Methods of Control Theory for the Analysis of Quantum Walks on Graphs

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***Abstract*— The goal of this paper is to summarize recent results on the analysis of quantum walks on graphs. These systems are used in quantum information theory as protocols to design quantum algorithms. By taking into account that some model variables can be changed with time, quantum walks can be looked at as control systems and several questions can be posed in control theoretic terms. In particular the set of states that can be reached for these systems can be characterized via controllability analysis. After setting up the model, the main results of the paper characterize the controllability of quantum walks both in algebraic and in combinatorial terms. Several examples are also discussed.**

I. INTRODUCTION

The study of quantum walks has recently developed into a rich and fruitful area of information theory and mathematics. These systems are the quantum counterpart of classical random walks which already have found several applications as tools for computational algorithms as well as models for natural phenomena. It was found in several papers that by considering the quantum counterpart of random walks, one can obtain improved performances, and in particular faster execution and lower complexity. Reviews on quantum walks and their algorithmic applications can be found in [5], [14], [15].

There are several aspects of these systems that are worth being studied, all of them interconnected: the design of better quantum algorithms, the complexity theory of these algorithms, the dynamics of these systems, and their physical implementation. An algorithm on a quantum walk can be looked at as an evolution from one state to a desired one. Moreover several proposed physical implementations (see e.g., [11]) involve parameters that can be changed at every step of the evolution (e.g., the duration of a laser pulse) which can therefore be considered as control variables. In this respect, a control point of view has the potential to make the study of these systems more systematic and embed it in a coherent framework. In this paper, we report on recent progress in this direction.

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There are different versions of quantum walks both continuous and discrete time. The relation between the various models is object of study and, as we shall see, some of our results have impact in connecting the discrete and continuous walks. Some relations among the various types of discrete quantum walks are also discussed in [7], [9]. In this paper we shall consider discrete time quantum walks on graph with coin, a model that will be described in mathematical terms in section II. In section III we give general controllability results for these systems by showing that the set of possible evolutions is a Lie group, with possibly more than one connected component. The calculation of an appropriate Lie algebra determines this group exactly. Although in principle always possible this calculation involves linear algebra manipulations possibly with very large matrices and it may be inefficient. For this reason, we propose combinatorial type of controllability tests in section IV based on the orbits of the set of permutations associated with the walk. In section V, we discuss several examples and special cases of quantum walks on graphs and their controllability. For the sake of brevity we shall refer for the proofs of our results to [2] and [3] which also present further results in particular for what concerns *constructive* controllability algorithms for quantum walks.

II. MODEL OF QUANTUM WALKS WITH COIN ON GRAPH

Let $G := \{V, E\}$ be a graph, where V denotes the set of vertices of cardinality N and E the set of edges. We assume that G is a regular graph and we denote by d its degree. G is also assumed to be connected and without self-loops.

Consider two quantum systems: a *walker system* whose state varies in an N-dimensional space $\mathcal{W}$ (the *walker space*) and a *coin system* whose state varies in a d dimensional space $\mathcal{C}$ (the *coin space*). We denote by $|0\rangle, \ldots, |N-1\rangle$, an orthonormal basis of the walker space $\mathcal{W}$ and by $|c_1\rangle, \ldots, |c_d\rangle$ an orthonormal basis of the coin space $\mathcal{C}$. The meaning of the state $|j\rangle$ is that if we measure the position of the walker we find the position j with certainty. Analogously, the meaning of the state $|c_j\rangle$ for the coin is that the (d-dimensional) coin is giving the result c_j.

With this notation, we define a *coin tossing operation* on $\mathcal{C} \otimes \mathcal{W}$ as an operation of the type

$$C := \sum_{j=0}^{N-1} Q_j \otimes |j\rangle\langle j|, \tag{1}$$

where $Q_j \in U(d)$. This operation applies a unitary evolution to the coin state which is allowed to depend on the current

