# One-dimensional three-state quantum walks: Weak limits and localization 

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We investigate one-dimensional three-state quantum walks. We find a formula for the moments of the weak limit distribution via a vacuum expectation of powers of a selfadjoint operator. We use this formula to fully characterize the localization of three-state quantum walks in one dimension. The localization is also characterized by investing the eigenvectors of the evolution operator for the quantum walk. As a byproduct we clarify the concepts of localization differently used in the literature. We also study the continuous part of the limit distribution. For typical examples we show that the continuous part is the same kind as that of two-state quantum walks. We provide with explicit expressions for the density of the weak limits of some three-state quantum walks.

Keywords: Three-state quantum walks; limit distribution; moments; localization.
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## 1. Introduction

Since the quantum walk (QW, hereafter) was introduced in mathematical way, the weak limit theory is nowadays well-known at least for one-dimensional two-state walks. When divided by a linear scale in time, the distribution of QW converges weakly. For details, we refer to Refs. 1, 4, 9-12, 16.

The linear scale of propagation in the QW, which is compared to the square root rate in the classical random walk, can be used to speed up a quantum algorithm. ${ }^{2}$ On the other hand, an opposite property, called localization, has also been observed in QWs, which causes exponential suppression of computations. See Refs. 5, 8, 13, 17 and 21.

In this paper we investigate one-dimensional three-state QWs in discrete time, which is motivated by Ref. 6 . By a three-state, it means that the intrinsic structure, or a coin space, has a degree of 3 . Two of them represent the left- and right-chirality, as usual, and the remaining one is for the central chirality. By this defining property, one guesses that there may occur a localization in this model and in fact it is shown to be true for the Grover walk in Refs. 3, 6, 15 and 19. The purpose of this paper is to discuss the distribution and localization property for the general one-dimensional three-state QWs. We remark here that we discuss the scaled limit distribution and therefore the localization is also understood in that point of view (Definition 4.1). However, it turns out that it is equivalent to the concept generally used in the literature. See Theorem 4.10.

We briefly summarize the contents of this paper. In Sec. 2, we introduce the definition of one-dimensional three-state QWs. In Sec. 3, we discuss the scaled limit distribution and moments. We represent the dynamics in the Fourier transform space and find a characteristic function of the scaled limit distribution. It is represented as a vacuum (or initial state) expectation. We consider some examples including a Grover walk and a natural extension of two-state walk to three-state walk. Section 4 deals with a localization problem, which is another main topic of this paper. We give necessity and sufficiency for the occurrence of a localization. For the characterization we use the representation formula for the moments and investigate the eigenvalues and eigenvectors of the generator of the QW evolution. We end with some examples.

## 2. Preliminaries

The definition of QWs in mathematical way can be found in several papers. See for example, Refs. 1, 4, 11, 12 and 16. Here we follow the description introduced in Ref. 9 modifying for three-state walks.

A quantum particle has an intrinsic degree of freedom, called chirality. This chirality is represented by a 3 -dimensional vector: we represent them in $\mathbb{C}^{3}$ and call the vectors $\left[\begin{array}{lll}1 & 0 & 0\end{array}\right]^{T}$, $\left[\begin{array}{lll}0 & 1 & 0\end{array}\right]^{T}$, and $\left[\begin{array}{lll}0 & 0 & 1\end{array}\right]^{T}$, the left, center, and right chirality, respectively, in that order. Here, and later, $\left[\begin{array}{lll}a & b & c\end{array}\right]^{T}$ denotes the transpose of the vector $\left[\begin{array}{lll}a & b & c\end{array}\right]$. The spatial movement of the particle is given as follows. At
time $n \in \mathbb{N}_{0}=\{0,1,2, \ldots\}$, the probability amplitude of finding the particle at site $x \in \mathbb{Z}$ with chirality state being left, center or right is given by a three-components vector

$$
\psi_{n}(x)=\left[\begin{array}{l}
\psi_{n}(1 ; x)  \tag{2.1}\\
\psi_{n}(2 ; x) \\
\psi_{n}(3 ; x)
\end{array}\right] \in \mathbb{C}^{3}
$$

After one unit of time the chirality is rotated by an a priori given unitary matrix $U$. According to the final chirality state, if the particle ends up with left chirality, then it moves one step to the left, if it ends up with central chirality, it stays at the present position, and if it ends up with right chirality, it moves one step to the right. For a detailed description, let a unitary $3 \times 3$ matrix $U$ be given by:

$$
\begin{align*}
U & =\left[\begin{array}{lll}
a_{11} & a_{12} & a_{13} \\
a_{21} & a_{22} & a_{23} \\
a_{31} & a_{32} & a_{33}
\end{array}\right]=: L+C+R  \tag{2.2}\\
L & =\left[\begin{array}{ccc}
a_{11} & a_{12} & a_{13} \\
0 & 0 & 0 \\
0 & 0 & 0
\end{array}\right], \quad C=\left[\begin{array}{ccc}
0 & 0 & 0 \\
a_{21} & a_{22} & a_{23} \\
0 & 0 & 0
\end{array}\right], \quad R=\left[\begin{array}{ccc}
0 & 0 & 0 \\
0 & 0 & 0 \\
a_{31} & a_{32} & a_{33}
\end{array}\right] . \tag{2.3}
\end{align*}
$$

Then the dynamics for $\psi_{n}=\left(\psi_{n}(x)\right)_{x \in \mathbb{Z}}$ is given by

$$
\begin{equation*}
\psi_{n+1}(x)=L \psi_{n}(x+1)+C \psi_{n}(x)+R \psi_{n}(x-1) \tag{2.4}
\end{equation*}
$$

Next we describe the dynamics in a Fourier transform space. For each $x \in \mathbb{Z}$, let $\mathcal{H}_{x}:=\mathbb{C}^{3}$ be a copy of the chirality space. Let

$$
\begin{equation*}
\mathcal{H}:=\oplus_{x \in \mathbb{Z}} \mathcal{H}_{x} \tag{2.5}
\end{equation*}
$$

be the direct sum Hilbert space, on which the evolution of a QW will be developed. Notice that $\mathcal{H}$ is isomorphic to the Hilbert spaces $l^{2}\left(\mathbb{Z}, \mathbb{C}^{3}\right)$ and $l^{2}(\mathbb{Z}) \otimes \mathbb{C}^{3}$. For each $x \in \mathbb{Z}$, let

$$
\begin{equation*}
e_{x}(k):=\frac{1}{\sqrt{2 \pi}} e^{i x k}, \quad k \in \mathbb{K}:=(-\pi, \pi] \tag{2.6}
\end{equation*}
$$

$\mathbb{K}$ being understood as a unit circle in $\mathbb{R}^{2}$. The set $\left\{e_{x}\right\}_{x \in \mathbb{Z}}$ defines an orthonormal basis in $L^{2}(\mathbb{K})$. For each $k \in \mathbb{K}$, let $\mathrm{h}_{k}$ be a copy of $\mathbb{C}^{3}$ and let

$$
\begin{equation*}
\widehat{\mathcal{H}}:=\int_{\mathbb{K}}^{\oplus} \mathrm{h}_{k} d k \approx L^{2}\left(\mathbb{K}, \mathbb{C}^{3}\right) \approx L^{2}(\mathbb{K}) \otimes \mathbb{C}^{3} \tag{2.7}
\end{equation*}
$$

be the direct integral of Hilbert spaces. The Fourier transform between $l^{2}(\mathbb{Z})$ and $L^{2}(\mathbb{K})$ naturally extends to a unitary map from $\mathcal{H}$ to $\widehat{\mathcal{H}}$ by

$$
\psi=\left\{\left[\begin{array}{l}
\psi(1 ; x)  \tag{2.8}\\
\psi(2 ; x) \\
\psi(3 ; k)
\end{array}\right]\right\}_{x \in \mathbb{Z}} \in \mathcal{H} \mapsto \widehat{\psi}=\left\{\left[\begin{array}{c}
\widehat{\psi}(1 ; k) \\
\widehat{\psi}(2 ; k) \\
\widehat{\psi}(3 ; k)
\end{array}\right]\right\}_{k \in \mathbb{K}} \in \widehat{\mathcal{H}}
$$

where

$$
\begin{equation*}
\widehat{\psi}(i ; k)=\sum_{x \in \mathbb{Z}} \psi(i ; x) e_{x}(k), \quad i=1,2,3 . \tag{2.9}
\end{equation*}
$$

