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Analysis of quantum walks with time-varying coin on *d*-dimensional lattices

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In this paper, we present a study of discrete time quantum walks whose underlying graph is a *d*-dimensional lattice. The dynamical behavior of these systems is of current interest because of their applications in quantum information theory as tools to design quantum algorithms. We assume that, at each step of the walk evolution, the coin transformation is allowed to change so that we can use it as a *control variable* to drive the evolution in a desired manner. We give an exact description of the possible evolutions and of the set of possible states that can be achieved with such a system. In particular, we show that it is possible to go from a state where there is probability 1 for the walker to be found in a vertex to a state where all the vertices have equal probability. We also prove a number of properties of the set of admissible states in terms of the number of steps needed to obtain them. We provide explicit algorithms for state transfer in low dimensional cases as well as results that allow to reduce algorithms on two-dimensional lattices to algorithms on the one-dimensional lattice, the cycle. © *2009 American Institute of Physics.*
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I. INTRODUCTION

Quantum walks are the quantum generalization of random walks and they are amenable of similar applications. In particular, they can be used as computational tools as well as mathematical models in several areas such as biology, physics, economics, etc. They are also a common model for general transport processes[3] and offer a paradigm to design quantum algorithms.[1,16,17] Quantum walks are of two types: continuous and discrete time. Given an undirected graph, a continuous time quantum walk is implemented as a quantum system which evolves according to an Hamiltonian H that respects the structure of the graph, i.e., $H_{jk} \neq 0$ if and only if there is an edge in the graph connecting the jth and kth vertices. The implementation of a discrete quantum walk requires the coupling of two quantum systems, a *walker system* and a *coin system*. An orthonormal basis of the Hilbert space associated with the walker (coin) system is in one to one correspondence with the vertices of the underlying graph, i.e., the positions of the walker (the directions of motion on the graph, i.e., the coin results). [As we will describe more in detail in Sec. II, this model requires the underlying graph to be regular. A different more general (decentralized) model can be given where the coin operation may depend on the walker position (see, e.g., Refs. 6 and 8 for the relation between the two models). We shall not consider this more general model here.] Each step of the evolution consists of an operation on the coin system followed by a conditional shift on the walker system, that is, an operation which changes the state of the walker according to the current state of the coin (following an edge of the underlying graph). This paper focuses on discrete time quantum walks (DTQWs).

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In many applications of quantum walks, one would like to obtain some desired dynamics. For example, one would like to transfer the state of the total system from a value where there is certainty to find the walker in a given position in the graph to a state where all the positions have the same probability. There are many types of problems in the literature, in many areas, which can be formulated as a state-to-state transfer control problem. To cite only one example, the quantum phase transition in an optical lattice treated in Ref. 5 can be formulated in this fashion. In practical implementations of quantum walks, one has some degree of freedom which can be used as control. For example, in DTQWs one can choose, at every step, the coin operation. This is the scenario we will consider here.

In this paper we shall present an analysis of DTQWs on d-dimensional lattice and, in particular, we shall explore the dynamical consequences of allowing a possible change in the coin dynamics. Quantum walks on d-dimensional lattices have been considered before in the context of quantum algorithms.[2,18] In particular, they were used to implement search algorithms on lattices. Some of the results we shall present are generalizations of the results presented for the case of the cycle ($d=1$) in Ref. 9.

In Sec. II, we discuss more in depth the mathematical model of DTQWs. We point out where the control variables appear and motivate this experimentally. We then specialize the graph underlying the walk to a d-dimensional lattice with periodic boundary condition and set up the notations used in the following sections. Since this graph is the Cartesian product of d cycles, the simple quantum walk on the cycle will play a prominent role. In Sec. III we start a study of the controllability of this model by calculating the dynamical Lie algebra (cf. Ref. 7) and therefore the set of all the unitary evolutions that can be achieved with this system. Having obtained the set of possible evolutions we then derive a description of the available states in Sec. IV. Instrumental in this treatment is a change in coordinates which amounts to a discrete Fourier transform. We prove, in particular, that it is always possible to go from a state where the probability of finding the walker is concentrated in one vertex to a state where all have the same probability. We prove some properties of the reachable sets in terms of the number of steps of the evolution in Sec. V. In Sec. VI, we give explicit algorithms for control for some low dimensional cases. These algorithms are optimal in the sense that they require the minimum number of steps. We also describe a general strategy which allows us to reduce a problem of control for a two-dimensional lattice to the one-dimensional case. In Sec. VII we discuss our results and indicate further research on these models.

II. MODEL DESCRIPTION; DTQWS ON *d*-DIMENSIONAL LATTICES

Consider an undirected regular graph $G:=\{V,E\}$ with a set of vertices V and a set of edges E. Let m denote the degree of the graph G. A DTQW on G is implemented with two quantum systems, a *walker system* whose associated Hilbert space $\mathcal{H}$ has dimension $|V|$ and a *coin system*, whose associated Hilbert space $\mathcal{C}$ has dimension m. (These might as well be two distinct degrees of freedom of the same physical systems, for example, spin and position of an atom, see below.) Each element of an orthonormal basis of $\mathcal{H}$, $\{|j_1\rangle,\ldots,|j_{|V|}\rangle\}$, represents a vertex of the graph, that is, a position of the walker. The coin space $\mathcal{C}$ is spanned by orthonormal states $\{|c_1\rangle,\ldots,|c_m\rangle\}$ each representing the result of a coin tossing. Denote by $n_j(c_k)$, $j=1,\ldots,|V|$, $k=1,\ldots,m$, an element in V if a coin result c_k induces a transition from j to it [clearly we will have that the edge $(j,n_j(c_k))$ is in E]. The state of the DTQW on G, $|\psi\rangle$, evolves on the Hilbert space $\mathcal{C}\otimes\mathcal{H}$. At each step the state $|\psi\rangle$ is transformed as $|\psi\rangle\to U|\psi\rangle$ where the unitary operator U has the form

$$U=S(C\otimes\mathbf{1}_{|V|}). \tag{1}$$

Here C is a unitary (coin tossing) operation on $\mathcal{C}$ and $\mathbf{1}_{|V|}$ is the identity on $\mathcal{H}$ (we always denote by $\mathbf{1}_w$ the $w\times w$ identity matrix) while S is a *controlled shift* defined by

$$S|c_k,j\rangle=|c_k,n_j(c_k)\rangle. \tag{2}$$

In many implementations of DTQWs it is possible to vary the coin operation C in (1) at every step. For example, the proposal put forward in Ref. 12 for the one-dimensional line and cycle places an atom in a periodic potential created by two laser waves. The internal state of the atom plays the role of the coin. The position of the atom gives the position of the walker in the quantum walk. A laser beam performs an operation of the type

$$C(t,\phi) = \begin{pmatrix} \cos(t) & -\sin(t)e^{-i\phi} \\ \sin(t)e^{i\phi} & \cos(t) \end{pmatrix}, \tag{3}$$

on the two-dimensional Hilbert space associated with the coin. This operation depends on the phase factor ϕ and the duration of the pulse t. By changing these two parameters (and possibly performing more than one operation in a cascade) one can obtain *all* the unitary transformations on the two-dimensional coin space. This available flexibility in the physical implementation gives several advantages in the performance of quantum walks in quantum algorithms. In this work, we shall consider this scenario and consider the coin operation C as a *control variable*.

In this paper, the focus is on DTQWs on d-dimensional lattices. Algorithms on these graphs have been proposed in Refs. 2 and 18. The set of vertices V is given by $V=\{0,1,\ldots,N-1\}^d$ (with $N>2$). If $\tilde{\mathcal{H}} := \mathrm{span}\{|0\rangle,|1\rangle,\ldots,|N-1\rangle\}$, then the associated state Hilbert space of the DTQW is $\mathcal{H}=\otimes^d\tilde{\mathcal{H}}$. This space is spanned by the orthogonal vectors $|j_1,\ldots,j_d\rangle$, with $j_i\in\{0,1,,\ldots,N-1\}$, which represent a vertex of the graph with coordinates $j_1,\ldots,j_d$. Each vertex of G, labeled by $(j_1,\ldots,j_d)$, has $2d$ neighbors each differing from $(j_1,\ldots,j_d)$ by only one coordinate and with (Hamming) distance of 1, i.e., of the form $(j_1,\ldots,j_k\pm 1,\ldots,j_d)$, where the ± 1 operation has to be intended mod N. This graph is the Cartesian product of d-cycles with N vertices (see, e.g., Ref. 11 for definitions and properties). The adjacency matrix is given by

$$A := \sum_{l=1}^{d} \tilde{A}^{(l)}. \tag{4}$$

Here $\tilde{A}^{(l)}$ is the tensor product of d, $N\times N$, identity matrices except in the lth position which is occupied by the adjacency matrix of the cycle $\tilde{A}$, where $\tilde{A}$ is given by $\tilde{A}=F+F^T$. The matrix F is the basic circulant[10] matrix defined as

$$F := \begin{pmatrix} 0 & 0 & \cdot & \cdot & \cdot & 0 & 1 \\ 1 & 0 & \cdot & \cdot & \cdot & 0 & 0 \\ 0 & 1 & \cdot & \cdot & \cdot & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot & 1 & 0 \end{pmatrix}. \tag{5}$$

The coin Hilbert space $\mathcal{C}$ is spanned by $2d$ basis vectors each corresponding to a different coin result. We choose the basis so that the vectors corresponding to the same dimension on the lattice are placed one after the other. For example, for a two-dimensional lattice, $\mathcal{C}$ is spanned by the ordered basis $\{|\rightarrow\rangle,|\leftarrow\rangle,|\uparrow\rangle,|\downarrow\rangle\}$, where the coin results induce a right, left, up, and down motions, respectively.

