POLYANDER VISUALIZATION OF QUANTUM WALKS

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ABSTRACT. We investigate quantum walks which play an important role in the modelling of many phenomena. The detailed and thorough description is given to the discrete quantum walks on a line, where the total quantum state consists of quantum states of the walker and the coin. In addition to the standard walker probability distribution, we introduce the coin probability distribution which gives more complete quantum walk description and novel visualization in terms of the so called polyanders (analogs of trianders in DNA visualization). The methods of final states computation and the Fourier transform are presented for the Hadamard quantum walk.

CONTENTS

1. INTRODUCTION	2
2. DISCRETE QUANTUM WALKS	2
3. POLYANDER VISUALIZATION OF QUANTUM WALKS	6
4. METHODS OF FINAL STATES COMPUTATION	8
4.1. Fourier transform and analytic solutions	8
5. GENERALIZATIONS OF DESCRETE-TIME QUANTUM WALKS	10
References	11

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1. INTRODUCTION

Quantum walks are the quantum counterpart of the classical random walks playing important role in the modelling of many phenomena, for instance information spreding in complex networks NOH AND RIEGER [2004], optimal search strategies LV ET AL. [2002], genetic sequence location VAN DEN ENGH ET AL. [1992], and chemical reactions GILLESPIE [1977]. The term "quantum walks" was introduced in AHARONOV ET AL. [1993], but the idea to incorporate quantum effects to stochastic calculus appeared in ICHE AND NOZIERES [1978], that is the coherence effects in evolution of Brownian quantum particle were first considered in SCHWINGER [1961]. Then the quantum analogies of classical random walks in discrete time and space were investigated in GODOY AND FUJITA [1992], the quantum cellular automata were introduced in GRÖSSING AND ZEILINGER [1988] which appeared to be equivalent to the construction of AHARONOV ET AL. [1993], which can be considered as one particle sector of the former, for a review, see ARRIGHI [2019] and more general VENEGAS-ANDRACA [2012]. The connections between correlated classical random walks and quantum walks were given in KONNO [2009] using matrix methods.

There are two models of quantum walks:

- 1) Discrete quantum walks consists of two systems, called a walker and a coin, and the evolution unitary operator acts on them in discrete time steps.
- 2) Continuous quantum walks consists of one quantum system called walker which "walks" without time restrictions, which is described by the evolution operator (Hamiltonian) and the Schrödinger equation CHILDS ET AL. [2002].

The general topology in both cases can be described by discrete graphs.

2. DISCRETE QUANTUM WALKS

In the case of discrete quantum walks on a line the total quantum state consists of quantum states of the walker and the coin, that is the total Hilbert state \mathcal{H}_{tot} becomes the direct product

$$\mathcal{H}_{tot} = \mathcal{H}_{coin} \otimes \mathcal{H}_{walk}.$$
(2.1)

The "position" of the walker is described by the vector from the computational basis of the walker Hilbert space $|\psi_{walk}\rangle \in \mathcal{H}_{walk}$ which is infinite-dimensional and countable, such that the walker state $|\psi_{walk}\rangle$ is the quantum superposition

$$|\psi_{walk}\rangle = \sum_{\ell \in \mathbb{Z}} w_{\ell} |\ell\rangle_{w}, \qquad \sum_{\ell \in \mathbb{Z}} w_{\ell}^{2} = 1, \quad w_{\ell} \in \mathbb{C}.$$
(2.2)

In distinction of the classical coin which can be in two states, the quantum *s*-state coin can be not only in *s* canonical basis states $|\mathbf{0}\rangle_c$, $|\mathbf{1}\rangle_c$, ..., $|\mathbf{s}-\mathbf{1}\rangle_c$, but also in their quantum superposition

$$|\psi_{coin}\rangle = \sum_{j=0}^{s-1} c_j |\mathbf{j}\rangle_c, \qquad \sum_{j=0}^{s-1} c_j^2 = 1, \quad c_j \in \mathbb{C}.$$
(2.3)

Usually, to be closer to the classical case, one puts s = 2. The total state of the quantum walk is given by

$$|\Psi_{tot}\rangle = |\psi_{coin}\rangle \otimes |\psi_{walk}\rangle, \tag{2.4}$$

and the initial total state, if to take $|\psi_{walk}\rangle_{initial} = |0\rangle_w$, becomes

$$|\Psi_{tot}\rangle_{initial} = |\psi_{coin}\rangle_{initial} \otimes |0\rangle_{w}$$
 (2.5)

In general, the total state can be written as

$$|\Psi_{tot}\rangle = \sum_{\ell \in \mathbb{Z}} \left(\varphi_{0,\ell} \left| \mathbf{0} \right\rangle_c \otimes \left| \ell \right\rangle_w + \varphi_{1,\ell} \left| \mathbf{1} \right\rangle_c \otimes \left| \ell \right\rangle_w \right), \tag{2.6}$$

$$\sum_{\ell \in \mathbb{Z}} \left(|\varphi_{0,\ell}|^2 + |\varphi_{1,\ell}|^2 \right) = 1 \quad \varphi_{0,\ell}, \varphi_{1,\ell} \in \mathbb{C}.$$

$$(2.7)$$

It follows from (2.2)–(2.3) that

$$\varphi_{j,\ell} = c_j w_\ell, \quad \ell \in \mathbb{Z}, \quad j = 0, 1, \tag{2.8}$$

and so the normalization condition (2.7) reduces one parameter from the set of ones describing the total state (2.6).

