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EXPLORING SCALAR QUANTUM WALKS ON CAYLEY GRAPHS

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A quantum walk, *i.e.*, the quantum evolution of a particle on a graph, is termed *scalar* if the internal space of the moving particle (often called the coin) has dimension one. Here, we study the existence of scalar quantum walks on Cayley graphs, which are built from the generators of a group. After deriving a necessary condition on these generators for the existence of a scalar quantum walk, we present a general method to express the evolution operator of the walk, assuming homogeneity of the evolution. We use this necessary condition and the subsequent constructive method to investigate the existence of scalar quantum walks on Cayley graphs of groups presented with two or three generators. In this restricted framework, we classify all groups – in terms of relations between their generators – that admit scalar quantum walks, and we also derive the form of the most general evolution operator. Finally, we point out some interesting special cases, and extend our study to a few examples of Cayley graphs built with more than three generators.

Keywords: Quantum walk

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1 Introduction

Within the traditional (discrete-time) model of quantum computation, there exist several definitions for a quantum walk on a given graph G over a set of vertices X. In general terms, a quantum walk simulates the evolution of a particle on the graph with some unitary operator as an evolution operator. The most studied model, the "coined model", defines the evolution operator as the product of two operators. One is a block diagonal operator which acts non-trivially only on some internal space of the particle, termed the "coin". The other operator is a permutation which moves the particle along the edges of the graph. In that model, the most common definition, which has been used for constructing existing quantum walk algorithms, is the one given by Aharonov *et al.* in [1]. Within this definition, the condition for the existence of such operators is that the graph G is a directed d-regular graph and that it is possible to "label each directed edge with a number between one and d such that for each possible label a, the directed edges labeled a form a permutation".

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Kendon gave another definition [2] which is valid for undirected graphs with a coin of dimension $|X|$, the number of vertices. In fact both definitions can be seen as particular cases of the definition given by Montanaro in [3]. Following the latter work, a necessary and sufficient condition to define a coined quantum walk is *reversibility*. When a graph is reversible, it has a certain number of cycles which may be used to define a coined quantum walk. The idea is that each cycle is associated to a basis state of the internal space, using the fact that cycles that do not have a vertex in common can be associated to the same basis state. The definition of Aharonov *et al.* requires the graph to be d-regular (and therefore reversible), with exactly d groups of disjoint cycles including all edges of the graph. Kendon's definition also requires a reversible graph, and in this case the cycles used are determined by each directed edge and the corresponding edge with opposite direction. Therefore, reversibility and the number of cycles in the graph may be used to classify the different possible definitions in a two operator (coined-shift) model of quantum walks.

If we restrict to the coined model (that is, we assume that the evolution operator factorizes into two operators), reversibility is a sufficient condition for the existence of a unitary evolution operator on a given graph. However, there exist other models that can be defined, where the evolution operator does not have the factorized (coined-shift) form, and for which no sufficient condition is known. In [4], quantum walks with one operator and with internal space (coin) are explored. It is shown how the existence of such walks is related to the properties of the graph and some examples are given. If the model has an internal space of dimension one, the one-operator model corresponds to the definition used in [5] and quantum walks become in this case equivalent to quantum cellular automata as defined by Meyer in [6]. Here, we will call this model (one operator and a one-dimensional internal space) a *scalar quantum walk*. When we will state that "a scalar quantum walk exists on some graph", it will be equivalent, in the language of [5], to the fact that "this graph is the pattern of a unitary matrix".

In [5], Severini gave a necessary condition for the existence of a scalar quantum walk on a directed graph (digraph), that he called *strong quadrangularity*, and which implies a weaker condition, namely *quadrangularity*. He also proved that when the graph satisfies another property, called *specularity*, strong quadrangularity becomes sufficient for the existence of a unitary evolution on the digraph. In general terms, a digraph is called *specular* if any two vertices are connected by outgoing edges to the same set of vertex or do not have any common first neighbor, the same being required for the ingoing edges. In [7], Severini also showed that specularity is equivalent to the condition that the operator may be expressed as the product of a permutation matrix and a block diagonal matrix. The underlying digraph of a coined quantum walk is therefore specular.

In this paper, we will address the general question of determining on which Cayley graphs a homogeneous scalar quantum walk can be defined. First, there is an obvious interest in this question from the point of view of quantum algorithmics. Indeed, the answer will help defining gates over digraphs, which could then be combined to construct quantum algorithms. Moreover, algorithms based on scalar quantum walks in the circuit model can also be compared in a more natural way to quantum walks in continuous-time models of quantum computation, such as adiabatic quantum computation. Apart from these algorithmic applications, there are also true conceptual differences between scalar and coined quantum walks, which make them both interesting topics of studies on their own. In the classical case, note that random walks using an internal state space exhibit a memory effect, which makes their classical evolution non-Markovian [8] in contrast to random walks with no internal space. In particular, the inclusion of an internal space by a procedure called lifting has been proved to modify the mixing time of classical random walks on some graphs [9]. The authors also suggest this procedure can have interesting algorithmic applications. In the quantum case, the behavior of scalar quantum walks is a more direct consequence of a purely quantum effect, namely phase interference, since adding an internal space necessarily prevents interferences between paths. Finally, we observe that the efficiency of the algorithms using quantum walks varies with the dimension of the internal space without any obvious reason [10], so that it seems to be important to investigate both scalar and coined quantum walks to solve an algorithmic problem on a given search space.