The dynamics of the DTQW on the Hilbert space $\mathcal{C}\otimes\mathcal{H}$ will be given, as in Eq. (1), by $S(C\otimes 1_{N^d})$, at every step. Here C, which is the coin transformation on $\mathcal{C}$, is a general matrix in SU($2d$) and S, which represents the controlled shift, is a $2dN^d\times 2dN^d$ matrix, and it has, in the chosen basis, a block diagonal structure. In fact, S is composed of d diagonal blocks $S^{(l)}$, $l=1,\ldots,d$, each of dimension $2N^d\times 2N^d$, and each corresponding to one a couple of successive basis states in the coin space (i.e., one dimension in the lattice). The lth block is given by

$$S^{(l)} = \begin{pmatrix} F^{(l)} & 0 \\ 0 & F^{(l)T} \end{pmatrix}, \tag{6}$$

where $F^{(l)}$ ($F^{(l)T}$) is the tensor product of d, $N\times N$ identity matrices, except in the lth position which is occupied by the matrix F (F^T) defined in Eq. (5). This represents a forward (backward) motion in the dimension identified by l.

The matrix C, i.e., the *coin tossing*, is in principle a general matrix in SU($2d$), and thus it depends on $(2d)^2-1$ parameters. In the next sections, we will treat this matrix (and so its parameters) as the *control*, and we will study the admissible evolutions and reachable sets of the DTQW where the coin tossing is used as a control to reach a desired configuration.

III. SET OF ADMISSIBLE STATE TRANSFORMATIONS

In this section we study the set of possible state transformations.

For a *general* DTQW, the set of available transformations $\mathbf{G}$ is, by definition, the set of finite products of the form $\Pi_j S(C_j\otimes \mathbf{1}_w)$ [cf. (1)], where $C_j \in \mathrm{SU}(m)$ (w is the dimension of the walker space and m the dimension of the coin space). This set is the group generated by S and $\mathrm{SU}(m)\otimes \mathbf{1}_w$. In fact, it contains both S [obtained by taking the product $S(\mathbf{1}_m\otimes \mathbf{1}_w)$] and $C\otimes \mathbf{1}_w$ for every $C_j \in \mathrm{SU}(m)$ [obtained by taking $(S(\mathbf{1}_m\otimes \mathbf{1}_w))^{r-1}S(C\otimes \mathbf{1})$, where r is the order of S as a permutation matrix]. Moreover, it is easily verified that it is a group (it is closed under the product and inversion operations).

In the case of the quantum walk on a d-dimensional lattice, which is the focus of this paper, the previous observation applies with r, the order of S, equal to N, the size of the lattice. We shall make the following important assumption which allows us to characterize $\mathbf{G}$ as a *Lie group*.

Assumption A: The size of the lattice, N, is **odd.**

Theorem 1: *Under the above Assumption A, consider the Lie algebra $\mathcal{L}$ generated by the set*

$$\mathcal{F} = \{(\mathrm{su}(2d)\otimes \mathbf{1}), S(\mathrm{su}(2d)\otimes \mathbf{1})S^{-1}, S^2(\mathrm{su}(2d)\otimes \mathbf{1})S^{-2}, \ldots, S^{N-1}(\mathrm{su}(2d)\otimes \mathbf{1})S\}, \tag{7}$$

where $\mathbf{1}=\mathbf{1}_{N^d}$ denotes the $N^d\times N^d$ identity matrix. Then $\mathbf{G}=\mathbf{e}^{\mathcal{L}}$, the connected Lie group associated with $\mathcal{L}$.

Proof: Let us first prove that $e^{\mathcal{L}}\subseteq \mathbf{G}$. Consider $X\in e^{\mathcal{L}}$, X is the finite product of elements of the form e^{At}, where A is in the generating set $\mathcal{F}$ and t is any real. Since $\mathbf{G}$ is a group, it is enough to show that $e^{At}\in \mathbf{G}$ for every $A\in \mathcal{F}$ and real t. Take $A\in \mathcal{F}$, $A := S^k(\tilde{A}\otimes \mathbf{1}_{N^d})S^{r-k}$, for some $k \in \{0,1,\ldots,r\}$ and $\tilde{A}\in \mathrm{su}(2d)$. ($r$ is the degree of S which, in this case, is equal to N.) We have $e^{At}=S^k(e^{\tilde{A}t}\otimes \mathbf{1}_{N^d})S^{r-k}$ which is in $\mathbf{G}$ because all the factors are in $\mathbf{G}$.

To prove that $\mathbf{G}\subseteq e^{\mathcal{L}}$, we need to prove that $C\otimes \mathbf{1}_{N^d}$ [for any $C\in \mathrm{SU}(2d)$] and S are both in $e^{\mathcal{L}}$. While this is obvious for $C\otimes \mathbf{1}_{N^d}$, we need Assumption A for S. Consider the matrix in $e^{\mathcal{L}}$,

$$\hat{S} := (P\otimes \mathbf{1}_{N^d})S^j(P^\dagger \otimes \mathbf{1}_{N^d})S^{-j}, \tag{8}$$

where P is a permutation matrix in SU($2d$) such that the transformation

$$S^j \to (P\otimes \mathbf{1}_{N^d})S^j(P^\dagger \otimes \mathbf{1}_{N^d})$$

interchanges all the pairs of blocks in (6). Therefore, each block of the matrix in (8) has the form $(S^{(l)})^{-2j}$. By choosing $j=(N-1)/2$ recalling that N is the order of S, we obtain $(S^{(l)})^{-2j}=S^{(l)}$ and therefore the matrix $\hat{S}$ in (8) is equal to S. ■

Remark 3.1: We notice that the assumption of N being odd is necessary in the above theorem. In fact, without this assumption the theorem does not hold because $S\notin e^{\mathcal{L}}$. To see this, consider for simplicity the case $d=1$, i.e., the case of the cycle. Assume N is even. Then the exponential of every element in $\mathcal{F}$ has the form $\begin{pmatrix} z\mathbf{1}_N & F^{2j}y \\ -y^*F^{-2j} & z^*\mathbf{1}_N \end{pmatrix}$, where z and y are two complex numbers with $|z|^2+|y|^2=1$ and j is any integer while F is the fundamental circulant matrix defined in (5). All elements of $e^{\mathcal{L}}$ are products of matrices of the above type. In particular, a straightforward induc-

tion argument shows that the (1,1) block is a linear combination of the form $\Sigma_{k=0}^{N/2-1} a_k F^{2k}$, with the a_k's complex coefficients, and this can never be equal to F because of the linear independence of the matrices F^l, $l=0,1,\ldots,N-1$. Therefore, no element in the Lie group $e^{\mathcal{L}}$ is equal to S.

Our task now is to characterize, in view of Theorem 1, more explicitly the Lie algebra $\mathcal{L}$. We will see that it is the direct sum of N^d Lie algebras su($2d$) and this will allow us to describe explicitly the set of admissible transformations. The first step is to make a change of coordinates which corresponds to a *discrete Fourier transform* on each factor of the walker space. The set of admissible transformations is much more easily described in these coordinates (that is, in the Fourier domain).

Recall that every circulant $N\times N$ matrix can be diagonalized by the Fourier matrix[10] Φ defined by

$$\Phi^{\dagger} := \frac{1}{\sqrt{N}} \begin{pmatrix} 1 & 1 & 1 & 1 & \ldots & 1 \\ 1 & \omega & \omega^2 & \omega^3 & \ldots & \omega^{N-1} \\ 1 & \omega^2 & \omega^4 & \omega^6 & \ldots & \omega^{2(N-1)} \\ 1 & \omega^3 & \omega^6 & \omega^9 & \ldots & \omega^{3(N-1)} \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ 1 & \omega^{N-1} & \omega^{2(N-1)} & \omega^{3(N-1)} & \ldots & \omega^{(N-1)(N-1)} \end{pmatrix}, \tag{9}$$

where ω is the Nth root of the unity, that is $\omega := e^{i(2\pi/N)}$. The Fourier matrix Φ is unitary. The map

$$X \to \Lambda X \Lambda^{\dagger}, \tag{10}$$

where

$$\Lambda := \mathbf{1}_{2d} \otimes \underbrace{\Phi \otimes \Phi \otimes \cdots \otimes \Phi}_{\text{d factors}}, \tag{11}$$

transforms S in a block diagonal matrix with d blocks, $\tilde{S}^{(l)}$, $l=1,\ldots,d$, of the form [cf. (6)]

$$\tilde{S}^{(l)} = \begin{pmatrix} T^{(l)} & 0 \\ 0 & T^{(l)T} \end{pmatrix}, \tag{12}$$