By analogy with the classical random walk, we need one operator to move the walker on the line and one operator to play the same role as the coin toss. As opposite to the classic case, where such an operator is represented by a stochastic matrix, in the case of the quantum walk evolution there is no room for randomness before measurement and it is represented by an unitary matrix which acts as an internal rotation in the internal state space. The goal of the coin operator is to render the coin state in a superposition, while the randomness is introduced by making a measurement on the system after both evolution operators have been applied to the total quantum system for many times.

Thus, the evolution of a quantum walk is driven by the special composite action of two unitary operators: 1) the first one, shift operator S acting in combined total position-coin space \mathcal{H}_{tot} ; 2) the other one is the coin operator C acting in the coin space \mathcal{H}_{coin} . In this way the total evolution is described by the unitary operator U defined by the main formula of the coined quantum walk concept

$$\mathbf{U} = \mathbf{S} \circ \left(\mathbf{C} \otimes \mathbf{I}_w \right), \tag{2.9}$$

$$\mathbf{S}: \mathcal{H}_{coin} \otimes \mathcal{H}_{walk} \to \mathcal{H}_{coin} \otimes \mathcal{H}_{walk}, \quad \mathbf{C}: \mathcal{H}_{coin} \to \mathcal{H}_{coin}, \quad \mathbf{U}: \mathcal{H}_{tot} \to \mathcal{H}_{tot},$$
(2.10)

where $\mathbf{I}_w \in \mathcal{H}_{walk}$ is the unity of the walker space \mathcal{H}_{walk} .

If we consider the two-state coin s = 2 (2.6), then the operator S should act on the total quantum state (2.4) by shifts which are dependent from the coin state

$$\mathbf{S} \circ (|\mathbf{0}\rangle_c \otimes |\ell\rangle_w) = |\mathbf{0}\rangle_c \otimes |\ell+1\rangle_w, \qquad (2.11)$$

$$\mathbf{S} \circ \left(\left| \mathbf{1} \right\rangle_{c} \otimes \left| \ell \right\rangle_{w} \right) = \left| \mathbf{1} \right\rangle_{c} \otimes \left| \ell - 1 \right\rangle_{w}.$$
(2.12)

This can be written in the unified form

$$\mathbf{S} \circ (|\mathbf{j}\rangle_c \otimes |\ell\rangle_w) = |\mathbf{j}\rangle_c \otimes \left|\ell + (-1)^j\right\rangle_w,$$
(2.13)

that is we have the shift operator depends on the coin state $S = S_j$. Therefore, in the computational basis S can be presented using two projections in \mathcal{H}_c as (the outer product representation)

$$\mathbf{S} = |\mathbf{0}\rangle_c \langle \mathbf{0}|_c \otimes \sum_{\ell \in \mathbb{Z}} |\ell + 1\rangle_w \langle \ell|_w + |\mathbf{1}\rangle_c \langle \mathbf{1}|_c \otimes \sum_{\ell \in \mathbb{Z}} |\ell - 1\rangle_w \langle \ell|_w, \qquad (2.14)$$

which satisfies the needed shifting properties in the walker space (2.11)–(2.12).

The coin operator C is an arbitrary element of the unitary group $\mathcal{U}(s)$, and for the two-state coin s = 2, and it can be represented by the 4 real parameter 2×2 complex matrix \hat{C} of the form

$$\hat{\mathbf{C}} = \hat{\mathbf{C}}_{\alpha,\beta,\gamma,\theta} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} = e^{i\gamma} \begin{pmatrix} e^{i\alpha}\cos\theta & e^{i\beta}\sin\theta \\ -e^{-i\beta}\sin\theta & e^{-i\alpha}\cos\theta \end{pmatrix}, \quad a,b,c,d \in \mathbb{C}, \quad \alpha,\beta,\gamma,\theta \in \mathbb{R}.$$
(2.15)

In the most cases, for quantum walks with two-state coin the Hadamard operator is widely used

$$\mathbf{C}_{H} = \frac{1}{\sqrt{2}} \left(\left| \mathbf{0} \right\rangle_{c} \left\langle \mathbf{0} \right|_{c} + \left| \mathbf{0} \right\rangle_{c} \left\langle \mathbf{1} \right|_{c} + \left| \mathbf{1} \right\rangle_{c} \left\langle \mathbf{0} \right|_{c} - \left| \mathbf{1} \right\rangle_{c} \left\langle \mathbf{1} \right|_{c} \right),$$
(2.16)

or in the matrix representation (2.15)

$$\hat{\mathbf{C}}_{H} = \hat{\mathbf{C}}_{\alpha = \frac{\pi}{2}, \beta = \frac{\pi}{2}, \gamma = \frac{\pi}{2}, \theta = \frac{\pi}{4}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$
(2.17)

The evolution of the total state (2.4) during the descrete time (= t) quantum walk after t steps $|\Psi_{tot}(t)\rangle$ is given by the application of the unitary operator (2.9) t times in the following way

$$|\Psi_{tot}(t)\rangle = \mathbf{U}^t |\Psi_{tot}(0)\rangle, \qquad (2.18)$$

where $|\Psi_{tot}(0)\rangle = |\Psi_{tot}\rangle_{initial}$ (2.5).

