Symmetries in discrete time quantum walks on Cayley graphs

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We address the question of symmetries of an important type of quantum walks. We introduce all the necessary definitions and provide a rigorous formulation of the problem. Using a thorough analysis, we reach the complete answer by presenting a constructive method of finding all solutions of the problem with minimal additional assumptions. We apply the results on an example of a quantum walk on a line to demonstrate the practical significance of the theory.

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I. INTRODUCTION

The search for symmetries is an important problem in all fields of physics. In both classical and quantum mechanics, the knowledge of symmetries of a given system can help significantly in finding a solution of its equations of motion, in reducing the number of parameters, or identifying the integrals of motion.

In this paper, we aim to find the symmetries of the time evolution equation of a broad class of discrete time quantum walks. We note that this important question has been addressed partly by other authors. Symmetries of particular quantum walk scenarios have been classified, e.g., in [1]. A special class of symmetries of discrete time quantum walks on Cayley graphs has been studied in [2] in relation to global analytic properties of the quantum walks. Symmetries have played an essential role in an approximate analytic solution of time evolution in the Shenvi-Kempe-Whaley algorithm [3] for quantum database searching. Another use of symmetries has been presented in a recent experimental realization of a quantum walk on a line [4] when a reduced set of parameters have been shown to cover all possible configurations of the model. However, no general study focused on the symmetries themselves has been presented so far.

The article is structured as follows. In Section II, we define the class of discrete time quantum walk to be studied in more detail. In Section III, we use a general method to find all symmetries of the time evolution equation which preserve measurement probabilities. In Section IV, we extend the result by generalizing the notion of symmetries of the system to allow automorphisms of the underlying graph. In Section V, we conclude and discuss our results.

II. QUANTUM WALKS ON CAYLEY GRAPHS

In the scope of this paper, we will restrict our study to discrete time quantum walks on Cayley graphs, with the quantum coin reflecting the graph structure. This class of graphs, however, covers all the most important cases used in algorithmic applications of quantum walks—lattices both with and without periodic boundary conditions [5], hypercube graphs [3], among many others.

In general, Cayley graphs are defined as follows:

Definition 1. Let $G$ be a discrete group finitely generated by a set $S$. The (uncolored) Cayley graph $\Gamma = \Gamma(G, S)$ is a directed graph $(G, E)$, where the set of vertices is identified with the set of elements of $G$ and the set of edges is

$$E = \{(g, gs) \mid g \in G, s \in S\}.$$ 

A discrete quantum walk on a given Cayley graph is defined as the time evolution of a particle confined to the vertices of the graph, and allowed to move along its edges, one per a discrete time step. Thus, the Hilbert space corresponding to the spatial degree of freedom of the particle is the space of $\ell^2$ functions defined on $G$, or equivalently, the space spanned by orthonormal basis states corresponding to the elements of $G$:

$$\mathcal{H}_S = \ell^2(G) = \text{Span}_\mathbb{C}\{ |x\rangle \mid x \in G \}. \quad (1a)$$

Besides the spatial degree of freedom, we will require the particle undergoing the walk (the walker) to have an internal degree of freedom whose dimension equals the cardinality of $S$.

$$\mathcal{H}_C = \ell^2(S) = \text{Span}_\mathbb{C}\{ |c\rangle \mid c \in S \}. \quad (1b)$$

This is in a direct analogy to [6] where quantum walks on general regular graphs have been introduced. The need for the presence of an internal degree of freedom has been shown to be crucial for quantum walks on Euclidean lattices [7] in order to reach nontrivial unitary time evolutions. A generalization of this “No-Go Lemma” to all Cayley graphs has been negated in [8]. In the scope of this article, however, we will keep the assumption about the internal degree of freedom as stated above.

Definition 2. The Hilbert spaces defined in Eqs. (1a) and (1b) are called position and coin Hilbert spaces, respectively. The full state space of the system is then

$$\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_C = \text{Span}_\mathbb{C}\{ |x, c\rangle \mid x \in G, c \in S \},$$
where \(|x,c⟩ = |x⟩_S ⊗ |c⟩_C\). We will refer to the systems \(\{ |x⟩ \mid x \in G\}, \{ |c⟩ \mid c \in S\}, \) and \(\{ |x,c⟩ \mid x \in G, c \in S\}\), as to geometrical bases of \(H_S, H_C\) and \(H\), respectively.

In the following, the symbols \(G, S, Γ, H_S, H_C, \) and \(H\) will always denote the objects introduced in Definitions 1 and 2. Moreover, a tensor product of two vectors or operators will be always understood to follow the factorization of \(H\) into \(H_S\) and \(H_C\).

This factorization of the state space plays a key role in the idea of a quantum walk. The general assumption is that operations which keep the position of the walker intact are generally available, whereas the position register can only be affected via controlled transitions of the walker on the underlying graph \(Γ\). We will formalize the former in the following definition:

**Definition 3.** Let \(A \in GL(H)\). We will call \(A\) a local operation if and only if there is a map \(ω_A : G → GL(H_C)\) such that \(A\) allows the following decomposition:

\[
A = \sum_{x \in G} |x⟩⟨x| ⊗ ω_A(x).
\]  

(2)

It trivially follows that for each local operation \(A\), the decomposition by Eq. (2) is unique. Moreover, if \(A \in U(H)\), then all the components \(ω_A(x)\) are elements of \(U(H_C)\), and vice versa. For a local operation \(A\), we will use notation \(A_x = ω_A(x)\) for the components in this decomposition.

We note that the set of local operations depends not only on the separation of \(H\) to a tensor product of \(H_S\) and \(H_C\) but also on the choice of the basis in \(H_S\). In any case, however, the local operations form a subgroup of \(GL(H)\).

It is important to distinguish local operations on \(H\) from operations acting only on \(H_C\), that is, operators of the form \(B = Id ⊗ B'\). The latter form a subgroup of the group of local operations: indeed, any such \(B\) is local with \(B_x = B'\) for all \(x \in G\).

Out of the other class of operations, altering the position of the walker, one representative is sufficient:

**Definition 4.** The step operator \(T\) is a controlled shift operator on \(H_S\) conditioned by the coin register, as prescribed by its action on the basis states \(|x,c⟩\),

\[
T|x,c⟩ = |xc,c⟩.
\]  

(3)

Clearly, \(T\) is defined by Eq. (3) on the whole of \(H\) via linearity and is a bounded operator. As the tensor product basis states, specified by Definition 2, are solely permuted under \(T\), it is obvious that \(T\) is an unitary operator on \(H\) and can thus form a time evolution operator in a discrete time quantum system.[10]

Before defining a quantum walk, we need one last supporting definition:

**Definition 5.** Let \(C = (C_n)_{n=0}^{+∞}\) is an infinite sequence of local unitary operations on \(H\). We call \(C\) a quantum coin.

If the sequence is constant, we call the quantum coin \(C\) time-homogeneous. If every term \(C_n\) of the sequence is a tensor product \(Id ⊗ C_n\), we call the quantum coin \(C\) space-homogeneous. In general, however, a quantum coin may be both time- and position-dependent.

We call a generic \(C\) a time- and position-dependent coin since, in accordance with Definition 3, we can find unitary operators \(C_{n,x} ∈ U(H_C)\) for each time \(n \in \mathbb{N}_0\) and position \(x \in G\) which alter the coin register in dependence on both the current time and the state of the position register, provided that the latter is well-defined.

The set of all quantum coins forms a group under element-wise composition.

The coin and step operators lead us to the definition of a discrete time quantum walk on a Cayley graph \(Γ\).