where $T^{(l)}$ ($T^{(l)T}$) is the tensor product of d, $N\times N$ identity matrices, except in the l-th position which is occupied by $T := \Phi F \Phi^{\dagger}$ ($\Phi F^T \Phi^{\dagger} = \bar{T}$). The matrix T is the Fourier transform of the fundamental circulant matrix F in (5) which becomes after diagonalization $T := \text{diag}\ (1, \bar{\omega}, \bar{\omega}^2, \ldots, \bar{\omega}^{N-1})$. Noticing that the change in coordinates (10) does not affect matrices of the form $C \otimes \mathbf{1}_{N^d}$, with $C \in \text{su}(2d)$, it follows that the set $\mathcal{F}$ in (7), in the Fourier coordinates, is composed by matrices of dimensions $2dN^d \times 2dN^d$ with a block structure. There are $2d\times 2d$ blocks of dimension $N^d \times N^d$ which are diagonal matrices. For example, for $d=1$ and $d=2$, we have matrices of the form

$$L_1 := \begin{pmatrix} D_{11} & D_{12} \\ -\bar{D}_{12} & D_{22} \end{pmatrix}, \quad L_2 := \begin{pmatrix} D_{11} & D_{12} & D_{13} & D_{14} \\ -\bar{D}_{12} & D_{22} & D_{23} & D_{24} \\ -\bar{D}_{13} & -\bar{D}_{23} & D_{33} & D_{34} \\ -\bar{D}_{14} & -\bar{D}_{24} & -\bar{D}_{34} & D_{44} \end{pmatrix}, \tag{13}$$

respectively. Here the D's matrices are diagonal matrices of dimension $N\times N$ in the case of L_1 ($d=1$) and $N^2\times N^2$ in the case of L_2 ($d=2$).

Moreover, fix k, $1\le k\le N^d$. The submatrix given by the $2d\times 2d$ principal minor corresponding to rows and columns $(k, k+N^d, k+2N^d, \ldots, k+(2d-1)N^d)$ is a matrix in su($2d$). This is because the whole matrix has to be skew-Hermitian and therefore so has to be every principal minor.

Furthermore, the diagonal blocks in all the elements in $\mathcal{F}$ are of the form $a_{jj}\mathbf{1}_{N^d}$, where the a_{jj}'s are the diagonal elements of a matrix in su$(2d)$ and therefore $\Sigma_{j=1}^{2d} a_{jj}=0$. Since these properties are preserved under the Lie bracket operation, the Lie algebra $\mathcal{L}$ generated by $\mathcal{F}$ is a subalgebra of the Lie algebra of block matrices of the previous form where one can assign to each k an arbitrary matrix in su$(2d)$. This latter Lie algebra is the direct sum (i.e., direct sum of vector spaces which commute with each other) of N^d, independent, su$(2d)$'s. We shall denote this Lie algebra by $\mathcal{L}_d$ and our discussion above says that (in the Fourier domain) $\mathcal{L}\subseteq\mathcal{L}_d$. Our next task is to show that *equality*, in fact, *holds* (under Assumption A). We shall prove this by induction on d.

For $d=1$, the case of the cycle, the result was already proven by direct computations in Ref. 9 and we shall not repeat this proof here (in this first step, Assumption A is used). We shall focus on the inductive step in the following.

Fixing $1\leq p<n$, su(n) has the vector space decomposition,

$$\text{su}(n)=\mathcal{K}\oplus\mathcal{P}, \tag{14}$$

where elements in $\mathcal{K}$ have the form $K=\left(\begin{smallmatrix} A & 0\\ 0 & B\end{smallmatrix}\right)$ with $A\in u(p)$ and $B\in u(n-p)$ and $\text{Tr}(A)+\text{Tr}(B)=0$, i.e., $\mathcal{K}$ is the subalgebra of block diagonal matrices. $\mathcal{P}$ is the subspace of block antidiagonal matrices. This is also known as the **AIII** Cartan decomposition of su(n) (cf., e.g., Ref. 13). It is easy to verify the following fact.

Lemma 3.2:

$$\text{span}\quad[\mathcal{P},\mathcal{P}]=\mathcal{K}. \tag{15}$$

That is, every block diagonal matrix in su(n) can be obtained as a linear combination of Lie brackets of block antidiagonal matrices.

To prove that $\mathcal{L}=\mathcal{L}_d$, we first separate the span of $\mathcal{F}$ in four subspaces

$$\text{span}\ \mathcal{F}:=\mathcal{F}_{\text{DU}}\oplus\mathcal{F}_{\text{DL}}\oplus\mathcal{F}_S\oplus\mathcal{F}_A.$$

[With some abuse of notation, we shall still denote by $\mathcal{F}$ the set in (7) even though we are now working in the Fourier domain, i.e., we assume that the change in coordinates (10) and (11) has taken place.] $\mathcal{F}_{\text{DU}}$ (diagonal upper) [$\mathcal{F}_{\text{DL}}$ (diagonal lower)] is the space of real linear combinations of matrices of the form in (7) where the matrices in su$(2d)$ that appear are restricted to be of the form $\left(\begin{smallmatrix} A & 0\\ 0 & 0\end{smallmatrix}\right)$ with A in su$(2(d-1))$ [or of the form $\left(\begin{smallmatrix} 0 & 0\\ 0 & A\end{smallmatrix}\right)$, respectively, with A in su(2)]. For the subspace $\mathcal{F}_S$ we restrict the matrices in su$(2d)$ to be multiples of $\left(\begin{smallmatrix} -i\mathbf{1}_{2(d-1)} & 0\\ 0 & i(d-1)\mathbf{1}_2\end{smallmatrix}\right)$, while for $\mathcal{F}_A$ (Antidiagonal) we restrict them to be of the form $\left(\begin{smallmatrix} 0 & A\\ -A^\dagger & 0\end{smallmatrix}\right)$ for an arbitrary $2(d-1)\times 2$ matrix A (we denote by $\mathbf{0}_k$ the square $k\times k$ matrix where all the entries are zeros and by $\mathbf{0}$ a not necessarily square matrix whose dimensions are clear from the context). Now, by the inductive assumption, the subalgebra generated by $\mathcal{F}_{\text{DU}}$ consists of matrices of the form $\left(\begin{smallmatrix} L_{d-1} & \mathbf{0}\\ \mathbf{0} & \mathbf{0}_{2N^{d-1}}\end{smallmatrix}\right)\otimes\mathbf{1}_N$, where the $2(d-1)N^{d-1}\times 2(d-1)N^{d-1}$ matrix L_{d-1} is any matrix in $\mathcal{L}_{d-1}$. We shall denote this subalgebra of $\mathcal{L}$ by $\mathcal{L}_{\text{DU}}$. Again, by the inductive assumption, the Lie subalgebra generated by $\mathcal{F}_{\text{DL}}$ consists of matrices of the form $\left(\begin{smallmatrix} \mathbf{0}_{2(d-1)N^d} & 0\\ 0 & (\mathbf{1}_2\otimes P_{1d})L_1\otimes\mathbf{1}_{N^{d-1}}(\mathbf{1}_2\otimes P_{1d}^T)\end{smallmatrix}\right)$, where P_{1d} is the $N^d\times N^d$ permutation matrix which exchanges the first and dth position in the Kronecker product of d, $N\times N$ matrices (cf., e.g., Ref. 14, Corollary 4.3.10) and L_1 is any matrix in $\mathcal{L}_1$. We shall denote the subalgebra spanned by matrices of this form by $\mathcal{L}_{\text{DL}}$. Our task is now to show that using matrices in $\mathcal{L}_{\text{DU}}$, $\mathcal{L}_{\text{DL}}$, $\mathcal{F}_S$, and $\mathcal{F}_A$, we can generate $\mathcal{L}_d$.

Fix a k, with $1\leq k\leq N^d$. We shall show that the Lie algebra generated by $\mathcal{L}_{\text{DU}}$, $\mathcal{L}_{\text{DL}}$, $\mathcal{F}_S$, and $\mathcal{F}_A$ contains matrices such that the principal $2d\times 2d$ minor corresponding to rows and columns $(k,k+N^d,k+2N^d,\ldots,k+(2d-1)N^d)$ is an arbitrary matrix in su$(2d)$, and the remaining entries are equal to zero. Since k is arbitrary, this proves our claim.

An arbitrary element in $\mathcal{L}_{\text{DL}}$ has the form

$$L_{\mathrm{DL}} = \begin{pmatrix} \mathbf{0}_{2(d-1)N^d} & \mathbf{0} \\ \mathbf{0} & \sum_{j=1}^{N} M_j \otimes \mathbf{1}_{N^{d-1}} \otimes E_j^N \end{pmatrix}, \tag{16}$$

with M_j arbitrary matrices in su(2). (This follows because an arbitrary matrix of the form L_1 can be written as [cf. (13)] $\Sigma_{j=1}^{N} M_j \otimes E_j^N$ with $M_j \in \mathrm{su}(2)$ and then applying the transformation $X \to (\mathbf{1}_2 \otimes P_{1d}) X (\mathbf{1}_2 \otimes P_{1d}^T)$, one obtains the matrix in the lower corner of (16).] Here and in the following, we use the notation E_j^p to denote the diagonal $p \times p$ matrix which has all entries equal to zero except the jth one on the diagonal which is equal to 1. Analogously, an arbitrary matrix in $\mathcal{L}_{\mathrm{DU}}$ has the form

$$L_{\mathrm{DU}} = \begin{pmatrix} \sum_{j=1}^{N^{d-1}} B_j \otimes E_j^{N^{d-1}} \otimes \mathbf{1}_N & \mathbf{0} \\ \mathbf{0} & \mathbf{0}_{2N^{d-1}} \end{pmatrix}, \tag{17}$$

with B_j arbitrary matrices in su$(2(d-1))$.