Example **2.1**. Using (2.9) and (2.16) we can get the first 3 steps for the Hadamard quantum walk with the two-state coin as

$$|\Psi_{tot}(1)\rangle = \frac{1}{\sqrt{2}} |\mathbf{0}\rangle_c \otimes |1\rangle_w + \frac{1}{\sqrt{2}} |1\rangle_c \otimes |-1\rangle_w, \qquad (2.19)$$

$$|\Psi_{tot}(2)\rangle = -\frac{1}{2}|1\rangle_c \otimes |-2\rangle_w + \frac{1}{2}(|0\rangle_c + |1\rangle_c) \otimes |0\rangle_w + \frac{1}{2}|0\rangle_c \otimes |2\rangle_w$$
(2.20)

$$= \frac{1}{2} |\mathbf{0}\rangle_c \otimes (|\mathbf{0}\rangle_w + |2\rangle_w) + \frac{1}{2} |\mathbf{1}\rangle_c \otimes (|0\rangle_w - |-2\rangle_w), \qquad (2.21)$$

$$|\Psi_{tot}(3)\rangle = \frac{1}{2\sqrt{2}} |\mathbf{1}\rangle_c \otimes |-3\rangle_w - \frac{1}{2\sqrt{2}} |\mathbf{0}\rangle_c \otimes |-1\rangle_w + \frac{1}{2\sqrt{2}} (2|\mathbf{0}\rangle_c + |\mathbf{1}\rangle_c) \otimes |1\rangle_w + \frac{1}{2\sqrt{2}} |\mathbf{0}\rangle_c \otimes |3\rangle_w$$
(2.22)

$$=\frac{1}{2\sqrt{2}}|\mathbf{0}\rangle_{c}\otimes\left(-\left|-1\right\rangle_{w}+2\left|1\right\rangle_{w}+\left|3\right\rangle_{w}\right) + \frac{1}{2\sqrt{2}}|\mathbf{1}\rangle_{c}\otimes\left(\left|1\right\rangle_{w}+\left|-3\right\rangle_{w}\right).$$
(2.23)

If the final state at the time t is known $\Psi_{tot}(t)$, the standard way to describe the quantum walk is the partial measurement of the walker state probabilities (see, e.g. PORTUGAL [2013]).

However, now we have the tensor product of two spaces (2.1), therefore to have the complete description of the quantum walk we propose to consider the partial measurement of the (s-) coin state probabilities as well.

Let the total state at the time t (2.18) has the general form (see (2.6)–(2.8))

$$\left|\Psi_{tot}\left(t\right)\right\rangle = \sum_{\ell \in \mathbb{Z}} \sum_{j=0}^{s-1} \varphi_{j,\ell}\left(t\right) \left|\mathbf{j}\right\rangle_{c} \otimes \left|\ell\right\rangle_{w}, \qquad (2.24)$$

$$\sum_{\ell \in \mathbb{Z}} |\varphi_{j,\ell}(t)|^2 = 1 \quad \varphi_{j,\ell} \in \mathbb{C}.$$
(2.25)

We denote the "doubly partial" probability of the state $|\mathbf{j}\rangle_c \otimes |\ell\rangle_w$ at the time t by

$$p_{j,\ell}(t) = |\varphi_{j,\ell}(t)|^2, \qquad \sum_{\ell \in \mathbb{Z}} \sum_{j=0}^{s-1} p_{j,\ell}(t) = 1.$$
 (2.26)

Now we propose to characterize the quantum walk by two partial probability distributions:

1) The walker probability distribution

$$p_{\ell}^{walk}(t) = \sum_{j=0}^{s-1} |\varphi_{j,\ell}(t)|^2, \qquad (2.27)$$

$$\sum_{\ell \in \mathbb{Z}} p_{\ell}^{walk}\left(t\right) = 1.$$
(2.28)

2) The coin probability distribution

$$p_j^{coin}\left(t\right) = \sum_{\ell \in \mathbb{Z}} |\varphi_{j,\ell}\left(t\right)|^2,$$
(2.29)

$$\sum_{j=0}^{s-1} p_j(t) = 1.$$
(2.30)

In the standard approach PORTUGAL [2013], only the first (walker) distribution (2.27) is usually considered: the time is fixed by $t = t_0$, and the graph $\{\ell, p_{\ell}^{walk}(t_0)\}$ is plotted. Nevertheless, the coin probability distribution (2.29) gives additional and information about the quantum walk. To observe the difference between (2.27) and (2.29) concretely, we continue the *Example* 2.1 in very details.

