Control by quantum dynamics on graphs

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We address the study of controllability of a closed quantum system whose dynamical Lie algebra is generated by adjacency matrices of graphs. We characterize a large family of graphs that renders a system controllable. The key property is a graph-theoretic feature consisting of a particularly *disordered* cycle structure. Disregarding efficiency of control functions, but choosing subfamilies of sparse graphs, the results translate into continuous-time quantum walks for universal computation.

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I. INTRODUCTION

The study of classical control theory is ubiquitous across engineering disciplines. The concept of controllability at the quantum level is a fundamental notion which expresses the ability of implementing *any* dynamics in a given quantum-mechanical setup (see [1] for an introductory monograph). From the practical point of view, the successful realization of quantum devices for a variety of information processing tasks strongly depends on the ability of manipulating systems with sufficient freedom. The design of protocols to control closed quantum systems mainly deals with schemes for efficient controllability by acting on subspaces [2].

A large number of systems have been shown to exhibit characteristics that allow controllability. For example, almost any pair of Hamiltonians that can be coherently applied to a finite-dimensional quantum system renders it controllable, and almost any quantum logic gate is universal [3]. However, controllability of large systems does not directly give an efficient implementation of control functions and, therefore, processes such as universal quantum computation. Moreover, control criteria are generally not computable for large systems and are not immediately scalable with the system size [4].

Here we consider controllability in relation to a class of dynamics that can be interpreted as Schrödinger evolutions of a particle hopping between the vertices of a graph. The corresponding Hamiltonians are matrices with nonzero entries only where transitions are permitted by the graph structure. This class naturally embraces continuous-time quantum walks (QWs) [5], and the evolution of a single (or multiple [6]) excitation subspace for systems of spin-half particles with various kinds of interaction (e.g., XY, XYZ, etc.) [7]. QWs have been shown to build gates by scattering off a set of small graphs attached to wires representing basis states [8]. QWs give examples of matrices for sufficient control, when we can arbitrarily modify edge weights (or, equivalently, strength of couplings) [9].

During our discussion, an n-level system is *controllable* by a given set of Hamiltonians (possibly acting on specific subsystems only) if every element of the unitary group $U(n)$ can be approximated by the matrices of the subgroup obtained via the dynamical Lie algebra of the set. This general definition is useful to isolate the main difference between the notions of controllability and universality. For instance, global evolution of a spin system may require complex protocols to implement two-qubit gates on distant sites, even if it permits complete controllability.

The specific problem addressed here is the following: we study controllability by the alternate application of two Hamiltonians. One of the Hamiltonians describes a nearest-neighbor interaction defined by some graph. The other Hamiltonian is a projector given by the characteristic vector of a subset of vertices. This describes an interaction between every two spins associated to the elements of the subset.

Our main result is to characterize a large family of graphs that give a pair of Hamiltonians implementing any quantum dynamics, thereby rendering a system controllable (Sec. II). The result can be seen as an analog of the Burgarth-Giovannetti infectivity criterion [10] in this setting involving two Hamiltonians. A comparison with the infectivity criterion, possibly with the use of the notion of zero forcing [11], remains an open question. It is also an open problem to determine the necessity of our condition.

The proofs follow easily from facts of Lie theory and algebraic properties of graphs. The members of this family present a particularly *disordered* cycle structure [12]. Specifically we require that the number of cycles of a certain length, starting from different vertices, cannot be written as a sum of the numbers of smaller cycles. We show that this is a property responsible for controllability when the Hamiltonian is the adjacency matrix of the graph. Indeed, we use powers of the adjacency matrix. These encode the cycles of a graph (see the definition of a walk matrix that follows). In analogy with a known result in quantum control theory of spin systems, the path graph turns out to be arguably the simplest example [1,4]. The setting is directly equivalent to a single excitation evolving on an XY spin chain with constant couplings (here XY means $XX + YY$, *à la* Bose [13]). The path is a connected graph with a minimal number of edges; therefore, it corresponds to a very sparse Hamiltonian. This is a fact that should be taken into account, since sparse Hamiltonians can be simulated efficiently in a quantum computer [14].

In general, if we focus only on the dynamics restricted to the n-dimensional subspace, the physical device for implementation consists of any machine realizing QWs (e.g., an optical waveguide lattice [15]). While we do not modify the circuitry for different tasks, an external clock is necessary, since we need to know the time of application of each Hamiltonian, even if the resulting operation is just a phase factor. We give evidence that our property is almost certain (Sec. II). This is parallel to the fact that almost every (generic) Hamiltonian gives sufficient control. For many types of graphs, the construction of an infinite family with a typical property may not be straightforward (e.g., expanders, small-diameter graphs, etc.). We present a method to construct infinite families of graphs (without special constraints) that satisfy our required property (Sec. III).

