Convergence theorems on multi-dimensional homogeneous quantum walks

Hiroki Sako¹

Received: 26 August 2019 / Accepted: 14 January 2021 / Published online: 6 March 2021
© The Author(s) 2021

Abstract

We propose a general framework for quantum walks on d -dimensional spaces. We investigate asymptotic behavior of these walks. We prove that every homogeneous walks with finite degree of freedom have limit distribution. This theorem can also be applied to every crystal lattice. In this theorem, it is not necessary to assume that the support of the initial unit vector is finite. We also pay attention on 1-cocycles, which is related to Heisenberg representation of time evolution of observables. For homogeneous walks with finite degree of freedom, convergence of averages of 1-cocycles associated with the position observable is also proved.

Keywords Quantum walk · Asymptotic behavior · Convergence theorem · Eigenvalue function

Mathematics Subject Classification 46L99 · 60F05 · 81Q99

1 Introduction

A quantum walk is a dynamical system given by a unitary operator U on a Hilbert space $\mathcal{H}$. The space $\mathcal{H}$ is often associated with some metric spaces like $\mathbb{Z}^d$ and $\mathbb{R}^d$. The first purpose of this paper is to propose a general framework for quantum walks on d -dimensional spaces. See Sect. 2.1. This new framework includes the quantum walks studied in [1–7], and in many other papers.

The second purpose is to observe asymptotic behavior of such walks. For an initial unit vector ξ in $\mathcal{H}$, we obtain a sequence $\{U^t \xi\}_{t \in \mathbb{N}}$ of unit vectors. It gives a sequence of probability measures $\{p_t\}_{t \in \mathbb{N}}$, which is related to the probability interpretation of quantum mechanics. It is proved in Theorem 3.10 that the probability measures are asymptotically concentrated on some small region. This theorem can be applied to

✉ Hiroki Sako
sako@eng.niigata-u.ac.jp

¹ Faculty of Engineering, Niigata University, Nishi-ku, Niigata 950-2181, Japan

walks which is not necessarily space-homogeneous. In this theorem, we need some very weak condition on the walk U called smoothness defined in Sect. 2.2.

The third purpose is to show existence of limit distributions for analytic homogeneous quantum walks with respect to an arbitrary initial unit vector in Theorem 4.3. Analyticity is so mild condition that almost all the known quantum walks satisfy it. For the proof, we study 1-cocycles of such a walk in Sect. 3.1. 1-cocycles are related to Heisenberg representation of time evolution of observables. Let U be a quantum walk acting on a Hilbert space $\mathcal{H}$, and let D be some observable of position. The sequence of observables $\{U^{-t}DU^t\}_t$ stands for the time evolution of the observable D . The sequence $\{c_t = U^{-t}DU^t - D\}_t$ is the most important example of 1-cocycle and is called a logarithmic derivative.

For more than 20 years, the most important subject of quantum walks is the following form of unitary operator:

$$U = \begin{pmatrix} S & 0 \\ 0 & S^{-1} \end{pmatrix} \begin{pmatrix} \alpha & -\bar{\beta} \\ \beta & \bar{\alpha} \end{pmatrix} \quad (1)$$

and their higher-dimensional version. Here, α and β are complex numbers satisfying $|\alpha|^2 + |\beta|^2 = 1$, and the operator S is the bilateral shift on the Hilbert space $\ell_2(\mathbb{Z})$ consisting of the square summable functions on the integer group $\mathbb{Z}$. The operator U acts on the Hilbert space $\ell_2(\mathbb{Z}) \otimes \mathbb{C}^2$. It has been already shown that several kinds of space-homogeneous quantum walks have limit distributions $\lim_{t \rightarrow \infty} p_t$. Although their argument was not rigorous, Grimmett, Janson, and Scudo presented an excellent idea to show such a convergence theorem in [3]. This paper improves their result in the following aspects:

- Our paper clarifies what kind of property of the operator U really works in the proof of the convergence theorem. It turns out that analyticity of the operator works.
- We no longer need smooth eigenvalue functions of the inverse Fourier transform of the quantum walk.¹
- Our theorem can be applied to many kinds of homogeneous quantum walks, because analyticity for the quantum walks is a weak condition. For example, a quantum walk on arbitrary crystal lattice with translation symmetry with finite propagation satisfies this condition.
- Our theorem does not require locality of its initial unit vector.

2 Definition of quantum walks and their regularity

2.1 Definition of multi-dimensional QWs

Throughout this paper, $\mathcal{B}(\mathcal{H})$ stands for the set of all the bounded linear operators on a Hilbert space $\mathcal{H}$.

¹ In fact, it is possible to construct a quantum walk whose eigenvalue function is not smooth. Because we need many pages for the construction, we omit. Our convergence theorem also works for such an example.

Definition 2.1 Let d be a natural number. A triple $(\mathcal{H}, (U^t)_{t \in \mathbb{Z}}, E)$ is said to be a d -dimensional quantum walk, if the following conditions hold:

- (1) $\mathcal{H}$ is a Hilbert space,
- (2) $(U^t)_{t \in \mathbb{Z}}$ is a unitary representation of $\mathbb{Z}$ on $\mathcal{H}$.
- (3) E is a Borel measure on $\mathbb{R}^d$ whose values are orthogonal projections in $\mathcal{B}(\mathcal{H})$ such that $E(\mathbb{R}^d) = \text{id}_{\mathcal{H}}$.

The measure E in the last item is called a spectral measure.

In many references, researchers concentrate on quantum walks on the Hilbert space $\ell_2(\mathbb{Z}^d) \otimes \mathbb{C}^d$.

Example 2.2 For the Hilbert space $\ell_2(\mathbb{Z}^d) \otimes \mathbb{C}^d$, the measure E is defined as follows: For every subset $\Omega \subset \mathbb{R}^d$, the operator $E(\Omega)$ is the orthogonal projection from $\ell_2(\mathbb{Z}^d) \otimes \mathbb{C}^d$ onto $\ell_2(\Omega \cap \mathbb{Z}^d) \otimes \mathbb{C}^d$. A unitary operator U on $\ell_2(\mathbb{Z}^d) \otimes \mathbb{C}^d$ defines a triplet $(\mathcal{H}, (U^t)_{t \in \mathbb{Z}}, E)$, which we call a *quantum walk* in this paper. $\square$

Throughout this paper, we often make use of the following items.

- For $i \in \{1, \dots, d\}$, a self-adjoint operator D_i on $\mathcal{H}$ is defined by

$$D_i = \int_{(x_i) \in \mathbb{R}^d} x_i E(dx_1 \cdots dx_i \cdots dx_d).$$

- We denote by $(\cdot, \cdot)$ the standard real-valued inner product on $\mathbb{R}^d$. The projection-valued measure E gives a unitary representation of $\mathbb{R}^d$:

$$\sigma : \mathbf{k} \mapsto \int_{\mathbf{x} \in \mathbb{R}^d} \exp(\mathbf{i}(\mathbf{k}, \mathbf{x})) E(d\mathbf{x}).$$

This representation is given by $\sigma((k_i)_i) = \prod_{i=1}^d \exp(\mathbf{i}k_i D_i)$. The representation σ is continuous with respect to the strong operator topology. Throughout this paper, $\mathbf{i}$ stands for the imaginary unit, and i is a natural number.

- We denote by $\alpha_{\mathbf{k}}$ the d -parameter automorphism group on $\mathcal{B}(\mathcal{H})$ defined by

$$\alpha_{\mathbf{k}}(X) = \sigma(\mathbf{k}) X \sigma(-\mathbf{k}).$$

In many cases, D_i stands for the position observable. However, Definition 2.1 allows us to treat quantum walks in more flexible manner. The self-adjoint operator D_i can be other quantum mechanical observables like momentum.

2.2 Regularity on bounded operators

Definition 2.3 Let X be a bounded operator on $\mathcal{H}$. The operator X is said to be uniform with respect to E , if the mapping $\mathbb{R}^d \ni \mathbf{k} \mapsto \alpha_{\mathbf{k}}(X) \in \mathcal{B}(\mathcal{H})$ is continuous with respect to the operator norm on $\mathcal{B}(\mathcal{H})$.

If the operator X is uniform, then the mapping $\mathbf{k} \mapsto \alpha_{\mathbf{k}}(X)$ is uniformly continuous. It is easy to see that the set of uniform operators is a closed subset $\mathcal{B}(\mathcal{H})$. Using the operator norm on $\mathcal{B}(\mathcal{H})$, we may consider partial derivatives.

Definition 2.4 For $i \in \{1, \dots, d\}$, define the partial derivative $\partial_i(X)$ by the norm limit

$$\partial_i(X) = \lim_{k \rightarrow 0} \frac{\exp(\mathbf{i}k D_i) X \exp(-\mathbf{i}k D_i) - X}{k}, \quad (2)$$

if it exists.

Example 2.5 Let $\ell_2(\mathbb{Z}^d)$ be the Hilbert space of all the square summable functions on $\mathbb{Z}^d$. For $\mathbf{x} \in \mathbb{Z}^d$, denote by $\delta_{\mathbf{x}}$ the definition function of $\{\mathbf{x}\} \subset \mathbb{Z}^d$. Let E be the standard spectral measure on $\mathbb{R}^d$ defined in Example 2.2. Let j be an element of $\{1, \dots, d\}$. Define the unitary operator S_j by $\delta_{\mathbf{x}} \mapsto \delta_{\mathbf{x} + \mathbf{e}_j}$, where $\{\mathbf{e}_1, \dots, \mathbf{e}_j, \dots, \mathbf{e}_d\}$ stands for the standard basis of $\mathbb{Z}^d$.

By the straightforward calculation, for every $\mathbf{k} = (k_1, \dots, k_j, \dots, k_d) \in \mathbb{R}^d$, we have

$$\alpha_{\mathbf{k}}(S_j) = \exp(\mathbf{i}k_j) S_j.$$

Since $\exp(\mathbf{i}k_j)$ is a continuous function on $\mathbb{R}^d$, it turns out that S_j is uniform.