Set

$$k := (f-1)N + g, \tag{18}$$

with $1 \le f \le N^{d-1}$ and $0 \le g \le N$. Choose $\tilde{L}_{\mathrm{DU}}$ in $\mathcal{L}_{\mathrm{DU}}$ as

$$\tilde{L}_{\mathrm{DU}} := \begin{pmatrix} B_f \otimes E_f^{N^{d-1}} \otimes \mathbf{1}_N & \mathbf{0} \\ \mathbf{0} & \mathbf{0}_{2N^{d-1}} \end{pmatrix}, \tag{19}$$

and $\tilde{L}_{\mathrm{DL}}$ in $\mathcal{L}_{\mathrm{DL}}$ as

$$\tilde{L}_{\mathrm{DL}} := \begin{pmatrix} \mathbf{0}_{2(d-1)N^d} & \mathbf{0} \\ \mathbf{0} & M_g \otimes \mathbf{1}_{N^{d-1}} \otimes E_g^N \end{pmatrix}. \tag{20}$$

For a general matrix $\begin{pmatrix} \mathbf{0}_{2(d-1)} & A \\ -A^\dagger & \mathbf{0}_2 \end{pmatrix} \in \mathrm{su}(2d)$, choose $Q \in \mathcal{F}_A$ as [this type of matrices belongs to the first type of the ones listed in (7)]

$$Q := \begin{pmatrix} \mathbf{0}_{2(d-1)N^d} & A \otimes \mathbf{1}_{N^d} \\ -A^\dagger \otimes \mathbf{1}_{N^d} & \mathbf{0}_{2N^d} \end{pmatrix}, \tag{21}$$

and calculate $[\tilde{L}_{\mathrm{DL}}, [\tilde{L}_{\mathrm{DU}}, Q]]$. A direct computation gives

$$[\tilde{L}_{\mathrm{DL}}, [\tilde{L}_{\mathrm{DU}}, Q]] := \begin{pmatrix} \mathbf{0}_{2(d-1)N^d} & -B_f A M_g \otimes E_f^{N^{d-1}} \otimes E_g \\ M_g A^\dagger B_f \otimes E_f^{N^{d-1}} \otimes E_g^N & \mathbf{0_{2N^d}} \end{pmatrix}. \tag{22}$$

In this matrix, the only elements that are possibly different from zero are the ones corresponding to the principal minor identified by k, according to (18). These form a matrix in $\mathcal{P}$ of the Cartan decomposition (14) of su$(2d)$ with $p := 2(d-1)$. Since A, M_g, and B_f are arbitrary, *every* matrix in $\mathcal{P}$ (antidiagonal), can be obtained this way. (It is enough to choose nonsingular B_f and M_g and then adjust A accordingly.) By using Lemma 3.2, we obtain that every matrix in su$(2d)$ can be obtained as linear combination of Lie brackets of these matrices. This completes the proof that $\mathcal{L} = \mathcal{L}_d$.

In conclusion, we have the following characterization of the set of admissible state transformations for the d-dimensional lattice which is more explicit than the one of Theorem 1.

Theorem 2: *Under Assumption A, in the Fourier domain, the set of admissible state transformations for a quantum walk on a d -dimensional lattice is the connected Lie group* $e^{\mathcal{L}}$ *corresponding to the Lie algebra,*

$$\mathcal{L} = \mathrm{span}\{A \otimes E_h^{N^d} | A \in \mathrm{su}(2d), 1 \leq h \leq N^d\}.$$

This Lie algebra is the direct sum of N^d $\mathrm{su}(2d)$ *'s. In particular, a state transformation can be achieved if and only if it belongs to the Lie groups,*

$$e^{\mathcal{L}} := \left\{ \sum_{h=1}^{N^d} R_h \otimes E_h^{N^d} | R_h \in \mathrm{SU}(2d) \right\}. \tag{23}$$

IV. SET OF ADMISSIBLE STATES

Having described the set of possible evolutions, we can now describe all the possible states that can be achieved for the system implementing the quantum walk on the d-dimensional lattice. This is more easily achieved by working in the Fourier domain first. We are always working under Assumption A, that is, we assume N to be odd. As we have seen in Sec. III, in the Fourier domain, the set of possible evolutions is given by matrices with $2d \times 2d$ blocks each of dimension N^d and each diagonal [cf. (13)]. Given a $1 \leq k \leq N^d$, the entries corresponding to the principal minor identified by $(k, k+N^d, k+2N^d, \ldots, k+(2d-1)N^d)$ are occupied by an arbitrary matrix in $\mathrm{SU}(2d)$. This is described in (23) of Theorem 2. Alternatively, by writing

$$k := (k_1 - 1)N^{d-1} + (k_2 - 1)N^{d-2} + \cdots + (k_{d-1} - 1)N + k_d,\ k_1, k_2, \ldots, k_d = 1, \ldots, N, \tag{24}$$

we can write any possible evolution as $\Sigma_{k_1,\ldots,k_d=1}^{N} B_{k_1,\ldots,k_d} \otimes E_{k_1}^N \otimes E_{k_2}^N \otimes E_{k_d}^N$, with arbitrary $B_{k_1,\ldots,k_d} \in \mathrm{SU}(2d)$.

Let us assume now that the initial condition is for the walker to be with certainty in position $(0,0,\ldots,0)$ and (without loss of generality) assume the coin is in the first possible state. Such an initial state can be written as $\psi_{\mathrm{in}} := \vec{e}_1^{2d} \otimes \vec{e}_1^N \otimes \vec{e}_1^N \otimes \cdots \otimes \vec{e}_1^N$, where the Kronecker product is taken d times and $\vec{e}_j^l$ denotes the (standard) vector of length l with all 0's except in the jth position which is occupied by 1. In the Fourier domain, this vector becomes, with Λ defined in (11) and (9),

$$\psi_{\mathrm{Fin}} = \Lambda \vec{e}_1^{2d} \otimes \vec{e}_1^N \otimes \vec{e}_1^N \otimes \cdots \otimes \vec{e}_1^N = \frac{1}{N^{d/2}} \vec{e}_1^{2d} \otimes \left(\sum_{l_1=1}^{N} \vec{e}_{l_1}^N \right) \otimes \cdots \otimes \left(\sum_{l_d=1}^{N} \vec{e}_{l_d}^N \right), \tag{25}$$

that is, except for the factor $1/N^{d/2}$ it is a $2dN^d$-vector with all 1's in the first N^d positions and zeros in the remaining positions. Combining this with the set of the possible evolutions, we obtain the set of admissible states in the Fourier domain, $\mathcal{O}_F$,

$$\begin{aligned} \mathcal{O}_F &= \left\{ \left(\sum\nolimits_{k_1,\ldots,k_d} B_{k_1,\ldots,k_d} \otimes E_{k_1}^N \otimes \cdots \otimes E_{k_d}^N \right) \psi_{\mathrm{Fin}} | B_{k_1,\ldots,k_d} \in \mathrm{SU}(2d) \right\} \\ &= \left\{ \frac{1}{N^{d/2}} \sum\nolimits_{k_1,\ldots,k_d} (B_{k_1,\ldots,k_d} \vec{e}_1^{2d}) \otimes \vec{e}_{k_1}^N \otimes \cdots \otimes \vec{e}_{k_d}^N | B_{k_1,\ldots,k_d} \in \mathrm{SU}(2d) \right\}. \end{aligned} \tag{26}$$

By denoting a general complex valued $2d$-vector by $\vec{b}_{k_1,\ldots,k_d}$, we can rewrite the set $\mathcal{O}_F$ as

$$\mathcal{O}_F = \left\{ \frac{1}{N^{d/2}} \sum_{k_1,\ldots,k_d} \vec{b}_{k_1,\ldots,k_d} \otimes \vec{e}_{k_1}^N \otimes \cdots \otimes \vec{e}_{k_d}^N | \| \vec{b}_{k_1,\ldots,k_d} \| = 1 \right\}. \tag{27}$$

By taking the antitransform of this expression, we obtain the admissible set in the standard domain, $\mathcal{O}$. We have [cf. (11)]

$$\mathcal{O} = \Lambda^\dagger \mathcal{O}_F = \left\{ \frac{1}{N^{d/2}} \sum_{k_1,\ldots,k_d} \vec{b}_{k_1,\ldots,k_d} \otimes \Phi^\dagger \vec{e}_{k_1}^N \otimes \cdots \otimes \Phi^\dagger \vec{e}_{k_d}^N | \| \vec{b}_{k_1,\ldots,k_d} \| = 1 \right\}. \tag{28}$$

Notice that the vector $\Phi^\dagger \vec{e}_{k_j}^N$ is the k_jth column of the Fourier matrix in (9). This observation will be important for what follows.

