How to Realize One-dimensional Discrete-time Quantum Walk by Dirac Particle

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One-dimensional discrete-time quantum walks (DTQWs) can simulate various quantum and classical dynamics and have already been implemented in several physical systems. This implementation needs a well-controlled quantum dynamical system, which is the same requirement for implementing quantum information processing tasks. Here, we consider how to realize DTQWs by Dirac particles toward a solid-state implementation of DTQWs.

KEYWORDS: discrete-time quantum walk, Dirac particle, physical implementation

1. Introduction

The discrete-time quantum walk (DTQW) is defined as the quantum-mechanical analogue of the discrete-time random walk and has many applications, especially in quantum information science. Recent progress on quantum complexity has been based on the quantum walk [1, 2], and other applications and insights have been reported in recent review papers [3–6] and books [7, 8]. It is remarked that the brief history of the DTQW was proposed by Feynman as the Feynman checkerboard [9] and thereafter independently formulated in quantum probability [10], quantum random walks [11], and quantum cellular automaton [12].

Owing to the developed quantum technology, there are several physical implementations [13–22]. However, it is emphasized that there is no implementation of the DTQW in a solid-state system. The simplest implementation in a photonic system is to use a polarized beam splitter or shifter and polarizers. Other experimental proposals of DTQWs have been demonstrated for an ion trap [23], cavity quantum electrodynamics [24], a non-Abelian anyon [25], Bose–Einstein condensation [26], angular momentum classical light [27], ensembles of nitrogen-vacancy centers in diamond coupled to a superconducting qubit [28], and an optomechanical system [29].

Various DTQWs can simulate the Dirac equation [30–34], the spatially discretized Schrödinger equation [35, 36], the Klein–Gordon equation [33, 37], or other various differential equations [38, 39]. Furthermore, classical dynamics can be simulated [40]. On the other hand, we have not yet shown how to realize the DTQW in natural classical/quantum dynamics. In this paper, we will show that the massive Dirac equation naturally has the structure of the DTQW by the discretization of the space and time.

2. Review of the Discrete-Time Quantum Walk

Let us recapitulate the discrete-time random walk. First, we prepare a particle, which is located at the origin at the beginning, and a coin. We repeatedly carry out the following procedures:

1. A coin flip,
2. A shift in the particle depending on whether the coin is tails or heads.

Finally, we calculate the probability distribution $Pr(n; t)$ at the position $n$ and step $t$.

Analogous to the discrete-time random walk, we define the DTQW [41]. First, we prepare the quantum particle, which is located in the origin at the beginning and is labeled with a position state denoted by $|0\rangle$, and the quantum coin with an orthogonal basis: $|\uparrow\rangle = (1, 0)^T$ and $|\downarrow\rangle = (0, 1)^T$, where $T$ is the transpose operator. We repeatedly carry out the following procedures:

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(1) A quantum coin flip: This operator is generally defined as
\[ C_i = \sum_n [(a_{n,i} |n, \uparrow\rangle + c_{n,i} |n, \downarrow\rangle)(n, \uparrow\rangle + (d_{n,i} |n, \downarrow\rangle + b_{n,i} |n, \uparrow\rangle)(n, \downarrow\rangle) \]
\[ = \sum_n [n\rangle \langle n| \otimes \left( \begin{array}{cc} a_{n,i} & b_{n,i} \\ c_{n,i} & d_{n,i} \end{array} \right) \] \]
\[ =: \sum_n [n\rangle \langle n| \otimes \hat{C}_{n,i}. \]  
where \( \hat{C}_{n,i} \in U(2) \), and \( \hat{C}_{n,i} \) expresses the coin operator at the position \( n \) and step \( t \).

(2) A shift depending on whether the coin is tails or heads: This operator is defined as
\[ W = \sum_n (|n-1, \uparrow\rangle (n, \uparrow\rangle + |n+1, \downarrow\rangle (n, \downarrow\rangle). \]

It is noted that these procedures should be described as unitary processes. One step of the quantum walk operator at the step \( t \) is defined as \( U_t = WC_t \). This representation is focused on the quantum coin.

On the other hand, as the quantum-particle representation, we define the quantum-particle state as
\[ \Psi(n, t) \equiv e_{n,i} |\uparrow\rangle + f_{n,i} |\downarrow\rangle \]
and its dynamics as
\[ \Psi(n, t + 1) = P_{n,i} \Psi(n + 1, t) + Q_{n,i} \Psi(n - 1, t) \]
with
\[ P_{n,i} + Q_{n,i} = C_{n,i}. \]
This representation is a good fit to the combinatorial approach of the DTQW to first show the weak limit theorem [42, 43].

As alluded to in the introduction, various DTQWs can simulate several dynamics. For example, the connection to the massive Dirac equation can be seen in the following theorem.

**Theorem 2.1** (Strauch [31]). The quantum coin is set as
\[ C(\epsilon) = \left( \begin{array}{cc} \cos \epsilon & -i \sin \epsilon \\ -i \sin \epsilon & \cos \epsilon \end{array} \right). \]
When the parameter \( \epsilon \) is sufficiently small, this DTQW can simulate the massive Dirac equation.

This analysis is similar to Ref. 30 and can be extended to the two-dimensional space [32]. It is emphasized that the DTQW can be implemented under well-controlled nonrelativistic quantum mechanics while the DTQW can simulate the relativistic quantum mechanics. This originates from the discrete structure of space and time in the DTQW. Therefore, DTQWs can simulate several quantum and classical dynamics to unify the concept as a quantum dynamical simulator [6]. However, there remains the question of whether or not the relativistic particle can experimentally implement several DTQWs. In the following section, we discuss this question.

