A quantum walk on a line and a Weyl equation in a space

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Abstract Discrete-time quantum walks are considered a discretization of Dirac equations and the study for them has been getting attention since around 2000. In this paper, we focus on a quantum walk on a line related to a Weyl equation in a space. The quantum walker with two inner states, also interpreted as a quantum particle with the down-spin and the up-spin state in physics, spreads on the line and we analyze the chance of finding the walker at each position after it carries out a unitary evolution a lot of times. The result is reported as a long-time limit distribution from which one can see an approximation to the finding probability.

Keywords Quantum walk · Weyl equation · Long-time limit distribution

1 Introduction

Quantum walks have been studied in physics, mathematics, and quantum information theory [1-3]. Since they are considered a discretization of Dirac equations, large attention is paid to the quantum walks in physics. While quantum walks are applied to quantum search algorithms in quantum information theory [5,6], physicists work on a possibility that quantum walks are applied to topological insulators [7]. In this paper, we see a discrete-time quantum walk on a line related to a Weyl equation in a space [8], and study a probability distribution with which the quantum walker is observed at each position on the line. The result for the probability distribution will be supplied in a long-time limit distribution. The study for the limit distributions of the quantum walks started in 2002 [9] which led to a Weyl equation in 2005 [10], and many types of limit distributions have been discovered [6]. Particularly, the long-time limit...
distributions play an important role to tell us approximations to the probability distributions when quantum walkers have repeated their evolutions a lot of times.

2 A quantum walk and a Weyl equation

Let us start with the description of a discrete-time quantum walk on a line. The quantum walker with the down-spin and the up-spin state locates at integer points on the line \( \mathbb{Z} = \{0, \pm 1, \pm 2, \ldots\} \) in superposition, and its system is described on a tensor Hilbert space \( \mathcal{H}_p \otimes \mathcal{H}_s \). The Hilbert space \( \mathcal{H}_p \) represents the integer points on the line and it is spanned by the orthogonal normalized basis \( \{ |x\rangle : x \in \mathbb{Z} \} \). Also, the Hilbert space \( \mathcal{H}_s \) represents the spin states and it is spanned by the orthogonal normalized basis \( \{ |0\rangle, |1\rangle \} \) in which \( |0\rangle \) is interpreted as the down-spin state and \( |1\rangle \) as the up-spin state. We are, for instance, allowed to define

\[
|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix},
\]

for the Hilbert space \( \mathcal{H}_s \). The system of quantum walk at time \( t (= 0, 1, 2, \ldots) \), represented by \( |\Psi_t\rangle \in \mathcal{H}_p \otimes \mathcal{H}_s \), updates with unitary operations \( U_1 \) and \( U_2 \) assigned a parameter \( \theta \in [0, \pi) \),

\[
|\Psi_{t+1}\rangle = \begin{cases} U_1 |\Psi_t\rangle \ (t = 0, 2, 4, \ldots) \\ U_2 |\Psi_t\rangle \ (t = 1, 3, 5, \ldots) \end{cases},
\]

where

\[
U_1 = \sum_{x \in \mathbb{Z}} |x - 2\rangle \langle x| \otimes (-\sin^2 \theta) |0\rangle \langle 1| \\
+ |x - 1\rangle \langle x| \otimes \cos \theta \sin \theta \left(|0\rangle \langle 0| - |1\rangle \langle 1|\right) \\
+ |x\rangle \langle x| \otimes \cos^2 \theta \left(|0\rangle \langle 1| + |1\rangle \langle 0|\right) \\
+ |x + 1\rangle \langle x| \otimes \cos \theta \sin \theta \left(|0\rangle \langle 0| - |1\rangle \langle 1|\right) \\
+ |x + 2\rangle \langle x| \otimes (-\sin^2 \theta) |1\rangle \langle 0|,
\]

