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Quantum walks on Cayley graphs

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Abstract

We address the problem of the construction of quantum walks on Cayley graphs. Our main motivation is the relationship between quantum algorithms and quantum walks. In particular, we discuss the choice of the dimension of the local Hilbert space and consider various classes of graphs on which the structure of quantum walks may differ. We completely characterize quantum walks on free groups and present partial results on more general cases. Some examples are given including a family of quantum walks on the hypercube involving a Clifford algebra.

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1. Introduction

Recently much effort has been devoted to the construction of new quantum algorithms. In particular, a question which has arisen is whether the known algorithms fully exploit the possibilities of quantum mechanics or if there could exist more efficient ones. A search for new ideas in this direction has been at the origin of a renewed study of quantum walks models [1], and a few results have already been obtained, showing that these are definitely relevant in this context.

The first general characterization of walks over graphs was presented in [2]. A possible construction for a walk operator is given, based on its classical equivalent, and some quantities relevant in the context of quantum algorithms are defined and computed. One of the principal results states that for bounded degree graphs the mixing time (defined also in the same work) is at most quadratically faster than the mixing time of the simple classical random walk on the same graph. Even if this general result is not so encouraging, some particular graphs have been shown to have properties intrinsically different from their classical equivalents. In particular, a symmetric quantum walk may get across a hypercube in a time linear with the dimension, while its classical counterpart would take an exponentially larger time.

In algorithmic applications, quantum walks have also shown interesting properties. The first important achievement has been the setting of the quantum search algorithm in the form of a quantum walk over a hypercube [3]. Some other similar quantum search algorithms were constructed after this. In one of them [4], the choice of the coin operator was revealed to be of crucial importance, since different operators may achieve different speed-ups (or no speed-up at all) without obvious reasons. A natural question which arises from this problem is whether there exist quantum walks different to those defined in [2] and if so, to what extent they could be the source of interesting new properties and algorithmic applications. Another problem lies in the dimension of the internal space: it is always possible to enlarge it, and in [5], it was shown that in an extremal case, the variance of the one-dimensional walk recovers the classical behaviour. In a similar direction in [6, 7], the authors have considered the evolution of a quantum particle governed by a quantum multi-baker map which can be settled as a quantum walk on a line with a multidimensional internal space; the classical limit is also recovered enlarging the dimension of the internal space. In contrast, an interesting and still open question is whether there exist quantum walks with local spaces of dimension smaller than that taken in the standard definition. In the context of quantum cellular automata, it is shown in [8] that for the simple lattice in d dimensions there is no nontrivial walk with an internal space of dimension 1, also known as the No-go theorem.

In this paper, we make a step in the direction of determining all possible quantum walks for general graphs and characterizing their structures. Starting from a general definition of a quantum walk we deduce necessary and sufficient conditions on the coin operators for the evolution to be unitary (section 2). The next section contains a discussion on the solutions of these equations (section 3). In particular, we characterize all possible walks on the Cayley graph of a free group. In the case of Abelian groups, the situation is somewhat more complicated, and after a general discussion we present particular solutions. We construct quantum walks over the two-dimensional and three-dimensional simple lattice with an internal space of dimension smaller than what was previously known and a generalization to arbitrary dimensions. We also consider the hypercube as a Cayley graph on which we construct a quantum walk where the coin operators are related to elements of the Clifford algebra. Finally, we propose a possible generalization of a quantum walk where we depart from the image of a particle moving on a lattice and which could be of interest in the context of quantum algorithms (section 4).

2. Model and unitary relations

A quantum algorithm is a sequence of transformations on a state of a quantum system. The quantum system is described by a tensor product of two-dimensional complex Hilbert spaces. There is a preferred basis of the elementary space where vectors are labelled with the integers 0 and 1 in correspondence to classical bits. Then a basis vector of the entire system is $|x_0\rangle \otimes \cdots \otimes |x_n\rangle$ where $x_i \in \{0, 1\}$ and in this way it is possible to associate with each base vector an integer whose binary decomposition coincides with the n-tuple $(x_0, \ldots, x_n)$. The total operator is the product of elementary operators. A presentation of possible sets as well as a demonstration of the universality of these sets may be found in [9].

A quantum walk is a model for the evolution of a particle over a graph. Many of the choices made in building the model may be explained by the aim of studying them as quantum algorithms. Let G be a directed graph with vertex set X and edge set E such that $G = (X, E)$. Let $\mathcal{H}$ be the Hilbert space defined by $\mathcal{H} = \mathcal{H}_I \otimes \mathcal{H}_G$. The space $\mathcal{H}_G = \ell^2(X)$ describes the position of the particle over the graph and the space $\mathcal{H}_I = \mathbb{C}^d$ describes some internal degrees of the particle. Let $\{|x\rangle\}_{x\in X}$ be a base of H_G and $\{|1\rangle, \ldots, |d\rangle\}$ a base of $\mathcal{H}_I$.

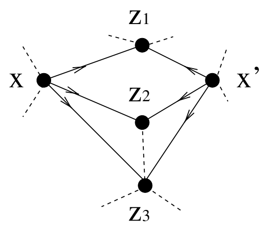

Figure 1. A pair of second neighbours and all paths of length 2 between them.