### 3. DTQW Implementation by Dirac Particle

Let us consider the massive Dirac equation as
\[ \partial_t \varphi(x, t) = -i(m \sigma_\xi + \sigma_\eta \partial_x) \varphi(x, t), \]  
where \( \varphi(x, t) \) represents the Dirac spinor. By the Lax method, we derive the discretized equation as
\[ \frac{\varphi(x, t + \Delta t) - \varphi(x, t)}{\Delta t} = -i \left( m \sigma_\xi \frac{\varphi(x + \Delta x, t) + \varphi(x - \Delta x, t)}{2} + \sigma_\eta \frac{\varphi(x + \Delta x, t) - \varphi(x - \Delta x, t)}{2 \Delta x} \right) + \Theta((\Delta t)^2, (\Delta x)^2). \]

To compare the discretized Dirac equation with the quantum-walk dynamics in (2.4), the quantum state can be rewritten as
\[ \varphi(x, t + \Delta t) = (1 - i \Delta t m \sigma_\xi) \varphi(x + \Delta x, t) + \varphi(x - \Delta x, t) \]
\[ \frac{\Delta t}{2} \sigma_\xi (\varphi(x + \Delta x, t) - \varphi(x - \Delta x, t)) + \Theta((\Delta t)^3, (\Delta x)^2) \]
\[ \approx \frac{1}{2} \left( 1 - i \Delta t m \sigma_\xi - i \frac{\Delta t}{\Delta x} \sigma_\xi \right) \varphi(x + \Delta x, t) \]
\[ \approx \frac{1}{2} \left( 1 - i \Delta t m \sigma_\xi - \frac{i \Delta t}{\Delta x} \sigma_\xi \right) \varphi(x + \Delta x, t) \]
\[ \approx \frac{1}{2} \left( 1 - i \Delta t m \sigma_\xi - \frac{i \Delta t}{\Delta x} \sigma_\xi \right) \varphi(x + \Delta x, t) \]
\[
+ \frac{1}{2} \left( 1 - i \Delta t m \sigma_x + i \frac{\Delta t}{\Delta x} \sigma_z \right) \phi(x - \Delta x, t) = P \phi(x + \Delta x, t) + Q \phi(x - \Delta x, t)
\]
(3.3)

with

\[
P \equiv \frac{1}{2} \left( -i \Delta t m \sigma_x - i \frac{\Delta t}{\Delta x} \sigma_z \right),
\]
\[
Q \equiv \frac{1}{2} \left( 1 - i \Delta t m \sigma_x + i \frac{\Delta t}{\Delta x} \sigma_z \right).
\]
(3.4)

Here, the one-step operator \( C \equiv P + Q \) is defined and \( \phi(x, t) \) is not normalized in general. Therefore, when the wavefunction \( \phi(x, t) \) is normalized to \( \tilde{\phi}(x, t) \), we define a new one-step operator \( \tilde{C} \) to satisfy

\[
\phi(x, t + \Delta t) \approx \tilde{P} \tilde{\phi}(x + \Delta x, t) + \tilde{Q} \tilde{\phi}(x - \Delta x, t).
\]
(3.5)

From Eq. (3.4), the quantum coin can be evaluated as

\[
\tilde{C} = \alpha (1 - i \Delta t m \sigma_x)
\]
(3.6)

with the complex constant \( \alpha \). To satisfy the unitary operator \( \tilde{C} \), the parameter \( \alpha \) should be set as

\[
\alpha = \frac{e^{i \theta}}{\sqrt{1 + (\Delta m \Delta t)^2}}
\]
(3.7)

with the arbitrary real parameter \( \theta \). Upon setting \( m = 1 \), this can be reduced to the specific quantum coin in (2.6).

Therefore, the discretized structure of the massive Dirac equation can simulate the one-dimensional DTQW. It is remarked that the massless Dirac equation can simulate the trivial DTQW. Note that similar approaches are well known as Dirac quantum cellular automata [44–47]. They have also exhibited various quantum dynamics by the massive Dirac equation.

This shows that the dynamical properties of a Dirac fermion is almost same as those of the DTQW, such as ballistic transport and the inverted-bell shape probability distribution. From Theorem 2.1, the Dirac fermion and DTQW have a one-to-one correspondence. Therefore, this result provides several experimental proposals in spintronics systems. Since spintronics systems have quantum-transport properties, this connection may reveal an efficient transport system. The Dirac particles in graphene and topological insulators are candidates for physical implementation of the DTQW. Since a topological insulator can be characterized by a topological phase, this must be one of the DTQW applications because the one-dimensional topological phase can be experimentally realized by a photonic implementation of the DTQW [17].

4. Conclusion

From the massive Dirac equation, we can derive the DTQWs with a specific coin. A spintronics system naturally has DTQW properties. However, higher-dimensional cases still remain unsolved — in particular, the correspondence to the chirality of the massive Dirac equation for more than three dimensions, whereas the one-dimensional case has been analyzed. The connection to the Majorana system has been discussed [48, 49]. Furthermore, a DTQW with an arbitrary coin has been not yet been shown by controlling the time-dependent potential. For experimental implementation, the decoherence process [50–55] should be considered, although there has been no systematic methodology for a spintronics system.

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