**Definition 6.** Let \(Γ\) is a Cayley graph, let \(C = (C_n)_{n=0}^{+∞}\) is a quantum coin on its corresponding Hilbert space \(H\). A discrete-time quantum walk on \(Γ\) with the coin \(C\) is a quantum protocol described by the following: an initial state \(|ψ_0⟩ \in H\) and the evolution operator

\[
W_C : \mathbb{N}_0 → U(H) : W_C(n) = TC_{n-1}TC_{n-2}...TC_0.
\]  

(4a)

For \(n ∈ \mathbb{N}_0\), we say that the state of the walker after \(n\) steps is

\[
|ψ_n⟩ = W_C(n)|ψ_0⟩.
\]  

(4b)

### III. SYMMETRIES PRESERVING MEASUREMENT PROBABILITIES

Symmetry of a system is an invariance of the system under some kind of transformation acting on its parameters and/or the initial state. Invariance does not necessarily mean that the time evolution is exactly the same, some variations may take place in the internal state as long as they do not influence the observable properties of the system, that is, the measurement probabilities of the spatial degree of freedom. Of all such transformations, we will be interested only in those which respect the unitary nature of quantum mechanics. Formally, we can state the requirement as follows:

**Definition 7.** Let \(T\) be an endomorphism on the Cartesian product of the set of quantum coins and initial states of a quantum walk on \(Γ\). We call \(T\) a unitary quantum walk symmetry on \(Γ\) if there is a sequence of local unitary operators \((U_n)_{n=0}^{+∞}\), such that for each quantum coin \(C = (C_n)_{n=0}^{+∞}\) and for each initial state \(|ψ_0⟩\),

\[
∀n ∈ \mathbb{N}_0 : W_C(n)|ψ_0⟩ = U_nW_C(n)|ψ_0⟩,
\]  

(5)

where \(\tilde{C} = (\tilde{C}_n)_{n=0}^{+∞}\) and \(|ψ_0⟩\) denote the image of \(C\) and \(|ψ_0⟩\) under \(T\).

The above definition is motivated by the fact that local unitary operations preserve measurement probabilities in
the geometrical basis of $\mathcal{H}_S$,

$$\sum_{c \in S} |\langle x, c|\phi \rangle|^2 =: \|\langle x|\psi \rangle\|^2 = \|\langle x|U_{\text{local}}|\psi \rangle\|^2.$$ 

**Lemma 1.** Let, in the notation of Definition 7, $(\tilde{C},|\tilde{\psi}_0\rangle) = T(C,|\psi_0\rangle)$. Then the condition of Eq. (5) is satisfied if and only if

$$|\tilde{\psi}_0\rangle = U_0|\psi_0\rangle,$$ (6a)

$$\forall n \in \mathbb{N}_0 : \quad T\tilde{C}_n = U_{n+1}TC_nU_n^\dagger,$$ (6b)

Proof. The first part is readily obtained by studying the special case of Eq. (5) where $n = 0$. Inserting Eq. (6a) back into Eq. (5), we get

$$\forall n \in \mathbb{N}_0 : \quad W_\tilde{C}(n)U_0|\tilde{\psi}_0\rangle = U_nW_C(n)|\psi_0\rangle$$ (7)

The generality of Eq. (7) with respect to $|\tilde{\psi}_0\rangle$ implies an equivalence of the operators,

$$W_\tilde{C}(n)U_0 = U_nW_C(n).$$

Substituting $n + 1$ for $n$, we get another identity,

$$W_\tilde{C}(n + 1)U_0 = U_{n+1}W_C(n + 1).$$

Comparing with

$$W_\tilde{C}(n + 1) = T\tilde{C}_nW_\tilde{C}(n),$$

$$W(n + 1) = TC_nW_C(n),$$

we obtain the relation

$$T\tilde{C}_nU_nW_C(n) = U_{n+1}TC_nW_C(n).$$

Due to the unitarity of the time evolution operators and $U_n$, this is equivalent to Eq. (6b).

**Lemma 2.** Let $T$ be a unitary quantum walk symmetry imposing a local unitary transform $(U_n)_{n=0}^{+\infty}$ on the instantaneous state of a quantum walk, as given by Definition 7. Then $U_{n,x}$ is diagonal in the geometrical basis of $\mathcal{H}_C$ for each $n \in \mathbb{N}$ (i.e. $n \geq 1$) and all $x \in G$, that is, there are complex units $u_{n,x,c}$ for each $n \in \mathbb{N}$, $x \in G$, and $c \in S$ such that

$$U_n = \sum_{x \in G} \sum_{c \in S} u_{n,x,c} |x,c\rangle \langle x,c|$$ (8)

Proof. Starting from Eq. (6b), we can rearrange the terms so that $U_{n+1}$ is isolated:

$$U_{n+1} = T\tilde{C}_nU_nC_n^\dagger T^\dagger.$$

Let $x \in G$ and $c, d \in S$. We can compare the corresponding matrix elements on both sides:

$$\langle x,c|U_{n+1}|x,d\rangle = \langle x,c|T\tilde{C}_nU_nC_n^\dagger T^\dagger|x,d\rangle.$$

From Definition 4 and the subsequent comment, we can derive that

$$T^\dagger|x,d\rangle = |xd^{-1},d\rangle$$ (9a)

and similarly

$$\langle x,c|T = (T^\dagger|x,c\rangle)^\dagger = (xc^{-1},c).$$ (9b)

Noting that all the other operators are local, we can factor out the position register to get

$$\langle x|x\rangle \langle c|U_{n+1,x}|d\rangle = \langle xc^{-1}|xd^{-1}\rangle \langle c|\tilde{C}_{n,xd^{-1}}U_{n,xd^{-1}}C_n^\dagger\tilde{C}_{n,xd^{-1}}|d\rangle$$

If $c \neq d$, the right hand side is zero due to its leftmost term. Since $\langle x|x\rangle = 1$, we obtain the implication

$$c \neq d \Rightarrow \langle c|U_{n+1,x}|d\rangle = 0,$$

meaning that $U_{n+1,x}$ is diagonal in the geometrical basis of $\mathcal{H}_C$ for all $n \in \mathbb{N}_0$.

The second part of the Lemma is a trivial application of the corresponding definitions.

**Theorem 1.** Let $T$ be a unitary symmetry of a quantum walk on $G$. Then there is a unique local unitary operation $U_0$ on $\mathcal{H}$ and a unique sequence of local unitary operations $(U_n)_{n=1}^{+\infty}$ diagonal in the geometrical basis of $\mathcal{H}$ such that for each quantum coin $C$ and each initial state $|\psi_0\rangle$, the transformed values read $|\psi_0\rangle = U_0|x,0\rangle$ and

$$\forall n \in \mathbb{N}_0 : \quad \tilde{C}_n = \sum_{x \in G} \left( \langle x| \otimes (V_{n,x}C_{n,x}U_{n,x}) \right),$$ (10a)

where $V_{n,x} \in U(\mathcal{H}_C)$ is related to $U_{n+1}$ by

$$V_{n,x} = \sum_{c \in S} u_{n+1,x,c,c} \langle c|c\rangle,$$ (10b)

using the notation of Eq. (8). Conversely, given any $U_0$ and $(U_n)_{n=1}^{+\infty}$ satisfying the aforementioned conditions, there is a unique symmetry $T$ yielding these values. Therefore, the symmetry group of Eq. (4) is $U(\mathcal{H}_C)^G \times U(1)^{G \times \mathbb{N} \times S}$.

Proof. The proof follows from Eq. (6b) and its equivalent form,

$$\tilde{C}_n = T^\dagger U_{n+1}TC_nU_n^\dagger.$$

Comparing the matrix elements, we obtain

$$\langle x,c|\tilde{C}_n|x,d\rangle = \langle x,c|T^\dagger U_{n+1}TC_nU_n^\dagger|x,d\rangle.$$

Using Eq. (3) and the locality of the $U$ and $C$ operations, we find that

$$\langle c|\tilde{C}_n|d\rangle = \langle xc,c|U_{n+1}T(|x\rangle \otimes C_{n,x}U_{n,x}^\dagger|d\rangle).$$
Using Lemma 2 and Eq. (9a),

$$\langle xc, c| U_{n+1}T = (T^{\dagger} U_{n+1}^\dagger |xc, c) \rangle =$$

$$= (u_{n+1, xc, c} T^\dagger |xc, c) \rangle = u_{n+1, xc, c} \langle xc, c |,$$

whence it follows that

$$\langle c| \tilde C_n |d = u_{n+1, xc, c} \langle x |c c_n^{\dagger} U_{n+1}^\dagger |d =$$

$$= \langle c| V_{n, xc, c} U_{n+1} x |d ,$$
as stated by the theorem.