To identify the Cayley graphs that accept a scalar quantum walk, we will first verify whether some necessary conditions are satisfied for various digraphs. First, we know that all Cayley graphs are reversible. The other known conditions are quadrangularity and strong quadrangularity. While the condition of strong quadrangularity depends on the number of subsets of the vertex set of the digraph, and thus requires an exponential time to be checked, the quadrangular condition depends on the number of pairs of vertices and may be checked in polynomial time. We will thus use quadrangularity as a necessary condition. This paper is organized as follows. In Section 2, we will derive the quadrangular condition and adapt it to homogeneous quantum walks on Cayley graphs. In Section 3, we will present a general method allowing us to determine whether a homogeneous scalar quantum walk exists on a given Cayley graph and, if so, to explicitly derive its evolution operator. In Section 4, we will apply the above necessary condition and constructive method in order to find new scalar quantum walks. We will consider a variety of Cayley graphs, built from two, three, and occasionally more than three generators.

2 Conditions on the existence of scalar quantum walks on Cayley graphs

2.1 Quadrangularity for general digraphs

Let $G(X,E)$ be a digraph with vertex set X and edge set E. A scalar quantum walk is a model of the evolution of a particle on the digraph G. The state of the particle is described by a unit vector in the Hilbert space $H = \ell^2(X)$ and we will use the set of states $\{|x\rangle\}_{x\in X}$ as a basis for H. The evolution operator W is a unitary operator on H. The evolution of $|\psi_t\rangle$, the state describing the position of the particle at time t, is given by the following equation:

$$|\psi_t\rangle = W^t|\psi_0\rangle, \tag{1}$$

where $|\psi_0\rangle$ is a given initial state. We denote as $W_{x,y}$ the matrix elements $\langle x|W|y\rangle$, corresponding to the amplitude transition from $|y\rangle$ to $|x\rangle$. A necessary condition for the existence of a scalar quantum walk on a digraph is called quadrangularity. It was first presented in [5], and can also be obtained as a consequence of the analysis presented in [4]. Let us recall it here.

Proposition 1 *Given a digraph $G(X,E)$, if a scalar quantum walk on this digraph exists then for each pair of different edges of the form (x,z) and (y,z) there exists another pair of different edges of the form (x,z') and (y,z').*

Proof. The equation $W^\dagger W = \mathrm{Id}_H$, where $W^\dagger$ is the conjugate transpose of W and Id_H is the identity on H, is equivalent to the set of equations:

$$\begin{cases} \sum_{z\in X} \overline{W}_{z,x} W_{z,y} = 0 & \forall\ x,y \in X, x \neq y \\ \sum_{z\in X} \overline{W}_{z,x} W_{z,x} = 1 & \forall\ x \in X \end{cases} \tag{2}$$

And the matrix equation $WW^\dagger = \mathrm{Id}_H$ is equivalent to

$$\begin{cases} \sum_{z\in X} W_{x,z} \overline{W}_{y,z} = 0 & \forall\ x,y \in X, x \neq y \\ \sum_{z\in X} W_{x,z} \overline{W}_{x,z} = 1 & \forall\ x \in X \end{cases} \tag{3}$$

where $\overline{\alpha}$ denotes the complex conjugate of α. Suppose that the sum in the first type of equation contains only one term for some pair (x, y). Then, the only possibility for the condition to be satisfied is to have one of the two coefficients equal to zero. This is equivalent to modifying the digraph, so that in this case, there is no scalar quantum walk for the original digraph G. $\square$.

This proposition can also be reformulated as follows:
Given a digraph $G(X, E)$, if a scalar quantum walk on this digraph exists then all consecutive edges in the digraph with different orientations belong to at least one closed path of length four with alternating orientations.

2.2 Quadrangularity for Cayley graphs

A Cayley graph is a digraph constructed using the relations of a group. More precisely, we have:

Definition 1 *Given a group Γ and a generating set Δ of elements of Γ, the Cayley graph $C_\Delta(\Gamma) = G(X, E)$ is defined by*

$$X = \Gamma, \tag{4}$$

$$E = \{(x, x\delta) : x \in \Gamma, \delta \in \Delta\}. \tag{5}$$

Let us note that we have assumed that Δ is a generating set for Γ, that is, all elements in Γ may be obtained by multiplication of elements and inverse elements of Δ. If this was not the case, the graph $C_\Delta(\Gamma)$ would not be connected.

