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Path-sum solution of the Weyl quantum walk in 3 + 1 dimensions

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We consider the Weyl quantum walk in 3 + 1 dimensions, that is a discrete-time walk describing a particle with two internal degrees of freedom moving on a Cayley graph of the group $\mathbb{Z}^3$, which in an appropriate regime evolves according to Weyl's equation. The Weyl quantum walk was recently derived as the unique unitary evolution on a Cayley graph of $\mathbb{Z}^3$ that is homogeneous and isotropic. The general solution of the quantum walk evolution is provided here in the position representation, by the analytical expression of the propagator, i.e. transition amplitude from a node of the graph to another node in a finite number of steps. The quantum nature of the walk manifests itself in the interference of the paths on the graph joining the given nodes. The solution is based on the binary encoding of the admissible paths on the graph and on the semigroup structure of the walk transition matrices.

This article is part of the themed issue 'Second quantum revolution: foundational questions'.

1. Introduction

Quantum walks (QWs) were originally introduced as the quantum analogue of classical random walks or Markov chains [1]. A discrete-time QW [2–4] describes a quantum particle jumping on a graph in discrete time steps, the 'direction' of the jumping being conditioned on the internal state of the particle. The latter is represented in a finite-dimensional Hilbert space—the *coin* space—while the Hilbert space associated with the positions on the lattice is generally infinite dimensional. The total Hilbert space of the walk is the tensor product of the above ones.

Since their first appearance, QWs have received an increasing attention in the literature, where their main

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application is the design of quantum algorithms [5–8]. As an example, efficient search algorithms [6,9,10] were devised exploiting the fact that the spread of a localized initial state after t steps is proportional to t, whereas for the classical random walk the spread is proportional to $\sqrt{t}$. Remarkably, any quantum circuit can be implemented as a QW on a graph, proving that QWs can be used for universal quantum computation [11].

Recently, in [12], the authors use QWs in a derivation of quantum field theory from principles, from which it follows that the graph of the QW is the *Cayley graph* of a finitely presented group G. The QWs reproducing free quantum field theory in Euclidean space correspond to group $G=\mathbb{Z}^d$ that is Abelian, which is the most common case in the literature. In particular, the simplest QW descending from the principles is the Weyl QW [12], reproducing the Weyl quantum field theory. The QW approach to quantum field theory has been successfully used in [12–20], where non-interacting field theories are studied in a simplified picture in terms of QWs.

In §2, we review the definition of QWs on Cayley graphs. In §3, we introduce the Weyl QW and solve its path-sum on the body-centred cubic (BCC), three-dimensional lattice.

2. Path-sum approach for quantum walks on Cayley graphs

In this section, we review the notion of a QW, focusing on the underlying graph structure, which for QWs representing a homogeneous dynamics is the Cayley graph of some group.

(a) Quantum walks on Cayley graphs

Every group can be described in terms of a set of generators. For example, the group S_n of permutations of n objects $\{1,2,\dots,n\}$ is generated by transpositions T_{ij}, namely those permutations that exchange the elements i and j and leave every other element untouched. Every permutation in S_n can be decomposed as a finite sequence of transpositions.

If the generators are viewed as an alphabet, each word over the alphabet is associated with an element of the group, and vice versa; given an element of the group, we can always find a word over the alphabet expressing the group element. To set the terminology, following [21], we define an alphabet as any non-empty set Σ, and a word over the alphabet Σ as a map $w\colon \{1,2,\dots,n\}\to\Sigma$, for some non-negative integer n. The length of a word $w\colon\{1,2,\dots,n\}\to\Sigma$ is $|w|:=l(w):=n$, and for $n=0$ there is a unique word denoted ε, called the *empty word* for the alphabet Σ. The set of finite strings over Σ, denoted by $\Sigma^\star$, is equipped with the associative operation of string concatenation, with ε as its unit.

We now come back to the idea of treating a set of generators of a group as an alphabet and make it more rigorous. We first introduce the set S^{-1} of formal inverses of S, and we say that a *word over* S is a word over the alphabet $S\cup S^{-1}$. When we consider a word over S, it may happen that the word contains, for example, the substring xx^{-1} for $x\in S$. In this case, clearly, xx^{-1} can be substituted by the empty string ε, thus shortening the length of the word by two, and the group element expressed by the shorter word is the same as the one expressed by the initial one. A word is called *reduced* if it does not contain substrings of the form xx^{-1}, with x in $S\cup S^{-1}$, i.e. it cannot be shortened further by the simplification rule above. The set of all reduced words $F(S)$ can be given a group structure where the group operation is represented by word juxtaposition, the unit is ε, and the inverse of a word w is the word consisting of the inverses of the symbols of w juxtaposed in the reverse order. The group $F(S)$ is called the *free group over the alphabet* S.

However, the free group $F(S)$ might be larger than the group that we are willing to present. For example, for the Abelian group $\mathbb{Z}^2$, one can choose two generators $S=\{a,b\}$. In this case, the two reduced words $aabb$ and $abab$ denote the same group element. In order to complete the presentation of the group, one then has to specify, besides the trivial simplification $xx^{-1}\mapsto\varepsilon$, a minimal set of rules that allow one to identify words expressing the same group element. These rules come as a set R of words that amount to the group identity e.

Any group G has then a presentation $\langle S|R\rangle$—S being a set of generators and R a subset of $F(S)$, whose elements are called *relators*. The group G with presentation $\langle S|R\rangle$ is the group isomorphic

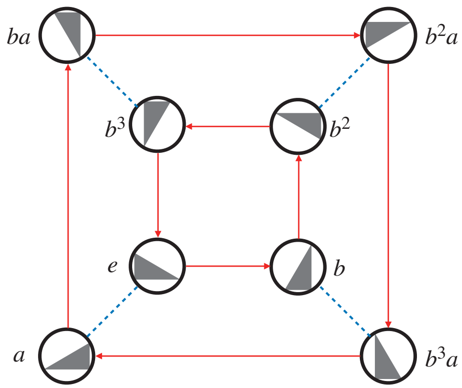

Figure 1. The Cayley graph of the dihedral group $D_4 = \langle a, b | a^2, b^4, abab \rangle$. The solid arrows represent b, while the dotted lines represent a. Note that a is represented without arrow heads because $a = a^{-1}$.

to $F(S)/\langle R^{F(S)} \rangle$, where $\langle R^{F(S)} \rangle$ denotes the normal closure[1] of R in $F(S)$. Knowing a presentation $\langle S|R \rangle$ of a group, we can give a graphical representation of it, called a Cayley graph, capturing both its algebraic and geometric properties. We have the following definition.