Its inverse is given by $\widehat{\psi} \mapsto \psi$ with

$$
\psi(x)=\int_{-\pi}^{\pi} \frac{1}{\sqrt{2 \pi}} e^{-i x k} \widehat{\psi}(k) d k \in \mathcal{H}_{x}
$$

Let us denote by $T$ the left translation in $l^{2}(\mathbb{Z})$ :

$$
\begin{equation*}
(T a)(x)=a(x+1), \quad \text { for } a=(a(x))_{x \in \mathbb{Z}} \tag{2.10}
\end{equation*}
$$

$T$ is a unitary map whose adjoint is the right translation:

$$
\begin{equation*}
\left(T^{*} a\right)(x)=a(x-1), \quad \text { for } a=(a(x))_{x \in \mathbb{Z}} \tag{2.11}
\end{equation*}
$$

The operator $T$ naturally extends to $\mathcal{H}=\oplus_{x \in \mathbb{Z}} \mathcal{H}_{x}$ and for the sake of simplicity we use the same notation $T$ for the extension. Given an operator ( $3 \times 3$ matrix) $B$ on $\mathbb{C}^{3}$, we let

$$
\begin{equation*}
\widetilde{B}:=\oplus_{x \in \mathbb{Z}} B \tag{2.12}
\end{equation*}
$$

be the bounded direct sum operator acting on $\mathcal{H}$.
With these preparations we can rewrite the dynamics of a QW as an evolution map in the Hilbert space $\mathcal{H}$. Notice that Eq. (2.4) is the same as

$$
\begin{equation*}
\psi_{n+1}(x)=L\left(T \psi_{n}\right)(x)+C \psi_{n}(x)+R\left(T^{*} \psi_{n}\right)(x), \quad x \in \mathbb{Z} \tag{2.13}
\end{equation*}
$$

which we can write in a single equation:

$$
\begin{equation*}
\psi_{n+1}=\left(\widetilde{L} T+\widetilde{C}+\widetilde{R} T^{*}\right) \psi_{n} \tag{2.14}
\end{equation*}
$$

It is not hard to see that the operator $\widetilde{L} T+\widetilde{C}+\widetilde{R} T^{*}$ is a unitary operator on $\mathcal{H}$. Thus the solution to (2.14) is easily seen to be

$$
\begin{equation*}
\psi_{n}=\left(\widetilde{L} T+\widetilde{C}+\widetilde{R} T^{*}\right)^{n} \psi_{0} \tag{2.15}
\end{equation*}
$$

This is the time evolution of the QW that we are looking for.
Now we find the evolution of the QW in a Fourier transform space. Notice that the translation operator $T$ is represented as a multiplication operator by $e^{-i k}$ in the Fourier transform space. Thus, the evolution in (2.15) has the representation in Fourier transform space as follows:

$$
\begin{equation*}
\widehat{\psi}_{n}(k)=U(k)^{n} \widehat{\psi}_{0}(k) \tag{2.16}
\end{equation*}
$$

where

$$
U(k):=\left[\begin{array}{ccc}
e^{-i k} & 0 & 0  \tag{2.17}\\
0 & 1 & 0 \\
0 & 0 & e^{i k}
\end{array}\right]\left[\begin{array}{lll}
a_{11} & a_{12} & a_{13} \\
a_{21} & a_{22} & a_{23} \\
a_{31} & a_{32} & a_{33}
\end{array}\right] .
$$

The probability density to find out the particle at a site $x \in \mathbb{Z}$ at time $n$ is simply

$$
\begin{equation*}
\left\|\psi_{n}(x)\right\|^{2}=\left|\psi_{n}(1 ; x)\right|^{2}+\left|\psi_{n}(2 ; x)\right|^{2}+\left|\psi_{n}(3 ; x)\right|^{2} \tag{2.18}
\end{equation*}
$$

or it can also be given by

$$
\begin{align*}
\| \int_{-\pi}^{\pi} & \frac{1}{\sqrt{2 \pi}} e^{-i x k} \widehat{\psi}_{n}(k) d k \|^{2} \\
= & \frac{1}{2 \pi}\left\{\left|\int_{-\pi}^{\pi} e^{-i x k} \widehat{\psi}_{n}(1 ; k) d k\right|^{2}+\left|\int_{-\pi}^{\pi} e^{-i x k} \widehat{\psi}_{n}(2 ; k) d k\right|^{2}\right. \\
& \left.+\left|\int_{-\pi}^{\pi} e^{-i x k} \widehat{\psi}_{n}(3 ; k) d k\right|^{2}\right\} \tag{2.19}
\end{align*}
$$

The matrix $U(k)$ in (2.17) is unitary and it is diagonalized as

$$
\begin{align*}
U(k) & =S(k)\left[\begin{array}{ccc}
e^{i \gamma_{1}(k)} & 0 & 0 \\
0 & e^{i \gamma_{2}(k)} & 0 \\
0 & 0 & e^{i \gamma_{3}(k)}
\end{array}\right] S(k)^{*} \\
& =: S(k) e^{i D(k)} S(k)^{*} \tag{2.20}
\end{align*}
$$

where $S(k)$ is a unitary matrix and

$$
D(k)=\left[\begin{array}{ccc}
\gamma_{1}(k) & 0 & 0  \tag{2.21}\\
0 & \gamma_{2}(k) & 0 \\
0 & 0 & \gamma_{3}(k)
\end{array}\right]
$$

## 3. Limit Distributions and Their Moments

In this section we discuss the limit distribution of the walk. We focus on the weak limit with a scaling by time $n$. We will find the characteristic function of the distribution. First, we derive the limit and then we give some examples.

### 3.1. Existence of weak limits

We start with some preparations. Let us define a self-adjoint matrix $H(k)$ by $H(k)=$ $S(k) D(k) S(k)^{*}$. Then we can write

$$
\begin{equation*}
U(k)=e^{i H(k)} \tag{3.1}
\end{equation*}
$$

Lemma 3.1. The eigenvalues of $U(k)$ are simple for all $k \in \mathbb{K}$ except at most finitely many points.

Proof. Define a function $D: \mathbb{C} \times \mathbb{K} \rightarrow \mathbb{C}$ by

$$
D(\lambda, k):=\operatorname{det}(U(k)-\lambda)
$$

The characteristic equation $D(\lambda, k)=0$ is written as

$$
\begin{equation*}
\lambda^{3}-a(k) \lambda^{2}+d \overline{a(k)} \lambda-d=0 \tag{3.2}
\end{equation*}
$$

with

$$
\begin{aligned}
a(k) & =e^{-i k} a_{11}+a_{22}+e^{i k} a_{33}, \\
d & =\operatorname{det} U(k)=\operatorname{det} U .
\end{aligned}
$$

Here we have used the unitarity of $U(k)$ to get the coefficient of $\lambda$ : that is, denoting it by $b(k)$ we have

$$
\begin{aligned}
b(k) & =e^{-i k}\left(a_{11} a_{22}-a_{12} a_{21}\right)+e^{i k}\left(a_{22} a_{33}-a_{23} a_{32}\right)+\left(a_{11} a_{33}-a_{13} a_{31}\right) \\
& =d \overline{a(k)}
\end{aligned}
$$

Notice that the coefficients are analytic as a function of the variable $z:=i k$. From the formula for the roots of polynomials of degree 3, it is easy to see that the characteristic equation (3.2) has simple roots for all $k \in \mathbb{K}$ but at most finitely many exceptional points.