\[
U_2 = \sum_{x \in \mathbb{Z}} |x - 2\rangle \langle x| \otimes \cos^2 \theta |1\rangle \langle 0| \\
+ |x - 1\rangle \langle x| \otimes \cos \theta \sin \theta \left(|0\rangle \langle 0| - |1\rangle \langle 1|\right) \\
+ |x\rangle \langle x| \otimes (-\sin^2 \theta) \left(|0\rangle \langle 1| + |1\rangle \langle 0|\right) \\
+ |x + 1\rangle \langle x| \otimes \cos \theta \sin \theta \left(|0\rangle \langle 0| - |1\rangle \langle 1|\right) \\
+ |x + 2\rangle \langle x| \otimes \cos^2 \theta \ |0\rangle \langle 1|.
\]
We assume in this study that the walker launches with a localized initial state $|\Psi_0\rangle = |0\rangle \otimes (\alpha |0\rangle + \beta |1\rangle)$ where the complex numbers $\alpha$ and $\beta$ are supposed to satisfy the constraint $|\alpha|^2 + |\beta|^2 = 1$. The quantum walker is observed at position $x \in \mathbb{Z}$ at time $t \in \{0, 1, 2, \ldots\}$ with probability

$$P(X_t = x) = \langle \Psi_t | \{ |x\rangle \otimes (|0\rangle \otimes |0\rangle + |1\rangle \langle 1|) \} |\Psi_t\rangle,$$

where $X_t$ denotes the position of the walker at time $t$.

Here, we see the Fourier transform of the quantum walk, which will be used to compute a limit distribution as $t \to \infty$. Let $i$ be the imaginary unit. Putting

$$\hat{U}_1(k) = 2 \cos \theta \sin \theta \cos k (|0\rangle \langle 0| - |1\rangle \langle 1|) + (\cos^2 \theta - e^{2ik\sin^2 \theta}) |0\rangle \langle 1| + (\cos^2 \theta - e^{-2ik\sin^2 \theta}) |1\rangle \langle 0|,$$

$$\hat{U}_2(k) = 2 \cos \theta \sin \theta \cos k (|0\rangle \langle 0| - |1\rangle \langle 1|) + (-\sin^2 \theta + e^{-2ik\cos^2 \theta}) |0\rangle \langle 1| + (-\sin^2 \theta + e^{2ik\cos^2 \theta}) |1\rangle \langle 0|,$$

we get the evolution of the Fourier transform $|\hat{\psi}_t(k)\rangle = \sum_{x \in \mathbb{Z}} e^{-ikx} \{ |x\rangle \otimes (|0\rangle \otimes |0\rangle + |1\rangle \langle 1|) \} |\Psi_t\rangle$ $(k \in [-\pi, \pi]),$

$$|\hat{\psi}_{t+1}(k)\rangle = \begin{cases} \hat{U}_1(k) |\hat{\psi}_t(k)\rangle & (t = 0, 2, 4, \ldots) \\ \hat{U}_2(k) |\hat{\psi}_t(k)\rangle & (t = 1, 3, 5, \ldots) \end{cases},$$

from which

$$|\hat{\psi}_{2t}(k)\rangle = \left(\hat{U}_2(k)\hat{U}_1(k)\right)^t |\hat{\psi}_0(k)\rangle,$$

$$|\hat{\psi}_{2t+1}(k)\rangle = \hat{U}_1(k) \left(\hat{U}_2(k)\hat{U}_1(k)\right)^t |\hat{\psi}_0(k)\rangle,$$

follow for $t = 0, 1, 2, \ldots$. Equation (8) has come up from Eq. (2). The initial state of the Fourier transform is computed to be $|\hat{\psi}_0(k)\rangle = \alpha |0\rangle + \beta |1\rangle$. We should note that the system is reproduced by inverse Fourier transform

$$|\Psi_t\rangle = \sum_{x \in \mathbb{Z}} |x\rangle \otimes \int_{-\pi}^{\pi} e^{ikx} |\hat{\psi}_t(k)\rangle \frac{dk}{2\pi}.$$

The Fourier transform of the quantum walk is actually interpreted as the solution to a Weyl equation in a space. Let $C$ be the set of complex numbers. The system of Weyl equation in the three-dimensional momentum space at time $\tau \in [0, \infty)$, represented by $|\Psi^W(\tau)\rangle \in C^2$, is defined by a periodic equation: For $t = 0, 1, 2, \ldots$,

$$i \frac{d}{d\tau} |\Psi^W(\tau)\rangle = \begin{cases} \frac{\nu}{2} H_1(k) |\Psi^W(\tau)\rangle & (2t \leq \tau < 2t + 1) \\ -\frac{\nu}{2} H_2(k) |\Psi^W(\tau)\rangle & (2t + 1 \leq \tau < 2t + 2) \end{cases},$$