Definition 2.1 (Cayley graph). Let G be a group and let $\langle S|R \rangle$ be a presentation of G. Then, the *Cayley graph of G* corresponding to the presentation $\langle S|R \rangle$, denoted $\Gamma(G, S)$, is the coloured directed graph $(G, E, \{c_h\}_{h \in S})$ such that the vertex set is G, the edge set is $E = \{(g, gh) \mid g \in G,\ h \in S\}$ and each $h \in S$ has an associated colour c_h.

As an example, in figure 1, we show the Cayley graph of the dihedral group D_4 on generators $S = \{a, b\}$, with relators $R = \{a^2, b^4, abab\}$.

We are interested in a discrete unitary evolution over such a graph. Formally, we have the following definition.

Definition 2.2 (quantum walk). Let V be a countable set, then a (discrete-time) QW on V is a local unitary operator W on the Hilbert space $\mathcal{H} = \ell^2(V) \otimes \mathbb{C}^s$, namely a unitary operator W such that there exists $k \in \mathbb{N}$ and

$$|\mathcal{N}_x| \leq k, \tag{2.1}$$

where the neighbourhood $\mathcal{N}_x$ of $x \in V$ is defined as the set

$$\mathcal{N}_x := \{y \in V \mid \exists \psi, \varphi \in \mathbb{C}^s, \langle y|\langle \psi|W|x\rangle|\varphi\rangle \neq 0 \vee \langle x|\langle \psi|W|y\rangle|\varphi\rangle \neq 0\}, \tag{2.2}$$

and $\{|x\rangle\}_{x \in V}$ is the canonical orthonormal basis in $\ell^2(V)$.

In this context, a QW on the set V can be specified providing the map $\mathcal{E}\colon V \times V \to \mathcal{M}_s(\mathbb{C})$ associating with each pair of sites (x, y) a $s \times s$-complex matrix, called *transition matrix* and representing the transition amplitude from x to y: in terms of the walk operator W, the map $\mathcal{E}$ can be defined as $\mathcal{E}(x, y) := \langle y|W|x\rangle$. The unitarity requirement in terms of transition matrices amounts to

$$\sum_{z \in V} \mathcal{E}(z, x)\mathcal{E}(z, y)^\dagger = \sum_{z \in V} \mathcal{E}(x, z)^\dagger \mathcal{E}(y, z) = \delta_{xy} I_s, \tag{2.3}$$

where I_s denotes the identity on $\mathbb{C}^s$. The locality constraint, on the other hand, becomes

$$\forall\, x \in V, \quad |\{y \in V | \mathcal{E}(x, y) \neq 0 \vee \mathcal{E}(y, x) \neq 0\}| \leq k. \tag{2.4}$$

[1]The normal closure $\langle R^G \rangle$ of a set R in a group G is the subgroup generated by gRg^{-1} with $g \in G$.

Furthermore, a sequence $\psi\colon \mathbb{N} \to \mathcal{H}$ is a solution of the QW W if it satisfies the following update rule for a given initial condition $\psi(0) \in \mathcal{H}$:

$$|\psi_x(t+1)\rangle = \sum_{y\in V} \mathcal{E}(y,x)|\psi_y(t)\rangle, \quad \forall x \in V, \forall t \in \mathbb{N}, \tag{2.5}$$

where $|\psi_x(t)\rangle \in \mathbb{C}^s$ is defined in such a way that $|\psi(t)\rangle = \sum_{x\in V} |x\rangle|\psi_x(t)\rangle$.

A QW W carries a natural graph structure defined by the non-null transition matrices, namely the directed graph (V, E) where V is the vertex set and E is the set of edges, $E = \{(x, y) \in V \times V | \mathcal{E}(x, y) \neq 0\}$. It has been shown [12] that the assumption of *homogeneity* of the QW W—i.e. the vertices cannot be distinguished by the walk dynamics—entails that the underlying graph is actually the Cayley graph $\Gamma(G, S)$ of a group G. The group G acts on $\ell^2(G)$ by means of the right-regular representation $g \mapsto T_g$ as $T_g|f\rangle := |fg^{-1}\rangle$. The homogeneity condition also entails that the transition matrices are independent of the location: $\mathcal{E}(gh, g) = \mathcal{E}(g'h, g')$, $\forall g, g' \in G$ and $\forall h \in S$, allowing the choice $\mathcal{E}(gh, g) = A_h \in \mathcal{M}_s(\mathbb{C})$. Hence, the walk operator W can be written as

$$W = \sum_{h\in S} T_h \otimes A_h. \tag{2.6}$$

The scope of this paper is the study of the QW evolution in terms of a path-sum, recalling the Feynman formulation of quantum mechanics. Such an approach has been effective to obtain the exact analytic solution in position space in a number of cases [22–25], giving a background for possible generalizations of the method on general graphs. In the present work, we will review the method in the setting of Cayley graphs and we will present a solution for the Weyl QW.

