain the optimal fidelity of transfer as

$$F_{\text{opt.}} = \sum_{k=0}^{5} |P_5(x_k)\gamma_k| = \frac{1 + \sqrt{3}}{3} \simeq 0.91.$$

4.2.2. Asymmetric G_n networks. Let us modify the G_n networks considered in subsection 4.1 in such a way that the QD parameters do not satisfy conditions (3.29). For example, one can change the QD parameters of the G_n networks as

$$\alpha_{n+1} = 1, \qquad \alpha_i = 0, \qquad i \neq n + 1; \qquad \omega_i = 2, \qquad i = 1, 2, \ldots, 2n.$$

See figure 3 for $n = 3$. Then, the recursion relations (2.15) and (2.17) give us the Stieltjes function and the spectral distribution for any given n (see the equations (2.16) and (2.19)). Since the conditions (3.29) are necessary but not sufficient conditions for PST, so in the networks for which the conditions (3.29) are not satisfied, one should evaluate $P_D(x_k)$ for $k = 0, 1, \ldots, D$.

In the following, we consider some values of n and investigate optimal state transfer over the corresponding asymmetric G_n networks:

The case $n = 2$:

In this case, we have

$$\alpha_3 = 1, \qquad \alpha_i = 0, \qquad i = 0, 1, 2, 4; \qquad \omega_1 = \omega_2 = \omega_3 = \omega_4 = 2.$$

Then the recursion relations (2.15) and (2.17) give us

$$Q_5(x) = x^5 - x^4 - 8x^3 + 4x^2 + 12x, \qquad Q_4^{(1)}(x) = x^4 - x^3 - 6x^2 + 2x + 4$$

so that x_l's (the roots of $Q_5(x)$) and γ_l's are given by

$$x_0 \simeq -2.2724, \quad x_1 \simeq -1.1573, \quad x_2 = 0, \quad x_3 \simeq 1.6295, \quad x_4 \simeq 2.8003;$$
$$\gamma_0 \simeq 0.1370, \quad \gamma_1 \simeq 0.2112, \quad \gamma_2 = \tfrac{1}{3}, \quad \gamma_3 \simeq 0.2868, \quad \gamma_4 \simeq 0.0316.$$

Then, from the fact that $P_{ij} = P_i(x_j) = \frac{1}{\sqrt{\omega_1 \ldots \omega_i}} Q_i(x_j)$, we obtain

$$P \simeq \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ -1.6069 & -0.8183 & 0 & 1.1522 & 1.9801 \\ 1.5820 & -0.3303 & -1 & 0.3276 & 2.9208 \\ -0.9352 & 1.0887 & 0 & -0.7748 & 3.8033 \\ 0.5820 & -1.3303 & 1 & -0.6724 & 1.9208 \end{pmatrix}.$$

Therefore, the conditions $P_4(x_k) = \pm 1$ are not fulfilled and hence PST cannot take place. By using result (3.28), one can obtain the following optimal coupling constants in order for optimal state transfer to be achieved:

$$J_0 \simeq -\frac{\phi/2 + 0.7823}{t_0}, \qquad J_1 \simeq -\frac{0.2474}{t_0}, \qquad J_2 \simeq -\frac{0.03794}{t_0},$$
$$J_3 \simeq -\frac{0.0123}{t_0}, \qquad J_4 \simeq \frac{0.7443}{t_0}.$$

The optimal fidelity of transfer is given by

$$F_{\text{opt.}} = \sum_{k=0}^{4} |P_4(x_k)\gamma_k| \simeq 0.94.$$

The case $n = 3$:

For $n = 3$, as is seen in figure 3, we have

$$\alpha_4 = 1, \qquad \alpha_i = 0, \qquad i = 0, 1, 2, 3, 5, 6; \qquad \omega_1 = \cdots = \omega_6 = 2.$$

Then recursion relations (2.15) and (2.17) give us

$$Q_7(x) = x^7 - x^6 - 12x^5 + 8x^4 + 40x^3 - 16x^2 - 32x + 8;$$
$$Q_6^{(1)}(x) = x^6 - x^5 - 10x^4 + 6x^3 + 24x^2 - 8x - 8.$$

Now, one can obtain

$$x_0 \simeq -2.4684, \quad x_1 \simeq -1.8729, \quad x_2 \simeq -1.0487, \quad x_3 \simeq 0.2390,$$
$$x_4 \simeq 1.1210, \quad x_5 \simeq 2.1060, \quad x_6 \simeq 2.9241;$$
$$\gamma_0 \simeq 0.0707, \quad \gamma_1 \simeq 0.0859, \quad \gamma_2 \simeq 0.2530, \quad \gamma_3 \simeq 0.2609,$$
$$\gamma_4 \simeq 0.1661, \quad \gamma_5 \simeq 0.1534, \quad \gamma_6 \simeq 0.0100.$$

