Path integral approach to one-dimensional discrete-time quantum walk

Karthik S. Joshi,1 S. K. Srivatsa,2,1 and R. Srikanth1

1Poornaprajna Institute of Scientific Research, Bengaluru, India.
2Dept. of Electrical and Electronics Engineering, PES University, Bengaluru, India.

Discrete-time quantum walk in one-dimension is studied from a path-integral perspective. This enables derivation of a closed-form expression for amplitudes corresponding to any coin-position basis of the state vector of the quantum walker at an arbitrary step of the walk. This provides a new approach to the foundations and applications of quantum walks.

I. INTRODUCTION

An approach to quantum mechanics via the generalization of the action principle in classical mechanics was established by Feynman [1], known as the path integral formulation. It assumes that a particle can take all possible paths to travel between two fixed points, say O, the origin, and T, the terminal point respectively. A probability amplitude is assigned to each path the particle can take and the propagator is obtained by taking the sum of all amplitudes corresponding to all paths for the particle to propagate from O to T.

Let C be a path from O to T, with an assigned probability amplitude $P(C)$, which in general is a complex number. The probability that the particle will take the path C is $|P(C)|^2$. The joint probability for the particle to take paths $C_1$ and $C_2$ is then $|P(C_1) + P(C_2)|^2$. Notice that the rule for obtaining joint probability deviates from its classical counterpart by an interference term of the form $P(C_1)P^*(C_2) + P^*(C_1)P(C_2)$. Further, in a path C made of two sub-paths say $C_1$ and $C_2$ meeting at an intermediate point M, the probability amplitude $P(C) = P(C_1)P(C_2)$.

The path integral approach has been applied to study various physical processes, including the quantum dynamics involving scalar potentials with singularities which were not amenable to the standard operator approach of Schrödinger [2]. It has also been extensively applied in the study of quantum field theory particularly for quantization, gauge fixing and phenomenon concerning elementary particles [3]. The problem of decoherence, central for realization of a quantum computer has been discussed via the path integral approach in [4].

A candidate system to study via Feynman approach is the quantum walk (QW). The QW is a process wherein the evolution of the walker is driven by a fixed unitary operator. QW process begins with the walker at the origin, and the evolution of the walker is obtained by taking the sum of all amplitudes corresponding to all paths for the particle to propagate from O to T.

We briefly present the Discrete Quantum walk scheme for completeness. Consider the walker to be initially in the state

\[ |\psi(t = 0)\rangle = (\alpha |0\rangle + e^{i\phi} \beta |1\rangle) \otimes |k\rangle. \] (1)

We assume $\alpha$ and $\beta$ to be real numbers without loss of generality. The Hilbert space of the walker is $\mathcal{H} = \mathcal{H}_{\text{coin}} \otimes \mathcal{H}_{\text{position}}$. One-step evolution of the walker is
achieved by applying a unitary operator $U \equiv C \otimes S$ on $|\psi(0)\rangle$, with coin operator $C$, given by:

$$C = \begin{pmatrix} \cos \theta & \sin \theta \\ \sin \theta & -\cos \theta \end{pmatrix},$$  \hspace{1cm} (2)

and the shift operator $S$ given by:

$$S = \Sigma_k |0\rangle \langle 0| \otimes |k-1\rangle \langle k| + \Sigma_k |1\rangle \langle 1| \otimes |k+1\rangle \langle k|. \hspace{1cm} (3)$$

Application of $U^n$ carries out a $n$ - step QW. Evolving the initial state $\langle 1 | \psi(1) \rangle$ by one step we obtain

$$|\psi(1)\rangle = \alpha \cos \theta |0, k-1\rangle + \alpha \sin \theta |1, k+1\rangle + e^{i\phi} \beta \sin \theta |0, k-1\rangle - e^{i\phi} \beta \cos \theta |1, k+1\rangle. \hspace{1cm} (4)$$

The basis vectors of $|\psi(1)\rangle$ represent the final state of the walker. Let the transitions $|k\rangle \rightarrow |k+1\rangle$ and $|k\rangle \rightarrow |k-1\rangle$ be labelled as forward ($F$) and backward ($B$) transition respectively. All possible one-step transitions are deduced from Eq.(4) and are illustrated in Fig. [1].