By Eq. (2), for $i \neq j$, we have

$$\partial_i(S_j) = \lim_{k \rightarrow 0} \frac{\exp(\mathbf{i}k D_i) S_j \exp(-\mathbf{i}k D_i) - S_j}{k} = 0.$$

We also have

$$\begin{aligned} \partial_j(S_j) &= \lim_{k_j \rightarrow 0} \frac{\exp(\mathbf{i}k_j D_j) S_j \exp(-\mathbf{i}k_j D_j) - S_j}{k_j} \\ &= \lim_{k_j \rightarrow 0} \frac{\exp(\mathbf{i}k_j) - 1}{k_j} S_j \\ &= \mathbf{i} S_j. \end{aligned}$$

We can also calculate the higher derivatives as above. It follows that the unitary operator S_j is smooth.

In particular, the bilateral shift S on $\ell_2(\mathbb{Z})$ is smooth. $\square$

Example 2.6 Consider the case that $d = 1$. Let U be the most famous 1-dimensional quantum walk presented in Eq. (1) acting on $\ell_2(\mathbb{Z}) \otimes \mathbb{C}^2$. Let E be the standard spectral measure on $\ell_2(\mathbb{Z}) \otimes \mathbb{C}^2$. Since the bilateral shift S on $\ell_2(\mathbb{Z})$ is smooth, U is smooth with respect to E . $\square$

Lemma 2.7 If $\partial_i(X)$ exists, then $X(\text{dom}(D_i)) \subset \text{dom}(D_i)$, and $\partial_i(X)$ is the unique extension of the commutator $[\mathbf{i}D_i, X] = \mathbf{i}(D_i X - X D_i)$ defined on the domain $\text{dom}(D_i)$. For every $\mathbf{k} \in \mathbb{R}^d$, $\partial_i(\alpha_{\mathbf{k}}(X))$ exists and is equal to $\alpha_{\mathbf{k}}(\partial_i(X))$.

Proof The first assertion is well known. See [8, Lemma 2.4] for example. We calculate $\partial_i(\alpha_{\mathbf{k}}(X))$ as follows:

$$\begin{aligned} & \lim_{k \rightarrow 0} \frac{\exp(\mathbf{i}k D_i) \sigma(\mathbf{k}) X \sigma(-\mathbf{k}) \exp(-\mathbf{i}k D_i) - \sigma(\mathbf{k}) X \sigma(-\mathbf{k})}{k} \\ &= \sigma(\mathbf{k}) \lim_{k \rightarrow 0} \frac{\exp(\mathbf{i}k D_i) X \exp(-\mathbf{i}k D_i) - X}{k} \sigma(-\mathbf{k}) = \alpha_{\mathbf{k}}(\partial_i(X)). \end{aligned}$$

□

Definition 2.8 Let X be an operator on $\mathcal{H}$ which is uniform with respect to E . The operator X is said to be smooth with respect to E , if for every sequence $\{i(m)\}$ of $\{1, \dots, d\}$, the higher-order partial derivatives

$$\partial_{i(1)}(X), \quad \partial_{i(2)}(\partial_{i(1)}(X)), \quad \partial_{i(3)}(\partial_{i(2)}(\partial_{i(1)}(X))), \quad \dots$$

exist and are uniform with respect to E .

Lemma 2.9 Suppose that $X, Y \in \mathcal{B}(\mathcal{H})$ are smooth with respect to E . Then, X^* and XY are also smooth and satisfy

$$\partial_i(X^*) = \partial_i(X)^*, \quad \partial_i(XY) = \partial_i(X)Y + X\partial_i(Y)$$

for every $i \in \{1, \dots, d\}$.

Proof By Eq. (2), we have the following equation of limits in norm topology:

$$\begin{aligned} \partial_i(X)^* &= \left(\lim_{k \rightarrow 0} \frac{\exp(\mathbf{i}k D_i) X \exp(-\mathbf{i}k D_i) - X}{k} \right)^* \\ &= \lim_{k \rightarrow 0} \left(\frac{\exp(\mathbf{i}k D_i) X \exp(-\mathbf{i}k D_i) - X}{k} \right)^* \\ &= \lim_{k \rightarrow 0} \frac{\exp(\mathbf{i}k D_i) X^* \exp(-\mathbf{i}k D_i) - X^*}{k} \\ &= \partial_i(X^*). \end{aligned}$$

Therefore, every partial derivatives of X^* exist. Since $\partial_i(X)$ is uniform, its adjoint is also uniform. Repeating this calculation of partial derivatives, every higher derivatives of X^* also exist and are uniform. This means that X^* is also smooth.

Since Y is uniform, the equation

$$Y = \lim_{k \rightarrow 0} \exp(\mathbf{i}k D_i) Y \exp(-\mathbf{i}k D_i)$$

holds. Combining with Eq. (2) for X and for Y , we have

$$\begin{aligned}
\partial_i(X)Y + X\partial_i(Y) &= \partial_i(X) \left(\lim_{k \rightarrow 0} \exp(\mathbf{i}k D_i) Y \exp(-\mathbf{i}k D_i) \right) + X\partial_i(Y) \\
&= \lim_{k \rightarrow 0} \frac{\exp(\mathbf{i}k D_i)XY \exp(-\mathbf{i}k D_i) - X \exp(\mathbf{i}k D_i)Y \exp(-\mathbf{i}k D_i)}{k} \\
&\quad + \lim_{k \rightarrow 0} X \frac{\exp(\mathbf{i}k D_i)Y \exp(-\mathbf{i}k D_i) - Y}{k} \\
&= \lim_{k \rightarrow 0} \frac{\exp(\mathbf{i}k D_i)XY \exp(-\mathbf{i}k D_i) - XY}{k} \\
&= \partial_i(XY).
\end{aligned}$$

Therefore, every partial derivatives of XY exist. Since $\partial_i(X)$, Y , X , $\partial_i(Y)$ are uniform, $\partial_i(XY)$ is also uniform. Repeating this calculation of partial derivatives, every higher derivatives of XY also exist and are uniform. This means that XY is also smooth. $\square$

Definition 2.10 Let X be a bounded operator on $\mathcal{H}$. The operator X is said to be analytic with respect to E , if the mapping $\mathbf{k} \mapsto \alpha_{\mathbf{k}}(X)$ can be extended to a holomorphic mapping defined on a neighborhood

$$\{(\kappa_1, \dots, \kappa_d) \in \mathbb{C}^d \mid -\delta < \operatorname{Im}(\kappa_i) < \delta \text{ for } 1 \leq i \leq d\}$$

of $\mathbb{R}^d$, where δ is some positive number.

Note that every analytic operator is smooth.

Definition 2.11 A d -dimensional quantum walk $(\mathcal{H}, (U^t)_{t \in \mathbb{Z}}, E)$ is said to be uniform (smooth, analytic), if U is uniform (smooth, analytic) with respect to E .

We note that analyticity on quantum walks is so weak that the class contains all the multi-dimensional quantum walks which have been studied.

Example 2.12 Let j be in $\{1, \dots, d\}$. Let S_j be the unitary operator on $\ell_2(\mathbb{Z}^d)$ given by the shift as in Example 2.5. The action $\alpha_{\mathbf{k}}(S_j)$ of $\mathbf{k} = (k_1, \dots, k_d) \in \mathbb{R}^d$ is given by Eq. (3), $\alpha_{\mathbf{k}}(S_j) = \exp(\mathbf{i}k_j)S_j$. This action can be extended to $\mathbf{k} = (k_1, \dots, k_d) \in \mathbb{C}^d$ by $\mathbf{k} \mapsto \exp(\mathbf{i}k_j)S_j$. This map is holomorphic. It follows that S_j is analytic. In particular, the bilateral shift S on $\ell(\mathbb{Z})$ is analytic. Therefore, the most famous 1-dimensional quantum walk presented in Eq. (1) is also analytic.

2.3 Similarity between multi-dimensional QWs

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces. For $i = 1, 2$, let E_i be a Borel measure on $\mathbb{R}^d$ whose values are orthogonal projections in $\mathcal{B}(\mathcal{H}_i)$. Define a new projection-valued measure $E_1 \oplus E_2$ by

$$E_1 \oplus E_2(\Omega) = E_1(\Omega) \oplus E_2(\Omega), \quad \text{a Borel subset } \Omega \subset \mathbb{R}^d$$

A bounded operator $X: \mathcal{H}_1 \rightarrow \mathcal{H}_2$ is said to be *smooth* with respect to E_1 and E_2 , if $\begin{pmatrix} 0 & 0 \\ X & 0 \end{pmatrix}: \mathcal{H}_1 \oplus \mathcal{H}_2 \rightarrow \mathcal{H}_1 \oplus \mathcal{H}_2$ is smooth with respect to $E_1 \oplus E_2$.

Definition 2.13 Two d -dimensional quantum walks $(\mathcal{H}_1, (U_1^t)_{t \in \mathbb{Z}}, E_1), (\mathcal{H}_2, (U_2^t)_{t \in \mathbb{Z}}, E_2)$ are said to be similar, if there exists a unitary operator $V: \mathcal{H}_1 \rightarrow \mathcal{H}_2$ satisfying the following conditions²:

- $VU_1 = U_2V$,
- V is smooth with respect to E_1 and E_2 .

Since V^{-1} is equal to V^* , by Lemma 2.9, similarity between quantum walks is a reflexive relation. To see similarity between quantum walks is transitive, assume that V_1 is a smooth unitary intertwiner from a quantum walk U_1 to a quantum walk U_2 , and that V_2 is a smooth unitary intertwiner from a U_2 to a quantum walk U_3 . Since we have

$$V_2V_1U_1 = V_2U_2V_1 = U_3V_2V_1,$$

V_2V_1 is a unitary intertwiner from U_1 to U_3 . Again by Lemma 2.9, the unitary V_2V_1 is also smooth. It follows that U_1 and U_3 are similar. Therefore, similarity is a equivalence relation. If two quantum walks are similar and if one of the walks is smooth, then the other walk is also smooth.

Remark 2.14 As in Proposition 3.12, if two quantum walks are similar, and if one of them has a limit distribution, then the other walk also has a limit distribution. Then, the limit is the same as that of the other. For the study of limit distributions of a quantum walk U , we can replace it with another walk which is similar to U . For a Hilbert space $\mathcal{H}$ with a d -dimensional coordinate system E , we can modify the information of position in the following sense.

