

Asymptotic velocity of a position-dependent quantum walk

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Abstract We consider a position-dependent coined quantum walk on \mathbb{Z} and assume that the coin operator $C(x)$ satisfies

$$\|C(x) - C_0\| \leq c_1|x|^{-1-\epsilon}, \quad x \in \mathbb{Z} \setminus \{0\}$$

with positive c_1 and ϵ and $C_0 \in U(2)$. We show that the Heisenberg operator $\hat{x}(t)$ of the position operator converges to the asymptotic velocity operator \hat{v}_+ so that

$$s\text{-}\lim_{t \rightarrow \infty} \exp\left(i\xi \frac{\hat{x}(t)}{t}\right) = \Pi_p(U) + \exp(i\xi \hat{v}_+) \Pi_{ac}(U)$$

provided that U has no singular continuous spectrum. Here $\Pi_p(U)$ (resp., $\Pi_{ac}(U)$) is the orthogonal projection onto the direct sum of all eigenspaces (resp., the subspace of absolute continuity) of U . We also prove that for the random variable X_t denoting the position of a quantum walker at time $t \in \mathbb{N}$, X_t/t converges in law to a random variable V with the probability distribution

$$\mu_V = \|\Pi_p(U)\Psi_0\|^2 \delta_0 + \|E_{\hat{v}_+}(\cdot)\Pi_{ac}(U)\Psi_0\|^2,$$

where Ψ_0 is the initial state, δ_0 the Dirac measure at zero, and $E_{\hat{v}_+}$ the spectral measure of \hat{v}_+ .

Keywords Quantum walk · Asymptotic velocity · Weak limit

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1 Introduction

The weak limit theorems for discrete time quantum walks have been studied in various models (for reviews, see [7, 12]). In his papers [5, 6], Konno first proved the weak limit theorem for a position-independent quantum walk on \mathbb{Z} . Grimmett et al. [4] simplified the proof and extended the result to higher dimensions. For position-dependent quantum walks on \mathbb{Z} , the weak limit theorems were obtained by Konno et al. [9], Endo and Konno [2], and Endo et al. [3].

We consider a position-dependent quantum walk on \mathbb{Z} given by a unitary evolution operator U :

$$(U\Psi)(x) = P(x + 1)\Psi(x + 1) + Q(x - 1)\Psi(x - 1), \quad x \in \mathbb{Z},$$

where Ψ is a state vector in the Hilbert space $\mathcal{H} = \ell^2(\mathbb{Z}; \mathbb{C}^2)$ of states and

$$P(x) = \begin{pmatrix} a(x) & b(x) \\ 0 & 0 \end{pmatrix}, \quad Q(x) = \begin{pmatrix} 0 & 0 \\ c(x) & d(x) \end{pmatrix}.$$

Let $C(x) = P(x) + Q(x) \in U(2)$ and S be a shift operator such that $U = SC$. Suppose that there exists a unitary matrix $C_0 = P_0 + Q_0 \in U(2)$ such that

$$\|C(x) - C_0\| \leq c_1|x|^{-1-\epsilon}, \quad x \in \mathbb{Z} \setminus \{0\} \tag{1.1}$$

with positive c_1 and ϵ independent of x . Here $\|M\|$ stands for the operator norm of a matrix $M \in M_2(\mathbb{C})$. A typical example is the quantum walks with one defect [1, 8, 9, 13], which clearly satisfies (1.1). We note that the condition (1.1) allows not only finite but also infinite defects, whereas the models introduced in [2, 3] do not satisfy (1.1). The unitary operator $U_0 = SC_0$ also defines an evolution of a position-independent quantum walk on \mathbb{Z} and satisfies

$$(U_0\Psi)(x) = P_0\Psi(x + 1) + Q_0\Psi(x - 1), \quad x \in \mathbb{Z}$$

with $C_0 = P_0 + Q_0$. Let \hat{x} be the position operator defined by $(\hat{x}\Psi)(x) = x\Psi(x)$, $x \in \mathbb{Z}$, and $\hat{x}_0(t) = U_0^{-t}\hat{x}U_0^t$ the Heisenberg operator of \hat{x} at time $t \in \mathbb{N}$ with the evolution U_0 . In Grimmett et al. [4] essentially proved that the operator $\hat{x}_0(t)/t$ weakly converges to the asymptotic velocity operator \hat{v}_0 so that

$$w\text{-}\lim_{t \rightarrow \infty} \exp\left(i\xi \frac{\hat{x}_0(t)}{t}\right) = \exp(i\xi \hat{v}_0), \quad \xi \in \mathbb{R}. \tag{1.2}$$