where $\nu$ is the momentum.
where
\[
H_1(k) = (\cos^2 \theta - \sin^2 \theta \cos 2k) \sigma_x + (\sin^2 \theta \sin 2k) \sigma_y + (2 \cos \theta \sin \theta \cos k) \sigma_z,
\]
(13)
\[
H_2(k) = (-\sin^2 \theta + \cos^2 \theta \cos 2k) \sigma_x + (\cos^2 \theta \sin 2k) \sigma_y + (2 \cos \theta \sin \theta \cos k) \sigma_z,
\]
(14)

with \( k \in [-\pi, \pi] \), in which \( \sigma_x, \sigma_y, \) and \( \sigma_z \) denote the Pauli operations \( \sigma_x = |0\rangle \langle 1| + |1\rangle \langle 0|, \sigma_y = -i |0\rangle \langle 1| + i |1\rangle \langle 0|, \) and \( \sigma_z = |0\rangle \langle 0| - |1\rangle \langle 1| \). We should note that the operations \( H_1(k) \) and \( H_2(k) \) are not only Hermitian operations but also unitary operations, that is, we indeed have \( H_1(k) = U_1(k) \) and \( H_2(k) = U_2(k) \).

Moving the parameter \( k \) on interval \([-\pi, \pi]\), we catch the traces of the triples \((\cos^2 \theta - \sin^2 \theta \cos 2k, \sin^2 \theta \sin 2k, 2 \cos \theta \sin \theta \cos k)\) and \((-\sin^2 \theta + \cos^2 \theta \cos 2k, \cos^2 \theta \sin 2k, 2 \cos \theta \sin \theta \cos k)\), as shown in Fig. 1. Given an initial state at time 0, we have the solution at the integer times: For

\[
|\Psi^W(2t)\rangle = \left( e^{i \frac{\pi}{2} H_2(k)} e^{-i \frac{\pi}{2} H_1(k)} \right)^t |\Psi^W(0)\rangle
\]
(15)
\[
|\Psi^W(2t+1)\rangle = e^{-i \frac{\pi}{2} H_1(k)} |\Psi^W(2t)\rangle
\]
(16)

Taking a look back at Eqs. \( \text{(13)} \) and \( \text{(14)} \), we realize that the system of Weyl equation at the integer times is equivalent to the Fourier transform of the quantum walk launching at time 0 with the initial state \( |\Psi^W(0)\rangle \) or \(-i |\Psi^W(0)\rangle\).
Back to the quantum walk, we assert a theorem for the finding probability defined in Eq. (15).

**Theorem 1** Assume that $\theta \neq 0, \pi/2$. Let $c$ and $s$ be the contractions of $\cos \theta$ and $\sin \theta$ respectively. For a real number $x$, we have

$$
\lim_{t \to \infty} \mathbb{P} \left( \frac{X_t}{t} \leq x \right) = \int_{-\infty}^{\infty} \left\{ f(y)\nu_+(\alpha, \beta; y)I_D(y) + f(-y)\nu_-(\alpha, \beta; y)I_D(-y) \right\} dy,
$$

where

$$
f(x) = \frac{\left(x + 2\sqrt{D(x)}\right)^2}{2\pi(4 - x^2)\sqrt{D(x)}\sqrt{W_+(x)}\sqrt{W_-(x)}},
$$

$$
D(x) = 1 - 16c^4s^4 + 4c^4s^4x^2,
$$

$$
W_+(x) = 2(1 + 4c^2s^2) - (1 + 2c^2s^2)x^2 - x\sqrt{D(x)}.
$$

The limit distribution is obtained from the convergence of the $r$-th moments \( \mathbb{E}[(X_t/t)^r] \) ($r = 0, 1, 2, \ldots$) as $t \to \infty$, and the convergence can be computed by Fourier analysis. The method for the computation of the long-time limit distributions by Fourier analysis was used to quantum walks in 2004 for the first time [11] and it has been useful to find limit theorems (e.g. [12]). The $r$-th moments of $X_t$ have a representation with the Fourier transform $|\tilde{\psi}_t(k)|$,

$$
\mathbb{E}[X_t^r] = \int_{-\pi}^{\pi} \langle \hat{\psi}_t(k) \rangle \left( i \frac{d}{dk} \langle \hat{\psi}_t(k) \rangle \right) \frac{dk}{2\pi}.
$$

Recalling Eqs. (9) and (10), we express the Fourier transform $|\tilde{\psi}_t(k)|$ on the eigenspace of the unitary operation $\hat{U}_2(k)\hat{U}_1(k)$. The operation $\hat{U}_2(k)\hat{U}_1(k)$ has two eigenvalues, represented by $\lambda_j(k) (j = 1, 2)$, and they are of the form $\lambda_j(k) = g(k) - (-1)^j i \sqrt{1 - g(k)^2}$ with $g(k) = 2c^2s^2\sin^22k + \cos2k$. 