Example 2.15 Let $X \subset \mathbb{R}^d$ is a discrete subset. Consider the case that for every $x \in X$, a Hilbert space $\mathcal{H}_x$ is given. Define a Hilbert space $\mathcal{H}_X$ by $\oplus_{x \in X} \mathcal{H}_x$. Let E_X be the spectral measure on $\mathbb{R}^d$ defined by the following: For $\Omega \subset \mathbb{R}^d$, $E_X(\Omega)$ is the orthogonal projection from $\mathcal{H}_X$ to $\oplus_{x \in \Omega \cap X} \mathcal{H}_x$.

Let $f: X \rightarrow \mathbb{R}^n$ be a map satisfying that there exists a constant $0 < R$ such that for every $x \in X$, the distance between x and $f(x)$ is at most R . The map f stands for the modification of position. Define Y by the image $f(X)$. For $y \in Y$, define $\mathcal{K}_y$ by $\oplus_{x \in f^{-1}(y)} \mathcal{H}_x$. Define $\mathcal{K}_Y$ by $\oplus_{y \in Y} \mathcal{K}_y$. Let E_Y be the spectral measure on $\mathbb{R}^d$ defined by the following: For $\Omega \subset \mathbb{R}^d$, $E_Y(\Omega)$ is the orthogonal projection from $\mathcal{K}_Y$ to $\oplus_{y \in \Omega \cap Y} \mathcal{K}_y$.

Define a unitary V from $\mathcal{H}_X = \oplus_{x \in X} \mathcal{H}_x$ to $\mathcal{K}_Y = \oplus_{y \in Y} \mathcal{K}_y = \oplus_{y \in Y} \oplus_{x \in f^{-1}(y)} \mathcal{H}_x$ by the direct sum of $\text{id}_{\mathcal{H}_x}: \mathcal{H}_x \rightarrow \mathcal{H}_x$. Then, the unitary V is smooth or more strongly analytic with respect to E_X and E_Y .

Let U be a quantum walk acting on $(\mathcal{H}_X, E_X)$. Then, we also have a walk VUV^{-1} acting on $(\mathcal{K}_Y, E_Y)$. Since V is analytic (therefore smooth and uniform), the walk VUV^{-1} is analytic (smooth, or uniform), if and only if U has the same regularity. Proposition 3.12 shows that asymptotic behavior of VUV^{-1} is the same as U .

² In this definition, we require that V is unitary. This condition can be relaxed. It is possible to replace the smooth unitary intertwiner V with a smooth *invertible* intertwiner. These definitions are equivalent. Because its proof is long, we omit the explanation.

We can apply this example to every crystal lattice. Let d be 2 or 3. Assume that $X \subset \mathbb{R}^d$ forms a crystal lattice. More precisely, there exists an additive subgroup $G \subset \mathbb{R}^d$ which is isomorphic to $\mathbb{Z}^d$ such that for every $g \in G$, $g + X = X$. We can choose some bounded fundamental domain $\Xi \subset \mathbb{R}^d$ of the additive action of G on $\mathbb{R}^d$; that is, the family $\{g + \Xi\}_{g \in G}$ is disjoint and its union is $\mathbb{R}^d$. The intersection of Ξ and X stands for the unit of the crystal structure. Choose a point y_0 in Ξ . Define $Y \subset \mathbb{R}^d$ by $\{g + y_0 \mid g \in G\}$. Define $f: X \rightarrow Y$ as follows: For every $x \in (g + \Xi) \cap X$, $f(x) = g + y_0$. This map f stands for the modification of position.

For a quantum walk U on a Hilbert space associated to X , we can consider a quantum walk VUV^{-1} on a Hilbert space associated with Y which is similar to U . In this way, we reduce the study of quantum walks on arbitrary crystal lattice to those on the integer lattice $(G + y_0) \cong \mathbb{Z}^d$. $\square$

3 General theory for asymptotic behavior of quantum walks

3.1 Logarithmic derivatives and their asymptotic behavior

Definition 3.1 Let $(U^t)_{t \in \mathbb{Z}}$ be a unitary representation of $\mathbb{Z}$ on a Hilbert space $\mathcal{H}$. A two-sided sequence $\{c_t\}_{t \in \mathbb{Z}}$ of bounded operators on $\mathcal{H}$ is called a 1-cocycle of $(U^t)_{t \in \mathbb{Z}}$, if for every $s, t \in \mathbb{Z}$, $c_{s+t} = U^{-t}c_sU^t + c_t$.

Lemma 3.2 If $\{c_t\}_{t \in \mathbb{Z}}$ is a 1-cocycle of $(U^t)_{t \in \mathbb{Z}}$, then for every $t \geq 1$, $\|c_t\| \leq t\|c_1\|$.

Proof For every $s, t \in \mathbb{Z}$, we have

$$\|c_{s+t}\| \leq \|U^{-t}c_sU^t\| + \|c_t\| = \|c_s\| + \|c_t\|. \quad (3)$$

Repeating this decomposition, we obtain $\|c_t\| \leq t\|c_1\|$. $\square$

Lemma 3.3 The limit $\lim_{t \rightarrow \infty} \frac{\|c_t\|}{t}$ exists and is less than $\|c_1\|$.

Proof By the inequality (3), the sequence $\{\|c_t\|\}$ is subadditive. For every subadditive sequence $\{\gamma_t\}_{t=1}^\infty$ of real numbers, the sequence $\{\gamma_t/t\}$ converges to its infimum. $\square$

For the rest of this paper, the 1-cocycle associated with the observable of position plays a key role. Let $(\mathcal{H}, (U^t)_{t \in \mathbb{Z}}, E)$ be a d -dimensional smooth quantum walk. Let $\mathbf{w} = (w_i)$ be a vector in $\mathbb{R}^d$. Denote by D the self-adjoint operator

$$\sum_{i=1}^d w_i D_i = \sum_{i=1}^d \int_{(x_i) \in \mathbb{R}^d} w_i x_i E(dx_1 \cdots dx_d).$$

Since U^t is smooth with respect to E , by Lemma 2.7, the commutator of U^t with $\mathbf{i}D_i$ is bounded. It follows that the operator

$$U^{-t}DU^t - D = -\mathbf{i} \sum_{i=1}^d U^{-t}w_i[\mathbf{i}D_i, U^t] \quad (4)$$

uniquely defines a bounded operator c_t on $\mathcal{H}$. We note that the sequence $U^{-t}DU^t$ stands for the time evolution of the observable D in the Heisenberg representation. The two-sided sequence $\{c_t\}_{t \in \mathbb{Z}}$ is a 1-cocycle of $(U^t)_{t \in \mathbb{Z}}$. By Lemma 2.7, and by Eq. (4), the 1-cocycle is equal to ³

$$c_t = -i \sum_i w_i U^{-t} \partial_i(U^t). \quad (5)$$

Definition 3.4 The 1-cocycle $\{c_t = U^{-t}DU^t - D\}$ is called the logarithmic derivatives of the quantum walk $(\mathcal{H}, (U^t)_{t \in \mathbb{Z}}, E)$ with respect to the operator $D = \sum_i w_i D_i$. The operator $\{c_t/t\}$ is called the average of logarithmic derivatives of the quantum walk.

In most cases, the norms of the logarithmic derivatives $\{\|c_t\|\}$ linearly increase. Asymptotic behavior of the average $\{c_t/t\}$ of the logarithmic derivatives is an important tool in the study of limit distribution of the quantum walk (Theorem 4.3). The following proposition means that if two walks are similar, then averages of logarithmic derivatives are similar.

Proposition 3.5 Let $(\mathcal{H}_1, (U_1^t)_{t \in \mathbb{Z}}, E_1)$ and $(\mathcal{H}_2, (U_2^t)_{t \in \mathbb{Z}}, E_2)$ be d -dimensional smooth quantum walks. Let $D_i^{(1)}$ be the self-adjoint operator $\int_{\mathbb{R}^d} x_i E_1(d\mathbf{x})$. Let $D_i^{(2)}$ be the self-adjoint operator $\int_{\mathbb{R}^d} x_i E_2(d\mathbf{x})$. Let $V: \mathcal{H}_1 \rightarrow \mathcal{H}_2$ be a smooth unitary operator which gives similarity between U_1 and U_2 . For $i = 1, \dots, d$, denote by $\partial_i^{(1)}$ the i -th partial derivative with respect to E_1 and denote by $\partial_i^{(2)}$ the i -th partial derivative with respect to E_2 . Then for $i = 1, \dots, d$, the sequence

$$\left\{ \frac{U_2^{-t} \partial_i^{(2)}(U_2^t)}{it} - V \frac{U_1^{-t} \partial_i^{(1)}(U_1^t)}{it} V^{-1} \right\}_t$$

converges to 0 in the norm topology.

Proof By Lemma 2.7, the operator $\frac{U_2^{-t} \partial_i^{(2)}(U_2^t)}{it}$ is equal to the closure of

$$\frac{V U_1^{-t} V^{-1} D_i^{(2)} V U_1^t V^{-1} - D_i^{(2)}}{t}.$$

Since V is smooth with respect to E_1 and E_2 , by Lemma 2.7 for $E_1 \oplus E_2$, the operator $D_i^{(2)} V - V D_i^{(1)}$ is bounded. This means that distance between $V^{-1} D_i^{(2)} V$ and $D_i^{(1)}$ is small. If t is large, the above operator is almost equal to

$$\frac{V U_1^{-t} D_i^{(1)} U_1^t V^{-1} - V D_i^{(1)} V^{-1}}{t} = \frac{V (U_1^{-t} D_i^{(1)} U_1^t - D_i^{(1)}) V^{-1}}{t}.$$

³ The equation is similar to the right-hand side of the following formula in calculus: $(\log f(t))' = f(t)^{-1} f'(t)$. This is the motivation of the definition of the logarithmic derivative.

This is equal to the operator $V \frac{U_1^{-t} \partial_i^{(1)}(U_1^t)}{it} V^{-1}$. $\square$

3.2 General theory for asymptotic behavior of the distribution p_t

For the quantum walk $(\mathcal{H}, (U^t)_{t \in \mathbb{Z}}, E)$, and for a unit vector $\xi \in \mathcal{H}$, a sequence $\{p_t\}_{t \in \mathbb{Z}}$ of Borel probability measures on $\mathbb{R}^d$ is defined by

$$p_t(\Omega) = \langle E(t\Omega)U^t\xi, U^t\xi \rangle, \quad \text{for every Borel subset } \Omega \subset \mathbb{R}^d. \quad (6)$$

The unit vector $\xi \in \mathcal{H}$ is called an *initial vector*. In many concrete examples of homogeneous quantum walks, the existence of the weak limit of $\{p_t\}$ has already been studied. See [4,5,7], for example.