(b) Quantum walk evolution as a path-sum

Let us consider now a QW whose transition matrices are given by the map $\mathcal{E}\colon V \times V \to \mathcal{M}_s(\mathbb{C})$ and whose associated graph is (V, E). From equation (2.5), one can readily write the evolution of a given initial configuration $|\psi(0)\rangle \in \mathcal{H}$ as a path-sum, which can be viewed as a discrete version of Feynman's path-integral [26,27]. The iteration of the one-step update rule (2.5) leads to an expression of the solution at time t in terms of the sum over all the paths σ of length t with fixed endpoints x' and x, that is $\sigma = (e_1, e_2, \ldots, e_t)$, where $e_i := (y_{i-1}, y_i)$ with the identifications $y_0 \equiv x'$ and $y_t \equiv x$. We denote the set of all such paths as $\Lambda_t(x', x)$, and $\mathcal{C}_t(x) := \{x' \in G | \Lambda_t(x', x) \neq \emptyset\}$ is the slice at time t of the past causal cone of x. In this way, the equation for the evolved state $|\psi_x(t)\rangle$ takes the form

$$|\psi_x(t)\rangle = \sum_{x'\in\mathcal{C}_t(x)} \sum_{\sigma\in\Lambda_t(x',x)} \mathcal{E}(e_t)\cdots\mathcal{E}(e_1)|\psi_{x'}(0)\rangle. \tag{2.7}$$

The situation of main interest for us is when the underlying graph of the walk is actually a Cayley graph $\Gamma(G, S)$. In such a case, the transition matrices depend only on the generators associated with the edges and, as before, we let $\mathcal{E}(xh, x) = A_h$. Note that a path σ is in $\Lambda_t(x', x)$ if and only if there exist $h_1, \ldots, h_t \in S$ such that $x'h_1 \cdots h_t = x$; therefore, we obtain the expression

$$|\psi_x(t)\rangle = \sum_{x'\in\mathcal{C}_t(x)} \sum_{h_1,\ldots,h_t\in S} \delta(x^{-1}x'h_1\cdots h_t)\mathcal{A}(h_1^{-1}, \ldots, h_t^{-1})|\psi_{x'}(0)\rangle, \tag{2.8}$$

where $\delta(x) = 1$ if $x = \varepsilon$ and 0 otherwise, ε being the identity element of G, and $\mathcal{A}(h_1, h_2, \ldots, h_t) = A_{h_t}A_{h_{t-1}}\cdots A_{h_1}$. The aim of this work is to provide an analytical expression for the propagator of the walk

$$\mathcal{K}(x, y; t) := \langle y|W^t|x\rangle = \sum_{h_1,\ldots,h_t\in S} \delta(y^{-1}xh_1\cdots h_t)\mathcal{A}(h_1^{-1}, \ldots, h_t^{-1}). \tag{2.9}$$

That is, we want to find an explicit expression for the transition amplitude from a site x to a site y in t time steps.

In the following section, we will present an application of the path-sum method in the specific case of the Weyl QW in $3 + 1$ dimensions deriving the solution in position space with the aid of a binary encoding of paths, an approach which has already proven its efficacy in the case of the Dirac QW in $1+1$ dimensions [24] and of the Weyl QW in $2+1$ dimensions [25].

3. Weyl quantum walk in 3 + 1 dimensions

In the following, we will use the vector notation to denote points $\mathbf{x} \in G = \mathbb{Z}^3$. The Weyl QW in $3+1$ dimensions, derived by D'Ariano & Perinotti [12], is a QW on the BCC lattice $\Gamma(G,S)$, where the vertex set can be chosen to be $G = 2\mathbb{Z}^3 \cup (2\mathbb{Z}^3 + (1,1,1))$ and the generators can be represented by the following vectors (and their inverses):

$$\mathbf{h}_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{h}_2 = \begin{pmatrix} 1 \\ -1 \\ -1 \end{pmatrix}, \quad \mathbf{h}_3 = \begin{pmatrix} -1 \\ 1 \\ -1 \end{pmatrix}, \quad \mathbf{h}_4 = \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix}. \tag{3.1}$$

The walk unitary operator is written as $W = \sum_{\mathbf{h}\in S} T_{\mathbf{h}} \otimes A_{\mathbf{h}}$, acting on $\ell^2(G) \otimes \mathbb{C}^2$, and the transition matrices are

$$\left.\begin{aligned}
A_{\mathbf{h}_1} &= \zeta^* \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, & A_{\mathbf{h}_{-1}} &= \zeta \begin{pmatrix} 0 & -1 \\ 0 & 1 \end{pmatrix}, \\
A_{\mathbf{h}_2} &= \zeta^* \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}, & A_{\mathbf{h}_{-2}} &= \zeta \begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix}, \\
A_{\mathbf{h}_3} &= \zeta^* \begin{pmatrix} 0 & -1 \\ 0 & 1 \end{pmatrix}, & A_{\mathbf{h}_{-3}} &= \zeta \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, \\
A_{\mathbf{h}_4} &= \zeta^* \begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix}, & A_{\mathbf{h}_{-4}} &= \zeta \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix},
\end{aligned}\right\} \tag{3.2}$$

with $\zeta = (1 \pm \mathrm{i})/4$ and $\mathbf{h}_{-l} = -\mathbf{h}_l$. The two possible choices for the coefficient ζ correspond to the two inequivalent QW solutions existing on the BCC lattice [12].

The intent of this paper is to provide an explicit expression for the propagator given in terms of sums over paths. To this end, it turns out to be very effective to adopt a binary description of paths, which amounts to finding a three-bits binary encoding $b_1b_2b_3$ for the generators. A suitable choice that simplifies the evaluation of the contribution to the transition amplitude of each path is given by

$$\left.\begin{aligned}
&\mathbf{h}_1\colon 011, \quad \mathbf{h}_2\colon 110, \quad \mathbf{h}_3\colon 101, \quad \mathbf{h}_4\colon 000, \\
&\mathbf{h}_{-1}\colon 100, \quad \mathbf{h}_{-2}\colon 001, \quad \mathbf{h}_{-3}\colon 010, \quad \mathbf{h}_{-4}\colon 111.
\end{aligned}\right\} \tag{3.3}$$