From (28), one can study the structure of the set of reachable states and, in particular, the type of probability distributions that can be achieved. For a state ψ of the total system, the probability of finding the walker in position $(l_1,\ldots,l_d)$ is the length square of the $2d$-vector $(\mathbf{1}_{2d}\otimes(\vec{e}^N_{l_1+1})^T \otimes(\vec{e}^N_{l_2+1})^T\otimes\cdots\otimes(\vec{e}^N_{l_d+1})^T)\psi$. If we impose that $\psi\in\mathcal{O}$, using formula (28), we have that an admissible probability distribution $p_{l_1,\ldots,l_d}$ is of the form

$$p_{l_1,\ldots,l_d}=\frac{1}{N^d}\left\|\sum_{k_1,\ldots,k_d}\vec{b}_{k_1,\ldots,k_d}((\vec{e}^N_{l_1+1})^T\Phi^\dagger\vec{e}^N_{k_1})((\vec{e}^N_{l_2+1})^T\Phi^\dagger\vec{e}^N_{k_2})\cdots((\vec{e}^N_{l_d+1})^T\Phi^\dagger\vec{e}^N_{k_d})\right\|^2$$
$$=\frac{1}{N^{2d}}\left\|\sum_{k_1,\ldots,k_d}\vec{b}_{k_1,\ldots,k_d}\omega^{(l_1)(k_1-1)}\omega^{(l_2)(k_2-1)}\cdots\omega^{(l_d)(k_d-1)}\right\|^2, \tag{29}$$

where we have used the formula [cf. (9)] $(\vec{e}^N_{l+1})^T\Phi^\dagger\vec{e}^N_k=(1/\sqrt{N})\omega^{(l)(k-1)}$. Therefore, a probability distribution $p_{l_1,\ldots,l_d}$ is obtainable if and only if there exist N^d, unit, $2d$-vectors, $\vec{b}_{k_1,\ldots,k_d}$, with

$$p_{l_1,\ldots,l_d}=\frac{1}{N^{2d}}\left\|\sum_{k_1,\ldots,k_d}\vec{b}_{k_1,\ldots,k_d}\omega^{(l_1)(k_1-1)}\omega^{(l_2)(k_2-1)}\cdots\omega^{(l_d)(k_d-1)}\right\|^2. \tag{30}$$

It is clear that the probability distribution,

$$p_{0,0,\ldots,0}=1,\quad p_{l_1,\ldots,l_d}=0\quad\text{otherwise}, \tag{31}$$

is achievable (it is, in fact, the probability distribution we started from) and can be obtained by using all the $b_{k_1,\ldots,k_d}$ equal to $(1/\sqrt{2d})[1,1,\ldots,1]^T$. [This follows easily from formula (30) recalling that for $l\neq 0 \pmod N$, $\Sigma_{k=1}^N\omega^{(l)(k-1)}=0$.] It is interesting to investigate other probability distributions. A particularly relevant case is the uniformly distributed probability. This is the extreme case with respect to the initial one. [One can see the problem of going from a probability concentrated in a vertex to the uniform distribution as a "mixing" problem and the time to achieve this as a "mixing time." Analogously, the problem of going from a uniform probability to a probability concentrated (or larger than a certain threshold) in a given vertex as a "hitting" problem and the time to achieve this as a "hitting time." In our control theoretic setting, there is a symmetry between these two problems, (cf. Theorem 4, part 3) The notions of mixing time and hitting time are among the ones most studied in the theory of random and quantum walks (see, e.g., Ref. 17). Many search algorithms on the lattice can also be formulated as going from a uniformly distributed probability to a concentrated one. However, these problems cannot be directly formulated as state transfer problems and our setting does not apply since the final target vertex is, in principle, unknown. To deal with search problems, one could, however, modify the model, for example, by allowing the coin transformation to depend on the vertex. This model incorporates a query of the current vertex in the evolution (cf., for example, Ref. 2). We believe similar techniques to the ones employed here can be used to analyze these modified models as well.] In order to show that a uniform probability distribution may be achieved, we pick a specific set of $2d$-vectors and show that they, in fact, lead to the desired probability distribution. In particular, choose

$$\vec{b}_{k_1,\ldots,k_d}=\prod_{j=1}^{d}\omega^{(k_j-1)(k_j-2)/2}\vec{e}^{2d}_1. \tag{32}$$

The corresponding probability distribution is

$$p_{l_1,\ldots,l_d}=\frac{1}{N^{2d}}\left|\sum_{k_1,\ldots,k_d}\prod_{j=1}^{d}\omega^{(k_j-1)(k_j-2)/2}\omega^{(l_j)(k_j-1)}\right|^2. \tag{33}$$

The sum in (33) is reminiscent of the Gauss' sums studied in number theory (cf., e.g., Ref. 4). Completing the square, (33) becomes

$$p_{l_1,\ldots,l_d} = \frac{1}{N^{2d}} \left| \sum_{k_1,\ldots,k_d} \prod_{j=1,\ldots,d} \omega^{(1/2)((k_j-1)+(l_j-1/2))^2} \prod_{j=1,\ldots,d} \omega^{-(1/2)(l_j-1/2)^2} \right|^2$$
$$= \frac{1}{N^{2d}} \left| \sum_{k_1,\ldots,k_d} \prod_{j=1,\ldots,d} \omega^{(1/2)((k_j-1)+(l_j-1/2))^2} \right|^2, \tag{34}$$

since the factor $\Pi_{j=1,\ldots,d}\omega^{-(1/2)(l_j-1/2)^2}$ has magnitude equal to 1. We now show that the right hand side of (34) does not depend on $l_1,\ldots,l_d$. Fix $\bar{j}\in\{1,\ldots,d\}$, we have (splitting the product)

$$v := \sum_{k_1,\ldots,k_d} \prod_{j=1}^{d} \omega^{(1/2)(k_j+l_j-3/2)^2} = \sum_{k_1,\ldots,k_d} \left(\prod_{j\neq\bar{j}} \omega^{(1/2)(k_j+l_j-3/2)^2} \right) \omega^{(1/2)(k_{\bar{j}}+l_{\bar{j}}-3/2)^2}$$
$$= \left(\sum_{k_1,\ldots,k_{\bar{j}-1},k_{\bar{j}+1},\ldots,k_d} \prod_{j\neq\bar{j}} \omega^{(1/2)(k_j+l_j-3/2)^2} \right) \left(\sum_{k_{\bar{j}}=1}^{N} \omega^{(1/2)(k_{\bar{j}}+l_{\bar{j}}-3/2)^2} \right). \tag{35}$$

Now,

$$\sum_{k_{\bar{j}}=1}^{N} \omega^{(1/2)(k_{\bar{j}}+l_{\bar{j}}-3/2)^2} = \sum_{h=1+l_{\bar{j}}}^{N+l_{\bar{j}}} \omega^{(1/2)(h-3/2)^2} = \sum_{h=1+l_{\bar{j}}}^{N} \omega^{(1/2)(h-3/2)^2} + \sum_{h=1}^{l_{\bar{j}}} \omega^{(1/2)(N+h-3/2)^2}. \tag{36}$$

The terms in the second sum can be written as

$$\omega^{(1/2)(N+h-3/2)^2} = \omega^{(1/2)(h-3/2)^2} \omega^{(1/2)(N(2(h-3/2)+N))}. \tag{37}$$

However, the term in the last exponent, $N\left(2\left(h-\frac{3}{2}\right)+N\right)$, is an even multiple of N, since N is odd, and therefore the last factor in (37) is 1.

Replacing this in (36), we obtain

$$\sum_{k_{\bar{j}}=1}^{N} \omega^{(1/2)(k_{\bar{j}}+l_{\bar{j}}-3/2)^2} = \sum_{h=1}^{N} \omega^{(1/2)(h-3/2)^2}, \tag{38}$$

thus the second factor of v, and therefore v itself, does not depend on $l_{\bar{j}}$. By the arbitrariness of $\bar{j}$, we have shown that v does not depend on $l_1,\ldots,l_d$. Therefore, the probability, $p_{l_1,\ldots,l_d}=|v|^2/N^{2d}$, must be uniform among the various vertices. This result extends (with a different proof) the result of reachability of the uniform distribution which was proven in Ref. 9 for the case of the cycle.

We summarize the discussion of this section in the following theorem.