Example 3.6 To see what the measure p_t means, let us look at a quantum walk U acting on $\ell_2(\mathbb{Z}^d) \otimes \mathbb{C}^n$. Take the spectral measure E as in Example 2.2. Express $U^t\xi \in \ell_2(\mathbb{Z}^d) \otimes \mathbb{C}^n$ by $(\Psi_t(\mathbf{x}))_{\mathbf{x} \in \mathbb{Z}^d}$, where $\Psi_t(\mathbf{x})$ is a vector in $\mathbb{C}^n$. By Eq. (6), for every subset Ω of $\mathbb{R}^d$, we have

$$p_t(\Omega) = \sum_{\mathbf{x} \in t\Omega \cap \mathbb{Z}^d} \|\Psi_t(\mathbf{x})\|^2 = \sum_{\mathbf{v} \in \Omega \cap \mathbb{Z}^d/t} \|\Psi_t(t\mathbf{v})\|^2.$$

Therefore, the measure p_t is a sum of scalar multiple of point masses $\{\delta_{\mathbf{v}}\}_{\mathbf{v} \in \mathbb{Z}^d/t}$, and the coefficient of $\delta_{\mathbf{v}}$ is $\|\Psi_t(t\mathbf{v})\|^2$. $\square$

Lemma 3.7 Let f be a bounded Borel function. The mean of f with respect to the measure p_t is given by

$$\int_{\mathbf{v} \in \mathbb{R}^d} f(\mathbf{v}) p_t(d\mathbf{v}) = \left\langle \int_{\mathbf{x} \in \mathbb{R}^d} f\left(\frac{\mathbf{x}}{t}\right) E(d\mathbf{x}) U^t\xi, U^t\xi \right\rangle. \quad (7)$$

Proof In the case that f is a definition function of a Borel subset of $\mathbb{R}^d$, the above equation holds, by the definition of p_t . It follows that for every Borel step function f , the above equation holds. For a general Borel function f , we have only to use a sequence f_n of Borel step functions which are uniformly close to f . $\square$

Definition 3.8 A vector ξ in $\mathcal{H}$ is said to be smooth, if it is in the domain of $D_{i(m)}D_{i(m-1)} \cdots D_{i(1)}$ for every natural number m and for every sequence $\{i(1), \dots, i(m)\}$ of $\{1, \dots, d\}$.

If the quantum walk $(\mathcal{H}, (U^t)_{t \in \mathbb{Z}}, E)$ is smooth and if the initial unit vector ξ is smooth, then $U^t\xi$ is also smooth. The proof is given by Lemma 2.7 and by the Leibniz rule: $D_i(U^t\xi) = -i\partial_i(U^t\xi) + U^t(D_i\xi)$.

Lemma 3.9 Suppose that the quantum walk $(\mathcal{H}, (U^t)_{t \in \mathbb{Z}}, E)$ is smooth and that the vector ξ is smooth. Let t be an arbitrary natural number. Then, every polynomial

function g on $\mathbb{R}^d$ is integrable with respect to p_t , and the integral is given by

$$\int_{\mathbf{v} \in \mathbb{R}^d} g(\mathbf{v}) p_t(d\mathbf{v}) = \left\langle \int_{\mathbf{x} \in \mathbb{R}^d} g\left(\frac{\mathbf{x}}{t}\right) E(d\mathbf{x}) U^t \xi, U^t \xi \right\rangle.$$

Proof We may assume that $g(x_1, x_2, \dots, x_d)$ is of the form $x_{i(m)} x_{i(m-1)} \cdots x_{i(1)}$. In this case, we have

$$\int_{\mathbf{x} \in \mathbb{R}^d} g\left(\frac{\mathbf{x}}{t}\right) E(d\mathbf{x}) = \frac{D_{i(m)}}{t} \cdots \frac{D_{i(1)}}{t}.$$

Since U and ξ are smooth with respect to E , $U^t \xi$ is in the domain of the above self-adjoint operator. Therefore, the right-hand side is well defined. There exists a countable sum $f(\mathbf{v})$ of scalar multiples of definition functions which is Borel and uniformly close to $g(\mathbf{v})$. Then, the difference between

$$\int_{\mathbf{x} \in \mathbb{R}^d} g\left(\frac{\mathbf{x}}{t}\right) E(d\mathbf{x}) \sim \int_{\mathbf{x} \in \mathbb{R}^d} f\left(\frac{\mathbf{x}}{t}\right) E(d\mathbf{x}),$$

is a bounded operator with small operator norm. Therefore, $U^t \xi$ is in the domain of $\int_{\mathbf{x} \in \mathbb{R}^d} f\left(\frac{\mathbf{x}}{t}\right) E(d\mathbf{x})$. For such f , it is easy to show that

$$\int_{\mathbf{v} \in \mathbb{R}^d} f(\mathbf{v}) p_t(d\mathbf{v}) = \left\langle \int_{\mathbf{x} \in \mathbb{R}^d} f\left(\frac{\mathbf{x}}{t}\right) E(d\mathbf{x}) U^t \xi, U^t \xi \right\rangle.$$

Since f is uniformly close to g , the integral $\int_{\mathbf{v} \in \mathbb{R}^d} f(\mathbf{v}) p_t(d\mathbf{v})$ is close to $\int_{\mathbf{v} \in \mathbb{R}^d} g(\mathbf{v}) p_t(d\mathbf{v})$. $\square$

Theorem 3.10 Suppose that the quantum walk $(\mathcal{H}, (U^t)_{t \in \mathbb{Z}}, E)$ is smooth and that the initial unit vector ξ is smooth. There exists a bounded subset K of $\mathbb{R}^d$ such that $\lim_{t \rightarrow \infty} p_t(K) = 1$.

Proof Let i be an arbitrary element of $\{1, \dots, d\}$. Let m be an arbitrary natural number. Note that the equation

$$\int_{(v_1, \dots, v_d) \in \mathbb{R}^d} v_i^m p_t(dv_1 \cdots dv_i \cdots dv_d) = \left\langle \frac{D_i^m}{t^m} U^t \xi, U^t \xi \right\rangle$$

holds, by Lemma 3.9.

The triplet $(\mathcal{H}, (U^t)_{t \in \mathbb{Z}}, D_i)$ is a one-dimensional quantum walk defined in [8, Definition 2.1]. Therefore, we can employ the theory of one-dimensional quantum walks developed in [8]. As proved in [8, Definition 2.27], for every $m \in \mathbb{N}$,

$$\limsup_t \left| \left\langle \frac{D_i^m}{t^m} U^t \xi, U^t \xi \right\rangle \right| \leq \| [D_i, U] \|^m.$$

Take and fix a positive number L_i larger than $\|[D_i, U]\|$. The inequality

$$\limsup_t \left| \int_{(v_1, \dots, v_d) \in \mathbb{R}^d} v_i^m p_t(dv_1 \cdots dv_i \cdots v_d) \right| \leq \|[D_i, U]\|^m.$$

implies that $\lim_t p_t(\mathbb{R}^{i-1} \times [-L_i, L_i] \times \mathbb{R}^{d-i}) = 1$. We conclude that $\lim_t p_t([-L_1, L_1] \times \cdots \times [-L_d, L_d]) = 1$. $\square$

Corollary 3.11 *Suppose that the quantum walk $(\mathcal{H}, (U^t)_{t \in \mathbb{Z}}, E)$ is smooth and that the initial unit vector ξ is smooth. Then, the following conditions are equivalent:*

- (1) (Convergence in Law). *There exists a Borel probability measure p_∞ on $\mathbb{R}^d$ such that for every polynomial function g on $\mathbb{R}^d$*

$$\lim_t \int_{\mathbf{v} \in \mathbb{R}^d} g(\mathbf{v}) p_t(d\mathbf{v}) = \int_{\mathbf{v} \in \mathbb{R}^d} g(\mathbf{v}) p_\infty(d\mathbf{v}).$$

- (2) (Weak convergence). *There exists a Borel probability measure p_∞ on $\mathbb{R}^d$ such that for every bounded continuous function f on $\mathbb{R}^d$*

$$\lim_t \int_{\mathbf{v} \in \mathbb{R}^d} f(\mathbf{v}) p_t(d\mathbf{v}) = \int_{\mathbf{v} \in \mathbb{R}^d} f(\mathbf{v}) p_\infty(d\mathbf{v}).$$

If the above conditions hold, then these limit distributions coincide and their support is compact.

Proof Let K be a compact subset of $\mathbb{R}^d$ in Theorem 3.10. Let ϵ be an arbitrary positive real number. For every polynomial function g on $\mathbb{R}^d$, there exists a bounded continuous function f on $\mathbb{R}^d$ such that $|f(\mathbf{x}) - g(\mathbf{x})| < \epsilon$ for arbitrary $\mathbf{x} \in K$. For every bounded continuous function f on $\mathbb{R}^d$, there exists a polynomial function g on $\mathbb{R}^d$ such that $|g(\mathbf{x}) - f(\mathbf{x})| < \epsilon$ for arbitrary $\mathbf{x} \in K$ by the theorem of Stone–Weierstrass. $\square$

Proposition 3.12 *Let $(\mathcal{H}_1, (U_1^t)_{t \in \mathbb{Z}}, E_1)$, $(\mathcal{H}_2, (U_2^t)_{t \in \mathbb{Z}}, E_2)$ be two d -dimensional smooth quantum walks. Suppose that there exists a smooth unitary operator $V: \mathcal{H}_1 \rightarrow \mathcal{H}_2$ which intertwines U_1 and U_2 . Let ξ be a unit vector in $\mathcal{H}_1$ which is smooth with respect to E_1 . Let $p_t^{(1)}$ be the sequence of probability measures on $\mathbb{R}^d$ given by $(\mathcal{H}_1, (U_1^t)_{t \in \mathbb{Z}}, E_1)$ and ξ . Let $p_t^{(2)}$ be the sequence of probability measures on $\mathbb{R}^d$ given by $(\mathcal{H}_2, (U_2^t)_{t \in \mathbb{Z}}, E_2)$ and $V\xi$. If $p_t^{(1)}$ converges in law, then $p_t^{(2)}$ also converges in law. Furthermore, these limit distributions coincide.*

Proof The proof is substantially the same as that of [8, Theorem 2.31]. $\square$

4 Convergence theorems on homogeneous QWs

4.1 Definition of homogeneous QWs

Definition 4.1 A quadruple $(\mathcal{H}, (U^t)_{t \in \mathbb{Z}}, E, \rho)$ is called a d -dimensional homogeneous quantum walk, if the following conditions hold:

- (1) $(\mathcal{H}, (U^t)_{t \in \mathbb{Z}}, E)$ is a d -dimensional quantum walk.
- (2) $\rho = (\rho(\mathbf{x}))_{\mathbf{x} \in \mathbb{Z}^d}$ is a unitary representation of the additive group $\mathbb{Z}^d$ on $\mathcal{H}$.
- (3) For every Borel subset $\Omega \subset \mathbb{R}^d$, $\rho(\mathbf{x})^{-1} E(\Omega) \rho(\mathbf{x}) = E(\Omega + \mathbf{x})$.
- (4) For every $\mathbf{x} \in \mathbb{Z}^d$, $U \rho(\mathbf{x}) = \rho(\mathbf{x}) U$.
- (5) The rank of $E([0, 1)^d)$ is finite.