Conversely, given the unitary operations $U_0$ and $(U_n)_{n=0}^{\infty}$, Eq. (6b) describes a way to construct a symmetry operation $T$.

According to Theorem 1, the sequence $(U_n)_{n=0}^{\infty}$ provides a full classification of all the unitary quantum walk symmetries. If there is no restriction on the homogeneity of the quantum coins $S$ and $\tilde C$ or the initial state, the choice of $U_n$ is free, up to the restriction of Lemma 2. More interesting cases arise when the coin has some global property that is required to be preserved under the symmetry.

Before stating the main theorem regarding homogeneous quantum coins, we introduce a means of classifying various walking spaces.

**Definition 8.** Let $G$ be a discrete group generated by a subset $S$, let $S^{-1}$ denote the set of inverses of all elements of $S$. The causal subgroup of $G$ with respect to $S$ is defined as

$$S^{(0)} = \left \langle \bigcup_{n \in \mathbb{Z}} S^n S^{-n} \right \rangle. \tag{11a}$$

The future causal subgroup of $G$ with respect to $S$ is defined as

$$S_+^{(0)} = \left \langle \bigcup_{n=1}^{+\infty} S^n S^{-n} \right \rangle. \tag{11b}$$

A Cayley graph $\Gamma = \Gamma(G, S)$ is called nonseparating if $S_+^{(0)} = S^{(0)}$.

In other words, the causal subgroup $S^{(0)}$ contains all the elements of $G$ which can be written as a product of generators and their inverses in such a way that the exponents add up to zero. The causal subgroup has several important properties, as shown in the following Theorem.

**Theorem 2.** The causal group $S^{(0)}$ is a normal subgroup of $G$. Moreover, $G/S^{(0)}$ is a cyclic group generated by the coset of any element in $S$.

**Proof.** Let $c \in S$, let $s \in S^n S^{-n}$ for some $n \in \mathbb{Z}$. Then it is simple to show that both $c s c^{-1}$ and $c^{-1} s c$ are elements of $S^{(0)}$. Indeed, let $n > 0$. Then $c s c^{-1} \in S S^n S^{-n} S^{-1} = S^{n+1} S^{-n-1} \subset S^{(0)}$. Similarly, $c^{-1} s c \in S^{-1} S^n S^{-n} S = (S^{-1} S^1)(S^n S^{-n}) \subset S^{(0)}$. The case $n < 0$ is analogous, $n = 0$ is trivial.

Using elementary algebra, this result can be generalized to any $c \in G$ and $s \in S^{(0)}$, which is one of the conditions equivalent to $S^{(0)}$ being normal in $G$.

For the second part, let $c_0$ be an arbitrary fixed element of $S$. We first show that the coset $c S$ equals $c_0 S$ for any $c \in S$. Indeed,

$$c S = (c_0 c_0^{-1}) c S = c_0 (c_0^{-1} c) S = c_0 S.$$

Analogously, $c^{-1} S = c_0^{-1} S$.

Let now $g$ be an arbitrary element of $G$. We can decompose $g$ into

$$g = c_1^{e_1} c_2^{e_2} \cdots c_k^{e_k},$$

where $c_i \in S$ and $e_i \in \mathbb{Z}$ for all $1 \leq i \leq k$. Using the above result, the coset $g S$ is equal to

$$g S = c_0^{e_1} c_0^{e_2} \cdots c_0^{e_k} S = c_0^{e_1 + e_2 + \cdots + e_k} S = (c_0 S)^{e_1 + e_2 + \cdots + e_k}.$$

This completes the proof.

**Remark.** The future causal subgroup $S_+^{(0)}$ generally does not share these properties. As they are extremely helpful for the theorems to follow, we will restrict the analysis below to quantum walks on nonseparating Cayley graphs, where there is no difference between $S_+^{(0)}$ and $S^{(0)}$.

We note without proof that a sufficient condition for the equality $S_+^{(0)} = S^{(0)}$ is that for each $c, d \in S, c d^{-1}$ is an element of $S_+^{(0)}$. This is satisfied automatically in, but not restricted to, all abelian groups. On the other hand, an example that this property is not universal is provided by the free group on 2 or more generators. In such cases, the quantum walk splits the initial excitation into a potentially unlimited number of mutually independent branches which never can interfere again.

In the following, we denote $[G : S^{(0)}] = \chi(G, S)$. This characteristic plays its role in an important corollary of Theorem 2.

**Corollary 1.** Let $c_0$ be a fixed element of $S$. For each $x \in G$, there are $\hat x \in S^{(0)}$ and $k \in \mathbb{Z}$ such that $x = \hat x c_0^k$. This decomposition is unique if and only if $[G : S^{(0)}]$ is infinite, otherwise $k$ is determined up to an integer multiple of $\chi(G, S)$.

Let $T$ be a unitary quantum walk symmetry, as defined in Definition 7. From Theorem 3, we know that the quantum coin and the initial state are transformed independently. The following theorem studies two important cases where the transformation of the coin is restricted.

Let $C$ denote a quantum coin and $\tilde C$ its image under $T$. We say that $T$ preserves time or space homogeneity of the quantum coin if the respective property of $\tilde C$ implies that the same property is held for $C$. 
Theorem 3. Let \( \mathcal{T} \) be a unitary symmetry of a quantum walk on a nonseparating Cayley graph, let \( (U_n)_{n=0}^{+\infty} \) be the transformation induced in the instantaneous state of the quantum walk.

- \( \mathcal{T} \) preserves space homogeneity of the quantum coin if and only if the unitary operators \( U_{n,x} \), forming the decomposition of \( U_n \), are of the form
  \[
  U_{n,x} = \rho(x) U_n, \quad \forall n \in \mathbb{N}_0,
  \]
  where \( \rho \) is an arbitrary doubly infinite sequence of complex units, periodic with the period \( \mathcal{H}(G,S) \) if the latter is finite, \( \rho(s) \) is a one-dimensional unitary representation of \( S(0) \) and the operators \( U_n \) act on \( H_C \) only. The group of symmetries preserving space homogeneity is \( \langle (U(1)^{\chi(G,S)}/[U(1)] \times \text{Rep}(S(0)) \times U(1)^{\chi(G,S)} \times U(1) \rangle \); \( \text{Rep}(S(0)) \) is the group of one-dimensional unitary representations of \( S(0) \) with pointwise multiplication.

- \( \mathcal{T} \) preserves time homogeneity of the quantum coin if and only if the unitary operations \( U_{n,x} \) are restricted by
  \[
  U_{n,x} = \eta_n - \epsilon \eta_n U_{n,x}, \quad \forall n \in \mathbb{N}_0,
  \]
  where \( \eta_n \) is defined the same way as above, \( \epsilon \) is an arbitrary complex unit and \( U_{x,n} \) are the components of a unitary operator \( U \in U(\mathcal{H}) \) diagonal in the geometrical basis of \( \mathcal{H} \). If \( \chi(G,S) \) is infinite, we can take \( \epsilon \) fixed at 1. The group of symmetries preserving space homogeneity is \( \langle (U(1)^{\chi(G,S)}/[U(1)] \times U(1) \times U(1) \rangle \); \( \chi(G,S) \) is \( \langle +\infty \rangle \) and \( (U(1)^{\chi(G,S)}/[U(1)] \times U(1) \rangle \) otherwise.