Note that the probability amplitudes are independent of the instantaneous position of the walker, $|k\rangle$ and the step number, $t$.

Two steps of the QW can be obtained by combining one-step transitions. For instance, a possible two step evolution can be obtained by combining $B$ and $F$ one-step transitions- a $BF$ transition, which indicates that the walker underwent a $|k\rangle \rightarrow |k-1\rangle$ transition at time $t=1$ followed by a $|k-1\rangle \rightarrow |k\rangle$ transition at time $t=2$. Similarly, an $n$ - step walk can be represented by a string of $F$s and $B$s of length $n$, which prompts the following definition:

**Definition 1** (Feynman string). Any $n$-bit string $S \in \{B,F\}^n$ represents the $n-1$ (one step) transitions in a Feynman path of an $n$ - step QW.

Strings starting with a $B$ are called $B$ - strings, likewise, strings starting with $F$ are called $F$ - strings. Given a string $S$, its dual $\bar{S}$, is obtained by interchanging $F$s and $B$s. Evidently, the dual of a $B$-string is an $F$-string and vice-versa.

For any path starting at the origin and terminating at position $|x\rangle$ (say), the corresponding Feynman string $S$ has $n+|x|$ $F$s and $n-|x|$ $B$s. Hence, the number of strings $N^*$ representing paths which start at the origin and terminate at $|x\rangle$ is given by the number of distinct permutations of $S$. Therefore:

$$N = \frac{n!}{(n+|x|)! (n-|x|)!} = \binom{n}{n+|x|}. \hspace{1cm} (5)$$

The walker has a certain initial coin state as shown in Eq. [1]. This obviously affects the evolution of the walker, as coin states $|0\rangle$ and $|1\rangle$ effect $B$ and $F$ translations respectively. This gives rise to the mapping $B \rightarrow |0\rangle$ and $F \rightarrow |1\rangle$. Each of the above $N$ strings are thus concatenated with a $B$ or an $F$, effectively giving rise to strings $B*S$ and $F*S$ for all $S$, leading to the following definition:

**Definition 2** (Feynman extended string). An $(n+1)$-bit string, denoted $S^*$, consisting of a Feynman string preceded by the initial coin state of the walker $B$ ($|0\rangle$) or $F$ ($|1\rangle$).

Note that each of the extended strings $S^*$ of an $n$ - step walk has $n$ one step transitions. Furthermore, $B*S$ and $F*S$ for all $N$ number of strings $S$, will result in $2N$ strings.

In the Feynman framework, each of the $2N$ paths are associated with a probability amplitude. Let the $m^{th}$ path string have a probability amplitude $P(S_m)$. The net probability amplitude, $P(x)$, for the walker to be found at position $|x\rangle$ is the sum of all these amplitudes:

$$P(x) = \sum_{m=1}^{2N} P(S_m). \hspace{1cm} (6)$$

On the other hand, for a given path represented by an $n + 1$ - bit string $S$, the corresponding probability amplitude $P(S)$ is given by the product of all the $n$ one step probability amplitudes $P(k)$:

$$P(S) = \prod_{k=1}^{n} P(k). \hspace{1cm} (7)$$

The discussion presented in the remainder of the article pertains to both Feynman string and its extended counterpart. They will be collectively referred to as Feynman strings unless otherwise specified.

Note that each one step transition introduces a $\sin \theta$ or a $\pm \cos \theta$ factor to the probability amplitude, therefore it is proportional to $\cos^i \theta \sin^j \theta$, with $i + j = n$.

**Definition 3** (Switch). In any $n$-bit Feynman string, $S \in \{B,F\}^n$, switch is defined as a $F \leftrightarrow B$ transition in the string.
It is easily seen from Fig. [1] that number of switches fixes the degree of sin \( \theta \) in the probability amplitude. Evidently, there are multiple strings, say \( \eta(n, x, j) \), with same number of switches, which needs to be accounted.