This choice is tantamount to the requirement

$$\tilde{A}_{b_1b_2b_3} = (\pm\mathrm{i})^{b_1 \oplus b_2 \oplus b_3} B_{b_1b_2}, \quad \tilde{A}_{b_1b_2b_3} := (\zeta^*)^{-1} A_{b_1b_2b_3}, \tag{3.4}$$

where $\oplus$ denotes the sum modulo 2 and $B_{b_1b_2}$ are the matrices

$$\left.\begin{aligned}
B_{00} &= \begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix}, & B_{10} &= \begin{pmatrix} 0 & -1 \\ 0 & 1 \end{pmatrix}, \\
B_{01} &= \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, & B_{11} &= \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix},
\end{aligned}\right\} \tag{3.5}$$

satisfying the product rule given by

$$B_{ab}B_{cd} = (-1)^{(c\oplus a)\cdot(d\oplus b)} B_{cb}, \tag{3.6}$$

where the notation $a \cdot b$ denotes the binary product of the two bits a and b; throughout this paper, all the bit operations are also extended element-wise to binary strings. One can note from equation (3.6) that the matrices $\tilde{A}_{b_1b_2b_3}$ generate, up to phases, a finite semigroup. The general product of t transition matrices is then given by

$$\begin{aligned}\tilde{A}\left(w^{(1)},w^{(2)},w^{(3)}\right) &:= \tilde{A}_{w_t^{(1)}w_t^{(2)}w_t^{(3)}}\cdots\tilde{A}_{w_1^{(1)}w_1^{(2)}w_1^{(3)}}\\ &= (-1)^{\iota((w^{(1)}\oplus Sw^{(1)})\cdot w^{(2)})}(\pm \mathrm{i})^{\iota(w^{(1)}\oplus w^{(2)}\oplus w^{(3)})}B_{w_1^{(1)}w_t^{(2)}},\end{aligned} \tag{3.7}$$

where $w^{(j)}\in\mathfrak{B}_t$ is the string made of the jth bits of the encoding equation (3.3), $\mathfrak{B}_t$ being the set of all binary strings of length t. Here, w_k denotes the kth bit of the string w. Finally, we introduced the function $\iota(w) := \sum_{k=1}^{|w|} w_k$ counting the number of 1-bits present in the string w and the left circular shift S defined by $(Sw)_i = w_{(i \bmod t)+1}$, for all $i = 1,\ldots,t$.

At this point, we need a characterization of the lattice paths in terms of their binary description. As shown in appendix A, the number of 1-bits in each one of the encoding strings $w^{(j)}\in\mathfrak{B}_t$ is fixed by the starting point $\mathbf{x}'$ and by the ending point $\mathbf{x}$ via the equations

$$\left.\begin{aligned}\iota(w^{(1)}) &= \frac{t-(x^3-x'^3)}{2},\\ \iota(w^{(2)}) &= \frac{t+(x^1-x'^1)}{2}\\ \text{and}\qquad \iota(w^{(3)}) &= \frac{t+(x^2-x'^2)}{2}.\end{aligned}\right\} \tag{3.8}$$

It is then convenient to define a special notation for the set of tuples of strings with a fixed number of 1-bits, which are indeed in bijective correspondence with paths connecting $\mathbf{x}'$ to $\mathbf{x}$ in t steps:

$$\mathfrak{S}_t^n(K_1,\ldots,K_n) := \{(w^{(1)},\ldots,w^{(n)})\in\mathfrak{B}_t^n \,|\, \iota(w^{(i)}) = K_i,\ \forall i = 1,\ldots,n\} \tag{3.9}$$

$$= \mathfrak{S}_t(K_1)\times\cdots\times\mathfrak{S}_t(K_n), \tag{3.10}$$

assuming for short $\mathfrak{S}_t(K)\equiv\mathfrak{S}_t^t(K)$. Thus, the path-sum of equation (2.8) can be rewritten as

$$|\psi_{\mathbf{x}}(t)\rangle = \zeta^{*t}\sum_{\mathbf{x}'\in\mathcal{C}_t(\mathbf{x})}\ \sum_{\mathbf{w}\in\mathfrak{S}_t^3(K_1,K_2,K_3)}\tilde{A}(\mathbf{w})|\psi_{\mathbf{x}'}(0)\rangle, \tag{3.11}$$

where $K_1 = (t+(x^3-x'^3))/2$, $K_2 = (t-(x^1-x'^1))/2$ and $K_3 = (t-(x^2-x'^2))/2$ (note that the signs here are consistent with equation (2.8) where the matrix associated to the step h is exactly $A_{h^{-1}}$). From equation (3.7), we see that the resulting matrix depends only on the first bit of $w^{(1)}$ and the last bit of $w^{(2)}$. Therefore, defining $\mathfrak{S}_{t,ab}^3(K_1,K_2,K_3)\subset\mathfrak{S}_t^3(K_1,K_2,K_3)$ as the subset of triads $(w^{(1)},w^{(2)},w^{(3)})$ with $w_1^{(1)} = a$ and $w_t^{(2)} = b$, we can rewrite equation (3.11) as

$$|\psi_{\mathbf{x}}(t)\rangle = \zeta^{*t}\sum_{\mathbf{x}'\in\mathcal{C}_t(\mathbf{x})}\ \sum_{a,b=0,1} c_{ab}B_{ab}|\psi_{\mathbf{x}'}(0)\rangle, \tag{3.12}$$

where the coefficients c_{ab} are defined by

$$c_{ab}(K_1,K_2,K_3) = \sum_{\mathbf{w}\in\mathfrak{S}_{t,ab}^3(K_1,K_2,K_3)}(-1)^{\iota((w^{(1)}\oplus Sw^{(1)})\cdot w^{(2)})}(\pm \mathrm{i})^{\iota(w^{(1)}\oplus w^{(2)}\oplus w^{(3)})}. \tag{3.13}$$

We seek now an explicit expression for the coefficients c_{ab}. As a first step, let us consider the sum $\sum_w(\pm \mathrm{i})^{\iota(v\oplus w)}$ alone with $\iota(w) = H$ for a given H and for some fixed $v\in\mathfrak{S}_t(K)$. In order to compute this sum, we have to classify the strings lying in the set $v\oplus\mathfrak{S}_t(H)$, according to the number of ones. It is convenient to define a canonical form for strings as follows.

Definition 3.1. We say that a binary string w is in *canonical form* if the following condition holds:

$$w_i \geq w_{i+1},\quad \forall\, i = 1,2,\ldots,|w|-1. \tag{3.14}$$

The computation of the coefficients c_{ab} in equation (3.13) is based on the next three results whose proofs are presented in appendix B.