Lemma 3.2. The eigenvalues and eigenvectors of $U(k)$ are continuously differentiable on $\mathbb{K}$ except at most finitely many points.

Proof. By Lemma 3.1 the eigenvalues of $U(k)$ are simple for all $k \in \mathbb{K}$ with at most finitely many exceptional points. Now the statements of the lemma can be proven by using an implicit function theorem. See for example Refs. 7 and 14.

Theorem 3.3. The weak limit $\mu^{\left(U ; \psi_{0}\right)}$ of the distribution $X_{n}^{\left(U ; \psi_{0}\right)} / n$ exists and there is a self-adjoint operator $B \in \mathcal{B}(\widehat{\mathcal{H}})$ such that

$$
\begin{equation*}
\int_{-\infty}^{\infty} e^{i t x} \mu^{\left(U ; \psi_{0}\right)}(d x)=\left\langle\widehat{\psi}_{0}, e^{i t B} \widehat{\psi}_{0}\right\rangle_{\widehat{\mathcal{H}}} \tag{3.3}
\end{equation*}
$$

The operator $B$ is given by

$$
\begin{equation*}
B=\int_{\mathbb{K}}^{\oplus} B(k) d k, \tag{3.4}
\end{equation*}
$$

where

$$
B(k)=S(k)\left[\begin{array}{ccc}
\gamma_{1}^{\prime}(k) & 0 & 0 \\
0 & \gamma_{2}^{\prime}(k) & 0 \\
0 & 0 & \gamma_{3}^{\prime}(k)
\end{array}\right] S(k)^{*}
$$

Proof. For the proof we adopt a method used in Ref. 10. For the reader's convenience we repeat here. Recall the random variables $\left\{X_{n}^{\left(U ; \psi_{0}\right)}\right\}_{n \geq 0}$. We start with the computation of the characteristic functions:

$$
\begin{align*}
\mathbb{E}\left(e^{i t X_{n}^{\left(U ; \psi_{0}\right)}}\right) & =\sum_{x \in \mathbb{Z}} e^{i t x}\left\|\psi_{n}(x)\right\|^{2} \\
& =\left\langle\psi_{n}, e^{i t \cdot} \psi_{n}\right\rangle_{l^{2}\left(\mathbb{Z}, \mathbb{C}^{3}\right)} \\
& =\left\langle\widehat{\psi_{n}}, \widehat{e^{i t \cdot} \psi_{n}}\right\rangle_{\widehat{\mathcal{H}}} \tag{3.5}
\end{align*}
$$

We see that $\widehat{e^{i t \cdot} \cdot \psi_{n}}(k)=\widehat{\psi}_{n}(k+t)$ by understanding $\widehat{\psi}_{n}(k)$ as a periodic function of period $2 \pi$ on the real line. Therefore, we have

$$
\begin{align*}
\mathbb{E}\left(e^{i t X_{n}^{\left(U ; \psi_{0}\right)}}\right) & =\int_{-\pi}^{\pi}\left\langle\widehat{\psi}_{n}(k), \widehat{\psi}_{n}(k+t)\right\rangle_{\mathbb{C}^{3}} d k \\
& =\int_{-\pi}^{\pi}\left\langle\widehat{\psi}_{0}(k), e^{-i n H(k)} e^{i n H(k+t)} \widehat{\psi}_{0}(k+t)\right\rangle_{\mathbb{C}^{3}} d k \tag{3.6}
\end{align*}
$$

where we have used (2.16) and (3.1) in the second line. Let us compute the limit

$$
\begin{align*}
\lim _{n \rightarrow \infty} & \mathbb{E}\left(e^{i t / n X_{n}^{\left(U ; \psi_{0}\right)}}\right) \\
& =\lim _{n \rightarrow \infty} \int_{-\pi}^{\pi}\left\langle\widehat{\psi}_{0}(k), e^{-i n H(k)} e^{i n H(k+t / n)} \widehat{\psi}_{0}(k+t / n)\right\rangle_{\mathbb{C}^{3}} d k \tag{3.7}
\end{align*}
$$

Using the diagonal matrix $D(k)$ in (2.21), we have

$$
\begin{align*}
& e^{-i n H(k)} e^{i n H(k+t / n)} \\
& \quad=S(k) e^{-i n D(k)} S(k)^{*} S(k+t / n) e^{i n D(k+t / n)} S(k+t / n)^{*} \tag{3.8}
\end{align*}
$$

By Lemma 3.2, we know that $S(k)$ and $D(k)$ are continuously differentiable on $\mathbb{K}$ except at most finitely many points. First we assume that they are continuously differentiable for all $k \in \mathbb{K}$. We see that

$$
\begin{align*}
S(k)^{*} S(k+t / n) & =I+S(k)^{*}(S(k+t / n)-S(k)) \\
& =I+S(k)^{*} S^{\prime}\left(k_{1}\right) t / n \tag{3.9}
\end{align*}
$$

where $k_{1} \in(k, k+t / n)$. Similarly,

$$
e^{-i n D(k)} e^{i n D(k+t / n)}=e^{i D^{\prime}\left(k_{2}\right) t}
$$

with $k_{2} \in(k, k+t / n)$. Using these relations we have

$$
e^{-i n H(k)} e^{i n H(k+t / n)}=S(k) e^{i D^{\prime}\left(k_{2}\right) t} S(k)^{*}+R_{n}(k),
$$

where $\lim _{n \rightarrow \infty} R_{n}(k)=0$ uniformly in $k \in \mathbb{K}$. Thus we get the limit in (3.7) as

$$
\begin{equation*}
\lim _{n \rightarrow \infty} \mathbb{E}\left(e^{i t / n X_{n}^{\left(U ; \psi_{0}\right)}}\right)=\int_{-\pi}^{\pi}\left\langle\widehat{\psi}_{0}(k), S(k) e^{i D^{\prime}(k) t} S(k)^{*} \widehat{\psi}_{0}(k)\right\rangle_{\mathbb{C}^{3}} d k \tag{3.10}
\end{equation*}
$$