The results of the paper may translate into valuable information in the perspective of designing schemes for scalable quantum computation via local control (e.g., help in the selection of the systems, the engineering of control functions, etc.; see [2,4] for extended treatments of this topic). From a wider angle, the results consist of a step toward a better and more general understanding of quantum evolution on networks. Additionally, we introduce concepts that propose an interface between control theory and graph theory. Section II contains the general result, examples are given in Sec. III, and we draw some brief conclusions and state open problems in Sec. IV.

II. CONTROLLABILITY

Let $X = (V(X),E(X))$ be a (simple) *graph* with a set of n vertices $V(X)$ and a set of edges $E(X) \subseteq V(X) \times V(X) - \{\{i,i\} : i \in V(X)\}$. The *adjacency matrix* of X, denoted by $A(X)$, is an $n \times n$ matrix with $A(X)_{i,j} = 1$ if $\{i,j\} \in E(X)$ and $A(X)_{i,j} = 0$, otherwise. The walk matrix of a graph contains information about its cycle structure [16]. Let X be a graph on n vertices and let $z \in \mathbb{R}^n$. We define and denote by $W_z(X) = (z\ A(X)z \cdots A(X)^{n-1}z)$ an $n \times n$ matrix with entries in $\mathbb{Z}^{\geqslant 0}$ associated to X. When z is the characteristic vector of some set $S \subseteq V(X)$, the matrix $W_z(X)$ is called a *walk matrix* of X with respect to S. In this case, we may write $W_S(X)$ instead of $W_z(X)$. Let X be a graph on n vertices and let $z \in \mathbb{R}^n$. The pair (X,z) is said to be *controllable* if the matrix $W_z(X)$ is invertible [i.e., $\det(W_z(X)) \neq 0$]. When z is the characteristic vector of some set $S \subseteq V(X)$, we may write (X,S) instead of (X,z). The definition of a controllable graph arises as a special case of a controllable pair. Let X be a graph and let $\mathbf{1}$ be the all-ones vector. This is also the characteristic vector of $V(X)$. The graph X is said be controllable if $(X,\mathbf{1})$ [or, equivalently, $(X,V(X))$] is controllable.

Let us recall that a *walk of length* l in a graph X is a sequence of vertices $1,2,\ldots,l,l+1$, such that $\{i,i+1\} \in E(X)$, for every $1 \leqslant i \leqslant l$. The ijth entry of the walk matrix, $[W_{\mathbf{1}}(X)]_{i,j} = \sum_{j=1}^{n} A_{i,j}^{l-1}(X)$, counts the number of all walks of length $l-1$ from vertex i. Let $d(i) := |\{j : \{i,j\} \in E(X)\}|$ be the *degree*of a vertex i. A graph X is *regular* if $d(i)$ is constant over $V(X)$. Notice that a controllable graph cannot be regular. In fact, the walk matrix of a regular graph has rank 1, because $\mathbf{1}$ is one of its eigenvectors. One can verify by exhaustive search that there are no controllable graphs on $n \leqslant 5$ vertices. Figure 1 contains drawings of all connected (nonisomorphic) controllable graphs on six vertices.

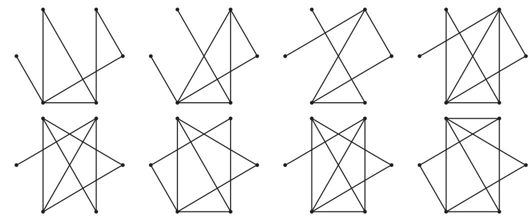

FIG. 1. Drawings of all connected nonisomorphic controllable graphs on six vertices. The vector $(d(i) : i \in V(X))$ is the *degree sequence* of X. The degree sequences of these graphs are particularly *irregular*. Top row, from left to right: (1,2,2,2,3,4), (1,1,2,3,3,4), (1,1,2,2,3,3), and (1,2,2,3,4,4). Bottom row, from left to right: (1,2,2,3,3,3), (2,2,2,3,3,4), (1,2,3,3,3,4), and (2,2,3,3,4,4). There are exactly 8, 85, and 2275 (connected) controllable graphs on 6, 7, and 8 vertices, respectively.