We also see that, by definition, Cayley graphs are directed graphs unless $\Delta = \Delta^{-1}$ (that is, $\forall \delta \in \Delta$, we also have $\delta^{-1} \in \Delta$). Moreover, assigning a colour to each of the $d = |\Delta|$ generators, we see that the associated Cayley graph is d-coloured: each outgoing edge $(x, x\delta)$ from a given vertex x has a different colour corresponding to the different generators δ. Following this, it will be natural to suppose that the transition amplitudes induced by the evolution operator W depend only on the colour of the edge that is followed, and not on the starting vertex, which can be interpreted as a homogeneity condition

$$W_{x\delta,x} = W_\delta. \tag{6}$$

In particular, we will use the following definition:

Definition 2 *A homogeneous scalar quantum walk (HSQW) on a Cayley graph $C_\Delta(\Gamma)$ is a unitary operator W acting on a Hilbert space $H = \ell^2(\Gamma)$, such that*

$$W = \sum_{\delta\in\Delta} W_\delta U_\delta, \tag{7}$$

where $W_\delta \neq 0$ ($\forall \delta \in \Delta$), and $U_\delta = \sum_x |x\delta\rangle\langle x|$ is the unitary operator that maps each group element to its right-product with δ.
Note that we do not allow W_δ to be zero since it would be equivalent to remove the edges corresponding to δ from the graph, or, in turn, to remove δ from the set of generators Δ.

Since the unitary operators U_δ are permutations and satisfies $U_{\delta_1} U_{\delta_2} = U_{\delta_2 \delta_1}$, they correspond to the regular representation of the group, except that the left- and right-products are interchanged. In the case of abelian groups, this is exactly the regular representation, and the fact that the operators U_δ commute allows us to directly deduce the spectral properties of the walk operator W. Indeed, the commuting operators U_δ admit a common basis of eigenstates, the Fourier basis,

$$|\chi_i\rangle = \frac{1}{\sqrt{|X|}} \sum_{x \in \Gamma} \bar{\chi}_i(x) |x\rangle, \tag{8}$$

where $\chi_i(x)$ are the characters of the group. Since $|\chi_i\rangle$ is an eigenstate of each operator U_δ with eigenvalue $\chi_i(\delta)$, it is also an eigenvector of W with eigenvalue $\sum_{\delta \in \Delta} W_\delta \ \chi_i(\delta)$. The spectrum of a quantum walk W is intimately related to its dynamical properties, so that this could prove useful for algorithmic applications.

For homogeneous scalar quantum walks over a Cayley graph, Proposition 1 translates into a necessary condition over the elements of the generating set Δ. More precisely, let us partition the set Δ^2 of pairs (δ_1, δ_2) of elements from Δ into subsets $\Delta^2_g = \{(\delta_1, \delta_2) \in \Delta^2 : \delta_1 \delta_2^{-1} = g\}$. We may then prove the following:

Proposition 2 *Let Γ be a group, Δ be a set of elements generating Γ, and Δ^2_g be as above. A necessary condition for the existence of a homogeneous scalar quantum walk $W = \sum_{\delta \in \Delta} W_\delta U_\delta$ on the Cayley graph $C_\Delta(\Gamma)$ is that there is no g in $\Gamma \setminus \{e\}$ for which Δ^2_g contains exactly one pair of generators, that is, $|\Delta^2_g| \neq 1 \ \forall g \in \Gamma \setminus \{e\}$ (where e is the identity element in Γ).*

Proof. In the case of a HSQW, the unitarity equations (2-3) become

$$\sum_{(\delta_1, \delta_2) \in \Delta^2_g} \overline{W}_{\delta_1} W_{\delta_2} = \delta_{g=e} \qquad \forall \ g \in \Gamma, \tag{9}$$

where $\delta_{g=e} = 1$ if $g = e$ and 0 otherwise. If the necessary condition is not satisfied, there exists some $g \in \Gamma$ for which there is only one pair (δ_1, δ_2) such that $\delta_1 \delta_2^{-1} = g$. For such an element g, Eq. (9) would read $\overline{W}_{\delta_1} W_{\delta_2} = 0$, and therefore one of the elements W_{δ_1} and W_{δ_2} should be zero, which would contradict Definition 2. $\square$.

It is interesting to note that the system of equations (9) only depends on the way the set Δ^2 of pairs of generators (δ_1, δ_2) is partitioned into subsets Δ^2_g. Therefore, when trying to build a HSQW on a given group, we should only bother about relations between generators of the type $\delta_1 \delta_2^{-1} = \delta_3 \delta_4^{-1}$.

Nevertheless, it is in principle impossible to solve the general problem of determining and classifying all groups obtained by the procedure of taking the quotient of a free group. This result is a consequence of the existence of finitely presented groups for which the word problem is unsolvable (see Theorem 7.2 in [11]). For this reason, it is probably hopeless to try solving the problem of determining and classifying all groups that satisfy the quadrangularity condition.

Here, we will instead consider groups with a small number of generators and build all possible minimal sets of relations satisfying the quadrangularity condition. For the resulting groups, we will completely solve the system of equations (9) arising from the unitarity condition, and thus derive the most general evolution operator for a HSQW on the associated Cayley graphs. The general method to solve this problem is exposed in the next section.