The full path string of length \( n \) and terminating at position \( |x| \) has \( N_F(n, x) = \frac{n + |x|}{2} \) dominant (say, forward) shifts and \( N_B(n, x) = \frac{n - |x|}{2} \) minority (say, backward) shifts. Note that for a fixed time step, \( n \) and \( |x| \) are both even or both odd.

The number of strings, for a fixed \( j \) switches, is equivalent to the problem of filling (i) \( \mathcal{N}_F(n, x) \) balls into \( \mu \equiv \lfloor (j + 1)/2 \rfloor \) urns and of \( \mathcal{N}_B(n, x) \) balls into \( \nu \equiv \lceil (j + 1)/2 \rceil \) urns; plus (ii) \( \mathcal{N}_F(n, x) \) balls into \( \nu \) urns and of \( \mathcal{N}_B(n, x) \) balls into \( \mu \) urns.

At the value of \( j \) where \( N_B(n, x) < \nu \) (i.e., when \( j = n - |x| \)), contribution (i) drops out. At precisely the next value of \( j \), \( N_B(n, x) < \mu \) (i.e., \( j = n - |x| + 1 \)), both (i) and (ii) have no more contributions. Thus, both (i) and (ii) contribute up to \( j = n - |x| - 1 \), and then at \( j = n - |x| \) there is a contribution from (ii) alone. For larger values of \( j \), there aren’t any more contributions.

Recall that the problem of filling \( n \) balls into \( k \) urns, such that no urn is empty, is the combinatorial problem of strong composition, and the number of ways are given by \( \binom{n-1}{k-1} \).

The total number of \( n \)-Feynman paths with \( j \) switches is given by:

\[
\eta(n, x, j) = \binom{n + |x|}{2} - 1 \left( \begin{array}{c} \frac{n - |x|}{2} \times (\frac{n - |x|}{2} - 1) \\ \frac{|x|}{2} \times (\frac{2|x|}{2} - 1) \end{array} \right) + \left( \begin{array}{c} \frac{n - |x|}{2} \times (\frac{n + |x|}{2} - 1) \\ \frac{|x|}{2} \times (\frac{2|x|}{2} - 1) \end{array} \right),
\]

(8)

assuming \( j \leq n - |x| - 1 \). If \( j = n - |x| \), then only the first summand in Eq. (8) contributes. The following identity can easily be verified:

\[
\binom{n}{\frac{n + |x|}{2}} = \sum_{j=1}^{n - |x| - 1} \eta(n, x, j) + \left( \begin{array}{c} \frac{n + |x|}{2} - 1 \\ \frac{n - |x| + |x| + 1}{2} - 1 \end{array} \right).
\]

(9)

Recall that the LHS of Eq. (9) is same as the total number of Feynman paths obtained in Eq. (5).

Note that in the case of equal forward and backward paths, where we set \( x = 0 \), the second summand in the RHS of Eq. (9) vanishes.

Further, when a \( B \)-string is concatenated with a \( F \) (or vice - versa), an additional switch is introduced. For example, a string with two switches \( BBFFB \), when concatenated with a \( F \) to obtain the extended string \( F \leftrightarrow BBFFB \), has three switches. The additional switch so introduced in the extended needs to be accounted for.

Let \( \eta^*(n + 1, x, j) \) denote the number of extended strings with \( j \) switches, then:

\[
\eta^*(n + 1, x, j) = \eta(n, x, j) + \eta(n, x, j - 1),
\]

(10)

for \( 1 < j < n - |x| \). For \( j = 1 \) and \( j = n - |x| + 1 \), we have:

\[
\eta^*(n + 1, x, j) = \eta(n, x, j).
\]

(11)

Definition 4 (Parity). Given an \( n \) bit Feynman (extended) string, the parity \( \epsilon \) takes the value \( +1 \) (resp., \( -1 \)) when the number of \( F \to F \) transitions in the string are even (resp. odd).

The parity of a Feynman extended string is obtained in the following lemma.