The rank of $E([0, 1)^d)$ is called the degree of freedom.

We note that the image of $E([0, 1)^d)$ is the fundamental domain of the action by $(\rho(\mathbf{x}))_{\mathbf{x} \in \mathbb{Z}^d}$. More precisely, $\{\rho(\mathbf{x})(\text{image}(E([0, 1)^d)))\}_{\mathbf{x} \in \mathbb{Z}^d}$ is mutually orthogonal and generates $\mathcal{H}$. We may consider a quadruple satisfying conditions (1), (2), (3), (4) which does not satisfy condition (5). In such a case, we call the quadruple *a homogeneous quantum walk with infinite degree of freedom*.

Let $(\mathcal{H}, (U^t)_{t \in \mathbb{Z}}, E, \rho)$ be a homogeneous quantum walk with finite degree of freedom. We denote by n the degree of freedom. There exists a unitary operator

$$V: \mathcal{H} \rightarrow \ell_2(\mathbb{Z}^d) \otimes \mathbb{C}^n$$

satisfying that V maps $\text{image}(E([0, 1)^n))$ onto $\delta_0 \otimes \mathbb{C}^n$ and that V is compatible with ρ and with the right regular representation $\tilde{\rho}$ on $\ell_2(\mathbb{Z}^d)$. Let $\tilde{E}$ be the projection-valued measure on $\mathbb{R}^d$ defined by

$$\tilde{E}(\Omega) = (\text{the orthogonal projection } \ell_2(\mathbb{Z}^d) \otimes \mathbb{C}^n \rightarrow \ell_2(\mathbb{Z}^d \cap \Omega) \otimes \mathbb{C}^n).$$

It is easy to show that V is smooth with respect to E and $\tilde{E}$. In fact, V is analytic with respect to E and $\tilde{E}$. Thus, we obtain a new homogeneous quantum walk

$$(\ell_2(\mathbb{Z}^d) \otimes \mathbb{C}^n, (V U^t V^{-1})_{t \in \mathbb{Z}}, \tilde{E}, \tilde{\rho}),$$

which is similar to the original walk in the sense of Definition 2.13. If the original walk is smooth, then new one is also smooth. If the original walk is analytic, then new one is also analytic. By Proposition 3.12, if the latter walk has limit distribution (as in Theorem 4.3), the original walk has the same limit distribution.

For the rest of this paper, we study d -dimensional *analytic homogeneous* quantum walks. Without loss of generality, we may concentrate on the homogeneous walks of the form $(\ell_2(\mathbb{Z}^d) \otimes \mathbb{C}^n, (U^t)_{t \in \mathbb{Z}}, \tilde{E}, \tilde{\rho})$.

4.2 The proof of the convergence theorem for homogeneous QWs

We often use the inverse Fourier transform $\mathcal{F}^{-1}: \ell_2(\mathbb{Z}^d) \otimes \mathbb{C}^n \rightarrow L^2(\mathbb{T}_{2\pi}^d) \otimes \mathbb{C}^n$. We express the Pontryagin dual $\mathbb{T}_{2\pi}^d$ of $\mathbb{Z}^d$ by $\{(k_1, \dots, k_d) \mid k_1, \dots, k_d \in \mathbb{R}/(2\pi\mathbb{Z})\}$. Via the inverse Fourier transform $\mathcal{F}^{-1}$,

- The analytic unitary operator U corresponds to a $(d \times d)$ -matrix $\hat{U}$ whose entries are analytic functions on $\mathbb{T}_{2\pi}^d$,

- and the diagonal operator

$$D_i = \int_{\mathbf{x} \in \mathbb{R}^d} x_i \tilde{E}(dx_1 \cdots dx_i \cdots dx_d) : \delta_{\mathbf{x}} \otimes \delta_y \mapsto x_i \delta_{\mathbf{x}} \otimes \delta_y$$

corresponds to the partial differential operator $-\mathbf{i} \frac{\partial}{\partial k_i}$.

Our main result (Theorem 4.3) relies on the following proposition.

Proposition 4.2 *Let $(U^t)_{t \in \mathbb{Z}}$ be a homogeneous analytic quantum walk acting on $\ell_2(\mathbb{Z}^d) \otimes \mathbb{C}^n$. Let $w_1, \dots, w_d$ be real numbers. Denote by D the operator $\sum_i w_i D_i$.*

- (1) *As t tends to infinity, the average $c_t/t = (U^{-t} D U^t - D)/t$ of the logarithmic derivative of $(U^t)_{t \in \mathbb{Z}}$ converges to some self-adjoint operator H in the strong operator topology.*
- (2) *Then, as t tends to infinity, the unitary operators defined by the commutators*

$$U^{-t} \exp\left(\mathbf{i} \frac{D}{t}\right) U^t \exp\left(-\mathbf{i} \frac{D}{t}\right)$$

converge to the unitary operator $\exp(\mathbf{i}H)$ in the strong operator topology.

For the case that the walk is one-dimensional ($d = 1$), the above two sequences converge in norm, and the limits are analytic operators.

To employ the analytic perturbation theory by Tosio Kato, we suppose analyticity. We denote by $\text{diag}(\alpha_i)_i$ the diagonal matrix whose diagonal entries are $\alpha_1, \dots, \alpha_n$.

Proof We make use of the Fourier transform $\widehat{U}(\mathbf{k})$, $\mathbf{k} \in \mathbb{T}_{2\pi}^d$ of the walk. The operator D corresponds to the operator $\widehat{D} = -\mathbf{i} \sum_i w_i \frac{\partial}{\partial k_i}$. Denote by $\mathbf{w}$ the real vector (w_i) . By Lemma 2.7, the average of the logarithmic derivative $c_t/t = U^{-t}[D, U^t]/t$ corresponds to

$$\widehat{c}_t/t = \frac{1}{t} \widehat{U}^{-t} [\widehat{D}, \widehat{U}^t] = \frac{1}{it} \widehat{U}^{-t} \sum_i w_i \frac{\partial \widehat{U}^t}{\partial k_i}. \quad (8)$$

We make use of the directional derivative $\frac{d}{ds} = \sum_i w_i \frac{\partial}{\partial k_i}$ along the curve of the form $\mathbb{R} \ni s \mapsto \mathbf{k}_0 + s\mathbf{w} \in \mathbb{T}_{2\pi}^d$. Choose an arbitrary base point $\mathbf{k}_0 \in \mathbb{T}_{2\pi}^d$. Let I be a closed interval in $\mathbb{R}$ whose interior part includes 0. For a while, we study the behavior of $\widehat{U}$ on the segment $\mathbf{k}_0 + I\mathbf{w} \subset \mathbb{T}_{2\pi}^d$. Making the interval I shorter, we may assume that the map

$$I \ni s \mapsto \mathbf{k}_0 + s\mathbf{w} \in \mathbb{T}_{2\pi}^d$$

is injective. Denote by $\widehat{u}(s)$ the unitary $\widehat{U}(\mathbf{k}_0 + s\mathbf{w})$. Note that the map $I \ni s \mapsto \widehat{u}(s)$ can be extended to a holomorphic map defined on a complex domain including I . By

Eq. (8), The average of the logarithmic derivative $\widehat{c}_t/t$ is equal to

$$\frac{\widehat{c}_t(\mathbf{k}_0 + s\mathbf{w})}{t} = \frac{1}{it} \widehat{u}^{-t}(s) \frac{d}{ds} (\widehat{u}^t(s)). \quad (9)$$

Let us make use of the analytic perturbation theory by T. Kato. The unitary $\widehat{u}(s)$ can be decomposed as follows

$$\widehat{u}(s) = \widehat{v}(s) \cdot \text{diag}(\lambda_1(s), \dots, \lambda_n(s)) \cdot \widehat{v}(s)^{-1}, \quad (10)$$

by [9, Theorem II.1.8 and II.1.10]. See also [9, Section II.4.6]. Here, $\widehat{v}$ is an analytic map to invertible matrices, and the eigenvalue functions $\lambda_1, \dots, \lambda_n$ are holomorphic functions defined on a complex domain including I .