The evolution equation is

$$|\psi_{t+1}\rangle = W|\psi_t\rangle, \tag{1}$$

where W is a discrete time evolution operator defined as

$$W = \sum_{x\in X}\sum_{z\in E_x} M_{x,z} \otimes T_{x\to z}, \tag{2}$$

where E_x denotes the set of neighbouring sites of x and $T_{x\to z}$ translates the particle from x to z. $T_{x\to z}$ is defined by

$$\langle x'|T_{x\to z}|\psi\rangle = \langle x'|z\rangle\langle x|\psi\rangle. \tag{3}$$

$M_{x,z} : H_I \to H_I$ are maps modifying the internal space at the same time as the translation from vertex x to vertex z is applied. Suppose $|\psi_t\rangle = |i\rangle \otimes |z\rangle$. Then after one time step the probability of finding the particle in at vertex y, a neighbour of z, will depend on the previous internal state:

$$P(y) = \sum_{j=1}^{d} |\langle j|M_{z,y}|i\rangle|^2. \tag{4}$$

One image commonly used to describe the local evolution is that of a coin attached to each vertex and flipped to decide which neighbour the particle will jump to (see for instance [2]) and accordingly the local map $M_{x,y}$ is termed the 'coin operator'. Here we follow this usage though our model is more general than the image: in fact, it is important to note that originally the internal state was identified to the set of possible outcomes of the coin flip, or equivalently to the set of neighbours, so that the dimension of the internal space at a given vertex was necessarily equal to the number of outgoing edges. Here we have not considered this identification.

Unitarity of W is satisfied if and only if

$$W^\dagger W = \mathbb{1} \quad \Leftrightarrow \quad \sum_{z\in E_x\cap E_{x'}} M^\dagger_{x,z} M_{x',z} = \delta_{x,x'}\mathbb{1}_{H_I} \tag{5}$$

$$W W^\dagger = \mathbb{1} \quad \Leftrightarrow \quad \sum_{z\in E_x\cap E_{x'}} M_{z,x} M^\dagger_{z,x'} = \delta_{x,x'}\mathbb{1}_{H_I} \tag{6}$$

$\forall x, x'$. When $x \neq x'$, in order to have a nontrivial equation, x and x' must be second neighbours and the number of terms in the sum is related to the number of closed paths of length 4 with alternating orientation.

In the example of figure 1, one condition equation of the form (5) with three terms is associated with the pair of second neighbours x and x':

$$M^\dagger_{x,z_1} M_{x',z_1} + M^\dagger_{x,z_2} M_{x',z_2} + M^\dagger_{x,z_3} M_{x',z_3} = 0. \tag{7}$$

3. Quantum walks on Cayley graphs

We will restrict our study from now on to quantum walks on Cayley graphs. We first recall their definitions and main properties. We follow the presentation given in [10]. Given a group Γ one considers a set Δ of elements in Γ such that Δ is a generating set for Γ. The Cayley graph $C_\Delta(\Gamma) = (X, E)$ is defined as the oriented graph with

$$X \equiv X(C_\Delta(\Gamma)) = \Gamma \tag{8}$$

$$E \equiv E(C_\Delta(\Gamma)) = \{(x, x\delta)_\delta | x \in \Gamma, \delta \in \Delta\}. \tag{9}$$

When associating a colour with each element of the generating family, the definition of $C_\Delta(\Gamma)$ makes it a coloured directed graph. In addition, a Cayley colour graph is vertex transitive, so that each site is equivalent. Thus, we consider internal operators which depend only on the edge colour and direction of the edge (x, y) (i.e. only on the generator $\delta = x^{-1}y$) and not on the starting vertex x:

$$M_{x,y} = M_{x^{-1}y} \qquad \text{for all} \quad (x, y) \in E. \tag{10}$$

Thus, the evolution operator W on $\mathcal{H}$ is

$$W = \sum_{\delta \in \Delta} M_\delta \otimes T_\delta, \tag{11}$$

where T_δ is the shift in the direction δ and is defined for all vertices by the group operation

$$T_\delta = \sum_{x \in X} T_{x \to x\delta}. \tag{12}$$

The problem is thus reduced to a local one on $\mathcal{H}_I$ and the unitarity conditions (5) and (6) now read

$$\sum_{\delta_1\delta_2^{-1}=u} M_{\delta_1}^\dagger M_{\delta_2} = \delta_{\{u=e\}} \mathbb{1} \tag{13}$$

$$\sum_{\delta_1\delta_2^{-1}=u} M_{\delta_1} M_{\delta_2}^\dagger = \delta_{\{u=e\}} \mathbb{1}, \tag{14}$$

where both sums run over all pairs of elements in Δ, u is any element in the set

$$\Delta_2 = \{\delta\delta'^{-1}; \delta, \delta' \in \Delta\} \tag{15}$$

and e is the neutral element in Γ. The number of equations is twice the cardinality of $|\Delta_2|$ and the number of terms in at least some of these equations will be larger than 1 as soon as there exist closed paths of length 4 on the graph with an alternating orientation, which in terms of the generators is

$$\delta_1\delta_2^{-1}\delta_4\delta_3^{-1} = e. \tag{16}$$

Because of this relation it will be sometimes useful to define the group Γ itself in terms of the 'free presentation',

$$\Gamma = \langle \Delta' | R \rangle, \tag{17}$$

where Δ' is a set of generators of a free group and R is the set (which may also be empty) of relations between the elements of Δ' and their inverses which defines the structure of the group. To define the Cayley graphs (8) and (9) in the following we will use the generating set Δ defined by

$$\Delta = \{\gamma : \gamma \in \Delta' \vee \gamma^{-1} \in \Delta'\}, \tag{18}$$

where Δ' is the generating set used in the free presentation of the group. In particular, Δ may contain at the same time a generator and its inverse.

We now list some generic cases of Cayley groups.

3.1. Cayley graphs of free groups

As its name suggests, a free group is a group generated with a (finite) number of generators with no relations between them:

$$\Gamma = \langle \Delta' | - \rangle. \tag{19}$$

Let us consider the Cayley graph $C_\Delta(\Gamma)$ of the precedent group defined by (8), (9) and (18). The two sets of equations (13) and (14) can be written as

$$M_{\delta_1}^\dagger M_{\delta_2} = M_{\delta_1} M_{\delta_2}^\dagger = 0 \qquad \text{for all} \quad \delta_1 \neq \delta_2 \tag{20}$$

$$\sum_{\delta \in \Delta} M_\delta M_\delta^\dagger = \sum_{\delta \in \Delta} M_\delta^\dagger M_\delta = \mathbb{1}. \tag{21}$$

Theorem 1. *On the Cayley graph of the free group (19), defined by (8), (9) and (18), the quantum walk evolution operator (2) is unitary if and only if the internal operators are of the form*

$$M_\delta = U P_\delta, \tag{22}$$

where U is a unitary matrix of dimension $\dim(\mathcal{H}_I)$ and $\{P_\delta\}_{\delta\in\Delta}$ is a complete family of orthogonal projectors,

$$\sum_{\delta \in \Delta} P_\delta = \mathbb{1}. \tag{23}$$

The internal space is of dimension larger than or equal to $|\Delta|$.