Fig. 2 The blue lines represent the probability distribution $P(X_t = x)$ at time $t = 500$ and the red points represent the right side of Eq. (36) as $t = 500$. The limit density function approximately reproduces the probability distribution as time $t$ becomes large enough. The walker launches with the localized initial state at the origin, $|\psi_0\rangle = |0\rangle \otimes (1/\sqrt{2}|0\rangle + i/\sqrt{2}|1\rangle)$.

We, moreover, hold one of the expressions for the normalized eigenvectors $|v_j(k)\rangle$ $(j = 1, 2)$ associated to the eigenvalues $\lambda_j(k)$,

$$|v_j(k)\rangle = \frac{1}{\sqrt{N_j(k)}} \left[ \begin{array}{c} (c^4 + s^4 - 2c^2s^2 \cos 2k) \sin 2k + (-1)^{j} \sqrt{1 - g(k)^2} \sin 2k \\ + \sqrt{1 - g(k)^2} \end{array} \right] |0\rangle,$$

$$+ \frac{1}{\sqrt{N_j(k)}} \left[ 2c \cos k \left( 1 - \cos 2k - i(c^2 - s^2) \sin 2k \right) \right] |1\rangle,$$

where the normalized factors are computed to be

$$N_j(k) = \left\{ (c^4 + s^4 - 2c^2s^2 \cos 2k) \sin 2k + (-1)^{j} \sqrt{1 - g(k)^2} \right\}^2$$

$$+ 4c^2s^2 \cos 2k \left\{ (1 - \cos 2k)^2 + (c^2 - s^2)^2 \sin^2 2k \right\}.$$

The decomposition of the initial state $|\psi_0(k)\rangle = \sum_{j=1}^{2} \langle v_j(k)|\phi\rangle |v_j(k)\rangle$ gives the representations

$$|\psi_{2t}(k)\rangle = \sum_{j=1}^{2} \lambda_j^t(k) \langle v_j(k)|\phi\rangle |v_j(k)\rangle,$$

$$|\psi_{2t+1}(k)\rangle = \hat{U}_1(k) \sum_{j=1}^{2} \lambda_j^t(k) \langle v_j(k)|\phi\rangle |v_j(k)\rangle.$$

from which
\[
\frac{d^r}{dt^r} |\bar{\psi}_{2r}(k)\rangle = \left\{ (t)^r \sum_{j=1}^{2} \lambda_j(k)^{t-r} (\lambda_j^*(k))^r \langle v_j(k)|\phi\rangle |v_j(k)\rangle \right\} + O(t^{r-1}),
\]
\[ (31) \]

\[
\frac{d^r}{dt^r} |\bar{\psi}_{2r+1}(k)\rangle = \bar{U}_1(k) \left\{ (t)^r \sum_{j=1}^{2} \lambda_j(k)^{t-r} (\lambda_j^*(k))^r \langle v_j(k)|\phi\rangle |v_j(k)\rangle \right\} + O(t^{r-1}),
\]
\[ (32) \]
follow with \((t) = t(t-1) \cdots (t-r-1)\). We finally reach the limits
\[
\lim_{t \to \infty} \mathbb{E} \left[ \left( \frac{X_{2t}}{2t} \right)^r \right] = \lim_{t \to \infty} \mathbb{E} \left[ \left( \frac{X_{2t+1}}{2t+1} \right)^r \right] = \int_{-\pi}^{\pi} \sum_{j=1}^{2} \frac{i\lambda_j(k)}{2\lambda_j(k)} \left\| \langle v_j(k)|\phi\rangle \right\|^2 \frac{dk}{2\pi},
\]
\[ (33) \]
where the function \(i\lambda_j(k)/2\lambda_j(k)\) is organized to be of the form
\[
\frac{i\lambda_j(k)}{2\lambda_j(k)} = (-1)^j \frac{\sin 2k}{\sin 2k} \frac{1 - 4c^2s^2 \cos 2k}{\sqrt{1 - 4c^2s^2(c^2s^2 \sin^2 2k + \cos 2k)}} \quad (j = 1, 2).
\]
\[ (34) \]
Putting \(i\lambda_j(k)/2\lambda_j(k) = x\), we achieve a desired representation of the convergence
\[
\lim_{t \to \infty} \mathbb{E} \left[ \left( \frac{X_t}{t} \right)^r \right] = \int_{-\infty}^{\infty} x^r \left\{ f(x)\nu_+(\alpha, \beta; x)I_D(x) + f(-x)\nu_-(\alpha, \beta; x)I_D(-x) \right\} dx,
\]
\[ (35) \]
and it guarantees the limit distribution Eq. (17). The limit density function reproduces the finding probability \(P(X_t = x)\) \((x \in \mathbb{Z})\) as \(t \to \infty\) in approximation,
\[
P(X_t = x) \sim \frac{1}{t} \left\{ f \left( \frac{x}{t} \right) \nu_+ \left( \alpha, \beta; \frac{x}{t} \right) I_D \left( \frac{x}{t} \right) + f \left( -\frac{x}{t} \right) \nu_- \left( \alpha, \beta; \frac{x}{t} \right) I_D \left( -\frac{x}{t} \right) \right\},
\]
\[ (36) \]
which is demonstrated in Fig. 2.