Lemma 1. The parity \( \epsilon(n, x, j) \) of Feynman \( B \) or \( F \)-strings with \( j \) switches is given by

\[
\epsilon(n, x, j) = (-1)^{\frac{n + x - 1}{2} + \frac{|x| + 1}{2}}
\]

(12)

and

\[
\epsilon(n, x, j) = (-1)^{\frac{n + x - 1}{2} - \frac{|x| + 1}{2}}
\]

(13)

respectively.

Proof. Let \( S \) be a \( B \)-string with \( j \) switches. Cut the string at points where switches occur. This process creates \( j + 1 \) sub-strings with \( \lfloor \frac{n + x}{2} \rfloor \) and \( \lceil \frac{|x|}{2} \rceil \) sub-strings of the same number of switches, which needs to be accounted.

The parity of a Feynman extended string is invariant under permutations which preserve the number of switches.

Lemma 2. A Feynman \( B \)-string (resp. \( F \)-string) with \( j \) switches determines the coin state in an eigen basis \( |b, x\rangle \): \( b = j + 1 \mod 2 \) (resp. \( b = j \mod 2 \)).

Proof. Let \( S \) be a \( B \)-string with \( j \) switches, where \( j \) is even. Cut the string at points where switches occur as described in lemma (1). As \( S \) is a \( B \)-string, the first of the \( j + 1 \) sub-strings contains only \( B \)s. This sub-string is followed by \( F \) sub-string which in turn is followed by a \( B \) sub-string and so on. It follows from this arrangement that the last sub-string contains \( B \)s. Every transition terminating with a \( B \) results in the coin state \( |0\rangle \) as evident from Fig. [1]. For an odd number of switches, \( j \), in a \( B \)-string, the above process of cutting and arranging the \( j + 1 \) sub-strings, where \( j + 1 \) is even, results in the \( (j + 1)\text{th} \) sub-string to contain only \( F \)s.
Every transition terminating with a $F$ results in the coin state $|1\rangle$ as evident from table Fig. [1].

The result can be similarly shown for $F$ - strings.

Hence, using the above results, the state vector component corresponding to a given Feynman extended string can expressly be written as:

$$|\xi(n, x, j, c)\rangle = e(n + 1, x, j) \cos^m \theta \sin^m \theta \times |(j + c \mod 2), x\rangle,$$

where, $c = 0$ for $B$- strings and $c = 1$ for $F$- strings.

We note that a $B$- string with $j$ switches and its dual have like parity when $j$ is even and unlike parity when $j$ is odd according to Eqs. [12] and [13].

Defining the summing operations:

$$\sum_1 \equiv \sum_{x=-n}^{n} \frac{1 + (-1)^{n+x}}{2} \sum_{m=1}^{n+|i|} \epsilon(n, x, 2m) \eta^{*}(n + 1, x, 2m)$$

we obtain the final state vector to be:

$$|\psi(n)\rangle = \left( \sum_1 \alpha N_B(n, x) (\cos \theta)^n - 2m (\sin \theta)^{2m} + \sum_2 \beta e^{i \phi} N_F(n, x) (\cos \theta)^n - 2m (\sin \theta)^{2m} \right) |0, x\rangle$$

$$+ \left( \sum_1 \beta e^{i \phi} N_F(n, x) (\cos \theta)^n - 2m (\sin \theta)^{2m} - \sum_2 \alpha N_B(n, x) (\cos \theta)^n - 2m (\sin \theta)^{2m} \right) |1, x\rangle,$$

which may be considered as an explicit representation of a QW parametrized by position. This allows us to circumvent a direct calculation of amplitudes at each position. Its application will be explored elsewhere.

### III. CONCLUSION

In this work, a closed form expression was obtained for the state vector corresponding to arbitrary time step for an $n$ - step QW in one dimension. The Feynman path integral approach was used to derive all possible (backward and forward) transition rules of the walker. The forward and backward transitions were mapped to a string of $F$s and $B$s respectively. A recipe for calculating the probability amplitude for a given string was provided using the properties of these strings.

The formalism presented in this work can be extended to QW in higher dimensions including walks by augmenting the QW “Feynman rules” presented in Fig. [1], which would allow us to accommodate QW in higher dimensions as well QW in arbitrary graphs. One can in principle extend this formalism to any Markovian process evolving under a fixed unitary operator.