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walker state. This may be referred as a 'decentralized' model. A 'centralized' model is a model where the coin evolution Q_j does not depend on j, i.e., it is the same for every walker state. In this case, the coin operation, has the form

$$C := Q \otimes \mathbf{1}, \tag{2}$$

where $\mathbf{1}$ is the $N \times N$ identity matrix and Q is a general $d \times d$ unitary matrix, i.e., an element of $U(d)$. Several other cases can be considered in between these two extreme cases. For example, in the search algorithms developed in [6], [20], the coin operation is uniform except at the searched for location(s). This is a way to distinguish the searched for location(s) from the others in the algorithm. We also define a *conditional shift* as an operation

$$S := \sum_{k=1}^{d} |c_k\rangle\langle c_k| \otimes P_k, \tag{3}$$

which applies to a state in $\mathcal{W}$ a permutation P_k depending on the current value of the coin system. In the basis $|c_k\rangle \otimes |j\rangle := e_{kj}$, $k = 1, \ldots, d$, $j = 0, \ldots, N-1$, S has the matrix representation

$$S = \begin{pmatrix} P_1 & 0 & \cdots & 0 \\ 0 & P_2 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & P_d \end{pmatrix}. \tag{4}$$

The conditional shift S has to be compatible with the graph underlying the walk. This means that for every permutation P_i, $i = 1, \ldots, d$, $P_i|j\rangle = |l\rangle$ implies that there exists an edge in the graph G connecting the vertices j and l. Moreover we will also have that for all $|j\rangle$, $i \neq k$ implies $P_i|j\rangle \neq P_k|j\rangle$, which means that different coin results have to induce different transitions on the graph. This requirement also implies that, if there is an edge in G connecting j and l there must be a permutation P_i such that $P_i|j\rangle = |l\rangle$ and a permutation P_k such that $P_k|j\rangle = |l\rangle$. Notice that the sum of the permutations P_i's is the adjacency matrix of the graph.

The state of the quantum walk is described by a vector $|\psi\rangle$ in $\mathcal{C} \otimes \mathcal{W}$, i.e., $|\psi\rangle := \sum_{k=1}^{d} \sum_{j=0}^{N-1} \alpha_{kj} |c_k\rangle \otimes |j\rangle$. The probability of finding the walker in position j, p_j , is found by tracing out the coin degrees of freedom, that is, $p_j = \sum_{k=1}^{d} |\alpha_{kj}|^2$.

The dynamics of the quantum walk is defined as follows. At every step $|\psi\rangle$ evolves as $|\psi\rangle \rightarrow SC|\psi\rangle$, i.e., a coin tossing operation C is followed by a conditional shift S. The coin tossing operation may change at any time step preserving however the structure (1) (or (2)). This leads to a point of view where the operations Q_j in (1) (or Q in (2)) are seen as *control variables* in the evolution of the system. In the following sections we shall study the set of possible evolutions for these systems.

III. CONTROLLABILITY; LIE ALGEBRAIC CHARACTERIZATION

The possible evolutions of a quantum walk are given by the set of all products of the form $\prod_{k=1}^{m} SC_k$ where C_k are arbitrary coin tossing operations of the form (1) (or (2)). We shall denote by $\mathcal{E}$ the set of possible evolutions. In the following we shall concentrate on the decentralized case and point out when similar results hold for the centralized or other cases.

We first set up some definitions. Recall that S being a permutation matrix has a certain order r, such that S^r is the identity on $\mathcal{C} \otimes \mathcal{W}$. Define the set of matrices

$$\mathcal{F} := \{\mathcal{A},\, S\mathcal{A}S^{r-1},\, \ldots,\, S^{r-1}\mathcal{A}S\}, \tag{5}$$

where $\mathcal{A}$ is the set of matrices of the form $\sum_{j=0}^{N-1} A_j \otimes |j\rangle\langle j|$ with $A_j \in u(d)$. The vector space $\mathcal{A}$ with the standard commutation relations is a Lie algebra, which is, in fact, the direct sum of N $u(d)$'s. [1] Let $\mathcal{L}$ be the Lie algebra generated by $\mathcal{F}$ defined as the smallest Lie algebra containing $\mathcal{F}$, and let $e^{\mathcal{L}}$ be the connected Lie group associated with $\mathcal{L}$, that is, the connected component containing the identity. Denote by $\mathbf{G}$ the Lie group generated by $e^{\mathcal{L}}$ and $\{S\}$. This Lie group will in general have various connected components and it has only one connected component if and only if $S \in e^{\mathcal{L}}$. The following result characterizes the controllability of quantum walks.

Theorem 1: The set of possible evolutions of the quantum walk $\mathcal{E}$ is given by

$$\mathcal{E} = \mathbf{G}. \tag{6}$$

Moreover, the quantum walk is completely controllable, i.e., $\mathcal{E} = U(dN)$ if and only if $\mathcal{L} = u(dN)$.