3 Solving the unitarity condition for the evolution operator

Let us suppose we want to build a scalar quantum walk on a Cayley graph satisfying the quadrangularity condition. When the homogeneity condition (6) is imposed in (2), the number of variables describing the evolution operator decreases considerably since it is reduced to $d = |\Delta|$, the number of elements in the generating set Δ. The number of (non-trivial) equations in the system (9) is also reduced, it is upper bounded by the number of different pairs of generators, that is, $\frac{d(d-1)}{2}$. More precisely, each non-empty set Δ_g^2 will correspond to a non-trivial equation that may be written as a bilinear equation

$$\begin{aligned} \boldsymbol{v}^\dagger P_g \boldsymbol{v} &= 0 \qquad \forall g \in \Gamma \setminus \{e\}, &(10)\\ \boldsymbol{v}^\dagger \boldsymbol{v} &= 1, &(11)\end{aligned}$$

where P_g is a $d \times d$ matrix with entries in $\{0,1\}$ (non-zero entries corresponding to the pairs in Δ_g^2) and $\boldsymbol{v} \in \mathbb{C}^d$ is a column vector having as components the elements W_i of the evolution operator. If we define as

$$\boldsymbol{e}_1 = \begin{pmatrix}1\\0\\\vdots\\0\end{pmatrix}, \boldsymbol{e}_2 = \begin{pmatrix}0\\1\\\vdots\\0\end{pmatrix}, \cdots, \boldsymbol{e}_d = \begin{pmatrix}0\\0\\\vdots\\1\end{pmatrix} \tag{12}$$

the vectors in the standard basis of $\mathbb{C}^d$, we have $\boldsymbol{v} = \sum_{i=1}^d W_i \boldsymbol{e}_i$. Let $\{\lambda_1, \ldots, \lambda_d\}$ be the d eigenvalues of P_g (with algebraic multiplicities). If the geometric multiplicities of these eigenvalues equal their algebraic multiplicities, we may build an orthonormal basis $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_d\}$ out of eigenvectors of P_g. Expanding $\boldsymbol{v}$ in this basis, we may write $\boldsymbol{v} = \sum_{j=1}^d \alpha_j \boldsymbol{v}_j$ so that Eq. (10) becomes

$$\sum_{j=1}^{d} \lambda_j |\alpha_j|^2 = 0, \tag{13}$$

whereas the normalization equation (11) is simply

$$\sum_{j=1}^{n} |\alpha_j|^2 = 1. \tag{14}$$

The relation between the new coefficients α_j and the evolution operator coefficients W_i is then given by

$$W_i = \sum_j \alpha_j \ \boldsymbol{e}_{\boldsymbol{i}}^\dagger \boldsymbol{v}_{\boldsymbol{j}}. \tag{15}$$

In the next section, we will use this approach to build HSQWs on groups with few generators, or prove that no such walk exists.

4 Application

Let us consider groups denoted as $\Gamma = \langle \Delta | R \rangle$, using the standard free group representation where Δ is a set of generators for the group Γ and R is a set of relations among these generators, and determine whether the associated Cayley graph admits a scalar quantum walk. Let us note that, for consistency, we will exclude the case where R implies that two elements of Δ are actually equal, which we will call a trivial reduction, so that the actual number of generators is really the cardinality of Δ.

4.1 Finitely presented groups with one generator

For the sake of completeness, let us first consider the simplest case of the free group with one generator $\Gamma = \langle x \rangle$ with $\Delta = \{x\}$. This admits a trivial scalar quantum walk, which acts as a shift operator on an infinite line. Adding a relation $x^n = e$, we obtain the cyclic group $C_n = \langle x | x^n = e \rangle$, and the associated Cayley graph becomes a cycle, which thus also accepts such a trivial scalar quantum walk.

4.2 Finitely presented group with two generators

Theorem 1 *Let $\Gamma = \langle x, y | R \rangle$ be a finitely presented group with a set of generators $\Delta = \{x, y\}$, R being a set of relations between these generators. There exists a homogeneous scalar quantum walk on $C_\Delta(\Gamma)$ iff R implies $xy^{-1} = yx^{-1}$. In this case, the general form of the walk operator W is given by*

$$W = \cos\phi \; U_x + i \sin\phi \; U_y, \tag{16}$$

where the operators U_x, U_y are as above and $\phi \in [0, 2\pi]$ is an arbitrary angle.

Proof. Let $g = xy^{-1}$, so that $(x, y) \in \Delta_g^2$. Since (y, x) is the only other possible pair of distinct generators, we need that $g = yx^{-1}$ as well to have $|\Delta_g^2| \neq 1$ and satisfies the necessary condition from Proposition 2. It remains to show that the unitarity equations (9) admits a solution when this condition is satisfied. We have

$$\begin{cases} \overline{W}_x W_y + \overline{W}_y W_x = 0 \\ \overline{W}_x W_x + \overline{W}_y W_y = 1, \end{cases} \tag{17}$$

which can be written as bilinear equations (10-11) with $\boldsymbol{v} = \begin{pmatrix} W_x \\ W_y \end{pmatrix}$ and $P_g = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. Expanding $\boldsymbol{v}$ in the basis formed by the eigenvectors of P_g, that is $\boldsymbol{v}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $\boldsymbol{v}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$, with respective eigenvalues $\lambda_1 = 1$ and $\lambda_2 = -1$, we see that Eq. (13-14) become

$$\begin{cases} |\alpha_1|^2 - |\alpha_2|^2 = 0 \\ |\alpha_1|^2 + |\alpha_2|^2 = 1, \end{cases} \tag{18}$$

so that the solution is up to a global phase

$$\begin{cases} W_x = \cos\phi \\ W_y = i \sin\phi \end{cases} \tag{19}$$

for $\phi \in [0, 2\pi]$. $\square$.