As in the previous case, the eigenvalue matrix P can be evaluated as

$$P \simeq \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1.7454 & -1.3244 & -0.7416 & 0.1690 & 0.7927 & 1.4892 & 2.0676 \\ 2.0466 & 0.7539 & -0.4501 & -0.9714 & -0.3717 & 1.2176 & 3.2751 \\ -1.8268 & 0.3259 & 1.0753 & -0.3332 & -1.0873 & 0.3241 & 4.7039 \\ 1.1419 & -1.1855 & -0.3473 & 0.9151 & -0.4902 & -0.7350 & 6.4509 \\ -0.9739 & 2.0825 & -0.5722 & -0.1592 & 1.0453 & -0.8989 & 4.0726 \\ 0.5510 & -1.5724 & 0.7716 & -0.9420 & 1.3188 & -0.6036 & 1.9697 \end{pmatrix}.$$

Therefore, the conditions $P_6(x_k) = \pm 1$ are not fulfilled and hence PST cannot be achieved. By using (3.28), the optimal coupling constants are obtained as

$$J_0 \simeq -\frac{\phi/2 + 0.7856}{t_0}, \qquad J_1 \simeq -\frac{0.2495}{t_0}, \qquad J_2 \simeq \frac{0.0029}{t_0}, \qquad J_3 \simeq \frac{0.0145}{t_0},$$
$$J_4 \simeq -\frac{0.0379}{t_0}, \qquad J_5 \simeq \frac{0.0009}{t_0}, \qquad J_6 \simeq \frac{0.7435}{t_0}.$$

The optimal fidelity of transfer is given by

$$F_{\text{opt.}} = \sum_{k=0}^{6} |P_6(x_k)\gamma_k| \simeq 0.95.$$

5. Conclusion

Optimal transfer of an arbitrary d-level quantum state over antipodes of pseudo-distance-regular networks was investigated. By using the spectral analysis techniques and algebraic structures of pseudo-distance-regular graphs an explicit formula for optimal coupling constants in the specific Hamiltonians was given so that the state of a particular qudit, initially encoded on one site, can be evolved optimally into the opposite site without any dynamical control. Moreover, for the specific Hamiltonians considered in the paper, the necessary conditions for PST over these networks were given, where it was shown that the networks with certain symmetry in their QD parameters allow PST.

Appendix A

Proof of equation (3.43). By using equation (3.14), we have

$$\sum_{m=0}^{d-2} H_m \otimes H_m = \sum_{m=0}^{d-2} \left\{ \frac{2}{(m+1)(m+2)} \sum_{p=0}^{m} E_{(p+1,p+1)} + \frac{2(m+1)}{m+2} E_{(m+2,m+2)} \right\}$$
$$+ \sum_{m=0}^{d-1} \left\{ \frac{2}{(m+1)(m+2)} \sum_{p,p'=0;\, p\neq p'}^{m} E_{(p'+1,p+1)} - \frac{2}{m+2} \sum_{p=0}^{m} [E_{(m+2,p+1)} + E_{(p+1,m+2)}] \right\}. \tag{A.1}$$

We evaluate the first sum in the above equation, the second one can be evaluated similarly.

$$\sum_{m=0}^{d-2} \left\{ \frac{2}{(m+1)(m+2)} \sum_{p=0}^{m} E_{(p+1,p+1)} + \frac{2(m+1)}{m+2} E_{(m+2,m+2)} \right\}$$
$$= \sum_{m=0}^{d-2} \frac{2}{(m+1)(m+2)} \sum_{p=0}^{m} E_{(p+1,p+1)} + \sum_{m=0}^{d-2} \frac{2(m+1)}{m+2} E_{(m+2,m+2)} = \sum_{p=0}^{0} E_{pd+p+1}$$
$$+ \frac{1}{3} \sum_{p=0}^{1} E_{pd+p+1} + \cdots + \frac{2}{d(d-1)} \sum_{p=0}^{d-2} E_{pd+p+1} + E_{d+2} + \frac{4}{3} E_{2d+3} + \cdots$$
$$+ \frac{2(d-1)}{d} E_{d^2} = E_1 \sum_{m=0}^{d-2} \frac{2}{(m+1)(m+2)} + E_{d+2} \sum_{m=1}^{d-2} \frac{2}{(m+1)(m+2)} + \cdots$$

$$+E_{d^2-d-1}\frac{2}{d(d-1)}+E_{d+2}+\frac{4}{3}E_{2d+3}+\cdots+\frac{2(d-1)}{d}E_{d^2}$$
$$=\sum_{\alpha=0}^{d-1}\left[\frac{2\alpha}{\alpha+1}+2\left(\frac{1}{\alpha+1}-\frac{1}{d}\right)\right]E_{\alpha d+\alpha+1}$$
$$=2(1-1/d)(E_1+E_{d+2}+\cdots+E_{d^2})=2(1-1/d)\sum_{p=0}^{d-1}E_{pd+p+1},$$

where we have used the identity $\sum_{m=\alpha}^{d-2}\frac{2}{(m+1)(m+2)}=2\sum_{m=\alpha}^{d-2}\left(\frac{1}{m+1}-\frac{1}{m+2}\right)=2\left(\frac{1}{\alpha+1}-\frac{1}{d}\right)$.