A direct calculation yields that

$$\begin{aligned} \frac{d}{ds} (\widehat{u}(s)^t) &= \frac{d\widehat{v}}{ds}(s) \cdot \text{diag}(\lambda_i(s)^t) \cdot \widehat{v}(s)^{-1} \\ &\quad + \widehat{v}(s) \cdot \text{diag}\left(\frac{d}{ds}(\lambda_i(s)^t)\right) \cdot \widehat{v}(s)^{-1} \\ &\quad - \widehat{v}(s) \cdot \text{diag}(\lambda_i(s)^t) \cdot \widehat{v}(s)^{-1} \cdot \frac{d\widehat{v}}{ds}(s) \cdot \widehat{v}(s)^{-1}. \end{aligned}$$

The second term is equal to

$$t \cdot \widehat{v}(s) \cdot \text{diag}\left(\lambda_i(s)^{t-1} \cdot \frac{d\lambda_i}{ds}(s)\right) \cdot \widehat{v}(s)^{-1}.$$

As t tends to infinity, the norm increases linearly. The norms of the first and the third terms are bounded. It follows that for the calculation of the average with respect to time, it suffices to see the second term. By Eq. (9), we have

$$\begin{aligned} \lim_{t \rightarrow \infty} \frac{\widehat{c}_t(\mathbf{k}_0 + s\mathbf{w})}{t} &= \widehat{v}(s) \cdot \text{diag}(\lambda_i(s)^t) \cdot \widehat{v}(s)^{-1} \cdot \widehat{v}(s) \cdot \text{diag}\left(\lambda_i(s)^{t-1} \cdot \frac{d\lambda_i}{ds}(s)\right) \cdot \widehat{v}(s)^{-1} \\ &= \widehat{v}(s) \cdot \text{diag}\left(\lambda_i(s)^{-1} \cdot \frac{d\lambda_i}{ds}(s)\right) \cdot \widehat{v}(s)^{-1}. \end{aligned} \quad (11)$$

The convergence is uniform on the closed interval I . Because $|\lambda_i(s)|^2 = 1$, $\lambda_i(s)^{-1} \cdot \frac{d\lambda_i}{ds}(s)$ is in $i\mathbb{R}$, as t tends to infinity, the average of logarithmic derivatives $\widehat{c}_t(\mathbf{k}_0)/t$ converges to a skew self-adjoint matrix $i\widehat{H}(\mathbf{k}_0)$, at each point $\mathbf{k}_0 \in \mathbb{T}_{2\pi}^d$. The operator norm is uniformly bounded by $\left\| \sum_i w_i \frac{\partial \widehat{U}}{\partial k_i} \right\|$ due to Lemma 3.2. This upper bound is independent of $\mathbf{k}_0$. Therefore, the convergence of $\widehat{c}_t(\mathbf{k}_0)/t$ at each point $\mathbf{k}_0$ yields that in the strong operator topology. Applying the Fourier transform, we obtain the first assertion.

Consider the case that d is one. Then, the convergence on each closed interval in $\mathbb{T}_{2\pi}$ is uniform, and the limit is given by a matrix-valued analytic function as in Eq. (11). Since the one-dimensional torus $\mathbb{T}_{2\pi}$ is a union of two segments, the average of logarithmic derivative converges in norm and the limit is analytic.

Let us consider general d again. The inverse Fourier transform of $U^{-t} \exp(\mathbf{i} \frac{D}{t}) U^t \exp(-\mathbf{i} \frac{D}{t})$ is

$$\widehat{U}^{-t} \exp\left(t^{-1} \sum_i w_i \frac{\partial}{\partial k_i}\right) \widehat{U}^t \exp\left(-t^{-1} \sum_i w_i \frac{\partial}{\partial k_i}\right).$$

For every $\mathbb{C}^n$ -valued analytic functions $\widehat{\xi}(\mathbf{k})$ defined on $\mathbb{T}_{2\pi}^d$, we calculate

$$\widehat{U}^{-t} \exp\left(t^{-1} \sum_i w_i \frac{\partial}{\partial k_i}\right) \widehat{U}^t \exp\left(-t^{-1} \sum_i w_i \frac{\partial}{\partial k_i}\right) \widehat{\xi}$$

as follows. The $\mathbb{C}^n$ -valued function $\exp\left(-t^{-1} \sum_i w_i \frac{\partial}{\partial k_i}\right) \widehat{\xi}$ is given by

$$\left[\exp\left(-t^{-1} \sum_i w_i \frac{\partial}{\partial k_i}\right) \widehat{\xi} \right](\mathbf{k}) = \sum_{m=0}^{\infty} \frac{1}{m!} t^{-m} \left[\left(\sum_i w_i \frac{\partial}{\partial k_i} \right)^m \widehat{\xi} \right](\mathbf{k}).$$

This is the Taylor expansion of $\widehat{\xi}(\mathbf{k} - t^{-1}\mathbf{w})$. Therefore, the unitary $\exp\left(-t^{-1} \sum_i \frac{\partial}{\partial k_i}\right)$ acts on analytic vectors by the translation of $t^{-1}\mathbf{w}$. Since analytic vectors are dense in the Hilbert space, the unitary $\exp\left(-t^{-1} \sum_i \frac{\partial}{\partial k_i}\right)$ acts on every vector in $L^2(\mathbb{T}_{2\pi}^d) \otimes \mathbb{C}^n$ by the translation of $t^{-1}\mathbf{w}$. By the same reason, the unitary $\exp\left(t^{-1} \sum_i \frac{\partial}{\partial k_i}\right)$ means the translation by $-t^{-1}\mathbf{w}$. It follows that for every $\widehat{\xi} \in L^2(\mathbb{T}_{2\pi}^d) \otimes \mathbb{C}^n$, the following equation holds:

$$\begin{aligned} & \left[\widehat{U}^{-t} \exp\left(t^{-1} \sum_i \frac{\partial}{\partial k_i}\right) \widehat{U}^t \exp\left(-t^{-1} \sum_i \frac{\partial}{\partial k_i}\right) \widehat{\xi} \right](\mathbf{k}) \\ &= \widehat{U}(\mathbf{k})^{-t} \cdot \widehat{U}(\mathbf{k} + t^{-1}\mathbf{w})^t \cdot \widehat{\xi}(\mathbf{k}). \end{aligned}$$

Since the vector $\widehat{\xi}$ in $L^2(\mathbb{T}_{2\pi}^d) \otimes \mathbb{C}^n$ is arbitrary, we obtain the following equation between two operators:

$$\begin{aligned} & \left[\widehat{U}^{-t} \exp\left(t^{-1} \sum_i \frac{\partial}{\partial k_i}\right) \widehat{U}^t \exp\left(-t^{-1} \sum_i \frac{\partial}{\partial k_i}\right) \right](\mathbf{k}) \\ &= \widehat{U}(\mathbf{k})^{-t} \cdot \widehat{U}(\mathbf{k} + t^{-1}\mathbf{w})^t. \end{aligned} \quad (12)$$

We make use of the restriction $\widehat{u}(s) = \widehat{U}(\mathbf{k} + s\mathbf{w})$ on the segment $\mathbf{k}_0 + I\mathbf{w} \subset \mathbb{T}_{2\pi}^d$ and its diagonal decomposition $\widehat{v}(s) \cdot \text{diag}(\lambda_i(s))_i \cdot \widehat{v}(s)^{-1}$ as in Eq. (10). Assume that

s is in I . Since I is simply connected, there exist real-valued analytic functions $l_1, l_2, \dots, l_n$ such that $\exp(\mathbf{i}l_i(s)) = \lambda_i(s)$.

Formula (12) is equal to $\widehat{u}(0)^{-t}\widehat{u}(t^{-1})^t$. If t is large, then the matrix $\widehat{v}(t^{-1})$ is close to $\widehat{v}(0)$ in norm. The unitary matrix $\widehat{u}(0)^{-t}\widehat{u}(t^{-1})^t$ is uniformly close to

$$\begin{aligned} & \widehat{v}(0) \cdot \text{diag}(\lambda_i(0)^{-t})_i \cdot \widehat{v}(0)^{-1} \cdot \widehat{v}(t^{-1}) \cdot \text{diag}(\lambda_i(t^{-1})^t)_i \cdot \widehat{v}(t^{-1})^{-1} \\ & \sim \widehat{v}(0) \cdot \text{diag}(\lambda_i(0)^{-t})_i \cdot \text{diag}(\lambda_i(t^{-1})^t)_i \cdot \widehat{v}(t^{-1})^{-1} \\ & = \widehat{v}(0) \text{diag} \left(\exp \left(\mathbf{i} \frac{l_i(t^{-1}) - l_i(0)}{t^{-1}} \right) \right)_i \widehat{v}(0)^{-1}. \end{aligned}$$

Note that the logarithms $l_1(s), \dots, l_n(s)$ are differentiable, since $\lambda_i(s)$ are analytic.

Therefore, we have

$$\begin{aligned} \lim_{t \rightarrow \infty} \widehat{u}(0)^{-t}\widehat{u}(t^{-1})^t &= \widehat{v}(0) \text{diag} \left(\exp \left(\mathbf{i} \frac{dl_i}{ds}(0) \right) \right)_i \widehat{v}(0)^{-1} \\ &= \widehat{v}(0) \text{diag} \left(\exp \left(\lambda_i(0)^{-1} \frac{d\lambda_i}{ds}(0) \right) \right)_i \widehat{v}(0)^{-1} \\ &= \exp \left(\widehat{v}(0) \text{diag} \left(\lambda_i(0)^{-1} \frac{d\lambda_i}{ds}(0) \right)_i \widehat{v}(0)^{-1} \right). \end{aligned}$$

By Eq. (11) and by the definition of the skew self-adjoint matrix $\mathbf{i}\widehat{H}(\mathbf{k}_0)$, we have the following convergence at each point $\mathbf{k}_0$:

$$\lim_{t \rightarrow \infty} \widehat{U}(\mathbf{k}_0)^{-t} \cdot \widehat{U}(\mathbf{k}_0 + t^{-1}\mathbf{w})^t = \exp(\mathbf{i}\widehat{H}(\mathbf{k}_0)).$$

Because the sequence consists of unitary operators, the convergence at each point implies that in the strong operator topology. Applying the Fourier transform, we obtain the second assertion.

In the case that d is one, the convergence is that in the operator norm topology, since the convergence is uniform on each segment included in the torus. $\square$

In case that d is one, the following theorem is proved in [10].