Thus we have for the weak limit $Z^{\left(U ; \psi_{0}\right)}$ of $X_{n}^{\left(U ; \psi_{0}\right)} / n$

$$
\begin{equation*}
\mathbb{E}\left(e^{i t Z^{\left(U ; \psi_{0}\right)}}\right)=\left\langle\widehat{\psi}_{0}, e^{i t B} \widehat{\psi}_{0}\right\rangle_{\widehat{\mathcal{H}}} \tag{3.11}
\end{equation*}
$$

with $B$ defined in (3.4).
Now suppose that the eigenvalues (and eigenvectors) have finite exceptional points where they are not continuously differentiable. Let $\mathbb{K}^{\prime}$ be the set $\mathbb{K}$ excluding
the finite exceptional points. By using the trick in (3.8) and (3.9), we see that

$$
\begin{aligned}
\mathbb{E}\left(e^{\left.i t / n X_{n}^{\left(U ; \psi_{0}\right)}\right)=}\right. & \int_{\mathbb{K}^{\prime}}\left\langle\widehat{\psi}_{0}(k), e^{-i n H(k)} e^{i n H(k+t / n)} \widehat{\psi}_{0}(k+t / n)\right\rangle_{\mathbb{C}^{3}} d k \\
= & \int_{\mathbb{K}^{\prime}}\left\langle\widehat{\psi}_{0}(k), S(k) e^{i D^{\prime}\left(k_{2}\right) t} S(k+t / n)^{*} \widehat{\psi}_{0}(k+t / n)\right\rangle_{\mathbb{C}^{3}} d k \\
& +\int_{\mathbb{K}^{\prime}}\left\langle\widehat{\psi}_{0}(k), S(k) e^{i n D(k)} S(k)^{*}(S(k+t / n)-S(k)) e^{i n D(k+t / n)}\right. \\
& \left.\cdot S(k+t / n)^{*} \widehat{\psi}_{0}(k+t / n)\right\rangle_{\mathbb{C}^{3}} d k \\
= & I_{1}(n)+I_{2}(n)
\end{aligned}
$$

where $k_{2} \in(k, k+t / n)$. Notice that $\lim _{n \rightarrow \infty} S(k+t / n)=S(k)$ and $\lim _{n \rightarrow \infty} \widehat{\psi}_{0}(k+$ $t / n)=\widehat{\psi}_{0}(k)$. Thus by using dominated convergence theorem, we see that

$$
\begin{aligned}
\lim _{n \rightarrow \infty} I_{1}(n) & =\int_{\mathbb{K}^{\prime}}\left\langle\widehat{\psi}_{0}(k), S(k) e^{i D^{\prime}(k) t} S(k)^{*} \widehat{\psi}_{0}(k)\right\rangle_{\mathbb{C}^{3}} d k \\
\lim _{n \rightarrow \infty} I_{2}(n) & =0
\end{aligned}
$$

This ends the proof.
Corollary 3.4. The moments of $\mu^{\left(U ; \psi_{0}\right)}$ are given by

$$
\begin{equation*}
\int_{-\infty}^{\infty} x^{n} \mu^{\left(U ; \psi_{0}\right)}(d x)=\left\langle\widehat{\psi}_{0}, B^{n} \widehat{\psi}_{0}\right\rangle_{\widehat{\mathcal{H}}}, \quad n=0,1, \ldots \tag{3.12}
\end{equation*}
$$

### 3.2. Examples

### 3.2.1. Grover walk

We first consider the Grover walk discussed in Ref. 6. The unitary operator $U$ is given by

$$
U=\frac{1}{3}\left[\begin{array}{rrr}
-1 & 2 & 2 \\
2 & -1 & 2 \\
2 & 2 & -1
\end{array}\right]
$$

The eigenvalues $\gamma_{1}(k), \gamma_{2}(k)$, and $\gamma_{3}(k)$ of $H(k)$ are $\theta(k), 0$, and $-\theta(k)$ with

$$
\cos \theta(k)=-\frac{1}{3}(2+\cos k)
$$

The corresponding normalized eigenvectors are

$$
\left|\Phi_{j}(k)\right\rangle=\sqrt{c_{k}\left(\gamma_{j}(k)\right)}\left[\begin{array}{c}
\frac{1}{1+e^{i\left(\gamma_{j}(k)+k\right)}} \\
\frac{1}{1+e^{i\left(\gamma_{j}(k)\right)}} \\
\frac{1}{1+e^{i\left(\gamma_{j}(k)-k\right)}}
\end{array}\right]
$$

where

$$
c_{k}(\gamma)=2\left\{\frac{1}{1+\cos (\gamma-k)}+\frac{1}{1+\cos \gamma}+\frac{1}{1+\cos (\gamma+k)}\right\}^{-1}
$$

Obviously, the eigenvalues and eigenvectors of $H(k)$ are continuously differentiable except at $k=0$.

### 3.2.2. Three-state walk from two-state walk

Let

$$
U_{2}:=\left[\begin{array}{ll}
a & b \\
c & d
\end{array}\right]
$$

be any $2 \times 2$ unitary matrix. Let $a_{22} \in \mathbb{C}$ be any complex number with $\left|a_{22}\right|=1$. Consider the unitary matrix

$$
U:=\left[\begin{array}{ccc}
a & 0 & b  \tag{3.13}\\
0 & a_{22} & 0 \\
c & 0 & d
\end{array}\right] .
$$

Let $\lambda_{ \pm}(k)$ be the eigenvalues of the matrix

$$
U_{2}(k):=\left[\begin{array}{cc}
e^{-i k} & 0 \\
0 & e^{i k}
\end{array}\right]\left[\begin{array}{ll}
a & b \\
c & d
\end{array}\right] .
$$

Then it is not hard to see that the eigenvalues of

$$
U(k):=\left[\begin{array}{ccc}
e^{-i k} & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & e^{i k}
\end{array}\right]\left[\begin{array}{ccc}
a & 0 & b \\
0 & a_{22} & 0 \\
c & 0 & d
\end{array}\right]
$$

are $\lambda_{ \pm}(k)$ and $a_{22}$. In fact, if $e_{ \pm}(k)=\left[\begin{array}{ll}a_{1}^{ \pm}(k) & a_{2}^{ \pm}(k)\end{array}\right]^{T}$ are the eigenvectors of $U_{2}(k)$ corresponding to the eigenvalues $\lambda_{ \pm}(k)$, then the eigenvectors of $U(k)$ corresponding to the eigenvalues $\lambda_{ \pm}(k)$ are given by $\widetilde{e}_{ \pm}(k):=\left[\begin{array}{lll}a_{1}^{ \pm}(k) & 0 & a_{2}^{ \pm}(k)\end{array}\right]^{T}$. And the eigenvector corresponding to the eigenvalue $a_{22}$ is $\left[\begin{array}{ccc}0 & 1 & 0\end{array}\right]^{T}$. The eigenvalues $\lambda_{ \pm}(k)$ and eigenvectors $e_{ \pm}(k)$ are continuously differentiable on $\mathbb{K}$, see e.g., Ref. 10.

## 4. Localization

In the two examples of the previous section, the eigenvalues of the operator $U(k)$ contain a constant, not depending on $k$. This results in a term that does not depend on the variable $t$ in the characteristic function $\varphi^{\left(U ; \psi_{0}\right)}(t)$ of $\mu^{\left(U ; \psi_{0}\right)}$. That is, the measure $\mu^{\left(U ; \psi_{0}\right)}$ has a portion of Dirac measure at the origin. This phenomenon has already been observed in other papers, see Refs. 3, 15, 18-20. In particular, in Refs. 18 and 20, the authors investigated the deformations of the Grover walk persisting to the stability of the point spectrum.

### 4.1. Localization

In this subsection, we thoroughly investigate the localization of the three-state QWs. Before going further, we remark that in the literature the localization is sometimes understood in the following sense ${ }^{3,6,15,19}$ :

$$
\begin{equation*}
\lim _{n \rightarrow \infty} \mathbb{P}\left(X_{n}^{\left(U, \psi_{0}\right)}=x\right)>0 \quad \text { for some } x \in \mathbb{Z} \tag{4.1}
\end{equation*}
$$

But, since we consider the scaled limit, the localization, when it occurs, is observed only as a Dirac measure at the origin. Moreover, as we will see later, localization depends not only on the unitary matrix $U$ that generates the QW but also on the initial conditions. Therefore, we make a precise definition of localization as follows.