Example 2.2 (*Example* 2.1 continued). Here we compute the walker and coin probabilities (2.27) and (2.29) for three steps t = 1, 2, 3 of the Hadamard walk $\Psi_{tot}(t)$ in (2.19)–(2.23). The formulas (2.19), (2.20) and (2.22) are convenient to use for the walker probabilities, and the formulas (2.19), (2.21) and (2.23) can be used for the coin probabilities. We derive the walker probabilities $p_{\ell}^{walk}(t)$ from (2.19)

$$p_{\ell=1}^{walk} \left(t = 1 \right) = p_{\ell=|1\rangle_w}^{walk} \left(t = 1 \right) = \left(\frac{1}{\sqrt{2}} \right)^2 = \frac{1}{2}, \tag{2.31}$$

$$p_{\ell=-1}^{walk} \left(t = 1 \right) = p_{\ell=|-1\rangle_w}^{walk} \left(t = 1 \right) = \left(\frac{1}{\sqrt{2}} \right)^2 = \frac{1}{2},$$
(2.32)

and from (2.20) we obtain the symmetric distribution

$$p_{\ell=-2}^{walk} \left(t=2\right) = p_{\ell=|-2\rangle_w}^{walk} \left(t=2\right) = \left(\frac{1}{2}\right)^2 = \frac{1}{4},$$
(2.33)

$$p_{\ell=0}^{walk} \left(t=2\right) = p_{\ell=|0\rangle_w}^{walk} \left(t=2\right) = \left(\frac{1}{2}\right)^2 + \left(\frac{1}{2}\right)^2 = \frac{1}{2},$$
(2.34)

$$p_{\ell=2}^{walk} \left(t=2\right) = p_{\ell=|2\rangle_w}^{walk} \left(t=2\right) = \left(\frac{1}{2}\right)^2 = \frac{1}{4}.$$
(2.35)

The probability distribution $p_{\ell}^{walk}(t)$ for the third step t = 3 is nonsymmetric (2.22)

$$p_{\ell=-3}^{walk} \left(t=3\right) = p_{\ell=|-3\rangle_w}^{walk} \left(t=3\right) = \left(\frac{1}{2\sqrt{2}}\right)^2 = \frac{1}{8},$$
(2.36)

$$p_{\ell=-1}^{walk} \left(t=3\right) = p_{\ell=|-1\rangle_w}^{walk} \left(t=3\right) = \left(-\frac{1}{2\sqrt{2}}\right)^2 = \frac{1}{8},$$
(2.37)

$$p_{\ell=1}^{walk} \left(t=3\right) = p_{\ell=|1\rangle_w}^{walk} \left(t=3\right) = \left(2\frac{1}{2\sqrt{2}}\right)^2 + \left(\frac{1}{2\sqrt{2}}\right)^2 = \frac{5}{8},\tag{2.38}$$

$$p_{\ell=3}^{walk} \left(t=3\right) = p_{\ell=|3\rangle_w}^{walk} \left(t=3\right) = \left(\frac{1}{2\sqrt{2}}\right)^2 = \frac{1}{8},$$
(2.39)

as well as for further steps (times) t > 3.

For the coin probabilities $p_{\ell}^{coin}(t)$ we have from (2.19)

$$p_{j=0}^{coin} \left(t=1\right) = p_{j=|\mathbf{0}\rangle_c}^{coin} \left(t=1\right) = \left(\frac{1}{\sqrt{2}}\right)^2 = \frac{1}{2},\tag{2.40}$$

$$p_{j=1}^{coin} \left(t=1\right) = p_{j=|\mathbf{1}\rangle_c}^{coin} \left(t=1\right) = \left(\frac{1}{\sqrt{2}}\right)^2 = \frac{1}{2},$$
(2.41)

and from (2.21) we have for the second step t = 2 the symmetric distribution

$$p_{j=0}^{coin} \left(t=2\right) = p_{j=|\mathbf{0}\rangle_c}^{coin} \left(t=2\right) = \left(\left(\frac{1}{2}\right)^2 + \left(\frac{1}{2}\right)^2\right) = \frac{1}{2},\tag{2.42}$$

$$p_{j=1}^{coin}\left(t=2\right) = p_{j=|\mathbf{1}\rangle_{c}}^{coin}\left(t=2\right) = \left(\left(\frac{1}{2}\right)^{2} + \left(-\frac{1}{2}\right)^{2}\right) = \frac{1}{2},$$
(2.43)

The probability distribution $p_j^{coin}(t)$ for the third step t = 3 is also nonsymmetric as $p_{\ell}^{walk}(t = 3)$, so from (2.23) we get

$$p_{j=0}^{coin}\left(t=3\right) = p_{j=|\mathbf{0}\rangle_{c}}^{coin}\left(t=3\right) = \left(\left(-\frac{1}{2\sqrt{2}}\right)^{2} + \left(2\frac{1}{2\sqrt{2}}\right)^{2} + \left(\frac{1}{2\sqrt{2}}\right)^{2}\right) = \frac{3}{4},$$
(2.44)

$$p_{j=1}^{coin}\left(t=3\right) = p_{j=|\mathbf{1}\rangle_{c}}^{coin}\left(t=3\right) = \left(\left(\frac{1}{2\sqrt{2}}\right)^{2} + \left(2\frac{1}{2\sqrt{2}}\right)^{2}\right) = \frac{1}{4},$$
(2.45)

and in the similar way for further steps (discrete times) t > 3.