Proof. In both cases, we start from Eq. (10). Let \( x \in G \) and \( c, d \in S \). Comparing matrix elements on both sides, we obtain

\[
\langle x, c \rangle \hat{C}_{n,x} |d\rangle = \langle c \rangle \hat{C}_{n,x} |d\rangle = \langle c \rangle |V_{n,x} C_{n,x} U_{n,x}^\dagger |d\rangle.
\]

Using the result of Lemma 2, the right hand side can be simplified substantially:

\[
\langle c \rangle \hat{C}_{n,x} |d\rangle = \frac{\eta_{n,x,c} \langle c \rangle \hat{C}_{n,x} |d\rangle}{\eta_{n,x,d}}.
\]

Let \( e \) be another element of \( S \). We compare the last equation with another matrix element equation,

\[
\langle c \rangle \hat{C}_{n,x} |e\rangle = \frac{\eta_{n,x,c} \langle c \rangle \hat{C}_{n,x} |e\rangle}{\eta_{n,x,e}}.
\]

As these formulas hold for any quantum coin \( C \), we select one for which all the matrix elements of \( C_{n,x} \) are nonzero for all \( n \in \mathbb{N} \) and \( x \in G \). We can then divide the above two equations to get

\[
\frac{\eta_{n,x,c}}{\eta_{n,x,d}} = \frac{\langle c \rangle \hat{C}_{n,x} |c\rangle \langle d \rangle \hat{C}_{n,x} |c\rangle}{\langle c \rangle \hat{C}_{n,x} |c\rangle \langle d \rangle \hat{C}_{n,x} |c\rangle}.
\]
By choosing $c = c_0$, the last equation becomes
\[ \alpha_{n+1,k+1}/\alpha_{n,k} = \beta_n, \]
whence we obtain
\[ \alpha_{n,k} = \beta_0 \beta_1 \ldots \beta_{n-1} \alpha_{0,n-k} = \gamma_n \tilde{\alpha}_{n-k}. \]

If $\chi(G,S)$ is a finite number, the decomposition of Corollary 1 is not unique. The value of $\chi(G,S)$ is then equal to the least positive power $l$ for which $c_0^l \in S^{(0)}$. Let $\tilde{x}_0 = \alpha_0^{\chi(G,S)}$. The equality
\[ \tilde{x}_0^k = \tilde{x}_0 x_c c_0^{-\chi(G,S)} \]
then imposes a condition on the choice of $\alpha_{n,k}$ and subsequently $\tilde{\alpha}_m$:
\[ \alpha_{n,k} \rho(\tilde{x}) = \alpha_{n,k-\chi(G,S)} \rho(\tilde{x}) \rho(\tilde{x}_0) \]
\[ \Rightarrow \alpha_{n,k+\chi(G,S)} = \alpha_{n,k} \rho(\tilde{x}_0) \]
\[ \Rightarrow \tilde{\alpha}_m - \chi(G,S) = \tilde{\alpha}_m \rho(\tilde{x}_0). \]

In this case, the freedom in choosing $\tilde{\alpha}$ is restricted to $\chi(G,S)$ independent complex units. If $\chi(G,S)$ is infinite, all elements of the doubly infinite sequence can be chosen freely.

Putting together all the above elements, we find that the complete solution of Eq. (14) with the right hand side independent of $x$ can be written as
\[ u_{n,x,c} = \gamma_n \tilde{\alpha}_{n-k} \rho(\tilde{x}) \delta_{n,c} \]
for $x = \tilde{x}_0^k$, where

- $\gamma_n$ and $\delta_{n,c}$ are any complex units for all $n \in \mathbb{N}$ and $c \in S$,
- $\tilde{\alpha}_m$ is a sequence of $\chi(G,S)$ independent complex units,
- $\rho$ is a one-dimensional unitary representation of $\mathbb{S}^{(0)}$.

Clearly, the sequence $\gamma_n$ can be absorbed into $\delta_{n,c}$. Besides that, only one degree of freedom is counted twice—a global phase factor, which can come from both $\tilde{\alpha}$ and $\delta$.

At this point, we emphasize that the parameter $n$ so far has been greater than or equal to 1; Lemma 2 puts no restriction on the form of $U_0$ except that it is local. Thus the case $n = 0$ must be studied separately. According to Lemma 1, the transformation of the quantum coin element $C_0$ reads
\[ \tilde{C}_0 = T^\dagger U_1 T C_0 U_0^\dagger. \]

Expressing $U_0$, we obtain
\[ U_0 = C_0^\dagger T^\dagger U_1 T C_0. \]

Comparing the corresponding matrix elements on both sides and expanding the matrix product on the right hand side while using the locality property of the $C$ and $U$ matrices gives
\[ \langle c | U_{0,x} | d \rangle = \sum_{a, \bar{a}} \langle c | C_0^\dagger | a \rangle u_{1,x,a,a} \langle a | C_0 | d \rangle. \]

This relates the components of $U_0$ to those of $U_1$, which are described by Eq. (17). Inserting the final form, we can see that
\[ \langle c | U_{0,x} | d \rangle = \sum_{a, \bar{a}} \langle c | C_0^\dagger | a \rangle \tilde{\alpha}_{1-k} \rho(\tilde{x}) \delta_{1,a} \langle a | C_0 | d \rangle = \alpha_{1-k} \rho(\tilde{x}) f(c, d), \]
where $x = \tilde{x}_0^k$ and $f$ represents the matrix elements of some unitary matrix (any matrix can be reached with a suitable choice of $C_0$). Therefore, the components of $U_0$ are complex unit multiples of one constant unitary operator on $\mathbb{H}_n$, where the dependence on $x$ follows the same rule as in the case of any other $U_n$, $n \geq 1$.

We conclude that the symmetry group under the aforementioned conditions is isomorphic to
\[ (U(1)^{\chi(G,S)} / U(1)) \times \text{Rep}(\mathbb{S}^{(0)}) \times U(1)^{N \times S} \times U(\mathbb{H}_n), \]
as stated by the theorem.

**Part B.** If $C$ and $\tilde{C}$ are simultaneously time-homogeneous, the right hand side of Eq. (14) is constant in $n$, which leads to a factorization
\[ u_{n,x,c} = u_{n,x} \tilde{\delta}_{x,c}, \]
where we again assume both terms to be complex units. Eq. (13) then gives for $w_{n,x}$ that the ratio $w_{n+1,x}/w_{n,x}$ does not depend on $n$ and thus for each $x \in G$ and $m, n \in \mathbb{N}_0$,
\[ \frac{w_{m+1,x}}{w_{m,x}} = \frac{w_{n+1,x}}{w_{n,x}} = \frac{w_{m,x}}{w_{n,x}}. \]

In a complete analogy to the above, we obtain for each $x \in G$, $n \in \mathbb{N}_0$, and $s \in S^+$,
\[ \frac{w_{m,x}}{w_{n,x}} = \frac{w_{n,x}}{w_{n,x}}. \]

This means that for each $m$ and $n$ in $\mathbb{N}_0$ and each right coset $x S_+^{(0)}$, the ratio between $w_{m,y}$ and $w_{n,y}$ is a constant complex unit for all $y \in x S_+^{(0)}$, so that we can factorize
\[ w_{n,x} = \alpha_n x S_+^{(0)} q_x. \]

Once more, we will require both factors to be unitary. If, by assumption, $S_+^{(0)} = S^{(0)}$, the cosets are identified by the power of one generator of $S$—that is $c_0^k S^{(0)}$, where $k \in \mathbb{Z}$, so that we obtain
\[ w_{n,x} = w_{n,x} c_0^k = \alpha_n k q_x. \]