Theorem 1 shows that there exists a HSQW on the Cayley graph $C_\Delta(\Gamma)$ for the group $\Gamma = \langle x, y | xy^{-1} = yx^{-1} \rangle$, but also for all finitely presented groups with two generators satisfying $xy^{-1} = yx^{-1}$, since adding other types of relation will not modify the system of equations (9). In particular, we can add some relations to the former infinite group in order to make it finite. Hence, we show that there is a HSQW for the dihedral group $D_n = \langle x, y | x^n = e, y^2 = e, (xy)^2 = e \rangle$, with generating set $\Delta = \{x, y\}$. The evolution operator coefficients are also given by Eqs. (19), and the corresponding Cayley graph is both strongly quadrangular and specular (it was first presented in [5]). Let us note that the hypercube of dimension 2 can be obtained as the Cayley graph of the $n = 2$ case of D_n, that is, $D_2 = \langle x, y | x^2 = e, y^2 = e, xy = yx \rangle$, with $\Delta = \{x, y\}$. We conclude that the hypercube of dimension 2 also accepts a HSQW. Finally, another example of a finite group admitting a scalar quantum walk was presented in [4], which can be obtained by adding the relation $xy = yx$ to the initial relation $xy^{-1} = yx^{-1}$.

4.3 Finitely presented groups with three generators

We know that the existence of a HSQW on a Cayley graph depends on the partition of the set Δ^2 of pairs of generators into subsets Δ_g^2. In the case of three generators there are six possible pairs, that may in principle be partitioned in 203 different ways ($203 = B_6$, where the Bell number B_n denotes the number of different partitions of a set of n elements).

We will use the following representation in order to simplify the counting of the possible sets of relations satisfying the necessary condition. We associate each pair of generators (δ_i, δ_j) to the vertex element $M_{i,j}$ of a 3×3 grid M (see Fig. 1). A relation $\delta_i \delta_j^{-1} = \delta_k \delta_l^{-1}$ may then be represented as an edge between vertices (δ_i, δ_j) and (δ_k, δ_l), meaning that both of these pairs lie in the same subset Δ_g^2.

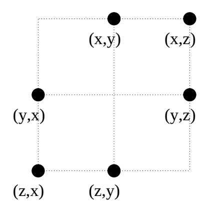

Fig. 1. Representation of the relations between generators as a grid. A relation $\delta_i \delta_j^{-1} = \delta_k \delta_l^{-1}$ will be represented as an edge between vertices (δ_i, δ_j) and (δ_k, δ_l).

Since the necessary condition requires that no Δ_g^2 (with $g \neq e$) has cardinality 1, we know that the grids corresponding to a valid graph are those where all vertices are connected with at least another vertex. Note that we do not need to consider the elements in the diagonal, since pairs of the form (δ_i, δ_i) are in C_e, for which the necessary condition does not apply. Moreover, the different edges are not independent, since $\delta_i \delta_j^{-1} = \delta_k \delta_l^{-1}$ is equivalent to $\delta_j \delta_i^{-1} = \delta_l \delta_k^{-1}$ (this implies a symmetry with respect to the diagonal axis), while by transitivity the relations $\delta_i \delta_j^{-1} = \delta_k \delta_l^{-1}$ and $\delta_k \delta_l^{-1} = \delta_m \delta_n^{-1}$ imply $\delta_i \delta_j^{-1} = \delta_m \delta_n^{-1}$. We also see that not all edges are interesting since a vertical or an horizontal edge implies a relation of the form $\delta_i = \delta_j$ and thus a trivial reduction of the number of generators.

Theorem 2 *Let $\Gamma = \langle x, y, z | R \rangle$ be a finitely presented group with a set of generators $\Delta = \{x, y, z\}$, R being a set of relations between these generators. There exists a homogeneous scalar quantum walk of the form $W = \sum_{\delta \in \Delta} W_\delta U_\delta$ on $C_\Delta(\Gamma)$ iff R implies, up to a* *permutation of* $\{x, y, z\}$*, either*

i) $\{xy^{-1} = yz^{-1}, xy^{-1} = zx^{-1}\}$*, in which case the walk operator is given by*

$$\begin{cases} W_x = \frac{1}{3}(1 + e^{i\phi_1} + e^{i\phi_2}) \\ W_y = \frac{1}{3}(1 + e^{i\frac{2\pi}{3}} e^{i\phi_1} + e^{-i\frac{2\pi}{3}} e^{i\phi_2}) \\ W_z = \frac{1}{3}(1 + e^{-i\frac{2\pi}{3}} e^{i\phi_1} + e^{i\frac{2\pi}{3}} e^{i\phi_2}), \end{cases} \tag{20}$$

for $\phi_1, \phi_2 \in [0, 2\pi]$*, or*

ii) $\{xy^{-1} = zx^{-1}, yz^{-1} = zy^{-1}\}$*, in which case the walk operator is given by*

$$\begin{cases} W_x = \cos\phi \\ W_y = \frac{1+i(-1)^q}{2} \sin\phi \\ W_z = -\frac{1-i(-1)^q}{2} \sin\phi, \end{cases} \tag{21}$$

for $\phi \in [0, 2\pi]$ *and* q *any integer.*

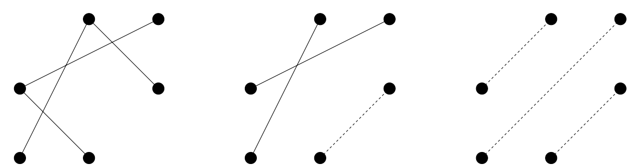

Fig. 2. Representation of the three sets of relations implying no reduction. Valid sets of relations are those for which any vertex is connected to at least one other vertex. Other sets of relations either reduce to one of the three sets represented here (possibly up to a permutation of the generators) or imply a reduction of the number of generators.