Theorem 4.3 *For any d -dimensional homogeneous analytic quantum walk with finite degree of freedom, and for any initial unit vector, the weak limit of probability measures $\{p_t\}$ defined in Sect. 3.2 exists.*

The limit distribution is described as follows. Let $(U^t)_{t \in \mathbb{Z}}$ be a homogeneous quantum walk acting on $\ell_2(\mathbb{Z}^d) \otimes \mathbb{C}^n$. Let $\xi \in \ell_2(\mathbb{Z}^d) \otimes \mathbb{C}^n$ be an initial unit vector. By Proposition 4.2, the limit of the average of logarithmic derivatives

$$H_i = \lim_{t \rightarrow \infty} \frac{1}{it} U^{-t} \partial_i(U^t)$$

exists and is a bounded self-adjoint operator. Since the self-adjoint operators $(D_1, \dots, D_d)$ mutually commute, the self-adjoint operators $(H_1, \dots, H_d)$ also mutually

commute. There exists a unique projection-valued Borel probability measure $\mathcal{E}$ on a compact subset of $\mathbb{R}^d$ satisfying that for every integers $m(1), \dots, m(d) \in \mathbb{Z}_{\leq 0}$,

$$\prod_i H_i^{m(i)} = \int_{\mathbf{v} \in \mathbb{R}^d} \prod_i v_i^{m(i)} \mathcal{E}(d\mathbf{v}).$$

The following argument shows that the limit distribution of the walk is equal to $p_\infty(\cdot) = \langle \mathcal{E}(\cdot) \xi, \xi \rangle$.

Proof We first assume that ξ is smooth. Via the inverse Fourier transform, the walk U corresponds to an $(n \times n)$ -matrix $\widehat{U}$ whose entries are analytic functions on $\mathbb{T}_{2\pi}^d$. The initial unit vector ξ corresponds to a smooth element $\widehat{\xi} \in L^2(\mathbb{T}_{2\pi}^d) \otimes \mathbb{C}^n$. For every $i = 1, \dots, d$, the self-adjoint operator $\widehat{D}_i$ is given by $-\mathbf{i} \frac{\partial}{\partial k_i}$. Define $\widehat{D}$ by $-\mathbf{i} \sum_i w_i \frac{\partial}{\partial k_i}$. By Eq. (7) in Lemma 3.7, the mean of the function $\exp(\mathbf{i}(\cdot, \mathbf{w})_{\mathbb{R}^d})$ on $\mathbb{R}^d$ with respect to p_t is equal to the following inner product:

$$\begin{aligned} & \int_{\mathbf{v} \in \mathbb{R}^d} \exp(\mathbf{i}(\mathbf{v}, \mathbf{w})_{\mathbb{R}^d}) p_t(d\mathbf{v}) \\ &= \left\langle \exp(\mathbf{i}t^{-1} \widehat{D}) \widehat{U}^t \widehat{\xi}, \widehat{U}^t \widehat{\xi} \right\rangle \\ &= \left\langle \widehat{U}^{-t} \exp(\mathbf{i}t^{-1} \widehat{D}) \widehat{U}^t \exp(-\mathbf{i}t^{-1} \widehat{D}) \widehat{\xi}, \widehat{\xi} \right\rangle. \end{aligned}$$

Let $\widehat{H}$ be the limit of the averages of logarithmic derivatives of $\widehat{U}^t$ with respect to the differential operator $-\mathbf{i} \sum w_i \frac{\partial}{\partial k_i}$. As in the proof of Proposition 4.2, define self-adjoint operators $\widehat{H}_i$ by

$$-\mathbf{i} \lim_{t \rightarrow \infty} \widehat{U}(\mathbf{k})^{-t} \frac{\partial \widehat{U}^t}{\partial k_i}(\mathbf{k}),$$

and $\widehat{H}$ by $\sum_{i=1}^d w_i \widehat{H}_i$. By Proposition 4.2, the operator

$$\widehat{U}^{-t} \exp(\mathbf{i}t^{-1} \widehat{D}) \widehat{U}^t \exp(-\mathbf{i}t^{-1} \widehat{D})$$

converges to $\exp(\mathbf{i}\widehat{H})$ in the strong operator topology. The vector $\exp(\mathbf{i}t^{-1} \widehat{D}) \widehat{\xi}$ is given by $[\exp(\mathbf{i}t^{-1} \widehat{D}) \widehat{\xi}](\mathbf{k}) = \widehat{\xi}(\mathbf{k} + t^{-1} \mathbf{w})$. It is uniformly close to $\widehat{\xi}(\mathbf{k})$. As t tends to infinity, the above integral converges to

$$\langle \exp(\mathbf{i}\widehat{H}) \widehat{\xi}, \widehat{\xi} \rangle_{L^2(\mathbb{T}_{2\pi}^d) \otimes \mathbb{C}^d} = \left\langle \prod_i \exp(\mathbf{i}w_i H_i) \xi, \xi \right\rangle.$$

We obtain

$$\begin{aligned}\lim_{t \rightarrow \infty} \int_{\mathbf{v} \in \mathbb{R}^d} \exp(\mathbf{i}(\mathbf{v}, \mathbf{w})_{\mathbb{R}^d}) p_t(d\mathbf{v}) &= \left\langle \prod_i \exp(\mathbf{i} w_i H_i) \xi, \xi \right\rangle \\ &= \left\langle \int_{\mathbf{v} \in \mathbb{R}^d} \exp(\mathbf{i}(\mathbf{v}, \mathbf{w})_{\mathbb{R}^d}) \mathcal{E}(d\mathbf{v}) \xi, \xi \right\rangle.\end{aligned}$$

We obtain that for every linear combination g of $\{\exp(\mathbf{i}(\cdot, \mathbf{w})_{\mathbb{R}^d}) \mid \mathbf{w} \in \mathbb{R}^d\}$,

$$\lim_{t \rightarrow \infty} \int_{\mathbf{v} \in \mathbb{R}^d} g(\mathbf{v}) p_t(d\mathbf{v}) = \left\langle \int_{\mathbf{v} \in \mathbb{R}^d} g(\mathbf{v}) \mathcal{E}(d\mathbf{v}) \xi, \xi \right\rangle.$$

By Theorem 3.10, there exists a compact subset K of $\mathbb{R}^d$ such that

$$\lim_{t \rightarrow \infty} p_t(K) = 1.$$

The linear span $\text{span}\{\exp(\mathbf{i}(\cdot, \mathbf{w})_{\mathbb{R}^d}) \mid \mathbf{w} \in \mathbb{R}^d\}$ is the space of trigonometric functions. By the theorem of Stone–Weierstrass, the linear span is dense in $C(K)$ with respect to the supremum norm. It follows that for every bounded continuous function f on $\mathbb{R}^d$,

$$\lim_{t \rightarrow \infty} \int_{\mathbf{v} \in \mathbb{R}^d} f(\mathbf{v}) p_t(d\mathbf{v}) = \left\langle \int_{\mathbf{v} \in \mathbb{R}^d} f(\mathbf{v}) \mathcal{E}(d\mathbf{v}) \xi, \xi \right\rangle.$$

In the special case that ξ is smooth, we finish the proof.

Let ξ be an initial unit vector in $\ell_2(\mathbb{Z}^d) \otimes \mathbb{C}^n = \ell_2(\mathbb{Z}^d \rightarrow \mathbb{C}^n)$ which is not necessarily smooth. Let $\tilde{p}_t$ be the sequence of probability measures defined by U^t and $\tilde{\xi}$. Let ϵ be an arbitrary positive number. Choose a smooth unit vector $\tilde{\xi} \in \ell_2(\mathbb{Z}^d \rightarrow \mathbb{C}^n)$ satisfying that $\|\xi - \tilde{\xi}\| < \epsilon$. For every element η of $\ell_2(\mathbb{Z}^d \rightarrow \mathbb{C}^n)$, define an ℓ_1 function $|\eta|^2$ on $\mathbb{Z}^d$ by

$$|\eta|^2(\mathbf{x}) = \|\eta(\mathbf{x})\|_{\mathbb{C}^n}^2,$$

By the inequality $\|U^t \xi - U^t \tilde{\xi}\| < \epsilon$, we have $\left\| |U^t \xi|^2 - |U^t \tilde{\xi}|^2 \right\|_{\ell_1} < 2\epsilon$. By Eq. (7), for every bounded Borel function f on $\mathbb{R}^d$, we have

$$\begin{aligned}\left| \int_{\mathbf{v} \in \mathbb{R}^d} f(\mathbf{v}) p_t(d\mathbf{v}) - \int_{\mathbf{v} \in \mathbb{R}^d} f(\mathbf{v}) \tilde{p}_t(d\mathbf{v}) \right| &\leq \sup_{\mathbf{v} \in \mathbb{R}^d} |f(\mathbf{v})| \cdot \left\| |U^t \xi|^2 - |U^t \tilde{\xi}|^2 \right\|_{\ell_1} \\ &\leq 2\epsilon \sup_{\mathbf{v} \in \mathbb{R}^d} |f(\mathbf{v})|.\end{aligned}$$

We also obtain

$$\begin{aligned}&\left| \left\langle \int_{\mathbf{v} \in \mathbb{R}^d} f(\mathbf{v}) \mathcal{E}(d\mathbf{v}) \xi, \xi \right\rangle - \left\langle \int_{\mathbf{v} \in \mathbb{R}^d} f(\mathbf{v}) \mathcal{E}(d\mathbf{v}) \tilde{\xi}, \tilde{\xi} \right\rangle \right| \\ &\leq 2 \left\| \int_{\mathbf{v} \in \mathbb{R}^d} f(\mathbf{v}) \mathcal{E}(d\mathbf{v}) \right\| \|\xi - \tilde{\xi}\| \leq 2\epsilon \sup_{\mathbf{v} \in \mathbb{R}^d} |f(\mathbf{v})|.\end{aligned}$$

It follows that for every bounded continuous function f on $\mathbb{R}^d$,

$$\lim_{t \rightarrow \infty} \int_{\mathbf{v} \in \mathbb{R}^d} f(\mathbf{v}) \tilde{p}_t(d\mathbf{v}) = \left\langle \int_{\mathbf{v} \in \mathbb{R}^d} f(\mathbf{v}) \mathcal{E}(d\mathbf{v}) \tilde{\xi}, \tilde{\xi} \right\rangle = \int_{\mathbf{v} \in \mathbb{R}^d} f(\mathbf{v}) \langle \mathcal{E}(d\mathbf{v}) \tilde{\xi}, \tilde{\xi} \rangle.$$

It follows that the sequence of probability measures $\{\tilde{p}_t\}$ weakly converges. $\square$

4.3 A quantum walk with an initial unit vector whose support is not localized

The convergence theorem (Theorem 4.3) holds true for an arbitrary initial unit vector. Let us consider an example, in which the support of the initial unit vector ξ is the whole space $\mathbb{Z}$. We define U by the 3-state Grover walk

$$U = \begin{pmatrix} S & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & S^{-1} \end{pmatrix} \cdot \frac{1}{3} \begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix}$$

acting on $\ell_2(\mathbb{Z}) \otimes \mathbb{C}^3$. We set the initial unit vector ξ by the infinite sum

$$\xi = \frac{1}{\sqrt{3}} \sum_{x \in \mathbb{Z}} \delta_x \otimes \begin{pmatrix} 0 \\ 2^{-|x|/2} \\ 0 \end{pmatrix}.$$

When we regard ξ as a map from $\mathbb{Z}$ to $\mathbb{C}^3$, the support of ξ is $\mathbb{Z}$. However, according to Theorem 3.10, the limit distribution of velocity $\{p_t\}_{t=1}^\infty$ defined in 3.2 should have compact support. To see what happens, let us look at the following results of numerical calculations.