Proof. First, it is easy to see that (22) is a solution for (20) and (21). Now suppose equations (20) and (21) imply the following relations between the images of the maps:

$$\mathcal{H}_I = \bigoplus_{\delta \in \Delta} \operatorname{Im}(M_\delta) \tag{24}$$

$$\mathcal{H}_I = \bigoplus_{\delta \in \Delta} \operatorname{Im}\big(M_\delta^\dagger\big). \tag{25}$$

The fact that a direct sum appears on the right-hand sides of (24) and (25) is just a consequence of equations (20) which make all subspaces pairwise orthogonal. The equality (rather than an inclusion) is due to (21). Define $U \equiv \sum_\delta M_\delta$, a unitary matrix by (20) and (21), and P_δ as the orthogonal projector on $\operatorname{Im}\big(M_\delta^\dagger\big)$, (22) follows by considering the elements of a vector basis compatible with decomposition (25). The claim that (22) is the general solution is thus proven. □

One should note however that the right-hand side of (22) could be written in many other ways, for instance with its factors written in the opposite order (which makes P_δ the projector on $\operatorname{Im}(M_\delta)$). When the rank of all matrices M_δ is fixed to 1, the dimension on the local Hilbert space takes its minimal value $\dim(\mathcal{H}_I) = |\Delta|$, and if a symmetric presentation for the group is chosen (i.e. $\delta \in \Delta$ implies $\delta^{-1} \in \Delta$), the standard definition of quantum 'coin' solution [2] is recovered. Besides these solutions, the only other possibility in the case of free groups consists in taking matrices M_δ of rank different from 1 and possibly varying with δ.

The case when the generating set that defines the Cayley graph contains the group identity e and at the same time some generators and their inverses are slightly more involved because the group identity e commutes with all the elements in the group. If both a generator δ and its inverse δ^{-1} are in Δ in addition to equations (20), one has

$$M_\delta^\dagger M_e + M_e^\dagger M_{\delta^{-1}} = 0 \tag{26}$$

$$M_e M_\delta^\dagger + M_{\delta^{-1}} M_e^\dagger = 0 \tag{27}$$

for all $\delta \neq e$. Summing all equations in (26), one gets $M_e^\dagger S = -S^\dagger M_e$ where $S = \sum_\delta M_\delta$. Adding again two instances of equations (26) for both a given δ and its inverse δ^{-1} gives

$$\big(M_e^\dagger S\big)(P_\delta + P_{\delta^{-1}}) = (P_\delta + P_{\delta^{-1}})\big(M_e^\dagger S\big) \tag{28}$$

for all $\delta \neq e$. Thus $M_e^\dagger S$ is block diagonal in the representation where all the orthogonal projectors P_δ are simultaneously diagonal. The problem can essentially be reduced to the one-dimensional case which we explore below. This is the first instance of a solution to equations (26) and (27) different to solution (22), in the case when there is more than one non-zero term.

3.1.1. One-dimensional walks. The simplest example is a quantum walk in one dimension. Let us consider the group generated by one element $\Gamma = \langle\delta|-\rangle$ and the Cayley graph obtained (8) and (9) using Γ and the set $\Delta = \{\delta, \delta^{-1}\}$. The minimal dimension of the internal space is 2 by the preceeding theorem and the form of the solution follows equation (22). The evolution operator defined in (11) reads in this case

$$W = (U \otimes Id)(P_\delta \otimes T_\delta + P_{\delta^{-1}} \otimes T_{\delta^{-1}}), \tag{29}$$

where U is a 2×2 unitary matrix. Two quantum walk evolution operators W and W' differing by a unitary transformation V would be equivalent, since this amounts to a change of basis for the initial and final states. We will suppose V of the form of a tensor product $A \otimes \mathbb{1}$. Thus equation (29) defines a family of inequivalent quantum walks indexed by four real parameters: the four parameters associated with the unitary matrix U while the projectors P_δ, $P_{\delta^{-1}}$ become the projectors over the spaces spanned by each of the basis vectors.

A quantum walk can also be left–right symmetric if it is invariant, up to a unitary transformation $S \otimes \mathbb{1}$, under the transformation $T_\delta \leftrightarrow T_{\delta^{-1}}$. The family of inequivalent and left–right symmetric quantum walks are of the reduced form described before with U,

$$U = e^{i\delta}\begin{pmatrix} \cos\frac{\theta}{2} & e^{i\alpha}\sin\frac{\theta}{2} \\ -e^{-i\alpha}\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}. \tag{30}$$

This defines then a three-parameter family of inequivalent left–right symmetric quantum walks. The unitary S depends also on the three parameters. When the identity appears in Δ, two kinds of solutions can be devised depending on whether the two terms appearing in (26) and (27) are separately zero or not. In the first case, one needs to add (at least) one state associated with the identity and the evolution operator becomes

$$W = (U \otimes Id)(P_\delta \otimes T_\delta + P_{\delta^{-1}} \otimes T_{\delta^{-1}} + P_e \otimes Id), \tag{31}$$

where U is a 3×3 unitary matrix, and appears just as a simple extension of the previous example. However, solutions exist with a two-dimensional local Hilbert space, and in such cases the evolution operator is

$$W = (U \otimes Id)\big(\cos(\theta)(P_\delta \otimes T_\delta + P_{\delta^{-1}} \otimes T_{\delta^{-1}}) + \sin(\theta) R_{\frac{\pi}{2}} \otimes Id\big), \tag{32}$$

where U is a 2×2 unitary matrix, and $R_{\frac{\pi}{2}} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$. Equivalent solutions with a two-dimensional local Hilbert space were presented first in [11]. In conclusion, we also note that solution (22) remains valid when adding relations between generators. Thus such solutions exist for all groups, in particular for free products of cyclic groups,

$$\Gamma = \left\langle \delta_1, \ldots, \delta_l \middle| \delta_1^{q_1} = \cdots \delta_l^{q_l} = e \right\rangle$$

and for free Abelian groups,

$$\Gamma = \left\langle \delta_1, \ldots, \delta_l \middle| \delta_i \delta_j \delta_i^{-1} \delta_j^{-1} = e \; \forall i, j \in \{1, \ldots, l\} \right\rangle,$$

which we consider in the next section.