Definition 4.1. Let us consider the QW driven by a unitary matrix $U$. We say that the QW has a strong localization if there is an initial state $\psi_{0}$ such that the relation (4.1) holds. We say that it has a weak localization if there is an initial state $\psi_{0}$ such that the weak limit $\mu^{\left(U ; \psi_{0}\right)}$ of the distribution $X_{n}^{\left(U ; \psi_{0}\right)} / n$ has a portion of Dirac measure at the origin. That is, we have a decomposition:

$$
\begin{equation*}
\mu^{\left(U ; \psi_{0}\right)}=\alpha \delta_{0}+(1-\alpha) \mu_{1} \tag{4.2}
\end{equation*}
$$

with $\alpha>0$.
Remark 4.2. As mentioned above, since we are considering the localization through scaled limit, by localization in this paper we always mean a weak localization and we omit the prefix "weak" for simplicity. However, in Theorem 4.10, it will be seen that the two concepts of localization are equivalent.

As mentioned before the existence of constant eigenvalue for $U(k)$ is closely related to the localization. Before investigating it we study when it has a constant eigenvalue.

Lemma 4.3. The unitary operator $U(k)$ has an eigenvalue $\lambda_{0}$ not depending on $k$ if and only if $\lambda_{0}$ satisfies the following two equations simultaneously.

$$
\begin{gathered}
a_{11} \lambda_{0}=d \overline{a_{33}} \\
\lambda_{0}^{3}-a_{22} \lambda_{0}^{2}+d \overline{a_{22}} \lambda_{0}-d=0
\end{gathered}
$$

Proof. We can rewrite the characteristic equation (3.2) as follows:

$$
\begin{equation*}
e^{-i k}\left(d \overline{a_{33}} \lambda-a_{11} \lambda^{2}\right)+e^{i k}\left(d \overline{a_{11}} \lambda-a_{33} \lambda^{2}\right)+\left(\lambda^{3}-a_{22} \lambda^{2}+d \overline{a_{22}} \lambda-d\right)=0 \tag{4.3}
\end{equation*}
$$

By the linear independence of the functions $\left\{e^{-i k}, e^{i k}, 1\right\}$ we see that Eq. (4.3) has a constant solution $\lambda_{0}$ if and only if it satisfies the equations in the statement of the lemma and $d \overline{a_{11}} \lambda-a_{33} \lambda^{2}=0$, but the last equation is equivalent to $d \overline{a_{33}} \lambda-$ $a_{11} \lambda^{2}=0$, and we are done.

The following proposition gives an equivalent condition to Lemma 4.3 in terms of matrix components of $U$, which is easier to check when the localization occurs.

Proposition 4.4. The unitary matrix $U(k)$ has a constant eigenvalue $\lambda_{0}$ if and only if the following equations are satisfied:

$$
\begin{aligned}
a_{11} \lambda_{0} & =d \overline{a_{33}}, \\
{\overline{a_{33}}}^{2} a_{12} a_{21} & =a_{11}^{2} \overline{a_{23}} \overline{a_{32}} .
\end{aligned}
$$

Proof. Suppose that $\lambda_{0}$ is a constant eigenvalue of $U(k)$. We may assume $a_{11} \neq$ $0 \neq a_{33}$. By Lemma $4.3 \lambda_{0}=d \overline{a_{33}} / a_{11}$ solves the second equation in Lemma 4.3:

$$
d^{3}\left(\frac{\overline{a_{33}}}{a_{11}}\right)^{3}-a_{22} d^{2}\left(\frac{\overline{a_{33}}}{a_{11}}\right)^{2}+d^{2} \overline{a_{22}} \frac{\overline{a_{33}}}{a_{11}}-d=0
$$

Multiplying by $a_{11}^{3}$ and factorizing we get

$$
d{\overline{a_{33}}}^{2}\left(d \overline{a_{33}}-a_{22} a_{11}\right)+a_{11}^{2}\left(d \overline{a_{22}} \overline{a_{33}}-a_{11}\right)=0 .
$$

Using the relations $d \overline{a_{33}}-a_{22} a_{11}=-a_{12} a_{21}$ and $d \overline{a_{22}} \overline{a_{33}}-a_{11}=d \overline{a_{23}} \overline{a_{32}}$ (which hold by the unitarity of $U$ ) we get the second relation in the statement. Conversely, if the two equations in the statement are satisfied, by reversing the argument, we see that $\lambda_{0}=d \overline{a_{33}} / a_{11}$ solves the equations in Lemma 4.3.

Let us turn our attention to the localization of the three-state QW. It is convenient to rewrite the moment generating operator in (3.3) in the following form:

$$
\begin{equation*}
e^{i t B}=S(k)\left(e^{i t \gamma_{1}^{\prime}(k)} P_{1}+e^{i t \gamma_{2}^{\prime}(k)} P_{2}+e^{i t \gamma_{3}^{\prime}(k)} P_{3}\right) S(k)^{*}, \tag{4.4}
\end{equation*}
$$

where $P_{i}, i=1,2,3$, are mutually commuting projections:

$$
P_{1}=\left[\begin{array}{lll}
1 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{array}\right], \quad P_{2}=\left[\begin{array}{lll}
0 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 0
\end{array}\right], \quad P_{3}=\left[\begin{array}{lll}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 1
\end{array}\right] .
$$

The following is a simple extension of Riemann-Lebesgue lemma.
Lemma 4.5. Suppose that $u(x)$ is differentiable and increasing (or decreasing) on an interval $(a, b)$ and $g(x)$ is integrable on $(a, b)$. Then,

$$
\lim _{t \rightarrow \infty} \int_{a}^{b} e^{i t u(x)} g(x) d x=0
$$

Proof. Take a change of variable $y=u(x)$ and use Riemann-Lebesgue lemma.

Theorem 4.6. The three-state $Q W$ driven by a unitary matrix $U$ has a localization if and only if the matrix $U(k)$ has a constant eigenvalue.

Proof. Suppose that the three-state QW has a localization. Then $\mu^{\left(U ; \psi_{0}\right)}$ has a decomposition as in (4.2) with $\alpha>0$. By (3.3) and (4.4) we have

$$
\begin{equation*}
\varphi^{\left(U ; \psi_{0}\right)}(t)=\left\langle\widehat{\psi}_{0}(k), S(k)\left(e^{i t \gamma_{1}^{\prime}(k)} P_{1}+e^{i t \gamma_{2}^{\prime}(k)} P_{2}+e^{i t \gamma_{3}^{\prime}(k)} P_{3}\right) S(k)^{*} \widehat{\psi}_{0}(k)\right\rangle_{\widehat{\mathcal{H}}} \tag{4.5}
\end{equation*}
$$

Since the limit measure has a portion of Dirac delta measure at the origin, from the formula (4.5) we can see that at least one of $\gamma_{i}(k)$ 's must be constant on a subinterval of $\mathbb{K}$. In fact, suppose the converse. Then on the intervals where $\gamma_{i}^{\prime}(k), i=1,2,3$, are constant (which are nonzero if the case occurs in any way), the R.H.S. of (4.5) results in an oscillating function of $t$. On the remaining region, $\gamma_{i}^{\prime}(k)$ 's are increasing or decreasing and in the limit $t \rightarrow \infty$ they converge to 0 by Lemma 4.5. Thus there is no term corresponding to the Dirac measure at the origin. Therefore there must be a subinterval $I \subset[0,2 \pi]$ on which one of $\gamma_{i}^{\prime}(k)$ 's, say $\gamma_{2}^{\prime}(k)$, is zero, that is, $\gamma_{2}(k)$ is a constant $\gamma_{2}$ on $I$. Notice that the functions $\left\{e^{-i k}, 1, e^{i k}\right\}$, considered to be defined on $I$, are linearly independent. Thus by the argument used in the proof of Lemma $4.3 \gamma_{2}$ solves the two equations in the statement of Lemma 4.3. But this in fact shows that $\gamma_{2}$ is a constant eigenvalue of $U(k)$ by that lemma.