Proof. By a straightforward (but tedious) inspection of all grids, it can be shown that among the 203 partitions of Δ^2, there are only three non-equivalent sets of relations of the type $\delta_i\delta_j^{-1} = \delta_k\delta_l^{-1}$ (excluding trivial reductions) that satisfy the necessary condition (see Fig. 2). There remains to check whether there actually exists a HSQW in these cases:

i) $\{xy^{-1} = yz^{-1}, xy^{-1} = zx^{-1}\}$
The unitarity condition equations (9) become

$$\begin{cases} \overline{W}_x W_y + \overline{W}_z W_x + \overline{W}_y W_z = 0 \\ \overline{W}_x W_x + \overline{W}_y W_y + \overline{W}_z W_z = 1, \end{cases} \tag{22}$$

which can be written as a bilinear hermitian form with $\boldsymbol{v} = \begin{pmatrix} W_x \\ W_y \\ W_z \end{pmatrix}$ and $P_g = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$.
Using the expansion of $\boldsymbol{v}$ in terms of the eigenvectors of P_g, the system reduces to

$$\begin{cases} |\alpha_1|^2 + e^{i\frac{2\pi}{3}}|\alpha_2|^2 + e^{-i\frac{2\pi}{3}}|\alpha_3|^2 = 0 \\ |\alpha_1|^2 + |\alpha_2|^2 + |\alpha_3|^2 = 1, \end{cases} \tag{23}$$

so that, up to a global phase, the solution is given by Eq. (20).

ii) $\{xy^{-1} = zx^{-1}, yz^{-1} = zy^{-1}\}$
Using a similar method, we find the general solution as in Eq. (21).

iii) $\{xy^{-1} = yx^{-1}, yz^{-1} = zy^{-1}, zx^{-1} = xz^{-1}\}$
We obtain that there is no solution (the proof is also based on the same method as above).

$\square$.

Considering a set R of relations of the type $\delta_i\delta_j^{-1} = \delta_k\delta_l^{-1}$ exclusively, Theorem 2 implies that there exists homogeneous scalar quantum walks on the Cayley graphs $C_\Delta(\Gamma)$ for

i) $\Gamma = \langle x, y, z | xy^{-1} = yz^{-1}, xy^{-1} = zx^{-1}\rangle$ and $\Delta = \{x, y, z\}$
(note that Γ may equivalently be written as $\langle x, y, z | z = xy^{-1}x, (xy^{-1})^3 = e\rangle$),

ii) $\Gamma = \langle x, y, z | xy^{-1} = zx^{-1}, yz^{-1} = zy^{-1}\rangle$ and $\Delta = \{x, y, z\}$,

but not for

iii) $\Gamma = \langle x, y, z | xy^{-1} = yx^{-1}, yz^{-1} = zy^{-1}, zx^{-1} = xz^{-1}\rangle$ and $\Delta = \{x, y, z\}$

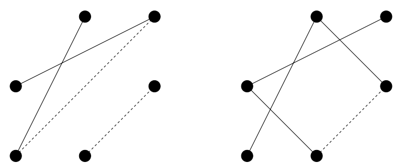

Fig. 3. Representation of the two sets of relations implying reductions of the number of generators. In the first case, we obtain $x = y$ (i.e. $|\Delta| = 2$), while in the second, we have $x = y = z$ (i.e. $|\Delta| = 1$). Note that other sets of relations may reduce to these cases, possibly up to some permutation of the generators.

If we add more relations of the type $\delta_i\delta_j^{-1} = \delta_k\delta_l^{-1}$ to these groups, reductions appear and we end up with groups with less than three generators (see Fig. 3). These were studied in Sections 4.1 (one generator) and 4.2 (two generators).

Of course, there exist other relations beyond these of the type $\delta_i\delta_j^{-1} = \delta_k\delta_l^{-1}$, so that we may build further groups by adding other relations. Nonetheless, as long as these additional relations do not imply relations of the previous type nor trivial reductions, they will have no influence on the possible existence of a HSQW on the associated Cayley graphs.

For instance, adding relations $x^2 = e$ and $y^2 = e$ to the above group (*i*), we obtain the symmetric group $S_3 = \langle x, y | x^2 = e, y^2 = e, (xy)^3 = e\rangle$ with two generators. This is the group of permutations of three elements, x corresponding to a permutation of the first two elements, y to a permutation of the last two elements, and xyx to a permutation of the first and third elements. Taking $\Delta = \{x, y, xyx\}$, the corresponding Cayley graph therefore admits a scalar quantum walk, with evolution operator coefficients given by Eq. (20).