3.2. Cayley graphs of free Abelian groups

One should note that the commutation relations between elements from the set of generators and their inverses, for instance

$$\delta_1 \delta_2^{-1} = \delta_2^{-1} \delta_1, \tag{33}$$

do not necessarily imply the existence of a closed path on the graph with alternate orientation of the edges (16), except in the case when the inverses of the elements of Δ are themselves in Δ. The group is defined by

$$\Gamma = \left\langle \delta_1, \ldots, \delta_n \middle| \delta_i \delta_j \delta_i^{-1} \delta_j^{-1} = e \; \forall i, j \in \{1, \ldots, n\} \right\rangle \tag{34}$$

and the set used to construct the Cayley graph is

$$\Delta = \left\{ \delta_1, \ldots, \delta_n, \delta_1^{-1}, \ldots, \delta_n^{-1} \right\}. \tag{35}$$

In such a case, equations (13) and (14) read

$$M_{\delta_i}^\dagger M_{\delta_j} + M_{\delta_j^{-1}}^\dagger M_{\delta_i^{-1}} = 0 \qquad \text{for all} \quad \delta_i \neq \delta_j \tag{36}$$

$$M_{\delta_i} M_{\delta_j}^\dagger + M_{\delta_j^{-1}} M_{\delta_i^{-1}}^\dagger = 0 \qquad \text{for all} \quad \delta_i \neq \delta_j \tag{37}$$

$$\sum_{\delta \in \Delta} M_\delta M_\delta^\dagger = \sum_{\delta \in \Delta} M_\delta^\dagger M_\delta = \mathbb{1}. \tag{38}$$

When $\delta_j = \delta_i^{-1}$, equations (36) and (37) contain a single term and read

$$M_{\delta_i}^\dagger M_{\delta_i^{-1}} = M_{\delta_i^{-1}} M_{\delta_i}^\dagger = 0. \tag{39}$$

These are much less restrictive conditions than (20) and (21), and we lack here the decomposition of $\mathcal{H}_I$ into orthogonal subspaces which allowed us to give a general answer in the case of free groups. We only note that equations (36) and (37) are equivalent to the following:

$$\left(\sum_{\delta \in A} \lambda_\delta M_\delta^\dagger \right) \left(\sum_{\delta \in A} \lambda_\delta M_\delta^{-1} \right) = \left(\sum_{\delta \in A} \lambda_\delta M_\delta^{-1} \right) \left(\sum_{\delta \in A} \lambda_\delta M_\delta^\dagger \right) = 0, \tag{40}$$

for all subset $A \in \Delta$ such that $\delta \in A \Rightarrow \delta^{-1} \notin A$ and for all families of real parameters $\{\lambda_\delta\}_{\delta \in A}$.

Equations (36) and (37) imply the following proposition which will help us classify the solutions.

Proposition 1. *Let $C_\Delta(\Gamma)$ be the Cayley graph of the free Abelian group with n generators ((34) and (35)). If a quantum walk operator (2) defined on G is unitary, then the image subspaces of any two internal operators M_{δ_i} and M_{δ_j} are either orthogonal or contain a* *common vector subspace. The same implication is valid for the image subspace of their conjugates $M_{\delta_i}^\dagger$ and $M_{\delta_j}^\dagger$:*

$$\big(\mathrm{Im}\big(M_{\delta_i}\big) \cap \mathrm{Im}\big(M_{\delta_j}\big) = \{0\}\big) \quad \Rightarrow \quad \mathrm{Im}\big(M_{\delta_i}\big) \perp \mathrm{Im}\big(M_{\delta_j}\big) \tag{41}$$

$$\big(\mathrm{Im}\big(M_{\delta_i}^\dagger\big) \cap \mathrm{Im}\big(M_{\delta_j}^\dagger\big) = \{0\}\big) \quad \Rightarrow \quad \mathrm{Im}\big(M_{\delta_i}^\dagger\big) \perp \mathrm{Im}\big(M_{\delta_j}^\dagger\big). \tag{42}$$

Proof. Using (37) for a pair δ_i, δ_j^{-1}, one has

$$\mathrm{Im}\big(M_{\delta_i} M_{\delta_j^{-1}}^\dagger\big) = \mathrm{Im}\big(M_{\delta_j} M_{\delta_i^{-1}}^\dagger\big) \tag{43}$$

and thus

$$\mathrm{Im}\big(M_{\delta_i} M_{\delta_j^{-1}}^\dagger\big) \subset \big(\mathrm{Im}\big(M_{\delta_i}\big) \cap \mathrm{Im}\big(M_{\delta_j}\big)\big). \tag{44}$$

Suppose now that $\mathrm{Im}\big(M_{\delta_i}\big)$ and $\mathrm{Im}\big(M_{\delta_j}\big)$ have no common vector subspace. Thus $M_{\delta_i} M_{\delta_j^{-1}}^\dagger = 0$, which can be written as

$$\mathrm{Im}\big(M_{\delta_i}^\dagger\big) \perp \mathrm{Im}\big(M_{\delta_j^{-1}}^\dagger\big) \tag{45}$$

and more particularly

$$\mathrm{Im}\big(M_{\delta_i}^\dagger M_{\delta_j}\big) \perp \mathrm{Im}\big(M_{\delta_j^{-1}}^\dagger M_{\delta_i^{-1}}\big). \tag{46}$$