Now suppose that $U(k)$ has a constant eigenvalue, say $\gamma_{2}:=\gamma_{2}(k)$ is a constant. Let us define the weights of the initial state to the direction of the eigenvectors by

$$
\begin{equation*}
\alpha_{i}:=\left\langle\widehat{\psi}_{0}(k), S(k) P_{i} S(k)^{*} \widehat{\psi}_{0}(k)\right\rangle_{\widehat{\mathcal{H}}}, \quad i=1,2,3 . \tag{4.6}
\end{equation*}
$$

Notice that $\alpha_{i} \geq 0$ and $\sum_{i=1}^{3} \alpha_{i}=1$. Let $\psi_{0}$ be any initial state such that $\alpha_{2}>0$, i.e. the weight of $\psi_{0}$ to the direction of the eigenvector corresponding to the eigenvalue $\gamma_{2}$ is positive. Let $\varphi(t):=\varphi^{\left(U ; \psi_{0}\right)}(t)$ be the characteristic function of the distribution $\mu^{\left(U ; \psi_{0}\right)}$. Since $\gamma_{2}^{\prime}(k)=0$, by (3.3) and (4.4) we have a decomposition:

$$
\begin{equation*}
\varphi(t)=\alpha_{2}+\left(1-\alpha_{2}\right) \varphi_{1}(t) \tag{4.7}
\end{equation*}
$$

where

$$
\begin{equation*}
\varphi_{1}(t)=\frac{1}{1-\alpha_{2}}\left\langle\widehat{\psi}_{0}(k), S(k)\left(e^{i t \gamma_{1}^{\prime}(k)} P_{1}+e^{i t \gamma_{3}^{\prime}(k)} P_{3}\right) S(k)^{*} \widehat{\psi}_{0}(k)\right\rangle_{\widehat{\mathcal{H}}} . \tag{4.8}
\end{equation*}
$$

(In the case $\alpha_{2}=1$, we have $\varphi(t)=1$ and the measure $\mu^{\left(U ; \psi_{0}\right)}$ is just a Dirac measure $\delta_{0}$.) Notice that the constant 1 is a characteristic function of Dirac measure $\delta_{0}$ and it is easy to see that $\varphi_{1}(t)$ is a characteristic function of a probability measure, say $\mu_{1}$. Therefore we obtained a decomposition

$$
\begin{equation*}
\mu^{\left(U ; \psi_{0}\right)}=\alpha_{2} \delta_{0}+\left(1-\alpha_{2}\right) \mu_{1} . \tag{4.9}
\end{equation*}
$$

We have shown that the QW has a localization and the proof is complete.
Example 4.7. Generalizing the Grover walk, Machida considered the following parametrized family of unitaries for three-state quantum walk ${ }^{15}$ :

$$
U=U(\theta):=\left[\begin{array}{ccc}
-\frac{1+c}{2} & \frac{s}{\sqrt{2}} & \frac{1-c}{2}  \tag{4.10}\\
\frac{s}{\sqrt{2}} & c & \frac{s}{\sqrt{2}} \\
\frac{1-c}{2} & \frac{s}{\sqrt{2}} & -\frac{1+c}{2}
\end{array}\right]
$$

where $c:=\cos \theta$ and $s:=\sin \theta$ for $\theta \in[0,2 \pi)$. Machida has shown that for all value $\theta \in[0,2 \pi)$, the unitary $U(k)$ has a constant eigenvalue 1 . He has also shown that for the value $\theta_{0}=\sin ^{-1}\left(-\frac{2 \sqrt{2}}{3}\right)+2 \pi$ the 3 -state quantum walk generated by $U\left(\theta_{0}\right)$ with initial condition $1 / \sqrt{3}[1,1,1]^{T}$ does not have a localization. One can show that in this case $\alpha_{2}=0$ in (4.6).

Example 4.8. (i) The two examples in Sec. 3.2 satisfy the conditions in Proposition 4.4. Hence by Theorem 4.6 the localizations occur in the examples. In fact, we can easily find initial conditions starting at the origin such that their weights to the direction of the constant eigenvector are positive, for instance we take $\psi_{0}=[0,1,0]^{T}$.
(ii) Consider a unitary matrix

$$
U=\left[\begin{array}{lll}
0 & 1 & 0 \\
1 & 0 & 0 \\
0 & 0 & 1
\end{array}\right]
$$

In this case

$$
U(k)=\left[\begin{array}{ccc}
0 & e^{-i k} & 0 \\
1 & 0 & 0 \\
0 & 0 & e^{i k}
\end{array}\right]
$$

and the eigenvalues of $U(k)$ are $e^{i k}, e^{-i k / 2}$ and $-e^{-i k / 2}$. Thus by Theorem 4.6 the QW generated by $U$ has no localization. See Fig. 1.

(a)

Fig. 1. (a) Grover walk, (b) three-state walk from two-state Hadamard walk, (c) Ex. 4.8 (ii).


Fig. 1. (Continued)

### 4.2. Localization and the eigenvectors

In the previous subsection we discussed localization in the viewpoint of eigenvalues. We observed that a localization occurs if and only if the matrix $U(k)$ has a constant eigenvalue. In this subsection we would like to see it in the viewpoint of eigenvectors. Let us denote the unitary operation for the QW given in (2.14) by $\widetilde{U}$. That is, the $n$-step walk is given by

$$
\begin{equation*}
\psi_{n}=\tilde{U}^{n} \psi_{0} \tag{4.11}
\end{equation*}
$$

We notice that $\widetilde{U}$ is the inverse image of the unitary $U(k)$ under the inverse Fourier transform. We say that a vector $\psi=(\psi(x))_{x \in \mathbb{Z}} \in l^{2}(\mathbb{Z}) \otimes \mathbb{C}^{3}$ is local or localized
if $\psi(x)=0$ except for finitely many $x \in \mathbb{Z}$. The following is a main result of this subsection.

Theorem 4.9. A three-state $Q W$ driven by the unitary matrix $U$ has a localization if and only if the unitary $\widetilde{U}$ has a localized eigenvector.

Proof. Sufficiency is easy to show. Suppose that $\widetilde{U}$ has a localized eigenvector. Let us run a QW with an initial state of local eigenvector. Then for all $n$, since the walk never diffuse, the limit distribution for $\psi_{n} / n$ is just a Dirac measure $\delta_{0}$.

We now show the necessity. Suppose that there occurs a localization in the walk. By Theorem 4.6 the matrix $U(k)$ has a constant eigenvalue which is given by $\lambda_{0}=d \overline{a_{33}} / a_{11}$ by Proposition 4.4. Let $\widehat{\xi}(k):=\left[\widehat{\xi}_{1}(k), \widehat{\xi}_{2}(k), \widehat{\xi}_{3}(k)\right]^{T}$ be the corresponding eigenvector. We solve the eigenvector equation:

$$
\left(U(k)-\lambda_{0}\right) \widehat{\xi}(k)=0
$$

After some computation, by utilizing the translation invariance of the walk, we can see that the (un-normalized) eigenvector is an element of

$$
\begin{equation*}
\mathcal{H}_{\mathrm{loc}}:=\operatorname{span}\left\{\widehat{\xi}_{m} \in \widehat{\mathcal{H}}: m \in \mathbb{Z}\right\} \tag{4.12}
\end{equation*}
$$