Let $X_t^{(0)}$ be the random variable denoting the position of a quantum walker at time $t \in \mathbb{N}$ with the evolution operator U_0 . Then, the characteristic function of $X_t^{(0)}/t$ is given by

$$\mathbb{E}\left(e^{i\xi X_t^{(0)}/t}\right) = \left\langle \Psi_0, e^{i\xi \hat{x}_0(t)/t} \Psi_0 \right\rangle, \quad \xi \in \mathbb{R},$$

where Ψ_0 is the initial state of the quantum walker. Hence, (1.2) means that the random variable $X_t^{(0)}/t$ converges in law to a random variable V_0 , which represents the linear spreading of the quantum walk: $X_t^{(0)} \sim tV_0$.

In this paper, we derive the asymptotic velocity \hat{v}_+ for the Heisenberg operator $\hat{x}(t) = U^{-t}\hat{x}U^t$ with the evolution U of the position-dependent quantum walk. The decaying condition (1.1) implies that $U - U_0$ is a trace class operator and allows us to prove the existence and completeness of the wave operator

$$W_+ = s\text{-}\lim_{t \rightarrow \infty} U^{-t}U_0^t\Pi_{\text{ac}}(U_0)$$

using a discrete analogue of the Kato–Rosenblum Theorem (see [11] for details), where $\Pi_{\text{ac}}(U_0)$ is the orthogonal projection onto the subspace of absolute continuity of U_0 . We also prove that

$$s\text{-}\lim_{t \rightarrow \infty} \exp\left(i\xi \frac{\hat{x}_0(t)}{t}\right) = \exp(i\xi \hat{v}_0), \quad \xi \in \mathbb{R}$$

under a reasonable condition, which is essentially the same as that of [4]. Furthermore, we assume that U has no singular continuous spectrum. Then, we prove that

$$s\text{-}\lim_{t \rightarrow \infty} \exp\left(i\xi \frac{\hat{x}(t)}{t}\right) = \Pi_{\text{p}}(U) + \exp(i\xi \hat{v}_+)\Pi_{\text{ac}}(U), \quad (1.3)$$

where $\Pi_{\text{p}}(U)$ is the orthogonal projection onto the direct sum of all eigenspaces of U and $\hat{v}_+ = W_+\hat{v}_0W_+^*$. We believe that the absence of a singular continuous spectrum can be checked with a concrete example such as the one-defect model. As a consequence of (1.3), we have the following weak limit theorem. Let X_t be the random variable denoting the position of a quantum walker at time $t \in \mathbb{N}$ with the evolution operator U and the initial state Ψ_0 . We prove that X_t/t converges in law to a random variable V with a probability distribution

$$\mu_V = \|\Pi_{\text{p}}(U)\Psi_0\|^2\delta_0 + \|E_{\hat{v}_+}(\cdot)\Pi_{\text{ac}}(U)\Psi_0\|^2,$$

where δ_0 is the Dirac measure at zero and $E_{\hat{v}_+}$ the spectral measure of \hat{v}_+ .

The remainder of this paper is organized as follows. In Sect. 2, we present the precise definition of the model and our results. Section 3 is devoted to the proof of the existence and completeness of the wave operator. In Sect. 4, we construct the asymptotic velocity.

2 Definition of the model

Let $\mathcal{H} = \ell^2(\mathbb{Z}; \mathbb{C}^2)$ be the Hilbert space of the square summable functions $\Psi : \mathbb{Z} \rightarrow \mathbb{C}^2$. We define a shift operator S and a coin operator C on \mathcal{H} as follows. For a vector

$\Psi = \begin{pmatrix} \Psi^{(0)} \\ \Psi^{(1)} \end{pmatrix} \in \mathcal{H}$, $S\Psi$ is given by

$$(S\Psi)(x) = \begin{pmatrix} \Psi^{(0)}(x+1) \\ \Psi^{(1)}(x-1) \end{pmatrix}, \quad x \in \mathbb{Z}.$$

Let $\{C(x)\}_{x \in \mathbb{Z}} \subset U(2)$ be a family of unitary matrices with

$$C(x) = \begin{pmatrix} a(x) & b(x) \\ c(x) & d(x) \end{pmatrix}.$$

$C\Psi$ is given by

$$(C\Psi)(x) = C(x)\Psi(x), \quad x \in \mathbb{Z}.$$

We define an evolution operator as $U = SC$. U satisfies

$$(U\Psi)(x) = P(x+1)\Psi(x+1) + Q(x-1)\Psi(x-1), \quad x \in \mathbb{Z}$$

with

$$P(x) = \begin{pmatrix} a(x) & b(x) \\ 0 & 0 \end{pmatrix}, \quad Q(x) = \begin{pmatrix} 0 & 0 \\ c(x) & d(x) \end{pmatrix}.$$