Since the two subspaces are equal (by (39) and orthogonal, they are equal to the null vector space and hence we have again $M_{\delta_i}^\dagger M_{\delta_j} = 0$, and finally

$$\mathrm{Im}\big(M_{\delta_i}\big) \perp \mathrm{Im}\big(M_{\delta_j}\big). \tag{47}$$

The implication (41) is thus proven. The proof of (42) is equivalent, beginning with equation (36) instead of (37). □

We can use proposition (1) to find solutions with an internal space dimension smaller than the number of generators in the following way. First we can write

$$\dim(\mathcal{H}_I) \geqslant \sup_{\delta_i, \delta_j} \left\{ \sum_{\epsilon_1, \epsilon_2 = \pm 1} \dim\big(\mathrm{Im}\big(M_{\delta_i^{\epsilon_1}}\big) \cap \mathrm{Im}\big(M_{\delta_j^{\epsilon_2}}\big)\big) \right\} \tag{48}$$

where the sup runs over all pairs δ_i, δ_j such that both $\delta_i \neq \delta_j$ and $\delta_i \neq \delta_j^{-1}$. This inequality is true since the four sets appearing on the right-hand side are pairwise orthogonal by (39). A similar equation could be written involving the $M^\dagger$'s. Suppose now that the supremum on the right-hand side of (48) is zero, hence giving no direct condition on the dimension of $\dim(\mathcal{H}_I)$. In such a case, all vector subspaces are orthogonal by (41), which imply $\dim(\mathcal{H}_I) \geqslant |\Delta|$. Hence, a necessary condition for the existence of quantum walks with a smaller internal space is that some of the intersections in the sum (48) are nonempty. In the following we give some examples.

3.2.1. A two-dimensional walk with a two-dimensional internal space. We consider here the group $\Gamma = \big\langle \delta_1, \delta_2 \big| \delta_1 \delta_2 \delta_1^{-1} \delta_2^{-1} = e \big\rangle$, a symmetric set $\Delta = \big\{\delta_1, \delta_1^{-1}, \delta_2, \delta_2^{-1}\big\}$ and define a quantum walk over the associated Cayley graph through the evolution operator (11) which reads here

$$W = M_{\delta_1} \otimes T_{\delta_1} + M_{\delta_1^{-1}} \otimes T_{\delta_1^{-1}} + M_{\delta_2} \otimes T_{\delta_2} + M_{\delta_2^{-1}} \otimes T_{\delta_2^{-1}}. \tag{49}$$

We suppose that the rank of each matrix M_{δ_i} is 1. In order to impose $\dim(\mathcal{H}_I) = 2$, we require that at least two terms on the right-hand side of (48) are zero for each possible pair of generators δ_i, δ_j. We obtain two solutions which transform one derived from the other by changing δ_1 and δ_1^{-1}. Up to a unitary transformation, the solution is

$$M_{\delta_1} = UP_1VP_1 \qquad M_{\delta_1^{-1}} = UP_2VP_2 \qquad M_{\delta_2} = UP_1VP_2 \qquad M_{\delta_2^{-1}} = UP_2VP_1,$$

where U and V are two unitary matrices and P_1, P_2 are two orthogonal projectors. The evolution operator factorizes into a product of two one-dimensional operators:

$$W = (U \otimes 1)\left(P_1 \otimes \left(T_{\delta_1}T_{\delta_2}\right)^{\frac{1}{2}} + P_2 \otimes \left(T_{\delta_1^{-1}}T_{\delta_2^{-1}}\right)^{\frac{1}{2}}\right) \\ \times (V \otimes 1)\left(P_1 \otimes \left(T_{\delta_1}T_{\delta_2^{-1}}\right)^{\frac{1}{2}} + P_2 \otimes \left(T_{\delta_1^{-1}}T_{\delta_2}\right)^{\frac{1}{2}}\right).$$

However, a quantum walk with a two-dimensional internal space which is symmetric by inversion of only one of the axes or by a rotation of angle $\frac{\pi}{2}$ does not exist. This solution generalizes in higher dimensions.

Proposition 2. *Let $C_\Delta(\Gamma)$ be the Cayley graph of the free Abelian group with n generators and symmetric presentation (34) and (35). Then there exists a unitary quantum walk operator (2) on G such that the dimension of the internal space is n if n is even and $n + 1$ if n is odd.*

Proof. Suppose n is even. We consider an internal space of dimension n and decompose it as a direct sum of two-dimensional subspaces. We associate with each of these subspaces one different pair of generators. For such a pair (δ_i, δ_j), the four operators $M_{\delta_i}, M_{\delta_j}, M_{\delta_i^{-1}}, M_{\delta_j^{-1}}$ act nontrivially only on the associated two-dimensional subspace and can be constructed in the same way as the internal operators of the previous example of a two-dimensional walk. The dimension of the internal space for such a quantum walk is then half the dimension of the free form solution. Suppose now n is odd. We can repeat the previous construction for $n - 1$ generators, and add a two-dimensional space where the internal operators associated with the last generator will have the form of the internal operators of a one-dimensional walk. All the internal operators then verify the condition equations (36)–(38). □