The second sum in (A.1) can be evaluated as

$$\sum_{m=1}^{d-1}\left\{\frac{2}{(m+1)(m+2)}\sum_{p,p'=0;\,p\neq p'}^{m}E_{(p'+1,p+1)}-\frac{2}{m+2}\sum_{p=0}^{m}[E_{(m+2,p+1)}+E_{(p+1,m+2)}]\right\}$$
$$=-\frac{2}{d}\sum_{p,p'=0;\,p\neq p'}^{d}E_{pd+p'+1}.$$

Therefore, we obtain

$$\sum_{m=0}^{d-2}H_m\otimes H_m=2\sum_{p=0}^{d-1}E_{pd+p+1}-\frac{2}{d}\sum_{p,p'=0}^{d-1}E_{pd+p'+1}=2\sum_{p=0}^{d-1}E_{pd+p+1}-\frac{2}{d}I.$$

□

Appendix B

In this appendix we show that for the pseudo-distance-regular graphs for which the QD parameters satisfy conditions (3.29), we have $P_D(x_k)=\pm1$ and hence the PST over the antipodes of these networks can be achieved. To this end, we use the Christoffel–Darboux identity from the theory of orthogonal polynomials, which is given by

Theorem (Christoffel–Darboux Identity)**.** *Let* $\{Q_n(x)\}$ *satisfy (2.15). Then*

$$\sum_{k=1}^{D}\frac{Q_k(x)Q_k(u)}{\omega_1\omega_2\ldots\omega_k}=(\omega_1\omega_2\ldots\omega_D)^{-1}\frac{Q_{D+1}(x)Q_D(u)-Q_D(x)Q_{D+1}(u)}{x-u}. \tag{B.1}$$

For the proof, the reader is referred to [26].

Now let $u\to x_l$ in the relation (B.1), then we obtain

$$\sum_{k=1}^{D}\frac{Q_k(x)Q_k(x_l)}{\omega_1\omega_2\ldots\omega_k}=(\omega_1\omega_2\ldots\omega_D)^{-1}\frac{Q_{D+1}(x)Q_D(x_l)-Q_D(x)Q_{D+1}(x_l)}{x-x_l}. \tag{B.2}$$

Multiplying two sides of equation (B.2) by $\frac{\gamma_l Q_D(x_l)}{\sqrt{\omega_1\ldots\omega_D}}$ and taking the sum over l, we obtain

$$\sum_{k=1}^{D}\frac{Q_k(x)}{\sqrt{\omega_1\omega_2\ldots\omega_k}}\underbrace{\sum_{l=0}^{D}\frac{Q_k(x_l)\gamma_l Q_D(x_l)}{\sqrt{\omega_1\omega_2\ldots\omega_k}\sqrt{\omega_1\omega_2\ldots\omega_D}}}_{\delta_{kD}}$$
$$=(\omega_1\omega_2\ldots\omega_D)^{-3/2}Q_{D+1}(x)\sum_{l=0}^{D}\frac{\gamma_l Q_D^2(x_l)}{x-x_l},$$

which indicates that

$$\frac{Q_D(x)}{Q_{D+1}(x)} = \sum_{l=0}^{D} \frac{\gamma_l \frac{Q_D^2(x_l)}{\omega_1 \ldots \omega_D}}{x - x_l}. \tag{B.3}$$

The above relation is similar to equation (2.16). If we assume that $Q_D(x) = Q_D^{(1)}(x)$, then we can conclude from relations (B.3) and (2.16) that

$$\frac{Q_D^2(x_l)}{\omega_1 \ldots \omega_D} = 1 \quad \rightarrow \quad Q_D(x_l) = \pm\sqrt{\omega_1 \ldots \omega_D} \quad \rightarrow \quad P_D(x_l) = \pm 1.$$

Now we show that if the QD parameters satisfy conditions (3.29), then the condition $Q_D(x) = Q_D^{(1)}(x)$ is fulfilled. To this end, we recall that

$$\frac{Q_D^{(1)}(x)}{Q_{D+1}(x)} = \frac{1}{x - \alpha_0 - \frac{\omega_1}{x-\alpha_1 - \frac{\omega_2}{x-\alpha_2-\frac{\omega_3}{x-\alpha_3-\cdots}}}}, \tag{B.4}$$

whereas

$$\frac{Q_D(x)}{Q_{D+1}(x)} = \frac{1}{x - \alpha_D - \frac{\omega_D}{x-\alpha_{D-1} - \frac{\omega_{D-1}}{x-\alpha_{D-2}-\frac{\omega_{D-2}}{x-\alpha_{D-3}-\cdots}}}}. \tag{B.5}$$

Then, one can easily see that the above two continued fractions are equal $\left(Q_D(x) = Q_D^{(1)}(x)\right)$ if conditions (3.29) are satisfied.

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