We note that if $\chi(G,S)$ is finite, then $\alpha_n + 1$ is $\chi(G,S)$ must be equal to $\alpha_n$ to retain consistency. Inserting this form into Eq. (19a), we find that the ratio
\[ \frac{\alpha_{n+1,k+1} q_x}{\alpha_{n,k} q_x} \]
should not depend on $n$. This is equivalent to the condition that $\alpha_{n+1,k+1}/\alpha_{n,k}$ depends on $k$ only. Denoting this ratio $\beta_k$, we find that
\[ \alpha_n k = \beta_{k-1} \alpha_{n-1,k-1} = \beta_{k-1} \beta_{k-2} \alpha_{n-2,k-2} = \ldots = \beta_{k-1} \beta_{k-2} \ldots \beta_{k-n} \alpha_{n-k}. \]
Denoting

\[ \gamma_K = \begin{cases} \prod_{k=0}^{K-1} \beta_k & \text{for } K \geq 0, \\ \prod_{k=1}^{K} \beta_{-k}^{-1} & \text{otherwise,} \end{cases} \]

we can write

\[ \alpha_{n,k} = \frac{\gamma_k}{\gamma_{k-n}} \alpha_{0,k-n}. \]

Unlike \( \alpha_{0,k} \), \( \gamma_k \) is not constant on the modular class mod \( \chi(G,S) \) for \( \chi(G,S) < +\infty \). Instead,

\[ \gamma_{m+1} \chi(G,S) = \prod_{k=0}^{m+1} \beta_k \gamma_m =: \varepsilon^{\chi(G,S)} \gamma_m. \]

In the case of infinite \( \chi \), let \( \varepsilon = 1 \). This allows us to write the solution uniformly as

\[ \alpha_{n,k} = \varepsilon^n \eta_{n-k} \gamma_k, \]

\[ u_{n,x,c} = \varepsilon^n \eta_{n-k} \gamma_k \delta_{x,c}, \quad (21) \]

where \( x = \tilde{x}_0^k \) and

- \( \delta_{x,c} \) are arbitrary complex units for all \( x \in G, c \in S \),
- \( \gamma_m \) and \( \eta_m \) are arbitrary sequences of \( \chi(G,S) \) complex units,
- \( \varepsilon \) is an arbitrary complex unit in the case of finite \( \chi(G,S) \) and 1 otherwise.

Again, as the term of \( \gamma_k \) depends only on \( x \), it can be immersed into \( \delta_{x,c} \). Also, a global phase factor can be factored out of \( \eta_m \) and put into \( \delta_{x,c} \).

As opposed to the previous case, it’s simple to determine the zeroth element \( U_0 \): starting from Eq. (18), we note that for time-homogeneous coins, there is a local unitary \( C \) such that \( C_n = C \) for all \( n \in \mathbb{N} \). Similarly, \( C_n = C \) for all \( n \in \mathbb{N} \). Thus,

\[ U_0 = \tilde{C}^T T^k U T C. \]

We can compare this equation with its equivalent for \( n = 1 \),

\[ U_1 = \tilde{C}^T T^k U T C. \]

Noting that by Eq. (21), \( U_2, \tilde{x}_0^k = \varepsilon^{n-k} U_{1, \tilde{x}_0^{k-1}} \), we obtain

\[ U_0, \tilde{x}_0^k = \varepsilon^{-1} U_{1, \tilde{x}_0^{k+1}} \]

so that the operator \( U_0 \) is also diagonal in the geometrical basis of \( \mathcal{H} \) and its matrix elements are given simply by extending the validity of Eq. (21) to the case \( n = 0 \).

We conclude the proof by establishing the group of time-homogeneity preserving symmetries. Taking into account Eq. (21) and the following notes, each symmetry is determined by specifying \( \delta_{x,c}, \eta_m \) (up to a global phase) and possibly \( \varepsilon \). As all of these parameters are just tuples of complex units, this immediately gives the group in the form stated by the theorem.

In the case of a both space- and time-homogeneous coin, we can easily combine the partial results given by Theorem 3 as follows.

**Corollary 2.** Let \( \Gamma \) be nonseparating, let \( \mathcal{T} \) be a unitary quantum walk symmetry described by a sequence of unitary operators \( (U_n)_{n=0}^{\infty} \). Then \( \mathcal{T} \) preserves both time and space homogeneity of the quantum coin if and only if the components of \( U_n \) are of the form

\[ U_{n,x} = \eta_{n-k} \varepsilon^n \gamma(x) U' \]

for all \( n \in \mathbb{N}_0 \), where \( \eta_m \) is defined the same way as in Theorem 3, \( \varepsilon \) is a complex unit, fixed at 1 in the case where \( \chi(\Gamma) \) is infinite, \( \gamma \) is a one-dimensional unitary representation of \( G \), and \( U' \in U(\mathcal{H}_C) \) is a unitary operation diagonal in the geometrical basis of \( \mathcal{H}_C \). The group of symmetries with this restriction is

\[ \mathcal{G}(\chi, \mathcal{H}_C) = \left( U(1)^{\chi(\mathcal{G}, S)/\chi(\mathcal{G}, \mathcal{S})} / U(1) \times \text{Rep}(S^{(0)}) \times U(1)^S \right) \]

if \( \chi(\mathcal{G}) < +\infty \) and

\[ \mathcal{G}(\chi, \mathcal{H}_C) = \left( U(1)^{\chi(\mathcal{G}, S)/\chi(\mathcal{G}, \mathcal{S})} / U(1) \times \text{Rep}(S^{(0)}) \times U(1)^S \right) \]

otherwise.

**Example.** In this example, we apply the above theory to a quantum walk on a line, where \( G \) is the additive group of integers, \( \mathbb{Z} \), generated by \( S = \{-1, 1\} \), with a homogeneous coin. Even in this simplest case the above theory produces useful results. Let \( \Gamma \) denote the Cayley graph \( \Gamma(\mathbb{Z}, S) \).

A general quantum coin with this property is given by \( C = (\text{Id} \otimes C)^{+\infty}_{\eta=0} \), where \( C \), expressed in the geometrical basis of \( \mathcal{H}_C \), is a general unitary matrix of rank 2,

\[ C = \omega \begin{pmatrix} \mu & 0 \\ 0 & \mu^* \end{pmatrix} \begin{pmatrix} \cos \psi \sin \psi \\ -\sin \psi \cos \psi \end{pmatrix} \begin{pmatrix} \nu & 0 \\ 0 & \nu^* \end{pmatrix}. \]

(23)

Here \( \omega, \mu, \nu, \psi, \phi \in \mathbb{C}, |\omega| = |\mu| = |\nu| = 1 \).

The causal subgroup is equal to \( 2\mathbb{Z} \), since any product of an odd number of generators is an even number, and 2 can be written as \( c + (-d) \in S + (-S) \subset S^{(0)} \) if \( c = 1, d = -1 \). The condition of \( \Gamma \) being nonseparating is a trivial property of any abelian walking space. We note that \( \chi(G, S) = 2 \) and the elements of \( G : S^{(0)} \) correspond to the subsets of even and odd integers. Indeed, walks started in either of these subsets never interfere.

A general form of a unitary representation of \( 2\mathbb{Z} \) on \( C \) is

\[ \gamma(x) = e^{i\phi x}, \quad \phi \in \mathbb{R}. \]

According to Corollary 2, the symmetries of the above system are classified by five continuous parameters: \( \eta_{\text{odd}}, \eta_{\text{even}}, \epsilon, \phi, \delta_{+, -} \). The transformed coin reads

\[ \tilde{C} = \omega e \begin{pmatrix} \epsilon^{i\phi} & 0 \\ 0 & e^{-i\phi} \end{pmatrix} \begin{pmatrix} \delta_{+1} & 0 \\ 0 & \delta_{-1} \end{pmatrix} \begin{pmatrix} \mu & 0 \\ 0 & \mu^* \end{pmatrix} \begin{pmatrix} \nu & 0 \\ 0 & \nu^* \end{pmatrix}. \]

(24a)
and the transformed initial state is
\[ U_0|\psi_0\rangle = \sum_{x \in \mathbb{Z}} \eta_{x \mod 2} e^{i\phi x} \begin{pmatrix} \delta_{+1} & 0 \\ 0 & \delta_{-1} \end{pmatrix} |x\rangle \langle x| \psi_0\rangle. \quad (24b) \]

Based on these formulas, some of the parameters assume a straightforward mathematical meaning:

- \( \epsilon \) is related to the invariance of the system with respect to multiplying \( C \) by a scalar. This is a phase that the system accumulates per every step of the quantum walk.
- A common prefactor of \( \delta \) is related to the freedom of global phase of the initial state.