Theorem 3: *Assume that Assumption A holds and assume the initial state of the quantum walk on the d -dimensional lattice is with certainty in position* $(0,0,\ldots,0)$. *Then the set of states that can be obtained by varying at each step the coin transformation is given by (27) in the Fourier domain and by (28) in the standard domain. A probability distribution* $p_{l_1,\ldots,l_d}$ *can be achieved if there exist* N^d, *unit*, $2d$ *-vectors* $\vec{b}_{k_1,\ldots,k_d}$, $k_1,\ldots,k_d=1,\ldots,N$, *such that (30) holds. In particular, it is always possible to reach a state where all the vertices of the walk have equal probability.*

V. PROPERTIES OF REACHABLE SETS

The above discussion concerns the set of admissible states without taking into account the number of steps needed to obtain a given state. In order to take this into account we have to study a different type of admissible sets which, following control theory terminology, we call *reachable sets*. We denote by $\mathcal{R}(t,\psi_{\text{in}})$ the set of states that can be reached starting with ψ_{in} with t steps. Clearly, we have $\mathcal{R}(0,\psi_{\text{in}})=\{\psi_{\text{in}}\}$. The corresponding set in the Fourier domain is $\mathcal{R}_F(t,\psi_{\text{in}})$ $:=\Lambda\mathcal{R}(t,\psi_{\text{in}})$, with Λ in (11). If we choose ψ_{in} as in Sec. III, we clearly have $\mathcal{O}=\cup_{t\geq 0}\mathcal{R}(t,\psi_{\text{in}})$ $[\mathcal{O}_F=\cup_{t\geq 0}\mathcal{R}_F(t,\psi_{\text{in}})]$. These definitions can be written as [cf. (25)]

$$\mathcal{R}(t,\psi_{\text{in}}) = \left\{ \left(\prod_{l=1}^{t} SC_l \otimes \mathbf{1}_{N^d} \right) \psi_{\text{in}} | C_l \in \text{SU}(2d) \right\},$$

$$\mathcal{R}_F(t,\psi_{\text{in}}) = \left\{ \left(\prod_{l=1}^{t} \Lambda S \Lambda^\dagger C_l \otimes \mathbf{1}_{N^d} \right) \Lambda \psi_{\text{in}} | C_l \in \text{SU}(2d) \right\}. \tag{39}$$

A probability distribution $p_{l_1,\ldots,l_d}$, $l_1,\ldots,l_d$, can be achieved at time t if it can be written as

$$p_{l_1,\ldots,l_d}(t) = \left\| \mathbf{1}_{2d} \otimes (\vec{e}_{l_1}^{N})^T \otimes (\vec{e}_{l_2}^{N})^T \otimes \cdots \otimes (\vec{e}_{l_d}^{N})^T \left(\prod_{l=1}^{t} SC_l \otimes \mathbf{1}_{N^d} \right) \psi_{\text{in}} \right\|^2 \tag{40}$$

for some C_l's $\in \text{SU}(2d)$. Although, in principle, one can study directly the reachable set in (39) by parametrizing the Lie group SU($2d$), this is a difficult task as the number of parameters grows very large with t and they appear in a complicated, nonlinear, fashion. It is possible, however, to give some general properties of the reachable sets $\mathcal{R}(t,\cdot)$, which we collect in the next theorem. (We state the results in the standard domain. Analogous results hold in the Fourier domain.)

Theorem 4: *The reachable sets satisfy the following properties.*

(1)

$$\mathcal{R}(t,\psi_{\text{in}}) \subseteq \mathcal{R}(t+2,\psi_{\text{in}}). \tag{41}$$

(2) There exists a finite T such that

$$\mathcal{R}(T,\psi_{\text{in}}) \cup \mathcal{R}(T-1,\psi_{\text{in}}) = \bigcup_{t\geq 0} \mathcal{R}(t,\psi_{\text{in}}). \tag{42}$$

(3) If $\psi_f \in \mathcal{R}(t,\psi_{\text{in}})$ then there exists a state $\tilde{\psi}_{\text{in}} \in \mathcal{R}(t,\psi_f)$, such that to $\tilde{\psi}_{\text{in}}$ there corresponds the same probability distribution as ψ_{in}.

We use Assumption A to prove property (2). This is done indirectly because we use the characterization of the set of available transformations as a Lie group which required this assumption. Properties (1) and (3) hold for every N and do not require Assumption A.

Proof:

(1) Let $\psi \in \mathcal{R}(t,\psi_{\text{in}})$ and let C be the matrix with d blocks, $C=\text{diag}(P,P,\ldots,P)$, where P is the matrix $P=\left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$ in SU(2). Then we have $(C^\dagger \otimes \mathbf{1}_{N^d}) S (C \otimes \mathbf{1}_{N^d}) = S^{-1}$, which implies that

$$S(C^\dagger \otimes \mathbf{1}_{N^d}) S (C \otimes \mathbf{1}_{N^d}) \psi = \psi, \tag{43}$$

and therefore $\psi \in \mathcal{R}(t+2,\psi_{\text{in}})$.

(2) Consider a set of linearly independent elements of $\mathcal{F}$ in (7), $\mathcal{G} := \{G_1,\ldots,G_h\}$. Using the product of a finite number n of exponentials of the form $e^{G_j t_j}$ with $t_j \in \mathbf{R}$ and $G_j \in \mathcal{G}$, it is possible to obtain every element in a neighborhood of the identity in $e^{\mathcal{L}}$ (cf. the proof of controllability in Appendix D of Ref. 7. There the proof is based on the idea of using similarity transformations $X \to e^{Ft} X e^{-Ft}$ to generate new directions in the Lie algebra $\mathcal{L}$. Once one has a number $\dim \mathcal{L}$ of linearly independent matrices in the Lie algebra $\mathcal{L}$, say $H_1,\ldots,H_{\dim \mathcal{L}}$, the set $\{X \in e^{\mathcal{L}} | X = \prod_{j=1}^{\dim \mathcal{L}} e^{H_j t_j}, t_1,\ldots,t_{\dim \mathcal{L}} \in \mathbf{R}\}$ contains an open neighborhood of the identity.) Moreover, each of these exponentials can be performed with a number of steps equal to N since $e^{G_j t} = S^{N-l} e^X \otimes \mathbf{1}_{N^d} S^l$ for some $0 \leq l \leq N-1$, and $X \in \text{su}(2d)$. Therefore, with nN steps we can obtain all the elements in a neighborhood U of the identity in $e^{\mathcal{L}}$. Write $e^{\mathcal{L}}$ as

$$e^{\mathcal{L}} = \bigcup_{x \in e^{\mathcal{L}}} xU. \tag{44}$$

Since $e^{\mathcal{L}}$ is the direct product of N^d SU($2d$)'s, which is compact, it is also compact and therefore the covering (44) has a finite subcover,

$$e^{\mathcal{L}} = \bigcup_{j=1}^{z} x_j U. \tag{45}$$

Moreover, because of compactness the exponential map is surjective and each x_j can be written as $x_j = e^{Y_j}$ with $Y_j \in \mathcal{L}$. For every j, we can choose a positive integer r_j (large enough) so that $e^{Y_j/r_j} \in U$ and therefore it can be obtained with at most nN steps. By repeating the same sequence r_j times we obtain x_j. By comparing with (45), we obtain that every element of $e^{\mathcal{L}}$ can be obtained in at most $((\max_j r_j)+1)nN$ steps. This means that there is a T, such that $\cup_{t\geq 0}^{T}\mathcal{R}(t,\psi_{\text{in}}) = \cup_{t\geq 0}\mathcal{R}(t,\psi_{\text{in}})$. However, from property (1) we have $\cup_{t\geq 0}^{T}\mathcal{R}(t,\psi_{\text{in}}) = \mathcal{R}(T,\psi_{\text{in}}) \cup \mathcal{R}(T-1,\psi_{\text{in}})$, which completes the proof. (Some arguments are in common with the proof of controllability for systems on Lie groups of Ref. 15.)

(3) Assume $\psi_f \in \mathcal{R}(t,\psi_{\text{in}})$. Therefore there exists a sequence of t transformations in SU($2d$), $C_1,\ldots,C_t$, such that

$$\psi_f = \left(\prod_{k=1}^{t} S(C_k \otimes \mathbf{1}_{N^d})\right)\psi_{\text{in}}. \tag{46}$$

Therefore, we have

$$\psi_{\text{in}} = \left(\prod_{k=t}^{1} (C_k^{\dagger} \otimes \mathbf{1}_{N^d})S^{-1}\right)\psi_f. \tag{47}$$

As we have seen in the proof of (1), there exists a matrix C such that $(C \otimes \mathbf{1}_{N^d})S(C^{\dagger} \otimes \mathbf{1}_{N^d}) = S^{-1}$. Replacing this in (47), we obtain

$$\psi_{\text{in}} = ((C_t^{\dagger}C) \otimes \mathbf{1}_{N^d})\left(\prod_{k=t-1}^{1} S((C^{\dagger}C_k^{\dagger}C) \otimes \mathbf{1}_{N^d})\right)S(C^{\dagger} \otimes \mathbf{1}_{N^d})\psi_f. \tag{48}$$

Therefore the state $((C^{\dagger}C_t) \otimes \mathbf{1}_{N^d})\psi_{\text{in}}$ is in $\mathcal{R}(t,\psi_f)$.