3.2.2. Two-dimensional walks with a four-dimensional internal space. The impossibility of having a fully symmetric quantum walk does not hold when taking a four-dimensional internal space. One possibility is to suppose that all the intersections involved in (48) are of dimension zero, in this case $\dim(\mathcal{H}_I) \geqslant |\Delta| = 4$ and the minimal choice of the dimension leads to an evolution operator $W = \sum_\delta P_\delta U \otimes T_\delta$ where U is a four-dimensional unitary matrix. The other possibility is to suppose that all the intersections involved in (48) are of dimension 1. In this case, the minimal dimension of the internal space is also 4. A simple choice of matrices of rank 2 verifying all the conditions (36)–(38) is

$$M_{\delta_1} = \frac{1}{\sqrt{2}}(|u_1\rangle\langle v_1| + |u_2\rangle\langle v_3|) \tag{50}$$

$$M_{\delta_1^{-1}} = \frac{1}{\sqrt{2}}(-|u_3\rangle\langle v_4| + |u_4\rangle\langle v_2|) \tag{51}$$

$$M_{\delta_2} = \frac{1}{\sqrt{2}}(|u_1\rangle\langle v_2| + |u_3\rangle\langle v_3|) \tag{52}$$

$$M_{\delta_2^{-1}} = \frac{1}{\sqrt{2}}(-|u_4\rangle\langle v_1| + |u_2\rangle\langle v_4|), \tag{53}$$

where $\{|u_i\rangle\}_{i=1,\dots,4}$ and $\{|v_i\rangle\}_{i=1,\dots,4}$ are two orthonormal bases of $\mathcal{H}_I$. In the following, we give the explicit form of the evolution operator supposing that the rank of the matrices M_δ is 1 and that the walk is symmetric. A permutation of the vertex set Π is associated with a spatial transformation. As in the one-dimensional case, the walk is symmetric under this transformation if there exists a unitary S such that $(S \otimes \Pi)^\dagger W(S \otimes \Pi) = W$. In other words, if the initial condition is modified by the transformation $S \otimes \Pi$, the wavefunction at any time can be deduced from the unmodified wavefunction by application of the same transformation. We impose invariance under the symmetries of the square lattice by considering the two transformations, $S_i \otimes \Pi_i$ and $S_r \otimes \Pi_r$, being respectively the representation of the inversion along the x axis and the rotation by $\frac{\pi}{2}$. The symmetry condition makes U reduce to a product $U = D^{-1}U_0 D$ where D is a diagonal unitary matrix depending on four real parameters and U_0 takes the form

$$U_0 = \begin{pmatrix} a & b & c & c \\ b & a & c & c \\ c & c & a & b \\ c & c & b & a \end{pmatrix}.$$

The matrix U_0 depends on three parameters by the unitarity condition. The matrices S_1 and S_2 depend on the same parameters as the matrix D. Then choosing these four parameters equal to 1 reduces the walk operator to $W = \sum_i P_i U_0 \otimes Ti$ and the matrices S_1 and S_2 are just the inverse permutation of the generators associated with the spatial transformation.

3.2.3. A three-dimensional walk with a four-dimensional internal space. It has been shown that no nontrivial solution exists in three dimensions with a two-dimensional internal space [12]. In the following, we give solutions on $\mathbb{Z}^3$ with a four-dimensional internal space. The starting point is again equation (48). Taking matrices of rank 2 would not break this condition for $\dim(\mathcal{H}_I)$ provided that each term on the left-hand side of (48) is 1. Here we thus give the general solution for rank 2 matrices. Let $\Delta = \{\delta_1, \delta_2, \delta_3, \delta_1^{-1}, \delta_2^{-1}, \delta_3^{-1}\}$. Defines two orthonormal bases $\{|u_i\rangle\}_{i=1,\cdot,4}$ and $\{|v_i\rangle\}_{i=1,\cdot,4}$. Now construct six matrices of rank 2 indexed by the elements of Δ in the form

$$M_{\delta_1} = \alpha_1|u_1\rangle\langle v_2| + \beta_1|u_2\rangle\langle v_1| \tag{54}$$
$$M_{\delta_1^{-1}} = \gamma_1|u_3\rangle\langle v_4| + \delta_1|u_4\rangle\langle v_3| \tag{55}$$
$$M_{\delta_2} = \alpha_2|u_1\rangle\langle v_3| + \gamma_2|u_3\rangle\langle v_1| \tag{56}$$
$$M_{\delta_2^{-1}} = \beta_2|u_2\rangle\langle v_4| + \delta_2|u_4\rangle\langle v_2| \tag{57}$$
$$M_{\delta_3} = \alpha_3|u_1\rangle\langle v_4| + \delta_3|u_4\rangle\langle v_1| \tag{58}$$
$$M_{\delta_3^{-1}} = \beta_3|u_2\rangle\langle v_3| + \gamma_3|u_3\rangle\langle v_2|. \tag{59}$$

It is clear that such a choice solves equations (39). The other equations are solved by taking

$$\alpha_2 = \lambda\alpha_1; \qquad \alpha_3 = \mu\alpha_1 \tag{60}$$
$$\beta_2 = \bar{\lambda}\nu\beta_1; \qquad \beta_3 = -\bar{\mu}\nu\beta_1 \tag{61}$$
$$\gamma_2 = -\lambda\bar{\nu}\gamma_1; \qquad \gamma_3 = -\bar{\mu}\gamma_1 \tag{62}$$
$$\delta_2 = -\bar{\lambda}\delta_1; \qquad \delta_3 = \mu\bar{\nu}\delta_1, \tag{63}$$

where $|\nu|^2 = 1$, $\lambda, \mu \in \mathbb{C}$ and

$$|\alpha_1| = |\beta_1| = |\gamma_1| = |\delta_1| = \frac{1}{\sqrt{1 + |\lambda|^2 + |\mu|^2}}. \tag{64}$$

3.3. Cayley graphs with multiply connected second neighbours

In this section, we consider Cayley graphs in which any second neighbour is connected by at least two alternating paths. They might be of interest since the condition equations contain at least two terms. Here, we only consider two examples in which each second neighbour is connected by at least two alternate paths. Both are interesting in their own right: the first one admits a scalar solution, while the other admits solutions in terms of a Clifford algebra.

3.3.1. A simple one-dimensional example. Let us consider the commutative group with two generators (34) with one more relation $\delta_1^2 = \delta_2^2$ in the presentation and as defining set for the Cayley graph $\Delta = \{\delta_1, \delta_2, \delta_1^{-1}, \delta_2^{-1}\}$.