Similarly, if we add the relation $y^2 = x$ to the group (*ii*), the set of relations imply $y^3 = z$ and $y^4 = e$, so that we obtain the cyclic group $C_4 = \langle y | y^4 = e\rangle$. Since we use as generators all the group elements except the identity e, that is, $\Delta = \{y, y^2, y^3\}$, the Cayley graph reduces to the complete graph over four vertices, which thus admits a scalar quantum walk with evolution operator coefficients given by Eq. (21).

Finally, if we impose the additional relations $x^2 = y^2 = z^2 = e$ to the group (*iii*), the associated Cayley graph becomes the hypercube in dimension 3. It follows that even though there exists a homogeneous scalar quantum walk on the hypercube in dimension 2, as we have seen above, there is no such walk in dimension 3 (actually, there exists *non-homogeneous* scalar quantum walks on the hypercube in any dimension, as shown in [12]). Moreover, the case (*iii*) may also be used to rule out the possibility of a HSQW on some Cayley graphs built with more than three generators.

Theorem 3 *Let $\Gamma = \langle \Delta | R \rangle$ be a finitely presented group with a set of generators Δ, R being a set of relations between these generators. If there exists $x, y, z \in \Delta$ such that*

$$\Delta^2_{x^{-1}y} = \{(x,y),(y,x)\}, \quad \Delta^2_{y^{-1}z} = \{(y,z),(z,y)\}, \quad \Delta^2_{z^{-1}x} = \{(z,x),(x,z)\}, \tag{24}$$

where Δ^2_g is as above, then there exists no homogeneous scalar quantum walk on $C_\Delta(\Gamma)$.

Proof. The system of equations (9) will have as subsystem the equations corresponding to the case (*iii*), which have no solution, so that the global system will have no solution as well. $\square$.

4.4 Examples with more than three generators

In this section, we will give some examples of HSQWs on Cayley graphs built with more than three generators. In particular, we will consider the cyclic group $C_n = \langle a | a^n = e \rangle$. We have already found a trivial way to define a scalar quantum walk on a cycle, which is the simplest Cayley graph of the cyclic group C_n (with only one generator). Here, we show how to build HSQWs on more general Cayley graphs of the cyclic group (see also [12]). The elements of C_n may be written as $\{a^i | i = 0, \ldots, n\}$. The necessary condition implies that if a^i and a^j are taken as generators to build the Cayley graph, we must also take some other pair of elements a^k and a^l such that $(i-j)-(k-l) \mod n = 0$. Let us consider two particular cases where this condition is satisfied.

i) Set of d generators, when n is a multiple of d.
If n is a multiple of d, the necessary condition may be satisfied if the generator set, with d elements, is taken as $\Delta = \{a^{j\frac{n}{d}+l} | j = 0, \ldots, d-1\}$, where l is some integer (l being prime to n/d so that Δ generates C_n). The unitarity condition equations (9) become

$$\sum_{j=0}^{d-1} \overline{W}_j W_{(j+i) \mod n} = \delta_{i,0} \tag{25}$$

for $i = 0, \ldots, d-1$ and the solution is

$$W_j = \frac{1}{d} \sum_{k=0}^{d-1} e^{i\theta_k} e^{i\frac{2\pi kj}{d}}. \tag{26}$$

Hence, there are $d-1$ real parameters that define the evolution operator for this family of Cayley graphs of the cyclic groups. The $d = n$ special case corresponds to the complete graph with self-loops (the self-loops come from the fact that we also take as generator the identity e, which maps any group element to itself). This graph trivially accepts scalar quantum walks since any unitary matrix without zero entries may be taken as a diffusion operator (note that here we give the general form of *homogeneous* scalar quantum walks). In particular, taking $\theta_0 = \pi$ and $\theta_k = 0$ for all $k \neq 0$ yields the usual diffusion operator from Grover's algorithm [13], with $W_0 = 1 - 2/n$ and $W_k = -2/n$ for all $k \neq 0$. The $d = 1$ special case reduces to the cycle, that we have already seen above in the context of the finitely presented groups with one generator.

ii) Set of 4 generators, when n is even.
In that case, the necessary condition is satisfied if we take $\Delta = \{a^j, a^{-j}, a^{\frac{n}{2}+j}, a^{\frac{n}{2}-j}\}$. Note that for Δ to be a generating set for C_n, j must be prime with respect to $n/2$. Defining $\delta_1 = a^j$ and $\delta_2 = a^{\frac{n}{2}+j}$ (so that, in particular $\delta_1 = \delta_2^2$), this set is simply $\Delta = \{\delta_1, \delta_1^{-1}, \delta_2, \delta_2^{-1}\}$, and the unitary equations (9) are given by:

$$\begin{cases} \overline{W}_{\delta_2} W_{\delta_1^{-1}} + \overline{W}_{\delta_2^{-1}} W_{\delta_1} + \overline{W}_{\delta_1} W_{\delta_2^{-1}} + \overline{W}_{\delta_1^{-1}} W_{\delta_2} = 0 \\ \overline{W}_{\delta_2} W_{\delta_1} + \overline{W}_{\delta_1^{-1}} W_{\delta_2^{-1}} = 0 \\ \overline{W}_{\delta_1} W_{\delta_1^{-1}} + \overline{W}_{\delta_2^{-1}} W_{\delta_2} = 0 \\ \overline{W}_{\delta_1} W_{\delta_1} + \overline{W}_{\delta_1^{-1}} W_{\delta_1^{-1}} + \overline{W}_{\delta_2} W_{\delta_2} + \overline{W}_{\delta_2^{-1}} W_{\delta_2^{-1}} = 1. \end{cases} \tag{27}$$