As it should be, both the above walker and coin probability distributions are correctly normalized satisfying (2.28) and (2.30) at each discrete time t.

3. POLYANDER VISUALIZATION OF QUANTUM WALKS

The coin probability distribution $p_j^{coin}(t)$ introducted in (2.29), from the first glance, can be also characterized at the fixed time $t = t_0$ by the graph $\{j, p_j^{coin}(t_0)\}$, as the walker probability distribution $p_\ell^{walk}(t_0)$. However, because the coin has a specific "physical" sense, we propose here another way of the quantum walk description, which has an origin from genome landscapes AZBEL' [1973, 1995], LOBRY [1996], one-dimensional DNA walks CEBRAT AND DUDEK [1998] and trianders DUPLIJ AND DUPLIJ [2005]. **Innovation 3.1.** We can consider the time evolution of the probability for the concrete quantum state, when we provide the corresponding measurements in the coin or walker subspaces. That is, we fix the states $\ell = \ell_0$ or $j = j_0$ and introduce the following time evolution graphs $\{t, p_{\ell=\ell_0}^{walk}(t)\}$ or $\{t, p_{j=j_0}^{coin}(t)\}$.

Definition 3.2. The polyander visualization of a quantum walk is its description by the time evolution graphs $\{t, p_{\ell}^{walk}(t)\}$ or $\{t, p_{j}^{coin}(t)\}$. Each line of the graph describing the probability evolution of the fixed quantum state $\ell = \ell_0$ for $|\ell_0\rangle_w$ or $j = j_0$ for $|\mathbf{j}\rangle_c$ is called a leg of the polyander.

It is obvious, that the walker polyander has finitely increasing number of legs and corresponding quantum states, while the *s*-side coin polyander has exactly *s* legs.

For the *Example* **2.1** we obtain

Example 3.3 (*Example* 2.1 continued). The walker polyander $p_{\ell}^{walk}(t)$ in the time range $1 \le t \le 3$ has 7 legs (quantum states) $-3 \le \ell \le 3$, which have the following probability evolutions

ℓ -leg\time t	1	2	3
$\left -3\right\rangle_{w}$	0	0	$\frac{1}{8}$
$\left -2\right\rangle_{w}$	0	$\frac{1}{4}$	0
$\left -1\right\rangle_{w}$	$\frac{1}{2}$	0	$\frac{1}{8}$
$\ket{0}_{w}$	0	$\frac{1}{2}$	0
$ 1\rangle_w$	$\frac{1}{2}$	0	$\frac{5}{8}$
$ 2\rangle_w$	0	$\frac{1}{4}$	0
$ 3\rangle_{m}$	0	0	$\frac{1}{2}$

(3.1)

The coin polyander $p_j^{coin}(t)$ in the time range $1 \le t \le 3$ has 2 legs (quantum states), j = 0, 1, which have the following probability evolutions

$ \mathbf{j}\rangle$ -leg $\langle time t \rangle$	1	2	3
$ 0\rangle_{c}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{3}{4}$
$ 1\rangle_{c}$	$\frac{\overline{1}}{2}$	$\frac{1}{2}$	$\frac{1}{4}$

Each leg can be presented as a horizontal strip of the width 1 on which the points corresponding to the probabilities $0 \le p(t) \le 1$ at times $t = 1, 2, 3 \dots$ are indicated. Then the probability behaviour of each quantum state can be visually seen and mutually compared in the same time points.

For the coin polyader it is important to consider the probability differences, because of the following

Definition 3.4. The total quantum state is called trivial at the time $t = t_{triv}$, if all the *s*-side coin states have equal probabilities $p_j^{coin}(t_{triv}) = \frac{1}{s}, j = 0, 1, ..., s - 1, s \ge 2$.

Definition 3.5. The quantum walk is called trivial, if the *s*-side coin states are trivial at all times.

In the case of the standard coin s = 2, the triviality means that the measurements of both sides give the same probability at the $t = t_{triv}$. Therefore, to describe triviality in detail, we should introduce the differences and search for nonzero ones.

Definition 3.6. The bias s-side coin polyander has (s-1) legs which are defined by

$$\Delta p_j^{coin}(t) = p_j^{coin}(t) - p_{j+1}^{coin}(t), \quad j = 0, \dots, s - 2.$$
(3.3)

Example 3.7 (*Example* 2.1 continued). The 2-side coin bias polyander in the time range $1 \le t \le 3$ has one leg which has the following probability evolution $\Delta p_0^{coin}(t) = \Delta p_{j=|0\rangle_c}^{coin}(t) - \Delta p_{j=|1\rangle_c}^{coin}(t)$ (see (3.2))

which can be nontrivial after the time t = 3 only.

In the higher times the walker and coin polyanders, as well as the bias coin polyander will have more complated behavior, which in any case needs the manifest form of the total quantum state (2.18). In *Example* 3.3 and *Example* 3.7, we considered for clarity only the time range $1 \le t \le 3$ and the 2-side coin to show in details, how to compute probability polyanders for finite times. The "physical sense" of the bias polyander is in the following: its nonzero values show nontriviality evolution along the quantum walk.

Thus, polyanders allow us to study further the "fine structure" and thorough characterization and visual presentation of quantum walks from different vieponts.