Numerics show that the ratio (number of graphs)/(number of controllable graphs) decreases with n (see caption of Fig. 1 for small examples). We expect that, asymptotically, almost surely every graph is controllable, also considering that the automorphisms fixing the vertices of a controllable graph are trivial.

A *(continuous-time) quantum walk* on a graph X, starting from a state $|\psi_0\rangle \in \mathbb{C}^n$, is the process induced by the rule $U_{M(X)}(t)|\psi_0\rangle \mapsto |\psi_t\rangle$, where $U_{M(X)}(t) := e^{-iM(X)t}$ $(t \in \mathbb{R}^+)$ and $M(X)$ is a symmetric matrix with nonzero entries corresponding to the edges of X (e.g., adjacency matrix, combinatorial Laplacian, etc.). A probability distribution supported by $V(X)$ is obtained by performing a projective measurement on the state $|\psi_t\rangle$. The matrix $M(X)$ can also be seen as governing the dynamics of a system of spin-half particles restricted to a single excitation subspace. The dimension of such a subspace is in fact n. Here we work with adjacency matrices only, but the results described are valid for any symmetric matrix. Studies of perfect state transfer and entanglement transfer in spin systems are often carried out with respect to this restriction [7]. QWs and their discrete analogs (e.g., coined quantum walks, scalar quantum walks, etc.) have found a number of algorithmic applications. The reviews [5] give a detailed perspective on this and related topics.

When choosing Hamiltonians of the form of $M(X)$, the question to ask about controllability is the following: can we obtain any quantum dynamics on an n-level system by performing repeated applications of QWs? Moreover, how much can we limit our resources (e.g., number of non-null interactions, number of different Hamiltonians, etc.)? In particular, can we use just a single QW (i.e., a fixed graph) plus an extra operation acting on a subspace of a relatively small dimension? The last question is linked to core questions in quantum control theory, where we are interested in driving global dynamics by directly modifying only a limited portion of the system under a parsimony criterion. In the quantum-mechanical setup, controllability occurs together with the ability of constructing with reasonable accuracy any unitary matrix of the appropriate dimension (see Chap. 3 of [1]). The corresponding property is expressed if we guarantee density in $U(n)$ of the group of unitaries realized as sequences of QWs. Lemma 1 describes a relation between controllable pairs and Lie algebras.

Lemma 1. Let X be a graph and let z be the characteristic vector of a set $S \subseteq V(X)$. Let us define the symmetric (0,1)-matrix $L = zz^T$. If (X,S) is a controllable pair then the real Lie algebra generated by the matrices $A(X)$ and L is $\mathrm{Mat}_{n\times n}(\mathbb{R})$, the algebra of all $n \times n$ real matrices. The real Lie algebra generated by $iA(X)$ and iL is the vector space of all skew-Hermitian matrices.

Proof. We prove by induction on k that the Lie algebra generated by $A = A(X)$ and L contains the matrices $A^{k-i}LA^i$, with $i = 0,\dots,k$. The first claim in the lemma follows at once from this. We note that there are integers c_r such that $LA^rL = c_rL$. If our Lie algebra contains the matrices $A^{k-i}LA^i$, then it contains the Lie products $A^{k+1-i}LA^i - A^{k-i}LA^{i+1}$, with $i = 0,\dots,k$, and the partial sums $A^{k+1-i}LA^i - LA^{k+1}$, for all i. In particular, it contains $A^{k+1}L - LA^{k+1-i}$ and, therefore, also

$$LA^{k+1}L - L^2A^{k+1} - A^{k+1}L^2 + LA^{k+1}L = 2c_{k+1}L - c_0(A^{k+1}L + LA^{k+1})$$

for all i. From this, it follows that it contains LA^{k+1} and, therefore, all the monomials $A^{k+1-i}LA^i$. Let us now consider the second claim of the lemma. We say a matrix is a *commutator of degree* $r+1$ if it can be written as $AX - XA$ or $LX - XL$ for some commutator of degree r, where the commutators of degree zero are the matrices in the span of A and L. Since A and L are symmetric, we see that all commutators of even weight are symmetric and all commutators of odd weight are skew-symmetric. The intersection of the space of symmetric matrices with the space of skew-symmetric matrices is the zero subspace, from which we deduce that the even-weight commutators span the space of real symmetric matrices and the odd-weight commutators span the space of skew-symmetric matrices. This implies that the even-weight commutators in iA and iL span the space of skew-symmetric matrices, with dimension $(n^2-n)/2$, while the odd-weight commutators span a complementary space of dimension $(n^2+n)/2$. This proves our second claim. ∎

We remark that it is not hard to show that the matrices

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

generate $\mathrm{Mat}_{2\times 2}(\mathbb{R})$, but the real Lie algebra they generate is $\mathfrak{sl}(2,\mathbb{R})$ rather than $\mathfrak{gl}(2,\mathbb{R})$. Lemma 1 is reminiscent of the Lie algebra rank condition in quantum control theory. The following result gives a sufficient condition to render a system controllable by a QW.