Using the previous method, we show that the general solution is

$$\begin{cases} W_{\delta_1} = \frac{1}{2} e^{i\phi} \\ W_{\delta_1^{-1}} = \frac{1}{2} \\ W_{\delta_2} = \frac{(-1)^q}{2} \\ W_{\delta_2^{-1}} = \frac{(-1)^{q+1}}{2} e^{i\phi} \end{cases} \tag{28}$$

for $\phi \in [0, 2\pi]$ and q any integer.

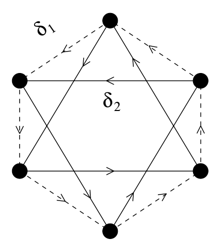

Fig. 4. Johnson graph $J(4, 2)$, which may be seen as the Cayley graph of the cyclic group $C_6 = \langle \delta_1 | \delta_1^6 = e \rangle$ with generating set $\Delta = \{\delta_1, \delta_1^{-1}, \delta_2, \delta_2^{-1}\}$, where $\delta_2 = \delta_1^2$. Note that we have only represented the oriented edges corresponding to δ_1 and δ_2, and not their inverses, corresponding to δ_1^{-1} and δ_2^{-1}.

The case $n = 6$ and $j = 1$ is of particular interest since the Cayley graph of the cyclic group of order six $C_6 = \langle \delta_1 | \delta_1^6 = e \rangle$ with $\Delta = \{\delta_1, \delta_1^{-1}, \delta_2, \delta_2^{-1}\}$, represented in Fig. 4, happens to coincide with the Johnson graph $J(4, 2)$. Let us recall that the Johnson graph $J(n, k)$ is defined as the graph having as vertices the C_n^k subsets of size k of a set of n elements, and such that two subsets are linked by an edge if they have $k - 1$ elements in common. Let us note that $J(n, n - k) = J(n, k)$.

In the context of quantum computation, quantum walks on the Johnson graph have been successfully used by Ambainis to solve a problem known as element distinctness [14]. While Ambainis makes use of a coined quantum walk, it would have been interesting to study the possibility of matching his result using scalar quantum walks. However, apart from some particular cases such as $J(4,2)$, our method does not apply to all Johnson graphs $J(n,k)$, since even though these graphs are vertex-transitive, they are in general not Cayley graphs. This is for example the case of the Johnson graph $J(5,2)$, being the complement of the Petersen Graph $K(5,2)$, a standard example of a vertex-transitive, non-Cayley graph [15]. Let us note that a possible extension of our method to all vertex-transitive (possibly non-Cayley) graphs could make use of the formalism of so-called Schreier coset graphs. We leave this possibility for further study.

5 Conclusion

We have obtained a simple necessary condition for the existence of a scalar quantum walk on Cayley graphs, as well as a general method to construct its evolution operator (or to conclude that no such walk exists) when the necessary condition is fulfilled. Even if the homogeneity of the evolution operator is required, scalar quantum walks often exist on Cayley graphs, and we have presented a series of examples for finitely presented groups (see Table 1).

Table 1. Summary of our results. The first two columns define the groups by giving their free group representation $\Gamma = \langle \Delta | R \rangle$, where Δ is the set of generators and R is the set of relations between these generators. The third column specifies whether there exists a homogeneous scalar quantum walk on the associated Cayley graph. The last column lists groups or graphs also concerned by this result.

Generators Δ	Relations R	Existence of HSQW	Groups or graphs
x	$\emptyset$	yes	Cycle graphs
x, y	$xy^{-1} = yx^{-1}$	yes	Dihedral groups D_n, Hypercube in dim. 2
x, y, z	$xy^{-1} = yz^{-1} = zx^{-1}$	yes	Symmetric group S_3
x, y, z	$xy^{-1} = zx^{-1}, yz^{-1} = zy^{-1}$	yes	Complete graph over 4 vertices
x, y, z	$xy^{-1} = yx^{-1}, xz^{-1} = zx^{-1}$, $yz^{-1} = zy^{-1}$	no	Hypercube in dim. 3
$a^{j\frac{n}{d}+l}$ $(j=0,\ldots,d-1)$	$a^n = e$	yes	Complete graph with self-loops, Cycle graphs
$a^j, a^{-j}, a^{\frac{n}{2}+j}, a^{\frac{n}{2}-j}$	$a^n = e$	yes	Johnson graph $J(4,2)$

We have unfortunately not been able to answer the open question of deriving a general necessary and sufficient condition for the existence of a scalar quantum walk on a digraph. We have shown, however, that assuming homogeneity significantly simplifies the problem and allows to solve it explicitly for a large class of Cayley graphs. For non Cayley graphs, there is no general procedure to assign equal coefficients to different edges in a non-arbitrary way. However, non-homogeneous quantum walks may also be used to construct quantum algorithms, so that exploring which general digraphs admit scalar quantum walks certainly deserves further investigation.

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