---

[1] R. P. Feynman. Space-time approach to non-relativistic quantum mechanics. *Rev. Mod. Phys.*, 20:367–387, Apr 1948.

[2] E. Nelson. Feynman Integrals and the Schrödinger Equation. *Journal of Mathematical Physics*, 5:332–343, March 1964.

[3] Das Ashok. *Field Theory: A Path Integral Approach*, volume 75. World Scientific, 2006.

[4] Sergio Albeverio, Laura Cattaneo, Sonia Mazzucchi, and Luca Di Persio. A rigorous approach to the feynman-vonbert influence functional and its applications. *Journal of Mathematical Physics*, 48(10):102109, 2007.

[5] C. Di Franco, M. Mc Gettrick, and Th. Busch. Mimicking the probability distribution of a two-dimensional grover walk with a single-qubit coin. *Phys. Rev. Lett.*, 106:080502, Feb 2011.

[6] Apoorva Patel, KS Raghunathan, and Pranaw Rungta.

Quantum random walks do not need a coin toss. *Physical Review A*, 71(3):032347, 2005.

[7] Renato Portugal, Raqueline AM Santos, Tharso D Fernandes, and Demerson N Gonçalves. The staggered quantum walk model. *Quantum Information Processing*, 15(1):85–101, 2016.

[8] R Srikanth, Subhashish Banerjee, and CM Chandrashekar. Quantumness in a decoherent quantum walk using measurement-induced disturbance. *Physical Review A*, 81(6):062123, 2010.

[9] SalvadorEls Venegas-Andraca. Quantum walks: a comprehensive review. *Quantum Information Processing*, 11(5):1015–1106, 2012.

[10] Kia Manouchehri and Jingbo Wang. *Physical Implementation of Quantum Walks*. Springer-Verlag, Berlin Heidelberg, 2014.

[11] B. C. Travaglione and G. J. Milburn. Implementing the
quantum random walk. *Phys. Rev. A*, 65:032310, Feb 2002.

[12] C. M. Chandrashekar. Implementing the one-dimensional quantum (hadamard) walk using a bose-einstein condensate. *Phys. Rev. A*, 74:032307, Sep 2006.

[13] Jozef Košík and Vladimír Bužek. Scattering model for quantum random walks on a hypercube. *Phys. Rev. A*, 71:012306, Jan 2005.

[14] G. S. Agarwal and P. K. Pathak. Quantum random walk of the field in an externally driven cavity. *Phys. Rev. A*, 72:033815, Sep 2005.

[15] Neil Shenvi, Julia Kempe, and K. Birgitta Whaley. Quantum random-walk search algorithm. *Phys. Rev. A*, 67:052307.

[16] Frédéric Magniez, Miklos Santha, and Mario Szegedy. Quantum algorithms for the triangle problem. *SIAM Journal on Computing*, 37(2):413–424, 2007.

[17] Andrew M Childs. Universal computation by quantum walk. *Physical review letters*, 102(18):180501, 2009.

[18] Neil B Lovett, Sally Cooper, Matthew Everitt, Matthew Trevers, and Viv Kendon. Universal quantum computation using the discrete-time quantum walk. *Physical Review A*, 81(4):042330, 2010.

[19] Pablo Arrighi, Vincent Nesme, and Marcelo Forets. The dirac equation as a quantum walk: higher dimensions, observational convergence. *Journal of Physics A: Mathematical and Theoretical*, 47(46):465302, 2014.

[20] C. M. Chandrashekar. Two-component dirac-like hamiltonian for generating quantum walk on one-, two- and three-dimensional lattices. *Scientific Reports*, 3:2829, Oct 2013.

[21] Arindam Mallick, Sanjoy Mandal, and C. M. Chandrashekar. Neutrino oscillations in discrete-time quantum walk framework. *The European Physical Journal C*, 77(2):85, Feb 2017.

[22] Ashwin Nayak and Ashvin Vishwanath. Quantum walk on the line. *arXiv preprint quant-ph/0010117*, 2000.