Lemma 3.2. *Given $t, K, H \in \mathbb{N}$, with $K, H \leq t$, let $v \in \mathfrak{S}_t(K)$ be in canonical form, then we have*

$$v \oplus \mathfrak{S}_t(H) = \bigsqcup_{n \in I} \mathfrak{W}(K, H, n) \tag{3.15}$$

and

$$\mathfrak{W}(K, H, n) := \begin{cases} \mathfrak{S}_K(K - H + n)\mathfrak{S}_{t-K}(n), & \text{if } K \geq H, \\ \mathfrak{S}_K(n)\mathfrak{S}_{t-K}(H - K + n), & \text{otherwise}, \end{cases} \tag{3.16}$$

with $I = \{0, 1, \ldots, \min\{K, H, t - K, t - H\}\}$. Defining $r = \vartheta(K - H)$, ϑ being the Heaviside step function, and $\bar{r} = 1 - r$, the size of each subset is given by

$$|\mathfrak{W}(K, H, n)| = D(t, \bar{r}t + (-1)^{\bar{r}}H, rt + (-1)^r K, n), \tag{3.17}$$

$$D(t, p, m, n) = \begin{cases} \binom{m}{n}\binom{t-m}{p-n}, & \text{if } 0 \leq n \leq m \leq t \text{ and } n \leq p, \\ 0, & \text{otherwise}, \end{cases}$$

and for all $w \in \mathfrak{W}(K, H, n)$, the set-bit count is given by $\iota(w) = |K - H| + 2n$.

Corollary 3.3. *Given $t, K, H \in \mathbb{N}$, with $K, H \leq t$, for all $v \in \mathfrak{S}_t(K)$ and for any π_v bitwise permutation of $\mathfrak{B}_t$ such that $\pi_v(v)$ is in canonical form, the following decomposition holds:*

$$v \oplus \mathfrak{S}_t(H) = \bigsqcup_{n \in I} \pi_v^{-1}(\mathfrak{W}(K, H, n)), \tag{3.18}$$

with $I = \{0, 1, \ldots, \min\{K, H, t - K, t - H\}\}$ and moreover

$$\left.\begin{aligned} |\pi_v^{-1}(\mathfrak{W}(K, H, n))| &= |\mathfrak{W}(K, H, n)| \\ \text{and} \qquad \iota(\pi_v^{-1}(\mathfrak{W}(K, H, n))) &= \iota(\mathfrak{W}(K, H, n)). \end{aligned}\right\} \tag{3.19}$$

Proposition 3.4. *Given $t, K, H \in \mathbb{N}$, with $K, H \leq t$, for all $v \in \mathfrak{S}_t(K)$ we have that*

$$\sum_{w \in \mathfrak{S}_t(H)} (\pm \mathrm{i})^{\iota(v \oplus w)} = f(K, H), \tag{3.20}$$

where

$$f(K, H) := (\pm \mathrm{i})^{|K-H|} \sum_{n \in I} (-1)^n D(t, \bar{r}t + (-1)^{\bar{r}}H, rt + (-1)^r K, n),$$

with $I = \{0, 1, \ldots, \min\{K, H, t - K, t - H\}\}$.

The expression of the coefficients c_{ab} of equation (3.13) can now be written as

$$c_{ab}(K_1, K_2, K_3) = \sum_{w^{(1)}, w^{(2)}} (-1)^{\iota((w^{(1)} \oplus S w^{(1)}) \cdot w^{(2)})} f(\iota(w^{(1)} \oplus w^{(2)}), K_3), \tag{3.21}$$

where, at this point, the sum is performed over the set $\mathfrak{S}^2_{t,ab}(K_1, K_2)$. In order to ease the calculation, we can study separately the values of $\iota((w^{(1)} \oplus Sw^{(1)}) \cdot w^{(2)})$ and their interplay with $f(K, H)$. The combinatorics for $\iota((w^{(1)} \oplus Sw^{(1)}) \cdot w^{(2)})$ is the same as that of [25] and is here reviewed for the convenience of the reader. The idea is to find a classification of the binary strings in terms of the values taken by $\iota((w^{(1)} \oplus Sw^{(1)}) \cdot w^{(2)})$. We first focus on the classification induced by $w^{(1)} \oplus Sw^{(1)}$ and then, as the contributions to the result come only from the 1-bits of both $w^{(1)} \oplus Sw^{(1)}$ and $w^{(2)}$, we use $w^{(2)}$ to select a given number of 1-bits from $w^{(1)} \oplus Sw^{(1)}$.

The combinatorics induced by $w^{(1)} \oplus Sw^{(1)}$ is provided by the following lemma (proved in appendix B).

Lemma 3.5. *Let $v \in \mathfrak{S}_t(K)$. Then, $v \oplus Sv \in \pi_v^{-1}(\mathfrak{S}_K(n)\mathfrak{S}_{t-K}(n))$, for some $n \in \{0, 1, \ldots, \min\{K, t - K\}\}$.*

The above classification is not sufficient in our case, because the summation of equation (3.21) requires the strings $w^{(1)}$ and $w^{(2)}$ to have, respectively, the first and the last bit fixed. This means that we have to refine the counting taking into account such a constraint: we denote $\mathfrak{T}_{aa'}(t,K,n)$ the set of strings $v \in \mathfrak{S}_t(K)$ such that $v \oplus Sv \in \pi_v^{-1}(\mathfrak{S}_K(n)\mathfrak{S}_{t-K}(n))$ with $v_1 = a$ and $v_t = a'$. The following lemma (also proved in appendix B) concludes the counting for strings with fixed endpoints.

Lemma 3.6. *The number $u_{aa'}(n)$ of binary strings $v \in \mathfrak{T}_{aa'}(t,K,n)$ is given by*

$$u_{aa'}(n) := |\mathfrak{T}_{aa'}(t,K,n)| = C_{K,n+aa'}C_{t-K,n+\bar{a}\bar{a}'}, \tag{3.22}$$

with $n_{\min}(K) \le n \le n_{\max}(K)$ and $n_{\min}(K) := \min\{1, K, t-K\}$,

$$n_{\max}(K) := \begin{cases} \min\{K - aa', t - K - 1 + aa'\}, & \text{if } 1 < K < t-1, \\ 1, & \text{if } K = 1 \text{ or } K = t-1, \\ 0, & \text{otherwise.} \end{cases} \tag{3.23}$$

Finally, we can focus on the joint classification given by the values of $\iota((v \oplus Sv) \cdot w)$ and of $\iota(v \oplus w)$. The final expression of the coefficients c_{ab} is summarized by the following proposition, whose proof is reported in appendix B.