Here $\widehat{\xi}_{m}(k):=e^{i m k} \widehat{\xi}_{0}(k)$ and $\widehat{\xi}_{0}(k)$ has the form:

$$
\widehat{\xi}_{0}(k)=e^{-i k} \lambda_{0}\left[\begin{array}{c}
-a_{12}  \tag{4.13}\\
a_{11} \\
0
\end{array}\right]+\left[\begin{array}{c}
\phi_{1} \\
\phi_{2} \\
\phi_{3}
\end{array}\right]+e^{i k} \lambda_{0}\left[\begin{array}{c}
0 \\
a_{33} \\
-a_{32}
\end{array}\right]
$$

where

$$
\left[\begin{array}{l}
\phi_{1} \\
\phi_{2} \\
\phi_{3}
\end{array}\right]=\left[\begin{array}{c}
a_{33} a_{12}-a_{13} a_{32} \\
-\lambda_{0}^{2}-a_{11} a_{33}+a_{31} a_{13} \\
a_{11} a_{32}-a_{31} a_{12}
\end{array}\right]=-\left[\begin{array}{c}
d \overline{a_{21}} \\
\lambda_{0}^{2}+d \overline{a_{22}} \\
d \overline{a_{23}}
\end{array}\right] .
$$

The inverse Fourier transform $\xi_{0}$ of $\widehat{\xi}_{0}$ is given by

$$
\begin{equation*}
\xi_{0}=\left(\left[\xi_{1}(x), \xi_{2}(x), \xi_{3}(x)\right]^{T}\right)_{x \in \mathbb{Z}} \tag{4.14}
\end{equation*}
$$

with

$$
\begin{align*}
& \xi_{1}(x)=\delta_{-1}(x)\left(-\lambda_{0} a_{12}\right)+\delta_{0}(x) \phi_{1} \\
& \xi_{2}(x)=\delta_{-1}(x)\left(\lambda_{0} a_{11}\right)+\delta_{0}(x) \phi_{2}+\delta_{1}(x)\left(\lambda_{0} a_{33}\right)  \tag{4.15}\\
& \xi_{3}(x)=\delta_{0}(x) \phi_{3}+\delta_{1}(x)\left(-\lambda_{0} a_{32}\right) \tag{4.16}
\end{align*}
$$

Now we see that $\xi_{0}$ (and also all the inverse Fourier transforms of $\widehat{\xi}_{m}$ 's) is a localized vector. By taking an initial state from the space $\mathcal{H}_{\text {loc }}$, we would get a localization. The proof is complete.

In Fig. 2, the evolution of the walk operated on a localized eigenvector is depicted graphically.


Fig. 2. The vectors $[1,0,0]^{T}$ and $[0,0,1]^{T}$ are depicted as left and right arrows, respectively. The self loop corresponds to $[0,1,0]^{T}$.

Combining Theorems 4.6 and 4.9 we can show that the two concepts of localization, strong and weak, are equivalent.

Theorem 4.10. In the three-state $Q W$ driven by a unitary matrix $U$, the weak localization and the strong localization are equivalent.

Proof. Suppose that the weak localization occurs. By Theorem 4.9 the operator $\widetilde{U}$ has a localized eigenvector. If we take it as an initial state for the walk, then it is obvious that the strong localization occurs. On the other hand, suppose that the strong localization occurs with an initial condition $\psi_{0}$. Then there is a $j \in \mathbb{Z}$ such that $\lim _{n \rightarrow \infty} P\left(X_{n}^{\left(U ; \psi_{0}\right)}=j\right)=c>0$. It is obvious to see that the limit measure $\mu^{\left(U ; \psi_{0}\right)}$ has a portion of Dirac measure at the origin with weight at least $c$, which says that the weak localization holds.

Example 4.7 and the next example show that when we say localization it is indispensable to mention the initial conditions.

Example 4.11. Consider the following unitary matrix for a 3-state QW:

$$
U:=\left[\begin{array}{lll}
0 & 0 & 1  \tag{4.17}\\
0 & 1 & 0 \\
1 & 0 & 0
\end{array}\right]
$$

The matrix $U(k)$ has constant eigenvalues $\pm 1$. Let us consider the initial condition $\psi_{0}:=[\alpha, \beta, \gamma]^{T}$ with all nonzero components starting at the origin. The walk does not escape the region $\{-1,0,1\}$. Thus we get $\mu^{\left(U ; \psi_{0}\right)}=\delta_{0}$ and the weak localization holds. But, there is no point $x \in \mathbb{Z}$ such that $\lim _{n \rightarrow \infty} \mathbb{P}\left(X_{n}^{\left(U ; \psi_{0}\right)}=x\right)>0$. However, let us consider the other initial condition

$$
\xi_{0}:=\left(\xi_{0}(x)\right)_{x \in \mathbb{Z}},
$$

with

$$
\xi_{0}(x)=\frac{1}{\sqrt{5}}\left(\delta_{-1}(x)[1,0,0]^{T}+\delta_{0}(x)[1,1,1]^{T}+\delta_{1}(x)[0,0,1]^{T}\right)
$$

We can easily check that $\xi_{0}$ is an eigenvector of $\widetilde{U}$ corresponding to the eigenvalue 1 and so $\lim _{n \rightarrow \infty} P\left(X_{n}^{\left(U ; \xi_{0}\right)}=x\right)>0$ for $x=-1,0,1$. That is, the strong localization holds.

### 4.3. Density functions

In this subsection we characterize the properties of the second term in (4.7), i.e. we find distributions that have characteristic functions $\varphi_{1}(t)$. It turns out that it is possible to get the density functions but it looks rather complicated, in some special cases we get a nice density function. Before going into typical examples we draw some general notions. In this subsection we assume that the walk has a localization at the origin, equivalently, we assume the $U(k)$ has a constant eigenvalue. By Proposition 4.4 we have $\left|a_{11}\right|=\left|a_{33}\right|=: r$.

Let $U(k)$ has eigenvalues $e^{i \gamma_{1}(k)}, e^{i \gamma_{3}(k)}$, and a constant $\lambda_{0}=d \overline{a_{33}} / a_{11}=$ : $e^{i\left(\delta-2 \sigma_{+}\right)}$, where we have put $\delta:=\arg d$ and $\sigma_{+}:=\frac{1}{2}\left(\arg a_{11}+\arg a_{33}\right)$. From the relation $d=\operatorname{det} U(k)=e^{i\left(\gamma_{1}(k)+\delta-2 \sigma_{+}+\gamma_{3}(k)\right)}$ we get

$$
\begin{equation*}
\gamma_{3}(k)=2 \sigma_{+}-\gamma_{1}(k) \tag{4.18}
\end{equation*}
$$

Now let us denote $\sigma_{-}:=\frac{1}{2}\left(\arg a_{11}-\arg a_{33}\right)$. From the relation $\operatorname{Tr}(U(k))=e^{i \gamma_{1}(k)}+$ $e^{i\left(\delta-2 \sigma_{+}\right)}+e^{i \gamma_{3}(k)}=a_{11} e^{-i k}+a_{22}+a_{33} e^{i k}$, using (4.18) we get the relation

$$
\begin{equation*}
\cos \left(\gamma_{1}(k)-\sigma_{+}\right)=r \cos \left(k-\sigma_{-}\right)+\frac{1}{2} e^{-i \sigma_{+}}\left(a_{22}-e^{i\left(\delta-2 \sigma_{+}\right)}\right) . \tag{4.19}
\end{equation*}
$$

By differentiating both sides w.r.t. $k$ we get the relation

$$
\begin{equation*}
\gamma_{1}^{\prime}(k)=\frac{r \sin \left(k-\sigma_{-}\right)}{\sin \left(\gamma_{1}(k)-\sigma_{+}\right)} . \tag{4.20}
\end{equation*}
$$

For convenience, which will be shown later, we take a random initial condition in the following way. Let $\Omega:=\{1,2,3\}$ and $\mathbb{Q}$ be the distribution on $\Omega$ with $\mathbb{Q}(\omega)=$ $1 / 3, \omega=1,2,3$. We denote the random initial condition by $\psi_{0}^{(\omega)}$ with $\psi_{0}^{(1)}=\mathbf{e}_{1}$, $\psi_{0}^{(2)}=\mathbf{e}_{2}, \psi_{0}^{(3)}=\mathbf{e}_{3}$, where $\mathbf{e}_{1}=[1,0,0]^{T}, \mathbf{e}_{2}=[0,1,0]^{T}, \mathbf{e}_{3}=[0,0,1]^{T}$. We call this a "mixed initial state".