For a matrix $M \in M(2, \mathbb{C})$, we use $\|M\|$ to denote the operator norm in \mathbb{C}^2 : $\|M\| = \sup_{\|x\|_{\mathbb{C}^2}=1} \|Mx\|_{\mathbb{C}^2}$. We suppose that:

(A.1) There exists a unitary matrix $C_0 = \begin{pmatrix} a_0 & b_0 \\ c_0 & d_0 \end{pmatrix} \in U(2)$ such that

$$\|C(x) - C_0\| \leq c_1|x|^{-1-\epsilon}, \quad x \in \mathbb{Z} \setminus \{0\}$$

with some positive c_1 and ϵ independent of x .

We denote by \mathcal{T}_1 the set of trace class operators.

Lemma 2.1 *Let U satisfy (A.1) and set $U_0 = SC_0$. Then, $U - U_0 \in \mathcal{T}_1$.*

Proof Let $T = U - U_0$ and $T(x) = C(x) - C_0$. Then,

$$T^*T = (C - C_0)^*(C - C_0) \tag{2.1}$$

is the multiplication operator by the matrix-valued function $T(x)^*T(x)$. Let $t_i(x)$ ($i = 1, 2$) be the eigenvalues of the Hermitian matrix $T(x)^*T(x) \in M(2, \mathbb{C})$ and take an orthonormal basis (ONB) $\{\tau_i(x)\}_{i=1,2}$ of corresponding eigenvectors for all $x \in \mathbb{Z}$.

We use $|\xi\rangle\langle\eta|$ to denote the operator on \mathcal{H} defined by $|\xi\rangle\langle\eta|\Psi = \langle\eta, \Psi\rangle\xi$. Then, we have

$$T^*T = \sum_{i=1,2} \sum_{x \in \mathbb{Z}} t_i(x) |\tau_{i,x}\rangle\langle\tau_{i,x}|, \quad (2.2)$$

where $\{\tau_{i,x}\}$ is the ONB given by

$$\tau_{i,x}(y) = \delta_{xy} \tau_i(x), \quad y \in \mathbb{Z}.$$

Since $T^*(x)T(x) \geq 0$, we have $t_i(x) \geq 0$. By (A.1), we know that

$$\max_{i=1,2} t_i(x) \leq c_1^2 |x|^{-2-2\epsilon}.$$

Hence, we have

$$\mathrm{Tr}|T| = \sum_{x \in \mathbb{Z}} \sum_{i=1,2} t_i(x)^{1/2} \leq 2c_1 \sum_{x \in \mathbb{Z}} |x|^{-1-\epsilon} < \infty,$$

which means that $T \in \mathcal{F}_1$. Since \mathcal{F}_1 is an ideal, $U - U_0 = ST \in \mathcal{F}_1$. \square

Example 2.1 (one-defect model) Let $C_0, C'_0 \in U(2)$ be unitary matrices with $C_0 \neq C'_0$ and set

$$C(x) = \begin{cases} C'_0, & x = 0 \\ C_0, & x \neq 0. \end{cases}$$

$U = SC$ satisfies (A.1), because $C(x) - C_0 = 0$ if $x \neq 0$.

Example 2.2 Let $C_0 \in U(2)$ be a unitary matrix and $\{C(x)\} \subset U(2)$ a family of unitary matrices. Assume that

$$\max_{i,j} |(C(x) - C_0)_{ij}| \leq c_1 |x|^{-1-\epsilon}, \quad x \in \mathbb{Z} \setminus \{0\},$$

where M_{ij} denotes the ij -component of a matrix M . Then, $U = SC$ satisfies (A.1), because all norms on a finite-dimensional vector space are equivalent.

We prove the following theorem in Sect. 3 using a discrete analogue of the Kato–Rosenblum theorem.

Theorem 2.1 *Let U and U_0 be as above and assume that (A.1) holds. Then,*

$$W_+ = s\text{-}\lim_{t \rightarrow \infty} U^{-t} U_0^t \Pi_{\mathrm{ac}}(U_0)$$

exists and is complete.