The proof of this result is presented in [3]. The proof can be easily adapted to the centralized case by replacing the generating set $\mathcal{F}$ in (5), with

$$\mathcal{F}_c := \{u(d) \otimes \mathbf{1},\, Su(d) \otimes \mathbf{1}S^{r-1},\, \ldots,\, S^{r-1}u(d) \otimes \mathbf{1}S\}, \tag{7}$$

i.e., replacing the Lie algebra $\mathcal{A}$ in (5) with the Lie algebra $u(d) \otimes \mathbf{1}$. Analogously it also extends to intermediate cases.

In quantum control theory, one considers different notions of controllability [1]. *State controllability* refers to the situation where it is possible to transfer between any two values of the state, and *complete controllability* refers to the situation where it is possible to obtain every unitary transformation (or special unitary transformation) between two states. These two notions are equivalent for quantum systems varying on a vector space of odd dimension but are not necessarily equivalent for systems of even dimension where one can have state controllability without having complete controllability. In the case of quantum walks the dimension of the state space is dN and it follows from the hand-shacking lemma of graph theory (see e.g., [4]) that

$$dN = 2|E|, \tag{8}$$

[1] There are several introductory books on Lie algebras and Lie groups (see e.g., [13], [17], [18]). The book [8] presents introductory notions with a view to applications to quantum systems.

where $|E|$ is the cardinality of the set of vertices. Therefore the dimension of the state space is always even and the distinction between state controllability and complete controllability has to be considered. Nevertheless, for the case of the decentralized walk we can prove that the two properties are equivalent (cf. [3]).

Theorem 2: A decentralized quantum walk is completely controllable if and only if it is state controllable.

The *dynamical Lie algebra* $\mathcal{L}$ plays a crucial role in the characterization of the set of available state transformations with the quantum walk and that is therefore the main object of study in the controllability analysis. This Lie algebra is also relevant in the approximation of continuous quantum walks with discrete ones as it gives the set of possible Hamiltonians that can be simulated on the space $\mathcal{C} \otimes \mathcal{W}$ (cf. [9], [19]). A direct calculation of the dynamical Lie algebra $\mathcal{L}$ from the definition, although in principle always possible, could be quite cumbersome especially in high dimensional cases. In fact one has to calculate many commutators of large matrices. In this calculation one might also loose the intuition about the actual dynamics of the walk. This motivates the treatment of the following section.

IV. COMBINATORIAL TESTS OF CONTROLLABILITY

In this section, we shall characterize the dynamical Lie algebra $\mathcal{L}$, for every quantum walk, in combinatorial terms, i.e., in terms of the permutations P_1,...,P_d characterizing the walk. We are assuming the decentralized case and we shall describe an algorithm which allows us to describe $\mathcal{L}$ in every case. The proof of the validity of this algorithm is given in [3].

Consider the permutations $\{P_1, \ldots, P_d\}$ and recall that r denotes the least common multiple of the order of these permutations. Consider all the pairs $\{P_l, P_m\}$ for $l < m$, and for each pair all the permutations $\mathcal{P}_{lm}^k := P_l^{-k} P_m^k$, for $k = 1, 2, \ldots, r-1$. It is helpful to use the cycle notation for the permutations (see, e.g., [12]) writing a permutation as the product of cycles of various lengths. For example, the permutation $P := (0123)(45)$, performs the transformation $0 \to 1$, $1 \to 2$, $2 \to 3$, $3 \to 0$, $4 \to 5$, $5 \to 4$. Now considering all the permutations $\mathcal{P}_{lm}^k$ and an auxiliary graph with N vertices each corresponding to a vertex of the original graph, we connect vertex j and i if and only if the sequence j, i appears in one of the cycles of the permutations $\mathcal{P}_{lm}^k$. If the resulting auxiliary graph is connected, then $\mathcal{L} = u(dN)$ and the system is completely controllable. If it is not connected, then it will have $s > 1$ connected components of size v_1,v_2,...,v_s, with $\sum_{n=1}^s v_n = N$. The Lie algebra $\mathcal{L}$ is isomorphic (in fact conjugate) to a direct sum of s copies of $su(v_n d)$ and a one dimensional Lie algebra spanned by multiples of the $dN \times dN$ identity, i.e.,

$$\mathcal{L} \simeq su(v_1 d) \oplus su(v_2 d) \oplus \cdots \oplus su(v_n d) \oplus \texttt{span}\{i\mathbf{1}_{dN}\}. \quad (9)$$

In linear algebra terms this means that we can find a similarity transformation to put all the matrices in $\mathcal{L}$ in block diagonal form where there are s blocks of dimensions $v_n d \times v_n d$, $n = 1, 2, \ldots, s$ each assuming an arbitrary value in $u(v_n d)$.