Remark 5.1: From a practical point of view, an interesting problem is to give estimates for the number of steps T of part (2) of the above theorem. This is, in general, a difficult problem in the theory of Lie groups in that one has not only to estimate the number of exponentials needed to obtain the open neighborhood U (n in the theorem) but also understand the size and shape of U. In fact, the main idea is to paste together translated copies of U as in (45) to cover the whole Lie group $e^{\mathcal{L}}$. It may be possible to give estimates for the time needed for a *specific evolution*. ■

VI. CONTROL ALGORITHMS FOR LOW DIMENSIONAL CASES

In this section, we first prove a reduction-type of result that provides an algorithm (we use the term (control) algorithm indicating a sequence of coin transformations) to reach the uniform probability distribution for a DTQW on a two-dimensional lattice for every N, if we are given an algorithm on the corresponding cycle ($d=1$) (see Theorem 5). Then we restrict ourselves to a DTQW on a cycle ($d=1$) with $N=3$ and $N=5$ vertices. If $N=3$, we provide a control algorithm for all the probability distributions which takes at most two steps (see Proposition 6.1), while, in the case $N=5$, we provide an explicit control to reach the uniform probability distribution in four steps (see Proposition 6.3). The algorithms in Propositions 6.1 and 6.3 are optimal in that the number of steps is the minimum required. By combining Theorem 5 with Propositions 6.1 and 6.3, we get algorithms to reach the uniform probability distribution in the planar lattice ($d=2$) with $N=3$ and $N=5$ (see Remark 6.5).

We will denote by $|+1\rangle$ and $|-1\rangle$ the two basis vectors of the coin space on the cycle ($d=1$) and with $|\rightarrow\rangle$, $|\leftarrow\rangle$, $|\uparrow\rangle$, and $|\downarrow\rangle$ the four basis vectors for the coin space on the planar lattice

($d=2$). The following theorem which is stated as an existence result provides, in its proof, a method to control to the uniform probability distribution for the two-dimensional lattice, once a method is known for the cycle $d=1$.

Theorem 5: *Assume that for the DTQW on the N -cycle it is possible from the initial state* $\psi_{\text{in}}^1=|+1\rangle\otimes|0\rangle$ *to reach in N steps a final state* ψ_f^1 *whose probability distribution is uniform. Then for the DTQW on the two-dimensional lattice it is always possible from the initial state* $\psi_{\text{in}}^2=|\rightarrow\rangle\otimes|0,0\rangle$ *to reach in 3N steps a final state* ψ_f^2 *whose probability distribution is the uniform one.*

Proof: Denote by $C_1,\ldots,C_N$ the N matrices in SU(2) which give the control algorithm steering ψ_{in}^1 to ψ_f^1. More precisely, this means that if $U_i=S(C_i\otimes\mathbf{1}_N)$, $i=1,\ldots,N$ (where S is the conditional shift on the cycle with N nodes) it holds

$$U_N\cdots U_1\psi_{\text{in}}^1=\psi_f^1=\sum_{k=0}^{N-1}(\alpha_k|+1\rangle+\beta_k|-1\rangle)\otimes|k\rangle \tag{49}$$

for some complex numbers α_k and β_k, $k=1,\ldots,N$, with $|\alpha_k|^2+|\beta_k|^2=1/N$.

We denote by $C_i^l\in\text{SU}(4)$, $l=1,2$ and $i=1,\ldots,N$, the block diagonal matrix which is composed by two blocks of dimension 2, where the lth block is equal to C_i, while the other one is the identity. More specifically, we have

$$C_i^1=\begin{pmatrix}C_i & 0\\ 0 & \mathbf{1}_2\end{pmatrix},\quad C_i^2=\begin{pmatrix}\mathbf{1}_2 & 0\\ 0 & C_i\end{pmatrix}. \tag{50}$$

We denote by $U_i^l=S(C_i^l\otimes\mathbf{1}_{N^2})$, where S is now the conditional shift on the two-dimensional lattice. Given the particular form of the matrices C_j^l in (50) and by using Eq. (49), we have that

$$U_N^1\cdots U_1^1(|\rightarrow\rangle\otimes|0,j\rangle)=\sum_{k=0}^{N-1}(\alpha_k|\rightarrow\rangle+\beta_k|\leftarrow\rangle)\otimes|k,j\rangle \tag{51}$$

for all $j\in\{0,\ldots,N-1\}$, where α_k and β_k are the same as (49). Moreover, since $S^N=\mathbf{1}_{N^2}$, we also have

$$U_N^1\cdots U_1^1((\gamma|\uparrow\rangle+\delta|\downarrow\rangle)\otimes|k,h\rangle)=((\gamma|\uparrow\rangle+\delta|\downarrow\rangle)\otimes|k,h\rangle) \tag{52}$$

for any constants γ, δ and any k, $h\in\{0,\ldots,N-1\}$. That is, the sequence $U_N^1U_{N-1}^1\cdots U_1^1$ does not modify the up-down part of the Hilbert space. Similarly, by replacing 1 with 2 and the basis vectors $|\rightarrow\rangle,|\leftarrow\rangle$ with $\uparrow,|\downarrow\rangle$, we will have

$$U_N^2\cdots U_1^2(|\uparrow\rangle\otimes|j,0\rangle)=\sum_{k=0}^{N-1}(\alpha_k|\uparrow\rangle+\beta_k|\downarrow\rangle)\otimes|j,k\rangle \tag{53}$$

and

$$U_N^2\cdots U_1^2((\gamma|\rightarrow\rangle+\delta|\leftarrow\rangle)\otimes|u,h\rangle)=((\gamma|\rightarrow\rangle+\delta|\leftarrow\rangle)\otimes|u,h\rangle), \tag{54}$$

again for any constants γ, δ, and for all j, u, $h\in\{0,\ldots,N-1\}$.

Now, given the initial state ψ_{in}^2, the control algorithm on the two-dimensional lattice first applies the N steps $U_N^1\cdots U_1^1$. From Eq. (51), we have

$$\psi_N:=U_N^1\cdots U_1^1\psi_{\text{in}}^2=\sum_{k=0}^{N-1}(\alpha_k|\rightarrow\rangle+\beta_k|\leftarrow\rangle)\otimes|k,0\rangle. \tag{55}$$

Let $\bar{C}\in\text{SU}(4)$ be the permutation matrix which exchanges $|\rightarrow\rangle$ with $|\uparrow\rangle$ and leave unchanged the other two basis vectors and denote by $\bar{U}_1^2=U_1^2(\bar{C}\otimes\mathbf{1}_{N^2})$. Then, since $(\bar{C}\otimes\mathbf{1}_{N^2})\psi_N=\Sigma_{k=0}^{N-1}(\alpha_k|\uparrow\rangle+\beta_k|\leftarrow\rangle)\otimes|k,0\rangle$, by using Eqs. (53) and (54), we have

$$\psi_{2N} := U_N^2 \cdots \bar{U}_1^2 \psi_N = \left[\sum_{k=0}^{N-1} \alpha_k \sum_{j=0}^{N-1} (\alpha_j |\uparrow\rangle + \beta_j |\downarrow\rangle) \otimes |k,j\rangle \right] + \sum_{k=0}^{N-1} \beta_k |\leftarrow\rangle \otimes |k,0\rangle. \tag{56}$$

Let $\hat{C} \in \mathrm{SU}(4)$ be the permutation matrix which makes the basis change,

$$\{|\rightarrow\rangle, |\leftarrow\rangle, |\uparrow\rangle, |\downarrow\rangle\} \Rightarrow \{|\downarrow\rangle, |\uparrow\rangle, |\rightarrow\rangle, |\leftarrow\rangle\}.$$

Notice that

$$(\hat{C} \otimes \mathbf{1}_{N^2}) \psi_{2N} = \left[\sum_{k=0}^{N-1} \alpha_k \sum_{j=0}^{N-1} (\alpha_j |\rightarrow\rangle + \beta_j |\leftarrow\rangle) \otimes |k,j\rangle \right] + \sum_{k=0}^{N-1} \beta_k |\uparrow\rangle \otimes |k,0\rangle.$$

Denote by $\hat{U}_1^2 = U_1^2(\hat{C} \otimes \mathbf{1}_{N^2})$. Then, as before, by using Eqs. (53) and (54), we have

$$\psi_f^2 := U_N^2 \cdots \hat{U}_1^2 \psi_{2N} = \sum_{k=0}^{N-1} \alpha_k \sum_{j=0}^{N-1} ((\alpha_j |\rightarrow\rangle + \beta_j |\leftarrow\rangle) \otimes |k,j\rangle + \sum_{k=0}^{N-1} \beta_k \sum_{j=0}^{N-1} ((\alpha_j |\uparrow\rangle + \beta_j |\downarrow\rangle) \otimes |k,j\rangle. \tag{57}$$

Now, we can verify that the probability distribution of ψ_f^2 is the uniform one, as desired, in fact, we have

$$p_{kj} = |\alpha_k|^2 |\alpha_j|^2 + |\alpha_k|^2 |\beta_j|^2 + |\beta_k|^2 |\alpha_j|^2 + |\beta_k|^2 |\beta_j|^2 = |\alpha_k|^2 (1/N) + |\beta_k|^2 (1/N) = 1/N^2.$$

■

A. Cycle with $N=3$

The following proposition provides a direct algorithm to obtain any probability distribution on a 3-cycle.

Proposition 6.1: It is always possible from the initial state $\psi_{\mathrm{in}} = |+1\rangle \otimes |0\rangle = \vec{e}_1^6$ to reach in at most two steps a final state ψ_f whose probability distribution is arbitrary.