In what follows, we introduce the asymptotic velocity \hat{v}_0 , obtained first in [4], of the quantum walk with the evolution U_0 as follows. Let

$$\hat{U}_0(k) = \begin{pmatrix} e^{ik} & 0 \\ 0 & e^{-ik} \end{pmatrix} C_0, \quad k \in [0, 2\pi).$$

Since $\hat{U}_0(k) \in U(2)$, $\hat{U}_0(k)$ is represented as

$$\hat{U}_0(k) = \sum_{i=1,2} \lambda_i(k) |u_j(k)\rangle \langle u_j(k)|,$$

where $\lambda_j(k)$ is an eigenvalue of $\hat{U}_0(k)$ and $u_j(k)$ is the corresponding eigenvector with $\|u_j(k)\| = 1$. The function $k \mapsto e^{ik}$ is analytic, and so is $\lambda_j(k)$. We need the following assumption on $u_j(k)$:

(A.2) The functions $k \mapsto u_j(k)$ are continuously differentiable in k with

$$\sup_{k \in [0, 2\pi)} \left\| \frac{d}{dk} u_j(k) \right\|_{\mathbb{C}^2} < \infty.$$

Let \mathcal{K} be the Hilbert space of square integrable functions $f: [0, 2\pi) \rightarrow \mathbb{C}^2$ with norm

$$\|f\|_{\mathcal{K}} = \left(\int_0^{2\pi} \frac{dk}{2\pi} \|f(k)\|_{\mathbb{C}^2}^2 \right)^{1/2}.$$

Let $\mathcal{F}_0: \mathcal{H} \rightarrow \mathcal{K}$ be the discrete Fourier transform given by

$$(\mathcal{F}\Psi)(k) = \sum_{x \in \mathbb{Z}} e^{-ik \cdot x} \Psi(x), \quad \Psi \in \mathcal{H}.$$

We also use $\hat{\Psi}(k) = \begin{pmatrix} \hat{\Psi}^{(0)}(k) \\ \hat{\Psi}^{(1)}(k) \end{pmatrix}$ to denote the Fourier transform of Ψ . The asymptotic velocity \hat{v}_0 is the self-adjoint operator defined by

$$\hat{v}_0 = \mathcal{F}^{-1} \left(\int_{[0, 2\pi)}^{\oplus} \frac{dk}{2\pi} \sum_{j=1,2} \left(\frac{i\lambda'_j(k)}{\lambda_j(k)} \right) |u_j(k)\rangle \langle u_j(k)| \right) \mathcal{F}$$

The position operator \hat{x} is a self-adjoint operator defined by

$$(\hat{x}\Psi)(x) = x\Psi(x), \quad x \in \mathbb{Z}$$

with domain

$$D(\hat{x}) = \left\{ \Psi \in \mathcal{H} \mid \sum_{x \in \mathbb{Z}} |x|^2 \|\Psi(x)\|_{\mathbb{C}^2}^2 < \infty \right\}.$$

Let $\hat{x}_0(t) = U_0^{-t} \hat{x} U_0^t$ be the Heisenberg operator of \hat{x} for the evolution U_0 .

Theorem 2.2 *Let \hat{v}_0 and \hat{x}_0 be as above. Suppose that (A.2) holds. Then,*

$$s\text{-}\lim_{t \rightarrow \infty} \exp\left(i\xi \frac{\hat{x}_0(t)}{t}\right) = \exp(i\xi \hat{v}_0), \quad \xi \in \mathbb{R}. \tag{2.3}$$

Proof By [10, Theorem VIII.21], (2.3) holds if and only if

$$s\text{-}\lim_{t \rightarrow \infty} \left(\frac{\hat{x}_0(t)}{t} - z\right)^{-1} = (\hat{v}_0 - z)^{-1}, \quad z \in \mathbb{C} \setminus \mathbb{R},$$

which is proved in Sect. 4.1. □

Example 2.3 (i) Let $C_0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. Then, $\hat{U}_0(k)$ has eigenvalues 1 and -1 , which are independent of k . By definition, $\hat{v}_0 = 0$. Hence, the random variable $X_t^{(0)}/t$ converges in law to a random variable V_0 with a probability distribution δ_0 .

(ii) Let $C_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. $\hat{U}_0(k)$ has eigenvalues e^{ik} and $-e^{-ik}$. Hence, \hat{v}_0 has eigenvalues -1 and 1 . The random variable $X_t^{(0)}/t$ converges in law to a random variable V_0 with a probability distribution $\|\Psi^{(0)}\|^2 \delta_{-1} + \|\Psi^{(1)}\|^2 \delta_1$.