4. METHODS OF FINAL STATES COMPUTATION

The main goal of studying the quantum walks is obtaining the analytical expression for the final quantum state (2.18) in discrete finite times $t \in \mathbb{Z}$, and then calculating the dynamical and statistical properties of various probability distributions and characteristics.

The main computational methods to find the total quantum state (2.18) are

- 1) The Schrödinger approach. Starting from an arbitrary state of the quantum walk with a certain walker position, to provide the discrete time Fourier transform AMBAINIS ET AL. [2001] and obtain the closed form of total amplitudes.
- 2) The combinatorial approach. The amplitude at any discrete time is derived as a sum of amplitudes of all paths starting from the initial state and ending up in the final state. This can be treated as reminiscent of the standard path integral technique.

In CARTERET ET AL. [2005] it was shown that both Schrödinger and combinatorial approaches are equivalent. Among less known methods we can mention the alternative description of quantum walks based on the scattering theory FELDMAN AND HILLERY [2007] and the analytic formulation of probability densities and moments FUSS ET AL. [2007].

4.1. Fourier transform and analytic solutions. In general, the usage of the Fourier transform is the standard way of simplification of computations by turning equations to the algebraic ones. In its application to quantum works and analysing the evolution (2.18) there two peculiarities:

- 1) The Fourier transform is applied to one subspace from the product (2.4), that is the walker one \mathcal{H}_{walk} .
- 2) Sometimes it is more simple to turn from transforming functions to transform the computational basis of the walker subspace.

Following 2) we transform the computational basis of the walker space \mathcal{H}_{walk} as

$$||\mathbf{k}\rangle\rangle_{w} = \sum_{\ell \in \mathbb{Z}} e^{i\mathbf{k}\ell} |\ell\rangle_{w}, \quad \ell \in \mathbb{Z}, \quad |\ell\rangle_{w}, \quad ||\mathbf{k}\rangle\rangle_{w} \in \mathcal{H}_{walk},$$
(4.1)

where the Fourier transformed vectors $||k\rangle_w$ are denoted by the double brackets and depend on the continuous real "wave number" $k \in \mathbb{R}, -\pi \leq k \leq \pi$. The inverse transformation is

$$\left|\ell\right\rangle_{w} = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\mathbf{k} e^{-i\mathbf{k}\ell} \left|\left|\mathbf{k}\right\rangle\right\rangle_{w}.$$
(4.2)

Let us introduce the Fourier transformation of the amplitudes $\varphi_{j,\ell}(t)$ at the time t from the decomposition (2.24) in the standard way by

$$\Phi_{j,\mathbf{k}}\left(t\right) = \sum_{\ell \in \mathbb{Z}} e^{-i\mathbf{k}\ell} \varphi_{j,\ell}\left(t\right), \quad -\pi \leq \mathbf{k} \leq \pi.$$
(4.3)

The inverse Fourier transform becomes

$$\varphi_{j,\ell}(t) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\mathbf{k} e^{i\mathbf{k}\ell} \Phi_{j,\mathbf{k}}(t) \,. \tag{4.4}$$

Then, instead of the computational basis $|\mathbf{j}\rangle_c \otimes |\ell\rangle_w$ in (2.24), using (4.1) and (4.4) and cancelling exponents, we can present the total state in the Fourier basis $|\mathbf{j}\rangle_c \otimes |\mathbf{k}\rangle_w$ as follows

$$\left|\Psi_{tot}\left(t\right)\right\rangle = \frac{1}{2\pi} \sum_{j=0}^{s-1} \int_{-\pi}^{\pi} \Phi_{j,\mathbf{k}}\left(t\right) \left|\mathbf{j}\right\rangle_{c} \otimes \left|\left|\mathbf{k}\right\rangle\right\rangle_{w}.$$
(4.5)

The action of the shift operator S on the Fourier basis can be derived from (2.13) and using (4.1) as follows

$$\mathbf{S} \circ (|\mathbf{j}\rangle_{c} \otimes ||\mathbf{k}\rangle\rangle_{w}) = \sum_{\ell \in \mathbb{Z}} e^{i\mathbf{k}\ell} \mathbf{S} \circ (|\mathbf{j}\rangle_{c} \otimes |\ell\rangle_{w}) = \sum_{\ell \in \mathbb{Z}} e^{i\mathbf{k}\ell} \mathbf{S} \circ (|\mathbf{j}\rangle_{c} \otimes |\ell\rangle_{w})$$
$$= \sum_{\ell \in \mathbb{Z}} e^{i\mathbf{k}\ell} \left(|\mathbf{j}\rangle_{c} \otimes \left|\ell + (-1)^{j}\right\rangle_{w} \right) = \sum_{\ell' \in \mathbb{Z}} e^{i\mathbf{k}\left(\ell' - (-1)^{j}\right)} (|\mathbf{j}\rangle_{c} \otimes |\ell'\rangle_{w})$$
$$= e^{-i\mathbf{k}(-1)^{j}} \sum_{\ell' \in \mathbb{Z}} e^{i\mathbf{k}\ell'} (|\mathbf{j}\rangle_{c} \otimes |\ell'\rangle_{w}) = e^{-i\mathbf{k}(-1)^{j}} |\mathbf{j}\rangle_{c} \otimes ||\mathbf{k}\rangle\rangle_{w},$$
(4.6)

where we used the substitution $\ell' = \ell + (-1)^j$ and the translation symmetry of the infinite sum.