Proposition 3.7. *For $t \ge 2$, the coefficients of equation (3.21) take the form*

$$c_{ab}(K_1,K_2,K_3) = \sum_{a'=0,1}\ \sum_{n=n_{\min}(K_1)}^{n_{\max}(K_1)}\ \sum_{J=b}^{K_2} u_{aa'}(n) w^{(0)}_{aa'b}(n,J) w^{(1)}_{aa'b}(n,J) f(\tau_J, K_3), \tag{3.24}$$

where, defining $r = \vartheta(K_1 - K_2)$, we have that $\tau_J = |K_1 - K_2| + 2J$, and

$$\left.\begin{aligned} w^{(s)}_{aa'b}(n,J) &= \sum_{k=0}^{n-\gamma^{(s)}_{aa'}} (-1)^{k+\gamma^{(s)}_{aa'}b} D(\eta^{(s)}_{a'}, \kappa^{(s)}_{a'b}(J), n - \gamma^{(s)}_{aa'}, k), \\ \kappa^{(s)}_{a'b}(J) &= (r \oplus \bar{s})K_2 + (-1)^{\bar{s}}(\bar{r}K_1 - J) - (\bar{s} \oplus a')b \\ \text{and} \qquad \eta^{(s)}_{a'} &= \bar{s}(t-1) + (-1)^{\bar{s}}(K_1 - a'), \quad \gamma^{(s)}_{aa'} = (s \oplus a)(\bar{s} \oplus a'). \end{aligned}\right\} \tag{3.25}$$

As a concluding remark of this section, we point out that, thanks to the binary encoding of paths, the counting is largely simplified, providing a powerful tool working in the general case.

4. Conclusion

In this paper, we provided an explicit analytical solution in position space of the propagator for the Weyl QW in $3+1$ dimensions. The method used here to analytically compute the Weyl QW path-sum is grounded on

(i) a combinatorial analysis for the characterization of the admissible paths connecting two fixed sites of the graph in a given number of steps and
(ii) the semigroup structure of the walk transition matrixes.

The semigroup structure allows us to classify the admissible paths (or binary strings according to the first point) into equivalence classes according to the global transition matrix of the path. To aid the calculation, we adopted here an extremely powerful approach consisting of the translation of the geometric properties of lattice paths into algebraic properties of binary strings. Such binary description of paths was also successful in the case of the Dirac QW in $1+1$ dimensions [24] and of the Weyl QW in $2+1$ dimensions [25]. In all these cases, the practical computation of the propagator relies on the semigroup property of the transition matrices which allows one to determine all the paths contributing with the same matrix.

As a future perspective, we propose the possibility to investigate such semigroup property of the transition matrices in the general non-Abelian case. It would also be interesting to derive the general hypotheses in the framework of QWs on Cayley graphs for which the semigroup structure is recovered.

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Appendix A. Relationship between lattice points and binary strings

The approach we follow here requires to find a binary description of paths: we provided such description by choosing a suitable binary encoding in equation (3.3) which also simplifies the evaluation of functions involving products of matrices giving the general formula of equation (3.7). Then, we also need to obtain a criterion telling us which paths have the same endpoints $\mathbf{x}'$ and $\mathbf{x}$; in order to do so, we employ the fact that the BCC lattice is Abelian: each path is described by a quadruple $(n_{\pm 1}, n_{\pm 2}, n_{\pm 3}, n_{\pm 4})$, where $n_{\pm l}$ counts the number of steps in direction $\mathbf{h}_{\pm l}$ and thus each path must satisfy the system

$$\left.\begin{aligned}&\sum_l (n_l - n_{-l}) h_l^i = x^i - x'^i\\ \text{and}\qquad &\sum_l (n_l + n_{-l}) = t.\end{aligned}\right\} \tag{A 1}$$

The binary encoding and the quadruple $(n_{\pm 1}, n_{\pm 2}, n_{\pm 3}, n_{\pm 4})$ are then related by the following constraints:

$$\left.\begin{aligned}&\iota(w^{(1)}) = n_{-1} + n_2 + n_3 + n_{-4},\\ &\iota(w^{(2)}) = n_1 + n_2 + n_{-3} + n_{-4}\\ \text{and}\qquad &\iota(w^{(3)}) = n_1 + n_3 + n_{-2} + n_{-4},\end{aligned}\right\} \tag{A 2}$$

where $\iota(w) := \sum_{k=1}^{|w|} w_k$ denotes the set-bit count of the string w. The relation we seek can be easily obtained by defining the number of steps in the positive- and negative-coordinate direction

$$x_+^i := \sum_l [\vartheta(h_l^i) n_l + \vartheta(h_{-l}^i) n_{-l}] \tag{A 3}$$

and

$$x_-^i := \sum_l [\vartheta(-h_l^i) n_l + \vartheta(-h_{-l}^i) n_{-l}], \tag{A 4}$$

ϑ being the Heaviside step function; then, for each i, it holds that

$$\left.\begin{aligned}&x_+^i + x_-^i = t\\ \text{and}\qquad &x_+^i - x_-^i = x^i - x'^i.\end{aligned}\right\} \tag{A 5}$$

Therefore, the set-bit counts of equation (A 2) are fixed by the coordinates through the equations

$$\left.\begin{aligned}&\iota(w^{(1)}) = x_-^3 = \frac{t - (x^3 - x'^3)}{2},\\ &\iota(w^{(2)}) = x_+^1 = \frac{t + (x^1 - x'^1)}{2}\\ \text{and}\qquad &\iota(w^{(3)}) = x_+^2 = \frac{t + (x^2 - x'^2)}{2}.\end{aligned}\right\} \tag{A 6}$$