Proof: As in (3), we use the notation

$$C(\theta,\phi) := \begin{pmatrix} \cos(\theta) & -\sin(\theta) e^{-i\phi} \\ \sin(\theta) e^{i\phi} & \cos(\theta) \end{pmatrix}. \tag{58}$$

Set $\phi=0$, and let $U(\theta) = S(C(\theta,0) \otimes \mathbf{1}_3)$. By direct computation, for any θ_1, θ_2, we have

$$\psi_f := U(\theta_2) U(\theta_1) \psi_{\mathrm{in}} = \begin{pmatrix} -\sin(\theta_2)\sin(\theta_1) \\ 0 \\ \cos(\theta_2)\cos(\theta_1) \\ \sin(\theta_2)\cos(\theta_1) \\ \cos(\theta_2)\sin(\theta_1) \\ 0 \end{pmatrix}.$$

Fix any arbitrary probability distribution (p_0, p_1, p_2). To prove our statement, we need to show that it is possible to choose θ_1 and θ_2, such that

$$p_0 = \sin^2(\theta_2),$$

$$p_1 = \sin^2(\theta_1)\cos^2(\theta_2),$$

$$p_2 = \cos^2(\theta_1)\cos^2(\theta_2).$$

In fact, if $p_0=1$ we can set $\theta_2=\pi/2$ and θ_1 arbitrary, while, if $p_0<1$ we choose θ_2 such that the first equation holds, and then θ_1 such that $\sin^2(\theta_1)=\sqrt{(p_1/(1-p_0))}$.

■

The sequence of coin transformations in the above proposition is optimal in the sense that there exist states (and probability distributions) that cannot be reached in a number of steps strictly less than 2. Using the results proven above and the symmetry property proven in Theorem 4, we obtain the following.

Corollary 6.2: Let (p_0^1,p_1^1,p_2^1) and (p_0^2,p_1^2,p_2^2) be two given probability distributions. Then it is always possible to find two states ψ_1 and ψ_2 whose probability distributions are the given one, and such that ψ_2 is reachable from ψ_1 in at most four steps.

B. Cycle with *N*=5

Proposition 6.3: It is possible from the initial state $\psi_{\text{in}}=|+1\rangle\otimes|0\rangle=\vec{e}_1^{10}$ to reach in four steps a final state ψ_f whose probability distribution is the uniform one.

Proof: In this proof we use again the notation $C(\theta,\phi)$ [see Eq. (58)] to denote matrices in SU(2). Let $\psi_f=[x_0,x_1,x_2,x_3,x_4,y_0,y_1,y_2,y_3,y_4]^T$ be the state reached from ψ_{in} in four steps by applying $U(\theta_i)=S(C(\theta_i,0)\otimes\mathbf{1}_5)$, with $i=1,\ldots,4$. Denote by $c_i=\cos(\theta_i)$ and by $T_i=\tan(\theta_i)$ for $i=1,\ldots,4$. A direct calculation of $U(\theta_1)U(\theta_2)U(\theta_3)U(\theta_4)\psi_{\text{in}}$ shows that we have

$$x_0 = c_4c_3c_2c_1(-T_3T_1 + T_4T_3T_2T_1 - T_4T_2),$$

$$x_1 = 0,$$

$$x_2 = c_4c_3c_2c_1(-T_2T_1 - T_3T_2T_1 - T_4T_3),$$

$$x_3 = c_4c_3c_2c_1(-T_4T_1),$$

$$x_4 = c_4c_3c_2c_1,$$

$$y_0 = c_4c_3c_2c_1(-T_4T_2T_1 - T_4T_3T_2 + T_3),$$

$$y_1 = c_4c_3c_2c_1(T_1),$$

$$y_2 = c_4c_3c_2c_1(T_4),$$

$$y_3 = c_4c_3c_2c_1(-T_4T_3T_1 - T_3T_2T_1 + T_2),$$

$$y_4 = 0. \tag{59}$$

We need to find θ_i, for $i=1,\ldots,4$, such that $p_j=x_j^2+y_j^2=1/5$ for all $j=0,\ldots,4$ (all quantities considered here are real).

One way to reach the uniform probability is to use the following constants:

$$c_1 = 1/\sqrt{2} \quad \text{and} \quad T_1 = 1,$$

$$|c_2| = |c_4| = \sqrt{2}/\sqrt{3} \quad \text{and} \quad |T_2| = |T_4| = 1/\sqrt{2}, \quad \text{with } T_2 = -T_4,$$

$$|c_3| = 3/\sqrt{(10)}, \quad \text{and} \quad T_3 = 1/3. \tag{60}$$

With this choice, we have

$$(c_4c_3c_2c_1)^2 = 1/5,$$

thus,

$$p_4 = x_4^2 = (c_4c_3c_2c_1)^2 = 1/5 \quad \text{and} \quad p_1 = y_1^2 = (c_4c_3c_2c_1)^2T_1^2 = 1/5.$$

Moreover, we also have

$$p_2 = x_2^2 + y_2^4 = 1/5T_2^2 + 1/5T_4^2 = 1/5$$

and

$$p_3 = x_3^2 + y_3^4 = 1/5T_4^2 + 1/5T_2^2 = 1/5.$$

It is also easy to see that by choosing $T_3=1/3$, we get $x_0=0$ and $y_0=c_4c_3c_2c_1$, while if we set $T_3=-1/3$, we get $x_0=c_4c_3c_2c_1$ and $y_0=0$. In any case, $p_0=1/5$, as desired. Notice that the choice is not unique.

The number of steps (4) in the previous proposition is optimal in the sense that no other algorithm will reach the uniform distribution with a number of steps less than 4. A direct analysis of the dynamics shows that after three steps the probability p_0 must be zero, after two steps p_1 and p_4 must be zero and after one step p_0, p_2, and p_3 must be zero.

Remark 6.4: It is not difficult to see that quantum walks can achieve different probability distributions and/or faster than classical random walks. There are several examples in the literature. The 5-cycle treated in this subsection offers another very simple example. By changing the coin operation in SU(2) at each step one directly verifies that, in two steps, from $\psi_{\text{in}}=|+1\rangle\otimes|0\rangle$, states can be reached with probability distributions $(p_0,0,p_2,p_3,0)$, with arbitrary (non-negative) values of p_0, p_2, and p_3, such that $p_0+p_2+p_3=1$. In the classical case, the evolution at each step (on a five-dimensional vector space) is given by $(1-r)F^T+rF$, where F defined in (5) is 5×5 and $0\leq r\leq1$. Starting with a probability concentrated in position 0, i.e., from $[1,0,0,0,0]^T$, and indicating by r_1 and r_2 the value of r at steps (1) and (2), respectively, the vector of probabilities after two steps is $[(1-r_2)r_1+r_2(1-r_1),0,r_1r_2,(1-r_1)(1-r_2),0]^T$. It is clear that $r_1r_2\neq0$ and $(1-r_1)(1-r_2)\neq0$ implies $(1-r_2)r_1+r_2(1-r_1)\neq0$ and therefore probability distributions with $p_0=0$, $p_2\neq0$, and $p_3\neq0$ cannot be reached in two steps. Other cases include $p_0=p_2=p_3=\frac{1}{3}$.

Remark 6.5: Propositions 6.1 and 6.3 give algorithms for the $N=3$ and $N=5$ cycles, in, respectively, *two* and *four* steps to reach a state whose probability distribution is the uniform one. To apply the result in Theorem 5 to get an algorithm to reach the uniform probability distribution in the corresponding planar lattice ($d=2$) for $N=3$ and $N=5$, we need to be able to reach the uniform probability distribution on the cycle in, respectively, *three* and *five* steps. This small discrepancy can be solved by adding an extra "dummy" step to the algorithms of Propositions 6.1 and 6.3. The evolution on the cycle at this step is of the form $S(\mathbf{1}_2\otimes\mathbf{1}_N)$ ($N=3$ or $N=5$). It performs a forward shift in the vertices of the cycle and does not modify the property of the probability distribution to be uniform. Therefore Propositions 6.1 and 6.3 can be used in conjunction with Theorem 5 to obtain algorithms on two-dimensional lattices with $N=3$ and $N=5$.

VII. CONCLUSION

The design of an algorithm using a quantum walk can be seen as a control problem consisting in driving the state of the walk from one value to another. For example, a search algorithm can start from a state where all the positions of the walker have the same probability and ends with a state where the probability is concentrated in one position. After the evolution has achieved the desired state transfer a measurement of the (walker) position observable reveals the (looked for)

eigenvalue corresponding to the desired position. The analysis of feasibility of quantum algorithms using quantum walks is therefore a *controllability analysis*.

In this paper, we have provided such controllability analysis for the quantum walk on a d-dimensional lattice, for general d, where the coin operation is allowed to change at each step. We have characterized the set of possible evolutions and seen that it is a Lie group which is the direct product on N^d, SU$(2d)$'s, where N is the number of vertices along one dimension of the lattice. We also described the set of achievable states and achievable probability distributions for this system. One important question is how the set of states and probabilities that can be achieved depends on the number of steps employed in the evolution. This study is formalized by defining reachable sets. We have described some general properties of these sets. Moreover, for low dimensional cases we were able to explicitly design the sequence of coin transformations leading to a desired state transfer (in minimum time). That is, we gave some results on constructive controllability. Further research in this area will focus on the extension of these control algorithms to general dimensions, the analysis of different graph topologies, and of different models, where the coin operation is allowed to change not only with time but also according to the position of the walker.

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