We first consider the example of Sec. 3.2.2; a 3-state walk coming from 2-state walk. Notice that in this example the localization occurs.

Proposition 4.12. In the example of Sec. 3.2.2, let us take a random initial condition mentioned above. Then the distribution corresponding to the characteristic function $\varphi_{1}(t)$ in (4.7) has a density of the form:

$$
f_{K}(x ; r):=\frac{\sqrt{1-r^{2}}}{\pi\left(1-x^{2}\right) \sqrt{r^{2}-x^{2}}} 1_{[-r, r]}(x) .
$$

Remark 4.13. We notice that the term $\frac{\sqrt{1-r^{2}}}{\pi\left(1-x^{2}\right) \sqrt{r^{2}-x^{2}}}$ is a typical factor in the density of two-state QWs. ${ }^{4,11,12}$

Proof. (of Proposition 4.12) The constant eigenvalue $\lambda_{0}$ is equal to $a_{22}$. Therefore the last term in (4.19) disappears resulting in:

$$
\begin{equation*}
\cos \left(\gamma_{1}(k)-\sigma_{+}\right)=r \cos \left(k-\sigma_{-}\right) \tag{4.21}
\end{equation*}
$$

Let $\varphi^{(\omega)}(t):=\varphi^{\left(U ; \psi_{0}^{(\omega)}\right)}(t)$ be the characteristic function of the distribution $\mu^{\left(U ; \psi_{0}^{(\omega)}\right)}$. Taking the expectation w.r.t. $\mathbb{Q}$ we get

$$
\begin{align*}
\mathbb{E}^{\mathbb{Q}}\left[\varphi^{(\omega)}(t)\right] & =\mathbb{E}^{\mathbb{Q}}\left[\left\langle\widehat{\psi}_{0}^{(\omega)}(k), e^{i t B} \widehat{\psi}_{0}^{(\omega)}(k)\right\rangle_{\widehat{\mathcal{H}}}\right] \\
& =\frac{1}{6 \pi} \int_{0}^{2 \pi} \operatorname{Tr}\left(e^{i t B} S^{*}(k)\left(\left|\mathbf{e}_{1}\right\rangle\left\langle\mathbf{e}_{1}\right|+\left|\mathbf{e}_{2}\right\rangle\left\langle\mathbf{e}_{2}\right|+\left|\mathbf{e}_{3}\right\rangle\left\langle\mathbf{e}_{3}\right|\right) S(k)\right) d k \\
& =\frac{1}{6 \pi} \int_{0}^{2 \pi}\left(e^{i t \gamma_{1}^{\prime}(k)}+1+e^{i t \gamma_{3}^{\prime}}\right) d k \\
& =\frac{1}{3}+\frac{1}{6 \pi} \int_{0}^{2 \pi}\left(e^{i t \gamma_{1}^{\prime}(k)}+e^{-i t \gamma_{1}^{\prime}(k)}\right) d k \tag{4.22}
\end{align*}
$$

where we have used the relation (4.18) in the last line. Now let us put

$$
\begin{equation*}
x=x(k):=\gamma_{1}^{\prime}(k)=\frac{r \sin \left(k-\sigma_{-}\right)}{\sin \left(\gamma_{1}(k)-\sigma_{+}\right)} . \tag{4.23}
\end{equation*}
$$

From (4.21) and (4.23) we have

$$
\begin{equation*}
\cos ^{2}\left(\gamma_{1}(k)-\sigma_{+}\right)=\frac{r^{2}-x^{2}}{1-x^{2}} \tag{4.24}
\end{equation*}
$$

By direct computation we can see that

$$
\begin{equation*}
x^{\prime}(k)=\frac{\left(1-r^{2}\right) \cos \left(\gamma_{1}(k)-\sigma_{+}\right)}{\left(1-\cos ^{2}\left(\gamma_{1}(k)-\sigma_{+}\right)\right)^{3 / 2}} \tag{4.25}
\end{equation*}
$$

Putting (4.23) into (4.22) and using (4.24)-(4.25) we finally get

$$
\begin{equation*}
\mathbb{E}^{\mathbb{Q}}\left[\varphi^{(\omega)}(t)\right]=\frac{1}{3}+\frac{2}{3} \int_{-r}^{r} e^{i t x} \frac{\sqrt{1-r^{2}}}{\pi\left(1-x^{2}\right) \sqrt{r^{2}-x^{2}}} d x \tag{4.26}
\end{equation*}
$$

This completes the proof.
We next consider another example. Let us rewrite (4.19) as

$$
\begin{equation*}
\cos \left(\gamma_{1}(k)-\sigma_{+}\right)=r \cos \left(k-\sigma_{-}\right)+\eta \tag{4.27}
\end{equation*}
$$

by denoting $\eta=\frac{1}{2} e^{-i \sigma_{+}}\left(a_{22}-e^{i\left(\delta-2 \sigma_{+}\right)}\right)$. Notice that we have $\eta=0$ if and only if the generating unitary matrix is of the form in (3.13).

Proposition 4.14. Suppose that the equality $r=1-|\eta|$ holds. By taking a random initial condition described in this subsection, the distribution corresponding to the characteristic function $\varphi_{1}(t)$ in (4.7) has a density of the form:

$$
f_{K}(x ; \sqrt{r})=\frac{\sqrt{1-r}}{\pi\left(1-x^{2}\right) \sqrt{r-x^{2}}} 1_{[-\sqrt{r}, \sqrt{r}]}(x) .
$$

Proof. The proof parallels that of Proposition 4.12. The key point here is that under the condition given in the proposition we get a factorization and many
computation reduces to simple forms. For example, if $\eta<0$ and we have $r^{2}=$ $(1+\eta)^{2}$, then we can compute to get

$$
x^{2}=\frac{2 \eta+1-\cos \left(\gamma_{1}(k)-\sigma_{+}\right)}{1-\cos \left(\gamma_{1}(k)-\sigma_{+}\right)} .
$$

Now we follow the same lines done in the proof of Proposition 4.12 to finish the proof.

Remark 4.15. (i) Štefaňák et al. ${ }^{19}$ considered the following parametrized coin (unitary) operators which generalize the Grover walk:

$$
U(\rho)=\left[\begin{array}{ccc}
-\rho^{2} & \rho \sqrt{2-2 \rho^{2}} & 1-\rho^{2} \\
\rho \sqrt{2-2 \rho^{2}} & 2 \rho^{2}-1 & \rho \sqrt{2-2 \rho^{2}} \\
1-\rho^{2} & \rho \sqrt{2-2 \rho^{2}} & -\rho^{2}
\end{array}\right], \quad \rho \in(0,1)
$$

It is easy to check that this class of operators fall into the category that satisfies the conditions of Proposition 4.14.
(ii) Machida has also obtained similar continuous measure for the three-state QW generated by a different class of unitary matrices given in Example 4.7. ${ }^{15}$

It is an interesting open question to see whether in the localization setting (see Proposition 4.4) the absolutely continuous part always has an $f_{K}$-type density or not.

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