Appendix B. Proofs of the results

Proof of lemma 3.2. Suppose for definiteness that $K \geq H$. Given a string $w \in \mathfrak{S}_t(H)$, we can define the two substrings $(L_K w)_i = w_i$, for $i = 1, \ldots, K$, and $(R_K w)_i = w_{K+i}$, for $i = 1, \ldots, t-K$: we have that $L_K w \in \mathfrak{S}_K(H-n)$, $R_K w \in \mathfrak{S}_{t-K}(n)$ and $w \in \mathfrak{S}_K(H-n)\mathfrak{S}_{t-K}(n)$. Here for A and B sets of strings, the set AB is formed by concatenating the elements of A and B. Moreover, if $n \neq m$, then $\mathfrak{S}_K(n) \cap \mathfrak{S}_K(m) = \emptyset$, which entails that the products $\mathfrak{S}_K(H-n)\mathfrak{S}_{t-K}(n)$ form a partition of $\mathfrak{S}_t(H)$, with $n \in I = \{0, 1, \ldots, \min\{H, t-K\}\}$:

$$\mathfrak{S}_t(H) = \bigsqcup_{n \in I} \mathfrak{S}_K(H-n)\mathfrak{S}_{t-K}(n). \tag{B 1}$$

Thus, the set $v \oplus \mathfrak{S}_t(H)$ decomposes as

$$v \oplus \mathfrak{S}_t(H) = \bigsqcup_{n \in I} v \oplus [\mathfrak{S}_K(H-n)\mathfrak{S}_{t-K}(n)] \tag{B 2}$$

$$= \bigsqcup_{n \in I} [L_K v \oplus \mathfrak{S}_K(H-n)][R_K v \oplus \mathfrak{S}_{t-K}(n)] \tag{B 3}$$

$$= \bigsqcup_{n \in I} \mathfrak{S}_K(K-H+n)\mathfrak{S}_{t-K}(n) \tag{B 4}$$

$$= \bigsqcup_{n \in I} \mathfrak{W}(K, H, n), \tag{B 5}$$

where in the third equation we have made use of the fact that v is in canonical form. The set-bit count of $w \in \mathfrak{W}(K, H, n)$ can be straightforwardly computed:

$$\iota(w) = \iota(L_K w) + \iota(R_K w) = K - H + 2n. \tag{B 6}$$

Finally, one can easily obtain the size of each factor:

$$|\mathfrak{W}(K, H, n)| = |\mathfrak{S}_K(K-H+n)\mathfrak{S}_{t-K}(n)| \tag{B 7}$$

$$= |\mathfrak{S}_K(K-H+n)| \cdot |\mathfrak{S}_{t-K}(n)| \tag{B 8}$$

$$= \binom{K}{H-n}\binom{t-K}{n}. \tag{B 9}$$

The case $K < H$ follows from a similar reasoning and we have the sought result. ■

Proof of corollary 3.3. Let $v \in \mathfrak{S}_t(K)$ and let π_v be a bitwise permutation such that $\pi_v(v)$ is canonical, then we have that

$$\pi_v(v \oplus \mathfrak{S}_t(H)) = \pi_v(v) \oplus \pi_v(\mathfrak{S}_t(H)) \tag{B 10}$$

$$= \pi_v(v) \oplus \mathfrak{S}_t(H). \tag{B 11}$$

Therefore, using the decomposition of lemma 3.2, we can write

$$v \oplus \mathfrak{S}_t(H) = \pi_v^{-1}\left(\bigsqcup_{n \in I} \mathfrak{W}(K, H, n)\right) \tag{B 12}$$

$$= \bigsqcup_{n \in I} \pi_v^{-1}(\mathfrak{W}(K, H, n)).$$

■

Proof of proposition 3.4. Suppose that $K \geq H$ and let $v \in \mathfrak{S}_t(K)$, $w \in \mathfrak{S}_t(H)$. From corollary 3.3, we know that $v \oplus w \in \pi_v^{-1}(\mathfrak{W}(K, H, n))$, for some $n \in I = \{0, 1, \ldots, \min\{H, t-K\}\}$, and $\iota(v \oplus w) = K -$

$H + 2n$. Therefore, we can compute the sum of equation (3.20), obtaining finally the result:

$$\sum_{w\in\mathfrak{S}_t(H)} (\pm \mathrm{i})^{\iota(v\oplus w)} = \sum_{n=0}^{\min\{H,t-K\}} \sum_{w\in\pi_v^{-1}(\mathfrak{W}(K,H,n))} (\pm\mathrm{i})^{\iota(w)} \tag{B 13}$$

$$= \sum_{n=0}^{\min\{H,t-K\}} |\mathfrak{W}(K,H,n)|\,(\pm\mathrm{i})^{K-H+2n} \tag{B 14}$$

$$= (\pm\mathrm{i})^{K-H} \sum_{n=0}^{\min\{H,t-K\}} (-1)^n \binom{K}{H-n}\binom{t-K}{n}.$$

■

Proof of lemma 3.5. Let $v \in \mathfrak{S}_t(K)$. From lemma 3.2 and corollary 3.3, we know that $v \oplus Sv \in \mathfrak{S}_t(2n)$, for some $n \in \{0, 1, \ldots, \min\{K, t-K\}\}$. We can split the string $\pi_v(v \oplus Sv) =: c \oplus \pi_v Sv$ as

$$L_K(c \oplus \pi_v Sv) = L_K c \oplus L_K \pi_v Sv = \overline{L_K \pi_v Sv} \tag{B 15}$$

and

$$R_K(c \oplus \pi_v Sv) = R_K c \oplus R_K \pi_v Sv = R_K \pi_v Sv. \tag{B 16}$$

Given that

$$\iota(L_K \pi_v Sv) + \iota(R_K \pi_v Sv) = \iota(v) = K, \tag{B 17}$$

the set-bit count of $c \oplus \pi_v Sv$ then reads

$$\begin{aligned}\iota(c \oplus \pi_v Sv) &= \iota(\overline{L_K \pi_v Sv}) + \iota(R_K \pi_v Sv)\\ &= 2K - 2\iota(L_K \pi_v Sv).\end{aligned} \tag{B 18}$$