In the case of the two-side coin j = 0, 1 and the Hadamard quantum walk (2.16)–(2.17), the action of operators can be expressed in the matrix form.

So we apply the total evolution operator U (2.9) in the matrix form to the Fourier basis $|\mathbf{j}\rangle_c \otimes ||\mathbf{k}\rangle\rangle_w$ using (2.17) to get

$$\hat{\mathbf{U}}\left(|\mathbf{j}'\rangle_{c}\otimes||\mathbf{k}\rangle\rangle_{w}\right) = \hat{\mathbf{S}}\left(\left(\sum_{j=0}^{1}\hat{\mathbf{C}}_{jj'}|\mathbf{j}\rangle_{c}\right)\otimes||\mathbf{k}\rangle\rangle_{w}\right) \\
= \left(\sum_{j=0}^{1}e^{-i\mathbf{k}(-1)^{j}}\hat{\mathbf{C}}_{jj'}|\mathbf{j}\rangle_{c}\right)\otimes||\mathbf{k}\rangle\rangle_{w} = \sum_{j=0}^{1}\bar{\mathbf{C}}_{jj'}\left(\mathbf{k}\right)|\mathbf{j}\rangle_{c}\otimes||\mathbf{k}\rangle\rangle_{w},$$
(4.7)

where

$$\bar{\mathbf{C}}\left(\mathbf{k}\right) = \begin{pmatrix} e^{-i\mathbf{k}} & 0\\ 0 & e^{i\mathbf{k}} \end{pmatrix} \hat{\mathbf{C}} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\mathbf{k}} & e^{-i\mathbf{k}}\\ e^{i\mathbf{k}} & -e^{i\mathbf{k}} \end{pmatrix}.$$
(4.8)

It follows from (4.7) that diagonalization of $\overline{\mathbf{C}}(\mathbf{k})$ leads to the spectral decomposition of the total operator $\hat{\mathbf{U}}$. Indeed, if $\lambda(\mathbf{k})$ is the eigenvalue of the matrix $\overline{\mathbf{C}}(\mathbf{k})$, then it is also the eigenvalue of $\hat{\mathbf{U}}$, as it is seen from (4.7). The corresponding $\lambda(\mathbf{k})$ eigenvector we denote by $||\mathbf{v}_{\lambda(\mathbf{k})}\rangle\rangle_c$, such that

$$\mathbf{\hat{U}} \circ \left(\left\| \left| \mathsf{v}_{\lambda(\mathsf{k})} \right\rangle \right\rangle_{c} \otimes \left\| \left| \mathsf{k} \right\rangle \right\rangle_{w} \right) = \left(\mathbf{\bar{C}} \left(\mathsf{k} \right) \circ \left\| \left| \mathsf{v}_{\lambda(\mathsf{k})} \right\rangle \right\rangle_{c} \right) \otimes \left\| \left| \mathsf{k} \right\rangle \right\rangle_{w} = \lambda \left(\mathsf{k} \right) \left\| \left| \mathsf{v}_{\lambda(\mathsf{k})} \right\rangle \right\rangle_{c} \otimes \left\| \left| \mathsf{k} \right\rangle \right\rangle_{w}.$$
(4.9)

The matrix $\bar{\mathbf{C}}\left(\mathsf{k}\right)$ (4.8) has two eigenvalues

$$\lambda_1 \left(\mathbf{k} \right) = e^{-i\alpha(\mathbf{k})}, \quad \lambda_2 \left(\mathbf{k} \right) = -e^{i\alpha(\mathbf{k})}, \tag{4.10}$$

$$\alpha\left(\mathsf{k}\right) = \arcsin\left(\frac{1}{\sqrt{2}}\sin\mathsf{k}\right), \quad -\frac{\pi}{2} \leqslant \alpha\left(\mathsf{k}\right) \leqslant \frac{\pi}{2},\tag{4.11}$$

and two corresponding normalized eigenvectors

$$\left\|\left|\mathbf{v}_{\lambda_{1,2}(\mathbf{k})}\right\rangle\right\rangle_{c} = \frac{1}{\sqrt{r_{1,2}}} \left(\begin{array}{c} e^{-i\mathbf{k}} \\ \pm\sqrt{2}e^{-i\alpha(\mathbf{k})} - e^{-i\mathbf{k}} \end{array}\right),\tag{4.12}$$

$$r_{1,2} = 2\left(1 + \cos^2 \mathbf{k} \mp \cos \mathbf{k} \sqrt{1 + \cos^2 \mathbf{k}}\right).$$
(4.13)