Theorem 1. Let X be a graph and let z be the characteristic vector of a set $S \subseteq V(X)$. If (X,S) is a controllable pair then the unitary matrices $U_{A(X)}(s) = e^{-iA(X)s}$ and $U_L(t) = e^{-iLt}$, $s,t \in \mathbb{R}^{\geqslant 0}$, generate a dense subgroup of the unitary group $U(n)$, $n \geqslant 2$.

Proof. Let G be the closed subgroup generated by the given elements. Then it is a Lie subgroup of $U(n)$, and its tangent space is the Lie algebra generated by $iA(X)$ and iL. Since X is controllable, by Lemma 1, this Lie algebra is the space of all skew-Hermitian matrices, which is the tangent space to the unitary group $U(n)$. It follows that $G = U(n)$. ∎

If $S = V(X)$ then $z = \mathbf{1}$ and the Hamiltonian $L = J$, the all-ones matrix. For its unitary, we have $U_J(t)_{k,l} = \frac{1}{n}(n + e^{-int} - 1)$ if $k = l$ and $U_J(t)_{k,l} = \frac{1}{n}(e^{-nit} - 1)$ otherwise. In fact, $U_M(t)$ is a polynomial in M with degree at most the degree of the minimal polynomial of M. Among adjacency matrices, this is the *fullest* possible Hamiltonian. Its implementation has been discussed in several works [17]. The matrix $U_J(t)$ is essentially the same as the Grover operator used in quantum search algorithms [18]. Turning our attention to different characteristic vectors, we can prove a similar result concerning the path graph. We denote by P_n the path of length $n-1$, that is, the graph on n vertices $\{1,2,\dots,n\}$ and edges $\{1,2\},\{2,3\},\dots,\{n-1,n\}$ (where 1 and n are called *end vertices*). Weighted paths are often used to model one-dimensional (1D) spin chains. A control criterion concerning the global space of 1D spin chains has been isolated in [4]. Controllability of these systems and scalable quantum computation has also been discussed in [4].

Corollary 1. Let P_n be the path on n vertices. The unitary matrix $U_{A(P_n)}(s) = e^{-iA(P_n)s}$ together with the diagonal unitary matrix $U_{e_1e_1^T}(t) = e^{-ie_1e_1^Tt} = [e^{-it},1,\dots,1]$, $s,t \in \mathbb{R}^{\geqslant 0}$, where $e_1 = (1,0,\dots,0)^T$ generates a dense subgroup of the unitary group $U(n)$, with $n \geqslant 2$.

Proof. We need to prove that $W(P_n) = (e_1 \;\; A(P_n)e_1 \cdots A(P_n)^{n-1}e_1)$ is invertible. Observe that the first entry of the vector $A^l(P_n)e_1$ is a Catalan number $C_{l/2} = \frac{2}{l+2}\binom{l}{l/2}$ if l is even and zero otherwise; the second entry behaves similarly, with $C_{(l+1)/2} = \frac{2}{l+3}\binom{l+1}{(l+1)/2}$, but for l odd [19]. For example, the first two rows of $W(P_7)$ are (1,0,1,0,2,0,5) and (0,1,0,2,0,5,0). Moreover, the matrix $W(P_n)$ is upper triangular. Since $C_k \succ \sum_{i=0}^{k} C_i$, for every $k \geqslant 3$, it follows that the rows of $W(P_n)$ are linearly independent. ∎

III. EXAMPLES

Given $S \subseteq V(X)$, the *cone* of X relative to S is the graph $\widehat{X}_S$ such that $V(\widehat{X}_S) = V(X) \cup \{0\}$, for a new vertex 0, and $E(\widehat{X}_S) = E(X) \cup \{\{0,i\} : i \in S\}$. We denote by $X\backslash i$ the graph obtained from X by deleting the vertex i and all its incident edges.