The four matrices M_δ have to be taken as solutions of the four equations:

$$M_{\delta_1}^\dagger M_{\delta_1^{-1}} + M_{\delta_2}^\dagger M_{\delta_2^{-1}} = M_{\delta_1^{-1}} M_{\delta_1}^\dagger + M_{\delta_2^{-1}} M_{\delta_2}^\dagger = 0 \tag{65}$$

$$M_{\delta_1}^\dagger M_{\delta_2^{-1}} + M_{\delta_2}^\dagger M_{\delta_1^{-1}} = M_{\delta_2^{-1}} M_{\delta_1}^\dagger + M_{\delta_1^{-1}} M_{\delta_2}^\dagger = 0 \tag{66}$$

$$M_{\delta_1}^\dagger M_{\delta_2} + M_{\delta_2}^\dagger M_{\delta_1} + M_{\delta_1^{-1}}^\dagger M_{\delta_2^{-1}} + M_{\delta_2^{-1}}^\dagger M_{\delta_1^{-1}} = 0 \tag{67}$$

$$M_{\delta_2} M_{\delta_1}^\dagger + M_{\delta_1} M_{\delta_2}^\dagger + M_{\delta_2^{-1}} M_{\delta_1^{-1}}^\dagger + M_{\delta_1^{-1}} M_{\delta_2^{-1}}^\dagger = 0 \tag{68}$$

$$\sum_\delta M_\delta^\dagger M_\delta = \sum_\delta M_\delta M_\delta^\dagger = \mathbb{1}. \tag{69}$$

This set of equations admits solutions with a one-dimensional internal space, and the evolution operator can be written as

$$W = \tfrac{1}{2}\left(\mathrm{e}^{\mathrm{i}\theta}(\tau_1 \pm \tau_2) + \mathrm{e}^{\mathrm{i}\varphi}\left(\tau_1^{-1} \mp \tau_2^{-1}\right)\right), \tag{70}$$

where τ_1 and τ_2 are the displacements in the directions δ_1 and δ_2. However, as can be seen from the form of the evolution operator, this example is equivalent to a quantum walk on $\mathbb{Z}$ with a two-dimensional internal space by grouping together pairs of second neighbours. What is interesting here is that even on a graph where all sites are equivalent, there may exist scalar solutions provided all second neighbours are multiply connected. The minimal dimension of the internal space would still however have to be questioned since it strongly depends on the choice of the graph and various descriptions appear to be equivalent.

3.3.2. The hypercube. We consider the group presentation

$$\Gamma = \left\langle \delta_1, \ldots, \delta_n \middle| \delta_i^2 = e\, \forall i;\, \delta_i \delta_j \delta_i^{-1} \delta_j^{-1} = e\, \forall i \neq j \right\rangle, \tag{71}$$

whose Cayley graph is the hypercube in n dimensions. The condition equations become

$$M_{\delta_i}^\dagger M_{\delta_j} + M_{\delta_j}^\dagger M_{\delta_i} = 0 \tag{72}$$

$$M_{\delta_i} M_{\delta_j}^\dagger + M_{\delta_j} M_{\delta_i}^\dagger = 0 \tag{73}$$

$$\sum_\delta M_\delta^\dagger M_\delta = \mathbb{1}. \tag{74}$$

Equations (72) and (73) are valid for all pairs of generators δ_i, δ_j. Solutions originating from those for a free group of n generators have been studied by various authors ([13]–[14]).

Proposition 3. *There exists a unitary quantum walk operator (2) on the Cayley graph of the group (71) such that the internal operators are of the form* $M_{\delta_i} = \frac{1}{\sqrt{n}}\sigma_i U$ *where* U *is a unitary matrix of dimension* $\dim(\mathcal{H}_I)$ *and* $\{\sigma_1 \cdots \sigma_n\}$ *is a set of anticommuting matrices.*

Proof. If one requires that all the matrices M_δ be Hermitian (or anti-Hermitian), then the first set of equations (72) and (73) takes the form of an anticommutation relation between all pairs of matrices. Hermitian anticommuting matrices generate a Clifford algebra; it is therefore natural to find solutions among their matrix representations. Let $\{\sigma_1 \cdots \sigma_n\}$ be such a set of anticommuting matrices and U a unitary matrix. A possible choice for the matrices M_δ is then $M_{\delta_i} = \frac{1}{\sqrt{n}}\sigma_i U$. □

For example, equations for $n = 3$ are solved by $M_i = \frac{1}{\sqrt{3}}\sigma_i U$ where each σ_i is one of the three Pauli matrices and U a unitary matrix in two dimensions. While the dimension of the matrix representation is rather large, (at least $2^{[\frac{n}{2}]}$), such solution may nevertheless be useful.

4. A generalized model of quantum walk

A quantum walk is a model for the motion of a quantum particle jumping (quantically) over a graph. A particle having a fixed number of internal degrees of freedom, one is naturally led to attach to each point x of the graph a copy of some Hilbert space $\mathcal{H}_I$ describing them. This is obviously not a necessary hypothesis in the context of a network of quantum processors, and even if we will retain here most of the terminology of quantum walks, we will not base our approach in this section on the interpretation of our quantum object as a physical particle. A second important property is the choice of a discrete time evolution, again motivated by the idea that quantum processors as their classical equivalents would exchange information at discrete times.

We will continue to consider discrete time evolution but we want to note that quantum walks with continuous time has also been introduced in the context of quantum algorithmics [15, 16]. As for the discrete time model, the success of these walks performing particular tasks is dependent on characteristics such as the initial vector state [17], thus indicating that a classification of this model may also be of some interest. Some properties of one-dimensional walks have been determined as for example the revival time [18] and a limit theorem demonstrated by [19].