Figure 1 shows the probability of position in $\mathbb{Z}$ according to the quantum state ξ . The left end stands for $x = -4$, and the right end stands for $x = 4$. Since the support of $\xi: \mathbb{Z} \rightarrow \mathbb{C}^3$ is $\mathbb{Z}$, the probability never vanishes.

Figure 2 shows the probability distribution on $\frac{1}{5}\mathbb{Z}$ defined by the unit vector $U^5\xi$. The left end stands for $x = -3$, and the right end stands for $x = 3$. The tails on the both sides become closer to the level of 0.

Figure 3 shows the probability distribution on $\frac{1}{100}\mathbb{Z}$ defined by the unit vector $U^{100}\xi$. The left end stands for $x = -1$, and the right end stands for $x = 1$. Although the support of $U^{100}\xi: \mathbb{Z} \rightarrow \mathbb{C}^3$ is not supported on a compact set, the distribution is very close to that with compact support and the difference is invisible. The probability on the interval $[-0.7, 0.7]$ is more than 0.999.

5 Interpretation of this paper from the view point of quantum physics

Many researchers have intensively studied quantum walks acting on the Hilbert space $\ell_2(\mathbb{Z}^d) \otimes \mathbb{C}^n$. The natural number d stands for the dimension of the space. The natural number n stands for the local degree of freedom at a point in $\mathbb{Z}^d$. This paper enables us

Fig. 1 The distribution of position according to the initial state ξ in Sect. 4.3

Fig. 2 The distribution of velocity p_5 given by the state $U^5\xi$

to generalize the framework of the theory of quantum walks. In the following, we see how our definitions and theorems in this paper enlarge the theory of quantum walks.

General n In the present study of quantum walks, the local degree of freedom is restricted to small natural numbers n such as 2. This is because researchers consider concrete physical observable such as the quantum spin. This observable can be

Fig. 3 The distribution of velocity p_{100} given by the state $U^{100}\xi$

described as a self-adjoint matrix acting on $\mathbb{C}^2$. In our new framework described in Definition 2.1, we can consider large finite-dimensional local Hilbert space $\mathbb{C}^n$. The results in Sect. 3 can be applied to the case that the local Hilbert spaces are infinite dimensional.

General d The space $\mathbb{Z}^d$ has a physical meaning in the case of $d = 1, 2, 3$. We no longer have to divide our studies into these three cases.

Quantum walks on more general spaces It is no longer necessary to stick to the concrete lattice $\mathbb{Z}^d$ inside $\mathbb{R}^3$. Let us consider the case that some devices or atoms are located on some discrete subset $X \subset \mathbb{R}^d$. In this paragraph, we put no requirement related to symmetry on X . Let us consider some Hilbert spaces $\mathcal{H}_x$ are attached to every point $x \in X$, where $\mathcal{H}_x$ may be infinite dimensional. Here, unit vectors in $\mathcal{H}_x$ describe quantum states at $x \in X$. The whole Hilbert space $\mathcal{H}$ is defined by the direct sum of Hilbert space $\bigoplus_{x \in X} \mathcal{H}_x$, and the spectral measure E is given by the orthogonal projections $E(\Omega)$ from $\mathcal{H}$ onto $\bigoplus_{x \in \Omega \cap X} \mathcal{H}_x$. Therefore, our new framework encompasses dynamical systems on arbitrary solid structures given by atoms and on those by devices.

Quantum walks without finite propagation Almost all the known quantum walks have *finite propagation*. The term “finite propagation” is defined as follows: The operator U on $\mathcal{H} = \bigoplus_{x \in X} \mathcal{H}_x$ is said to have finite propagation, if there exists a positive number R such that for every $x, y \in X$, if $\text{dist}(x, y) > R$, then $U\mathcal{H}_x$ and $\mathcal{H}_y$ are perpendicular. The meaning of this condition is that if x, y are distant, and $\xi \in \mathcal{H}$ is located at $\mathcal{H}_x$ and $\eta \in \mathcal{H}$ is located at $\mathcal{H}_y$, then the transition probability $|\langle U\xi, \eta \rangle|^2$ is zero. It is easy to show that having finite propagation implies analyticity defined in Definition 2.10. The converse does not hold. The theory in this paper uses analyticity or more mild conditions. Thus, we obtain a wider framework.

Quantum walks on arbitrary crystal lattices Preparing a general framework is not the only goal of this paper. Let us apply our mathematical argument to quantum walks on crystal lattices. For every crystal lattice $X \subset \mathbb{R}^d$, there exists an additive subgroup $G \subset \mathbb{R}^d$ which is isomorphic to $\mathbb{Z}^d$ such that X is invariant under the addition by G . Here, d is 2 or 3. The Hilbert space $\mathcal{H} = \bigoplus_{x \in X} \mathcal{H}_x$ also has translation symmetry under the action of G ; in other words, for every $g \in G$ and $x \in X$, $g + x \in X$ and $\mathcal{H}_{g+x} = \mathcal{H}_x$. Let U be a unitary operator on $\mathcal{H}$. The unitary operator satisfies a convergence theorem, if the following assumption holds:

- All the local Hilbert spaces $\mathcal{H}_x$ are finite dimensional.
- The unitary operator U has the *translation symmetry* with respect to G . More precisely, if we denote by $\rho(g)$ the unitary operator on $\mathcal{H}$ given by the shift $g \in G$, then $U\rho(g) = \rho(g)U$.
- The unitary operator U has *finite propagation*.

Almost all the known quantum walks with translation symmetry on crystal lattices satisfy these conditions.

Corollary 5.1 *For any initial unit vector $\xi \in \mathcal{H}$, and for the quantum walk $(\mathcal{H}, (U^t)_{t \in \mathbb{Z}}, E)$ on arbitrary crystal lattice satisfying above conditions, the weak limit of the distribution of velocity $\{p_t\}$ defined in Sect. 3.2 exists.*

Proof A quantum walk with *finite propagation* is *analytic*. The quantum walk U is space-homogeneous with respect to the additive group $G \cong \mathbb{Z}^d$. This corollary is a direct conclusion of Theorem 4.3. $\square$

Physical meaning of 1-cocycles and logarithmic derivatives of quantum walks Let A be an observable described by a self-adjoint operator acting on a dense subspace of $\mathcal{H} = \bigoplus_{x \in X} \mathcal{H}_x$. Let $(U^t)_{t \in \mathbb{Z}}$ be a dynamical system acting on $\mathcal{H}$. According to the Heisenberg representation of time evolution, the sequence $(U^{-t}AU^t)_{t \in \mathbb{Z}}$ stands for the evolution of the observable with time. The $U^{-t}AU^t - A$ stands for the difference between two observables A and $U^{-t}AU^t$, where the latter represents the observable after t . Let us consider the case that $U^{-1}AU - A$ is bounded. In this case, the possible values of the observable $U^{-1}AU - A$ are restricted to some closed interval. The family of bounded self-adjoint operators $(c_t)_{t \in \mathbb{Z}} = (U^{-t}AU^t - A)_{t \in \mathbb{Z}}$ forms a 1-cocycle introduced in Definition 3.1. Thus, using 1-cocycle, we can treat the difference of the observable A and that after t . Proposition 4.2 means that the average of the 1-cocycle $\frac{1}{t}(U^{-t}AU^t - A)$ converges if the quantum walk is analytic and homogeneous. This can be applied to analytic quantum walks on crystal lattices with translation symmetry.

In our mathematical argument for the convergence theorem (Theorem 4.3), a 1-cocycle called the logarithmic derivative plays a key role.

Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit <http://creativecommons.org/licenses/by/4.0/>.

References

1. Mackay, T.D., Bartlett, S.D., Stephenson, L.T., Sanders, B.C.: Quantum walks in higher dimensions. *J. Phys. A* **35**(12), 2745–2753 (2002)
2. Tregenna, B., Flanagan, W., Maile, R., Kendon, V.: Controlling discrete quantum walks: coins and initial states. *N. J. Phys.* **5**, 83–83 (2003)
3. Grimmett, G., Janson, S., Scudo, P.F.: Weak limits for quantum random walks. *Phys. Rev. E* **69**, 026119 (2004)
4. Inui, N., Konishi, Y., Konno, N.: Localization of two-dimensional quantum walks. *Phys. Rev. A* **69**, 052323 (2004)
5. Konno, N.: A new type of limit theorems for the one-dimensional quantum random walk. *J. Math. Soc. Jpn.* **57**(4), 1179–1195 (2005)
6. Oliveira, A.C., Portugal, R., Donangelo, R.: Decoherence in two-dimensional quantum walks. *Phys. Rev. A* **74**, 012312 (2006)
7. Watabe, K., Kobayashi, N., Katori, M., Konno, N.: Limit distributions of two-dimensional quantum walks. *Phys. Rev. A* **77**, 056112 (2008)
8. Sako, H.: Intertwining operators between one-dimensional homogeneous quantum walks. preprint, [arxiv:1902.02479](https://arxiv.org/abs/1902.02479), (2019)
9. Kato, T.: *Perturbation Theory for Linear Operators*. Classics in Mathematics. Springer, Berlin (1995). Reprint of the 1980 edition
10. Saigo, H., Sako, H.: Space-homogeneous quantum walks on $\mathbb{Z}$ from the viewpoint of complex analysis. *J. Math. Soc. Jpn.* **72**(4), 1201–1237 (2020)

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.