Theorem 2. Given a graph X and a vertex $1 \in V(X)$, the pair $(\widehat{X}_1,\{0\})$ is controllable if $(X,\{1\})$ is.

Proof. We show that if $u \in V(Z)$ for some graph Z, then $(Z,\{u\})$ is controllable if and only if the characteristic polynomials (of the adjacency matrices) $\phi(Z,t)$ and $\phi(Z\backslash u,t)$ are coprime. From the properties of $\widehat{X}_1$, one can prove that $\phi(\widehat{X}_1,t) = t\phi(X,t) - \phi(X\backslash 1,t)$. From this, we deduce that if $\phi(X,t)$ and $\phi(X\backslash 1,t)$ are coprime then so are $\phi(\widehat{X}_1,t)$ and $\phi(X,t)$. Now we derive our characterization of controllability. Assume $n = |V(X)|$. Let e_1 be the first vector of the standard basis, and let E_θ denote the idempotent in the spectral decomposition of $A = A(X)$ that corresponds to θ (see [20], pp. 186–187); it follows that

$$\frac{\phi(X\backslash 1,t)}{\phi(X,t)} = [(tI - A)^{-1}]_{1,1} = \sum_\theta (t-\theta)^{-1} e_1^T E_\theta e_1.$$

We observe that the number of poles in the rational function here is equal to the number of eigenvalues θ such that

$e_1^T E_\theta e_1 \neq 0$; in other words, it is equal to the number of eigenvalues θ such that the projection $E_\theta e_1 \neq 0$. Note also that this number is n if and only if $\phi(X,t)$ and $\phi(X\backslash 1,t)$ are coprime. To complete the argument, consider the walk matrix $W_{e_1}(X)$. By spectral decomposition (again), $A^r e_1 = \sum_\theta E_\theta e_1$, from which it follows that the column space of $W_{e_1}(X)$ lies in the span of the nonzero vectors $E_\theta e_1$. Since each projection E_θ is a polynomial in A, we conclude that rk(W) is equal to the number of eigenvalues θ of X such that $E_\theta e_1 \neq 0$. This proves our characterization. ■

A method based on the theorem can be used to construct infinite families of controllable graphs, as follows.

Corollary 2. Let (X,S) be a controllable pair. If Y is the graph obtained by joining one end vertex of the path to each vertex in S, then Y is controllable.

IV. CONCLUSIONS

We have considered controllability and QWs. As a technical tool, we have introduced the combinatorial notion of a controllable pair. A graph and a subset of its vertices form a controllable pair, when the structure of the graph exhibits a certain type of disorder. The disorder is expressed by the cycle structure of the graph, encoded in the entries of powers of the adjacency matrix. We have proved that a QW involving a such a pair renders a system controllable. By this result, we can *in principle* perform universal quantum computation as an alternating sequence of QWs on two graphs, or on the same graph, but interspersed with phase factors. Including fault tolerance in this picture would encounter hard obstacles because of the sensitivity to phenomena linked to decoherence and Anderson localization [21]. An issue related to the more abstract aspects is the lack of transparency when trying to design algorithms with a logic that requires operations on specific subsystems. We conclude by stating four problems:

1. Let G be a subgroup of $U(n)$ which fixes $|\psi\rangle \in \mathbb{C}^n$ ($n \geqslant 3$) and let $V \in U(n) - G$. Then, the group $\langle G, V\rangle$ [i.e., the subgroup of $U(n)$ generated by G and V] is dense in $U(n)$ (see, e.g., Lemma 20 in [22]). Is there an analog to this statement for dynamical Lie algebras generated by adjacency matrices? In particular, let z be the characteristic vector of $S \subseteq V(X)$ and let P be a permutation matrix corresponding to an automorphism of X. When $Pz = z$, it follows that $PW_S(X) = W_S(X)$ and then $P = I$ because $\det(W_S(X)) \neq 0$. This means that the automorphisms of X fixing S are trivial if (X,S) is controllable. Is this the most general condition for controllability?

2. Can we lift the combinatorial criterion for controllability introduced in this paper to general criteria for controllability of spin systems?

3. In the study of controllability by adjacency matrices, when the time of application of each Hamiltonian is constrained, determining relations between quantum control by nearest-neighbor interaction on graphs and classical simulatability of the associated dynamics is an open problem.

4. What can be said about controllability by acting only on a connected induced subgraph? If the number of vertices is constrained, the optimum may be difficult to compute. This would be parallel to the Burgarth-Giovannetti criterion, whose optimum is difficult even to approximate [23].

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