The global phase can be completely moved from \( \delta \) into \( \eta \) by introducing a constraint \( \delta_{-1} = \delta_{+1} \) and making \( \eta_{\text{even}} \) and \( \eta_{\text{odd}} \) two independent parameters.

In general, any continuous symmetry can be used to reduce the number of parameters determining nonequivalent instances of a given physical system. In our example, by choosing appropriate values of \( \epsilon, \phi, \) and \( \delta_{\pm1} \), we can find a quantum walk equivalent with \( W_C \) in which the coin is simplified to

\[ \tilde{C} = \begin{pmatrix} \cos \psi & \sin \psi \\ -\sin \psi & \cos \psi \end{pmatrix} \]

and thus determined by a single parameter. The rest of the information about the particular quantum walk can be encoded into the initial state.

Besides this result, Eq. (25) has one nontrivial consequence: the transformed coin is a real-valued matrix and so is the infinite matrix of the step operator in the geometrical basis of \( \mathcal{H} \). Therefore, an initial state with real coefficients in the geometrical basis will stay real-valued during the whole time evolution and an analogous result holds for a pure imaginary-valued initial vector.

As a consequence, the real and imaginary parts of the transformed initial state define two quantum walks which never interfere, although visiting the same set of vertices. The contributions to measurement probabilities can be computed separately in the field of real numbers and classically summed.

Moreover, if the initial state of the walker is localized at a vertex \( x_0 \), i.e., of the form

\[ |\psi_0\rangle = |x_0\rangle \otimes |\chi_0\rangle, \]

then this property is kept under the transformation Eq. (24b). If we also neglect the global phase, which can be done using \( \eta \) with no effect on the coin, the initial state is completely determined by two parameters (the spherical angles on the Bloch sphere). Thus any quantum walk on a line with position- and time-independent coin starting from a state localized at a given position is completely determined by a total of three degrees of freedom. This particular result has been exploited in a recent experimental realization [4] where there was only one adjustable parameter of the quantum coin, corresponding precisely to \( \psi \) in this example, and a full control of the initial chirality \( \chi_0 \) (up to a global phase) using two adjustable optical elements.

### IV. Symmetries Involving Permutation of the Measurement Probabilities

In order to extend the applicability of the theory, we generalize the notion of quantum walk symmetries. According to Definition 7, the probability distribution of a complete measurement of the position register was required to stay invariant under a symmetry transformation. We obtain a broader class of solutions if we allow transformations which do affect the probability distribution, but in such a way that the original distribution is easily reconstructible—more precisely, such that the probabilities merely undergo some fixed permutation. In order to respect the underlying group structure of the Cayley graph, we assume that the permutation is given by an automorphism on \( G \) and an optional multiplication by a fixed element of \( G \), and define a wider class of symmetries which impose this kind of transformation on the measurement probability.

**Definition 9.** Let \( \phi \) be an automorphism of \( G \) such that \( \phi(S) = S \), let \( g \in G \). We call the map \( g\phi : G \rightarrow G : x \mapsto g \cdot \phi(x) \) a shifted \( S \)-preserving automorphism on \( G \). We associate three operators with \( g\phi \): a spatial permutation operator \( P_{g\phi}^{(S)} \) on \( \mathcal{H}_S \), defined by its action on geometrical basis states

\[ P_{g\phi}^{(S)}|x\rangle = |\phi(x)\rangle \quad (26a) \]

for all \( x \in G \); a coin permutation operator \( P_{g\phi}^{(C)} \) on \( \mathcal{H}_C \), defined by

\[ P_{g\phi}^{(C)}|c\rangle = |\phi(c)\rangle \quad (26b) \]

for all \( c \in S \); and a total permutation operator

\[ P_{g\phi} = P_{g\phi}^{(S)} \otimes P_{g\phi}^{(C)} \quad (26c) \]

on \( \mathcal{H} \).

Note that the automorphism part \( \phi \) of a shifted \( S \)-preserving automorphism \( g\phi \), needed in the definition of \( P_{g\phi}^{(C)} \), can be extracted using

\[ \phi(c) = (g\phi(e))^{-1}(g\phi(c)). \]

**Definition 10.** Let \( T \) be an endomorphism on the Cartesian product of the set of quantum coins and initial states of a quantum walk on \( \Gamma \). We call \( T \) a generalized unitary quantum walk symmetry on \( \Gamma \) if there is a sequence of local unitary operators \( (U_n)^{+\infty}_{n=0} \) and a shifted automorphism \( g\phi \) such that for each quantum coin \( \mathcal{C} = (C_n)^{+\infty}_{n=0} \) and for each initial state \( |\psi_0\rangle \),

\[ \forall n \in \mathbb{N}_0 : \quad W_C(n)|\psi_0\rangle = P_{g\phi}U_n W_C(n)|\psi_0\rangle, \quad (27) \]
where $\tilde{C}$ and $|\tilde{\psi}_0\rangle$ have the same meaning as in Definition 7 and $P_{g\phi}$ denotes the total permutation operator associated with the shifted $S$-preserving automorphism $g\phi$.

The (unshifted) automorphisms to be considered have to preserve the generating set $S$ in order to preserve the edges of the Cayley graph $\Gamma(G, S)$. We note, however, that the automorphism group of $\Gamma(G, S)$ may be more general.[11] As shown by the following Lemma, the shifted $S$-preserving automorphisms form a subgroup of the automorphism group of $\Gamma$.

**Lemma 3.** The set of all automorphisms on $G$ which preserve $S$ forms a subgroup $\text{Aut}(G | S)$ of $\text{Aut}(G)$. The set of all shifted $S$-preserving automorphisms on $G$ with the operation of map composition forms a group isomorphic to $G \rtimes \text{Aut}(G | S)$.

**Proof.** For the first part, it suffices to show that for any pair $\phi_1, \phi_2$ of automorphisms on $G$ preserving $S$, $\phi_1^{-1} \circ \phi_2$ preserves $S$. This is simple as both $\phi_1$ and $\phi_2$ act as permutations when restricted to $S$.

To show that the shifted $S$-preserving automorphisms constitute a group, we have to prove that the four group axioms are satisfied.

**Closure.** Let $\phi_1, \phi_2 \in \text{Aut}(G | S)$ and $g_1, g_2 \in G$. The composition of $g_1\phi_1$ and $g_2\phi_2$ is a map $G \rightarrow G$ prescribed by

$$ (g_1\phi_1 \circ g_2\phi_2)(x) = g_1\phi_1(g_2\phi_2(x)) = g_1\phi_1(g_2 \cdot (\phi_1 \circ \phi_2)(x)). \quad (28a) $$

Noting that $g_1\phi_1(g_2) \in G$ and that $\phi_1 \circ \phi_2 \in \text{Aut}(G | S)$, the composed map is by definition a shifted $S$-preserving automorphism.

**Associativity.** Associativity is granted by the operation of composition.

**Identity.** The identity element is the shifted $S$-preserving automorphism $e \cdot Id$, where $e$ is the identity element in $G$. Indeed, this is the identity map on $G$ and thus the neutral element with respect to map composition.