Therefore, as $\iota(c \oplus \pi_v Sv) = 2n$, we have precisely

$$\iota(\overline{L_K \pi_v Sv}) = \iota(R_K \pi_v Sv) = n$$

and the result follows. ■

Proof of lemma 3.6. A string in $\mathfrak{T}_{aa'}(t, K, n)$ can be constructed by first arranging the K 1-bits in $n + aa'$ slots and then by arranging the $t - K$ 0-bits in $n + \bar{a}\bar{a}'$ slots; the problem is then the same as counting the number of compositions of an integer [28]. We denote here as $C_{K,n}$ the number of n-compositions of an integer K:

$$C_{K,n} = \begin{cases} \binom{K-1}{n-1}, & \text{if } K \geq n > 0,\\ 1, & \text{if } K = n = 0,\\ 0, & \text{otherwise.}\end{cases} \tag{B 19}$$

As the $n + aa'$ slots can be filled independently from the $n + \bar{a}\bar{a}'$ ones, the cardinality of $\mathfrak{T}_{aa'}(t, K, n)$ is simply given by the product

$$u_{aa'}(n) := |\mathfrak{T}_{aa'}(t, K, n)| = C_{K,n+aa'} C_{t-K,n+\bar{a}\bar{a}'}. \tag{B 20}$$

■

Proof of proposition 3.7. Let us consider the case where $K_1 \geq K_2$ as the other one is a simple variation of the following construction. First of all, recall the expression for the coefficients (3.21), implementing the result of proposition 3.4:

$$c_{ab} = \sum_{v,v'} (-1)^{\iota((v\oplus Sv)\cdot v')} f(\iota(v\oplus v'), K_3) \tag{B 21}$$

$$= \sum_{a'=0,1} \sum_{n=n_{\min}(K_1)}^{n_{\max}(K_1)} \sum_{v_n} \sum_{w} (-1)^{\iota((av_na'\oplus v_na'a)\cdot wb)} f(\iota(av_na'\oplus wb), K_3), \tag{B 22}$$

where $av_na' \in \mathfrak{T}_{aa'}(t, K_1, n)$ and $w \in \mathfrak{S}_{t-1}(K_2 - b)$. For ease of discussion, we consider from now on the case where $a = a' = 0$, as the others can be treated in a very similar way.

We already know that the sum modulo 2 of a pair of strings $0v_n0$ and wb can be parametrized as $\iota(0v_n0 \oplus wb) = |K_1 - K_2| + 2J$ for some J; yet, we need to find a finer classification taking into account the values of $\iota((0v_n0 \oplus v_n00)\cdot wb)$, for each fixed v_n. To such end, we consider the partition

$$\mathfrak{S}_{t-1}(K_2 - b) = \bigsqcup_{J=b}^{\min\{K_2, t-K_1-1\}} \bigsqcup_{k=0}^{n} \bigsqcup_{k'=0}^{n} \mathfrak{Z}_b^{(1)}(J,k)\mathfrak{Z}_b^{(0)}(J,k'),$$

$$\mathfrak{Z}_b^{(1)}(J,k) = \mathfrak{S}_n(k)\mathfrak{S}_{K_1-n}(K_2 - J - k) \tag{B 23}$$

and

$$\mathfrak{Z}_b^{(0)}(J,k') = \mathfrak{S}_n(k')\mathfrak{S}_{t-K_1-n-1}(J - k' - b); \tag{B 24}$$

this particular construction corresponds to choosing as reference strings

$$p_L = \underbrace{11\cdots1}_{n}\underbrace{00\cdots0}_{K_1-n}, \quad p_R = \underbrace{11\cdots1}_{n}\ \underbrace{00\cdots0}_{t-K_1-n-1}, \tag{B 25}$$

where the text under braces denotes the length of the substring.

As $\mathfrak{S}_t(K_2)$ can be constructed by concatenating strings picked from the sets $\mathfrak{Z}_b^{(1)}(J,k)$ and $\mathfrak{Z}_b^{(0)}(J,k')$, we can study separately the binary product and binary sum on them. Multiplying p_L and p_R with $\mathfrak{Z}_b^{(1)}(J,k)$ and $\mathfrak{Z}_b^{(0)}(J,k')$, respectively, we obtain

$$p_L\cdot \mathfrak{Z}_b^{(1)}(J,k) = \mathfrak{S}_n(k)\underbrace{00\cdots0}_{K_1-n}, \tag{B 26}$$

$$p_R\cdot \mathfrak{Z}_b^{(0)}(J,k') = \mathfrak{S}_n(k')\ \underbrace{00\cdots0}_{t-K_1-n-1} \tag{B 27}$$

and

$$\iota((p_Lp_R)\cdot w) = k + k', \tag{B 28}$$

for all $w \in \mathfrak{Z}_b^{(1)}(J,k)\mathfrak{Z}_b^{(0)}(J,k')$, whereas for the binary sum, we get

$$\iota\left(\underbrace{11\cdots1}_{K_1}\oplus \mathfrak{Z}_b^{(1)}(J,k)\right) = K_1 - K_2 + J, \quad \iota(\mathfrak{Z}_b^{(0)}(J,k')) = J - b. \tag{B 29}$$

In conclusion, the total number of ones for the sum modulo 2 turns out to be

$$\iota([\pi_{t-2}(v_n)00] \oplus [\mathfrak{Z}_b^{(1)}(J,k)\mathfrak{Z}_b^{(0)}(J,k')b]) = K_1 - K_2 + 2J, \tag{B 30}$$

which corresponds to the parameter τ_J of the statement of the proposition. Furthermore, as $f(\iota(0v_n0 \oplus wb), K_3)$ does not depend on k or k', we can sum separately over the strings in equations (B 24) and (B 23) obtaining the function $w^{(s)}_{00b}$ of equation (3.25):

$$w^{(s)}_{00b}(n, J) = \sum_{k=0}^{n} (-1)^k |\mathfrak{Z}^{(s)}_b(J, k)|. \tag{B 31}$$

■

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