This algorithms allows us, in the decentralized case, to check controllability without calculating Lie brackets. It should be also emphasized that, in typical cases, one needs very few of the permutations $\mathcal{P}_{lm}^k$ to check whether the auxiliary graph is connected or not. Moreover in the case where controllability is not verified the above algorithm describes the structure of the Lie algebra $\mathcal{L}$ from which one can determine whether a certain state transfer is possible. The algorithm is in the same spirit of graph theoretic methods to test controllability such as the ones in [21]. In fact, its proof [3] uses some of the results of [21].

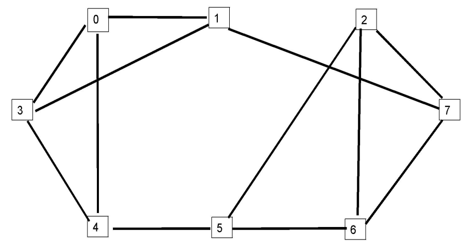

Fig. 1. Example of graph of degree 3 for quantum walk with 8 nodes.

As an example, on the graph of Figure 1, we can consider the walk determined by the three permutations $P_1 := (03172654)$, $P_2 := (01)(25)(34)(67)$, $P_3 := (04562713)$. We can see immediately that the permutation $\mathcal{P}_{12}^1 = (03572614)$ is a full cycle so that the auxiliary graph is connected and the system is controllable.

V. SPECIAL CASES

Some stronger results can be obtained if we consider special cases of graphs. For a *decentralized* quantum walk on a *complete* graph we always have complete controllability.[2] In fact a stronger result can be obtained ([3]).

Proposition 5.1: If $d > \frac{N}{2}$ the quantum walk is completely controllable.

Another interesting case is the one of walks on cycles, i.e., connected regular graphs of degree 2, and their generalizations, periodic lattices in every dimension, which are Cartesian products of cycles. It is possible to prove [3] that there are only three possible cases for quantum walks on the cycle, up to label changing of vertices and or coin:

1) N is odd and $P_1 = P_2^{-1} := (012 \cdots N-1)$.
2) N is even and $P_1 = P_2^{-1} := (012 \cdots N-1)$
3) N is even and $P_1 := (01)(23) \cdots ((N-2)(N-1))$, $P_2 := (12)(34) \cdots ((N-3)(N-2))\,((N-1)0)$

In the first case above the system is always controllable. To see this notice that $\mathcal{P}_{12} = P_1^{-2}$ is a full cycle and therefore

[2] We are assuming here and always $N \geq 3$ to avoid trivial cases.

the auxiliary graph is connected. In the second case however, for every k, $\mathcal{P}_{12}^k = P_1^{-2k}$ is always either the identity or the product of two cycles, each of length $\frac{N}{2}$ and containing, respectively, the odd and even vertices. In the third situation above, $\mathcal{P}_{12}^k := P_1^{-k} P_2^k$ is the identity for k even and for k odd is $\mathcal{P}_{12} = (135 \cdots N-1)(024 \cdots N-2)$. This shows that controllability is never verified in both of the last cases.

The centralized case was considered in [2], [10] and the Lie algebra was described there for cycles and lattices of any dimensions. Lattices are of particular interest. In fact, finding efficient search algorithms on lattices is an open problem in the current research in quantum information theory (see, e.g., [16] for a recent paper). It follows from the results in [2], [10] that these systems are not controllable. However some important state transfers can be achieved. An example is the transfer from a state with probability concentrated in one vertex to a state with uniform probability. The latter state is such that, upon measurement of the walker position, one may obtain any value with equal probability.

VI. CONCLUSIONS AND FUTURE WORK

Quantum walks provide a rich set of models that can be studied with methods of control theory. In particular, the set of states that can be obtained by these systems can be described using the concept of controllability and controllability tests. In this paper we have proposed several controllability conditions for a large class of quantum walk systems. These tests are both of Lie algebraic nature and of combinatorial, graph theoretic, nature. In the future, it will be of interests to extend these controllability conditions to different classes of quantum walks and, at the same time, deepen our understanding on how this dynamical analysis impact the applications of quantum systems. This concerns in particular the design of quantum algorithms.

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