**Inverse.** Let $\phi \in \text{Aut}(G | S)$, let $g \in G$. Then the inverse element of the shifted $S$-preserving automorphism $g\phi$ with respect to composition is a map $G \rightarrow G$ defined by

$$ (g\phi)^{-1}(x) = \phi^{-1}(g^{-1}x) = \phi^{-1}(g^{-1} \cdot \phi^{-1}(x)) \quad (28b) $$

This is a shifted $S$-preserving automorphism as $\phi^{-1}(g^{-1}) \in G$ and $\phi^{-1} \in \text{Aut}(G | S)$.

Let us denote this group $\mathcal{G}$. In order to show that $\mathcal{G} \cong G \rtimes \text{Aut}(G | S)$, we first identify $G$ with a subgroup $G'$ of $\mathcal{G}$ using the monomorphism

$$ \gamma : G \rightarrow \mathcal{G} : g \mapsto g\cdot Id $$

and similarly identify $\text{Aut}(G | S)$ with a subgroup $A'$ of $\mathcal{G}$ using the monomorphism

$$ \alpha : \text{Aut}(G | S) \rightarrow \mathcal{G} : \phi \mapsto \psi \cdot \phi. $$

It follows directly from the definition that $\mathcal{G} = G' A'$ and that $G' \cap A' = \{e\}$. In order to show that the product is semidirect, we show that $G'$ is a normal subgroup of $\mathcal{G}$.

Let $h\cdot Id \in G'$, let $g\phi$ be an arbitrary element of $\mathcal{G}$. Using Eq. (28a) and Eq. (28b), we simplify the composition

$$ g\phi \circ h\cdot Id \circ (g\phi)^{-1} = g\phi \circ h\cdot Id \circ \phi^{-1}(g^{-1}) \phi^{-1} = \\
= g\phi \circ (h\phi^{-1}(g^{-1})) \phi^{-1} = \\
= (g\phi(h))^{-1} \cdot Id \in G'. $$

This proves that $\mathcal{G} = G' \rtimes A' \cong G \rtimes \text{Aut}(G | S)$.

**Lemma 4.** In the notation of Definition 10, the condition of Eq. (27) is satisfied for each $C$ and each $|\psi_0\rangle$ if and only if

$$ |\tilde{\psi}_0\rangle = P_{g\phi}\tilde{U}_0|\psi_0\rangle, $$

$$ \forall n \in \mathbb{N}_0 : \quad TC_n = P_{g\phi}U_{n+1}T C_n U_{n+1}^\dagger P_{g\phi}^\dagger. \quad (29) $$

Here, $\tilde{C}$ and $|\tilde{\psi}_0\rangle$ denote the image of $C$ and $|\psi_0\rangle$ under $T$.

**Proof.** The proof is done in a straightforward analogy to the proof of Lemma 1.

**Lemma 5.** Let $\phi \in \text{Aut}(G | S)$, let $g \in G$. Then the total permutation operator $P_{g\phi}$ commutes with the step operator $T$. Furthermore, let $U$ be a local unitary operation. Then $P_{g\phi}^\dagger U P_{g\phi}$ is a local unitary operation. If $U$ is of the form $Id \otimes U'$, then $P_{g\phi}^\dagger U P_{g\phi}$ is of the form $Id \otimes (P_{g\phi}^C)^\dagger U' P_{g\phi}^C$.

**Proof.** To show the commutation of $T$ and $P_{g\phi}$, we compare the action of both $TP_{g\phi}$ and $P_{g\phi}T$ on the same basis state $|x, c\rangle$.

$$ TP_{g\phi}|x, c\rangle = T|g\phi(x), \phi(c)\rangle = |g\phi(x)\phi(c), (c)\rangle $$

$$ P_{g\phi}T|x, c\rangle = P_{g\phi}|xc, c\rangle = |g\phi(xc), \phi(c)\rangle $$

The equality $\phi(x)\phi(c) = \phi(xc)$ follows from the fact that $\phi$ is a group automorphism.

In order to prove the second part of the Lemma, we first note that all the operators $P_{g\phi}^C$, $P_{g\phi}^{S}$, and $P_{g\phi}$ are unitary. This can be shown promptly from the fact that the operators act as permutations in the corresponding geometrical basis systems. Thus for any unitary operator $U$, $P_{g\phi}^\dagger UP_{g\phi}$ is also unitary.

If $U$ is local, we can show using Eq. (26c)

$$ \tilde{U} := P_{g\phi}^\dagger \left( \sum_{x \in G} |x\rangle \langle x| \otimes U_x \right) P_{g\phi} = \\
= \sum_{x \in G} \left( \left( P_{g\phi}^{S}\right) |x\rangle \langle x| P_{g\phi}^{S}\right) \otimes \left( P_{g\phi}^{C}\right) U_x P_{g\phi}^{C}\right). $$

If we change the summation variable from $x$ to $y = \phi^{-1}(g^{-1}x)$, such that $g\phi(y) = x$, we obtain

$$ \tilde{U} = \sum_{y \in G} \left( P_{g\phi}^{S}\right) |g\phi(y)\rangle \langle g\phi(y)| P_{g\phi}^{S}\right) \otimes \left( P_{g\phi}^{C}\right) U_{g\phi(y)} P_{g\phi}^{C}\right). $$
We used the fact that the composition of an automorphism and left multiplication is a bijection on $G$.

Using the unitarity of $P^{(S)}_{\phi\phi}$, from which it follows that

$$P^{(S)}_{\phi\phi} |g\phi(y)\rangle = \left(P^{(S)}_{\phi\phi}\right)^{-1} |g\phi(y)\rangle = |y\rangle$$

and

$$\langle g\phi(y)|P^{(S)}_{\phi\phi} = \left(P^{(S)}_{\phi\phi}\right)^\dagger = \langle y|,$$

we can simplify $\tilde{U}$ to the form

$$\tilde{U} = \sum_{y \in G} |y\rangle \langle y| \otimes \left(P^{(C)}_{\phi\phi} I_d \ P^{(S)}_{\phi\phi}\right),$$

which proves that $\tilde{U}$ is a local operator.

Similarly, let $U = I_d \otimes U'$. Then

$$P^{(S)}_{\phi\phi}(I_d \otimes U')P^{(S)}_{\phi\phi} =
\left(P^{(S)}_{\phi\phi} I_d \ P^{(S)}_{\phi\phi}\right) \otimes \left(P^{(C)}_{\phi\phi} U' = P^{(C)}_{\phi\phi}\right) =
I_d \otimes \left(P^{(C)}_{\phi\phi} U' P^{(C)}_{\phi\phi}\right).$$

As shown by the following Theorem, the search for generalized unitary quantum walk symmetries can be reduced to the problem already solved in Section III.

**Theorem 4.** Let $\mathcal{T}$ be an endomorphism on the Cartesian product of the set of quantum coins and initial states of a quantum walk on $\Gamma$, let $\mathcal{T}(C, |\psi_0\rangle) = (\tilde{C}, |\psi_0'\rangle), \tilde{C} = (C_n)_{n=0}^{\infty}$. Then $\mathcal{T}$ is a generalized unitary quantum walk symmetry if and only if there is an ordinary unitary quantum walk symmetry $\mathcal{T}' : (C, |\psi_0\rangle) \mapsto (C', |\psi_0'\rangle), C' = (C_n')_{n=0}^{\infty}$, and a shifted $S$-preserving automorphism $\phi$ such that

$$|\psi_0'\rangle = P^{(S)}_{\phi\phi} |\psi_0\rangle \quad \forall n \in \mathbb{N}_0 : \quad C''_n = P^{(S)}_{\phi\phi} C'_n P^{(S)}_{\phi\phi}. \quad (30)$$

Theorem 4 solves in general the problem of symmetries without any assumptions about the coin. The restricted problems with position- and/or time-independent coins can also be addressed. As a direct consequence of Lemma 5, the restriction is transferred from the quantum coin $C$ to the quantum coin $C'$ of the original problem, where we can use Theorem 3 or Corollary 2 to find all solutions.