Thus, in the total evolution operator can be written in terms of eigenvalues and eigenvectors of C(k) (4.8)

$$\hat{\mathbf{U}} = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\mathbf{k} \left[\left(e^{-i\alpha(\mathbf{k})} \left\| |\mathbf{v}_{\lambda_{1}(k)} \right\rangle \right)_{c} \left\langle \left\langle \mathbf{v}_{\lambda_{1}(k)} \right\| \right|_{c} - e^{i\alpha(\mathbf{k})} \left\| |\mathbf{v}_{\lambda_{2}(k)} \right\rangle \right\rangle_{c} \left\langle \left\langle \mathbf{v}_{\lambda_{2}(k)} \right\| \right|_{c} \right) \otimes \left\| \mathbf{k} \right\rangle \right\rangle_{w} \left\langle \left\langle \mathbf{k} \right\| \right\|_{w} \right].$$
(4.14)

Using orthogonality the basis eigenvectors, the power of the evolution operator can be presented as

$$\hat{\mathbf{U}}^{t} = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\mathbf{k} \left[\left(e^{-i\alpha(\mathbf{k})t} \left\| \left| \mathbf{v}_{\lambda_{1}(k)} \right\rangle \right\rangle_{c} \left\langle \left\langle \mathbf{v}_{\lambda_{1}(k)} \right\|_{c} + (-1)^{t} e^{i\alpha(\mathbf{k})t} \left\| \left| \mathbf{v}_{\lambda_{2}(k)} \right\rangle \right\rangle_{c} \left\langle \left\langle \left| \mathbf{v}_{\lambda_{2}(k)} \right\|_{c} \right\rangle \otimes \left\| \mathbf{k} \right\rangle \right\rangle_{w} \left\langle \left\langle \mathbf{k} \right\|_{w} \right].$$

$$(4.15)$$

Now we can use the main quantum evolution formula (2.18) to obtain the total quantum state at any time from an initial quantum state (2.5). For instance, if $|\Psi_{tot}\rangle_{initial} = |\mathbf{0}\rangle_c \otimes |0\rangle_w$, then using (4.5) and (4.12), we derive the Fourier transformed amplitudes

$$\Phi_{j=0,k}(t) = \frac{1}{2\sqrt{1+\cos^2 k}} \left[\left(\sqrt{1+\cos^2 k} + \cos k \right) e^{-i\alpha(k)t} + \left(\sqrt{1+\cos^2 k} - \cos k \right) e^{i(\pi+\alpha(k))t} \right],$$

$$\Phi_{j=1,k}(t) = \frac{e^{ik}}{2\sqrt{1+\cos^2 k}} \left(e^{-i\alpha(k)t} - e^{i(\pi+\alpha(k))t} \right).$$
(4.16)

Then applying the reverse Fourier transform (4.4) and taking into account symmetries of integrand, we get the amplitudes in the computational basis at the arbitrary time t as

$$\varphi_{j=0,\ell}(t) = \begin{cases} \frac{1}{2\pi} \int_{-\pi}^{\pi} d\mathbf{k} e^{i(\mathbf{k}\ell - \alpha(\mathbf{k})t)} \left(\frac{\cos \mathbf{k}}{\sqrt{1 + \cos^2 \mathbf{k}}} + 1\right), & t+\ell = even, \\ 0, & t+\ell = odd, \end{cases}$$

$$\varphi_{j=1,\ell}(t) = \begin{cases} \frac{1}{2\pi} \int_{-\pi}^{\pi} d\mathbf{k} e^{i(\mathbf{k}\ell - \alpha(\mathbf{k})t + \mathbf{k})} \frac{1}{\sqrt{1 + \cos^2 \mathbf{k}}}, & t+\ell = even, \\ 0, & t+\ell = odd. \end{cases}$$
(4.17)
$$(4.18)$$

Finally, using the partial probability formulas (2.27) and (2.29) one can plot the time evolution graphs $\{t, p_{\ell=\ell_0}^{walk}(t)\}$ and $\{t, p_{j=j_0}^{coin}(t)\}$, that is to provide the polyander visualization (see Section 3).

5. GENERALIZATIONS OF DESCRETE-TIME QUANTUM WALKS

There are plenty of various generalizations of the above constructions. Nevertheless, the main procedures remain the nearly same.

- **Coin operator:** The most general form of the two-sided (s = 2) coin operator C is given by the complex matrix (2.15) from the unitary group $\mathcal{U}(2)$. That is other than the Hadamard matrix (2.17) can be considered, for instance the Fourier coin PORTUGAL [2013].
- **Higher dimensions:** The main quantum walk equation (2.9) can be extended to higher dimension the *s*-sided coin, when \mathcal{H}_{coin} is 2*s*-dimensional Hilbert space and \mathcal{H}_{walk} is the Hilbert

space corresponding to the direct product $\mathbb{Z} \otimes \ldots \otimes \mathbb{Z}$. The common choice for *s*-sided coin is the Grover operator described by the corresponding 2*s*-dimensional matrix \hat{C}_{Grover} proposed in MOORE AND RUSSELL [2002].

Anyonic quantum walks: To include the braiding interaction one includes the additional Hilbert space (fusion space) \mathcal{H}_{fusion} where the generators of the braid group act. Then the total space becomes $\mathcal{H}_{tot} = \mathcal{H}_{coin} \otimes \mathcal{H}_{fusion} \otimes \mathcal{H}_{walk}$, and the time evolution contains the additional braid operator in some representation LEHMAN ET AL. [2011].

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