Due to the limits \(\lim_{x \to +\sqrt{1 + 4c^2s^2}} W_+(x) = 0\) and \(\lim_{x \to -\sqrt{1 + 4c^2s^2}} W_-(x) = 0\), the limit density function generally has four singular points, except for \(\theta = \pi/4, 3\pi/4\), that is,
\[
\lim_{x \to +\sqrt{1 + 4c^2s^2}} \frac{d}{dx} \lim_{t \to \infty} P \left( \frac{X_t}{t} \leq x \right) = \begin{cases} +\infty & (\theta \neq \frac{\pi}{4}, \frac{3\pi}{4}) \\ \frac{2}{\pi^2} & (\theta = \frac{\pi}{4}, \frac{3\pi}{4}) \end{cases},
\]
\[ (37) \]
\[
\lim_{x \to -\sqrt{1 + 4c^2s^2}} \frac{d}{dx} \lim_{t \to \infty} P \left( \frac{X_t}{t} \leq x \right) = \begin{cases} +\infty & (\theta \neq \frac{\pi}{4}, \frac{3\pi}{4}) \\ \frac{2}{\pi^2} & (\theta = \frac{\pi}{4}, \frac{3\pi}{4}) \end{cases},
\]
\[ (38) \]
\[
\lim_{x \to \pm \sqrt{1 + 4c^2s^2}} \frac{d}{dx} \lim_{t \to \infty} P \left( \frac{X_t}{t} \leq x \right) = +\infty, \quad (39)
\]

\[
\lim_{x \to \pm \sqrt{1 + 4c^2s^2}} \frac{d}{dx} \lim_{t \to \infty} P \left( \frac{X_t}{t} \leq x \right) = +\infty. \quad (40)
\]

Equations (37)–(40) are true for any complex numbers \(\alpha\) and \(\beta\) which satisfy the constraint \(|\alpha|^2 + |\beta|^2 = 1\) and determine the initial state of the quantum walk. Also, we should note that if the value \(\pi/4\) or \(3\pi/4\) is assigned to the parameter \(\theta\), the edges of compact support \(\pm \sqrt{1 - 4c^2s^2}\) take the value 0 and then the gap around the origin in the probability distribution closes. These facts are confirmed in Fig. 2.

3 Summary

Let us summarize this paper. We took care of a quantum walk on a line related to a Weyl equation in a space and analyzed the finding probability as \(t \to \infty\). As a result, one can say that the probability distribution \(P(X_t = x)\) as \(t \to \infty\) holds a gap around the position where the walker localizes at the initial time. In the past studies, two quantum walks whose probability distributions could have a gap, were also reported [13,14]. Both papers were studies for limit distributions of time-dependent quantum walks on a line. Grünbaum and Machida [13] analyzed a quantum walk with two inner states and Machida [14] handled a quantum walk with three inner states. The quantum walk in this study was a different type from the time-dependent quantum walks, but we observed a gap in its probability distribution and the fact was surely demonstrated as the limit law in Theorem 1. Such a discovery could lead to applications of quantum walks, for instance, the band gap theory in material science.

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