It also trivially follows that the symmetry group is in all cases simply augmented by the group of shifted $S$-preserving automorphisms.

**Proof.** Let us define $|\psi_0'\rangle$ and $C'_{\mu}$ such that Eq. (30) is held. Then, according to Eq. (29), these objects must satisfy

$$|\psi_0'\rangle = U_0 |\psi_0\rangle \quad (31a)$$

and

$$TP^{(S)}_{\phi\phi} C'_n P^{(S)}_{\phi\phi} = P^{(S)}_{\phi\phi} U_{n+1} T C_n U_n^\dagger P^{(S)}_{\phi\phi}. \quad (31b)$$

Using the commutativity of $T$ and $P^{(S)}_{\phi\phi}$, Eq. (31b) becomes

$$TC_n = U_{n+1} T C_n U_n^\dagger. \quad (31c)$$

However, Eq. (31a) and Eq. (31c) are exactly the conditions of Lemma 1. Therefore $\mathcal{T}$ is a generalized unitary quantum walk symmetry if and only if the map $(C, |\psi_0\rangle) \mapsto (C', |\psi_0'\rangle)$ is an ordinary unitary quantum walk symmetry.

**Example.** We show an application of the generalized quantum walk symmetries again on a quantum walk on a line with a homogeneous coin. Given a coin $C = (I_d \otimes C)_{n=0}^{\infty}$ and an initial state $|\psi_0\rangle$, we can use Theorem 4 to find a new homogeneous quantum coin $\tilde{C} = (I_d \otimes \tilde{C})_{n=0}^{\infty}$ and an initial state $|\psi_0'\rangle$ such that the evolution of the new quantum walk is a mirror image of the original one.

Taking the $S$-preserving automorphism $\mathcal{P} : x \mapsto -x = 0 \pm (-1)x$, we construct the tuple of permutation operators $P^{(S)}_{\mu}$ easily. We note that the matrix of the coin permutation operator is the Pauli $X$-matrix, or the quantum NOT gate.

In the simplest case, we can choose to only perform the permutation, choosing the identity transform as $\mathcal{T}'$ in Theorem 4. Doing so, not only the measurement probabilities but also the amplitudes are preserved, they only undergo the permutation in both position and coin geometrical bases. In this case, the transformed coin is described by the matrix

$$\tilde{C} = X C X^\dagger = X C X$$

and the transformed initial state satisfies

$$|x\rangle |\psi_0\rangle = X (-x\rangle |\psi_0\rangle$$

for all $x \in \mathbb{Z}$.

If we use the general form of the coin as described by Eq. (23), after the transformation we obtain

$$\tilde{C} = \omega \begin{pmatrix} \mu^* & 0 \\ 0 & \mu \end{pmatrix} \begin{pmatrix} \cos \psi - \sin \psi \\ \sin \psi \cos \psi \end{pmatrix} \begin{pmatrix} \nu^* \\ 0 \end{pmatrix} = \begin{pmatrix} \mu \cos \psi - \nu \sin \psi \\ \mu \sin \psi \cos \psi \end{pmatrix} \begin{pmatrix} \nu^* \\ 0 \end{pmatrix}. \quad (32)$$

We note that it is now possible, if desired, to transform the coin back to its original state, using the results of Section III only. This way, the probability distribution stays unchanged, i.e. mirrored with respect to the original quantum walk, thus we obtain a new initial state $|\psi_1\rangle$ for the original coin $C$ for which the time evolution has flipped sides.

We can do so by the following transform:

$$C = \omega \begin{pmatrix} \mu^* & 0 \\ 0 & \mu \end{pmatrix} \begin{pmatrix} \mu^2 \nu^2 & 0 \\ 0 & (\mu^2 \nu^2)^* \end{pmatrix} \begin{pmatrix} -i \nu^2 & 0 \\ 0 & i \nu^2 \end{pmatrix} \begin{pmatrix} \cos \psi - \sin \psi \\ \sin \psi \cos \psi \end{pmatrix} \begin{pmatrix} \nu^* \\ 0 \end{pmatrix}. \quad (33)$$

This corresponds to choosing $\delta_\mu = \delta_\nu = i \nu^2$, $\epsilon = \mu^2 \nu^2$, and $\epsilon = 1$ in the notation of the Example in Section III. The choice of $\nu_{\text{even}}$ and $\nu_{\text{odd}}$ is free, so we can let them be 1. The transformed initial state is then given by

$$|\psi_1\rangle = \sum_{x \in \mathbb{Z}} (-i \nu^2 \nu \cos \psi \sin \psi - \nu \cos \psi \sin \psi) X (-x\rangle |\psi_0\rangle.$$
If the initial state $|\psi_0\rangle$ is localized at $x = 0$, the transition to $|\psi_1\rangle$ is simply a linear transformation of the initial chirality, described in the geometrical basis by the matrix

$$Q = \begin{pmatrix} -i\nu^2 & 0 \\ 0 & i\nu^2 \end{pmatrix} X = \begin{pmatrix} 0 & -i\nu^2 \\ i\nu^2 & 0 \end{pmatrix}$$

Having this result enables us to find initial states which produce a symmetric probability distribution at each iteration of the quantum walk. These are simply the eigenstates of the matrix $Q$, tensor multiplied by $|0\rangle$ in the position register. The eigenvalues of $Q$ are $\pm 1$ and the corresponding normalized eigenvectors are

$$|\chi_0\rangle_{\pm} = \frac{1}{\sqrt{2}} \left( \nu^* \right)$$

in the coin space basis. Except for the degenerate cases of $\psi = k\pi, k \in \mathbb{Z}$, the parameter $\nu$ is defined uniquely up to a sign and therefore there are exactly two localized initial states producing a symmetric probability distribution and these are orthonormal.

**V. CONCLUSIONS**

We used analytic and algebraic methods to study the symmetries of discrete time quantum walks on Cayley graphs, where the quantum coin was allowed to transform along with the initial state. We constructed a general way of obtaining transformations which preserve the measurement probabilities, and our results grant that we obtained the complete set of such transformations in a uniform manner. We described the symmetry group of the quantum walk time evolution operator using the results of the analysis.

Some of the symmetries found this way correspond to trivial properties of any discrete time quantum system, but most of the symmetries are specific to quantum walks. Once the symmetry group is found, any continuous symmetry can be used to reduce the problem. We have demonstrated this fact on the quantum walk on a line with a constant coin, where the result was that two out of three physical parameters of the quantum coin could be dropped without loss of generality. Quantum walks on more complicated graphs allow even more significant reduction.

An open question is how the results change if we drop the condition that the Cayley graph is nonseparating. An example where this condition is not held is a quantum walk on any group which contains the free group of order 2 or higher. Counterexamples to the forms provided by Theorem 3 can be found for such graphs, indicating that a more general treatment is necessary to cover all Cayley graphs.

However, the most important open question, which could be addressed in a subsequent work, is how the results change if the definition of a quantum walk is generalized such that the dimension of the coin space is different from the out-degree of the Cayley graph.

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[10] We note that the above definition of a step operation on the Hilbert space $\mathcal{H}$ is not the only possible one; as shown in [9], the concept of quantum coin can be altered so that the basis coin states do not imply the transition over individual edges from the vertex $x$ in a one-to-one manner. Throughout the text, however, we will stay with Definition 4.
[11] Consider, for example, a free group over three generators, $a$, $b$, and $c$. The elements are uniquely described by words in the alphabet $A = \{a, b, c, a^{-1}, b^{-1}, c^{-1}\}$. Define a map $A^* \rightarrow A^*$ which substitutes $b$ for $c$ and vice versa for words beginning with an $a$ and leaves all other words intact. Such a map induces a graph automorphism of the Cayley graph but is not a group automorphism itself.