We consider an oriented graph $G = (X, E)$, where X is the set of vertices, and E is the set of oriented edges. To each vertex $x \in X$, we attach a (finite) Hilbert space $\mathcal{H}_x$, and define the quantum evolution over $\mathcal{H} = \oplus_{x\in X}\mathcal{H}_x$ as follows. For each oriented pair (x, y), we define a linear map $M_{x,y}$ from $\mathcal{H}_x$ to $\mathcal{H}_y$, extend it on $\mathcal{H}$ by setting $M_{x,y} = 0$ on $\mathcal{H}_x^\perp$. We define its conjugate $M_{x,y}^\dagger$ as the map such that

$$\langle \Psi' | M_{x,y}\Psi\rangle = \left\langle M_{x,y}^\dagger \Psi' \middle| \Psi\right\rangle \tag{75}$$

for all $|\Psi\rangle, |\Psi'\rangle$ in $\mathcal{H}$. Then, we define the evolution of the quantum walk over $\mathcal{H}$ as

$$|\Psi(t+1)\rangle = W|\Psi(t)\rangle, \tag{76}$$

where $|\Psi(t)\rangle$ is the state of the system at time t and W is the unitary operator

$$W = \sum_{(x,y)\in E} M_{x,y}. \tag{77}$$

In order to restrict the sum to the pairs of neighbouring sites and impose W to be unitary we require the following three properties:

$$M_{x,y} \neq 0 \qquad \text{if and only if} \qquad (x, y) \in E \tag{78}$$

$$\sum_y M^\dagger_{x,y} M_{z,y} = \sum_y M_{y,x} M^\dagger_{y,z} = 0 \qquad \text{for all} \qquad x \neq z \tag{79}$$

$$\sum_y M^\dagger_{x,y} M_{x,y} = \sum_y M_{y,x} M^\dagger_{y,x} = \mathbf{1_x}, \tag{80}$$

where $\mathbf{1_x}$ is the projector over $\mathcal{H}_x$. Conditions (79) and (80) are necessary and sufficient conditions for W to be unitary. Here, it is already interesting to note that even in this more general context quantum 'coin' solutions exist provided that on each site the number of incoming edges equals the number of outgoing ones. The construction can be done in the following way: we first set the dimension of all local Hilbert spaces equal to the number of incoming (or equivalently outgoing) neighbours,

$$\dim(\mathcal{H}_x) = \left|E^{\text{in}}_x\right| = \left|E^{\text{out}}_x\right|, \tag{81}$$

where we have set

$$E^{\text{in}}_x = \{y \in X : (y, x) \in E\} \tag{82}$$

$$E^{\text{out}}_x = \{y \in X : (x, y) \in E\}. \tag{83}$$

For all $x \in X$, we fix two orthonormal bases $\mathcal{B}^{\text{in}}_x$ and $\mathcal{B}^{\text{out}}_x$ in $\mathcal{H}_x$ an label its elements using the list of neighbours,

$$\mathcal{B}^{\text{in}}_x = \left\{\left|\varphi^{\text{in}}_x(y)\right\rangle\right\}_{y \in E^{\text{in}}_x} \tag{84}$$

$$\mathcal{B}^{\text{out}}_x = \left\{\left|\varphi^{\text{out}}_x(y)\right\rangle\right\}_{y \in E^{\text{out}}_x}. \tag{85}$$

Now setting

$$M_{x,y} = \left|\varphi^{\text{in}}_y(x)\right\rangle\left\langle\varphi^{\text{out}}_x(y)\right| \tag{86}$$

just satisfies all conditions (79), (80) and defines a general quantum 'coin' solution even outside the context of a quantum particle on a lattice. In fact, we get some more insight into how such solutions work from the point of view of a quantum network: first, each node splits the (partial) wavefunction along the vectors of a fixed basis $\mathcal{B}^{\text{out}}_x$ and send the resulting complex number to each of its neighbours; then a (partial) wavefunction is recomposed using the received numbers and the other fixed basis $\mathcal{B}^{\text{in}}_x$. We now want to recover the previous definition of quantum walks on a Cayley graph, so we naturally suppose that the properties of the graph are transferred to the walk. In particular, all local Hilbert spaces are copies of the same space

$$\mathcal{H}_x = \mathcal{H}_0 \tag{87}$$

for all x in X and the complete Hilbert space is equivalent to the direct product of the local space $\mathcal{H}_0$ with a position space $\mathcal{H}_X$:

$$\mathcal{H} \approx \mathcal{H}_0 \otimes \mathcal{H}_X. \tag{88}$$

Furthermore, the maps $M_{x,y}$ will depend only on the edge colour and direction of the edge (x, y) (i.e. only on the generator $\delta = x^{-1}y$) and not in the starting vertex x:

$$M_{x,y} = T_{0,y} M_{x^{-1}y} T_{x,0} \qquad \text{for all} \qquad (x, y) \in E \tag{89}$$

where $M_{x^{-1}y}$ is a map on $\mathcal{H}_0$ and $T_{x,y}$ is the canonical shift map sending $\mathcal{H}_x$ onto $\mathcal{H}_y$. Thus, the evolution operator W on $\mathcal{H}$ as a product space reads

$$W = \sum_{\delta \in \Delta} M_\delta \otimes T_\delta. \tag{90}$$

5. Conclusion

We have considered quantum walks on Cayley graphs of groups and addressed the problem of classifying them as a function of the group presentation and the choice of the internal space. A first result is that the smallest possible dimension of the internal space depends strongly on the generating set chosen for constructing the Cayley graph. In the case of free groups, we succeeded in classifying all possible solutions. Standard quantum walk definition is recovered and corresponds to an internal space of dimension equal to the number of neighbours (its smallest value) and a free group with a set of generators containing elements of the group different from the identity. When the identity element is present in the generating set used to define the Cayley graph of a free group, or on other Cayley graphs, we showed that different solutions do exist for which we give a partial characterization. We presented a few examples of solutions which do not enter in the previously known solutions and which become available as soon as there exist closed paths of length 4 on the graph, with alternating orientation. In particular, we found solutions with a smaller internal dimension that is usually expected and a new kind of quantum walks on the hypercube based on Clifford algebra representation. We hope that these new possibilities will prove useful in the context of the relationship between quantum walks and quantum algorithms.

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