(iii) Let C_0 be the Hadamard matrix. The eigenvalues of $\hat{U}_0(k)$ are given by $\lambda_j(k) = ((-1)^j w(k) + i \sin k) / \sqrt{2}$ ($j = 1, 2$), where $w(k) = \sqrt{1 + \cos^2 k}$. Hence, \hat{v}_0 has no eigenvalue. The corresponding eigenvectors

$$u_j(k) = \sqrt{\frac{w(k) + (-1)^j \cos k}{2w(k)}} \begin{pmatrix} e^{ik} \\ (-1)^j w(k) - \cos k \end{pmatrix}$$

form an ONB of \mathbb{C}^2 and satisfy (A.2). The random variable $X_t^{(0)}/t$ converges in law to a random variable V_0 with a probability distribution $\|E_{\hat{v}_0}(\cdot)\Psi_0\|^2$, where $E_{\hat{v}_0}$ is the spectral measure of \hat{v}_0 . Let us consider the Hadamard walk starting from the origin. Let the initial state Ψ_0 satisfy $\Psi_0(0) = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ ($|\alpha|^2 + |\beta|^2 = 1$) and $\Psi(x) = 0$ if $x \neq 0$. Then,

$$d\|E_{\hat{v}_0}(v)\Psi_0\|^2 = (1 - c_{\alpha,\beta}v) f_K\left(v; \frac{1}{\sqrt{2}}\right) dv,$$

where $c_{\alpha,\beta} = |\alpha|^2 - |\beta|^2 + \alpha\bar{\beta} + \bar{\alpha}\beta$,

$$f_K(v; r) = \frac{\sqrt{1-r^2}}{\pi(1-v^2)\sqrt{r^2-v^2}} I_{(-r,r)}(v)$$

is the Konno function, and I_A is the indicator function of a set A . For more details, the reader can consult [4, 7].

Let $\hat{x}(t) = U^{-t}\hat{x}U$ be the Heisenberg operator of \hat{x} and define the asymptotic velocity \hat{v}_+ for the evolution U by

$$\hat{v}_+ = W_+ \hat{v}_0 W_+^*.$$

We need the following assumption:

(A.3) The singular continuous spectrum of U is empty.

We are now in a position to state our main result, which is proved in Sect. 4.2.

Theorem 2.3 *Let $\hat{x}(t)$ and \hat{v}_+ be as above. Suppose that (A.1)–(A.3) hold. Then,*

$$s\text{-}\lim_{t \rightarrow \infty} \exp\left(i\xi \frac{\hat{x}(t)}{t}\right) = \Pi_p(U) + \exp(i\xi \hat{v}_+) \Pi_{ac}(U), \quad \xi \in \mathbb{R}.$$

Let X_t be the random variable denoting the position of the walker at time $t \in \mathbb{N}$ with the initial state Ψ_0 . We use $\Pi_p(U)$ to denote the orthogonal projection onto the direct sum of all eigenspaces of U and E_A to denote the spectral projection of a self-adjoint operator A .

Corollary 2.4 *Let X_t be as above. Suppose that (A.1)–(A.3) hold. Then, X_t/t converges in law to a random variable V with a probability distribution*

$$\mu_V = \|\Pi_p(U)\Psi_0\|^2 \delta_0 + \|E_{\hat{v}_+}(\cdot)\Pi_{ac}(U)\Psi_0\|^2,$$

where δ_0 is the Dirac measure at zero.

Proof From Theorem 2.1, $s\text{-}\lim_{t \rightarrow \infty} U_0^{-t} U^t \Pi_{ac}(U)$ exists and is equal to W_+^* . Then, W_+ is unitary from $\text{Ran}W_+^* = \text{Ran}\Pi_{ac}(U_0)$ to $\text{Ran}W_+ = \text{Ran}\Pi_{ac}(U)$. Since, by Lemma 4.1, U_0 is strongly commuting with \hat{v}_0 , we know, from the intertwining property $UW_+ = W_+U_0$, that U is also strongly commuting with \hat{v}_+ . Hence, \hat{v}_+ is strongly commuting with $\Pi_{ac}(U)$ and $e^{i\xi \hat{v}_+} \Pi_{ac}(U) = \Pi_{ac}(U) e^{i\xi \hat{v}_+}$. Hence, by Theorem 2.3, $\exp(i\xi \hat{x}(t)/t)\Psi_0$ converges strongly to $\Pi_p(U)\Psi_0 + e^{i\xi \hat{v}_+} \Pi_{ac}(U)\Psi_0$ and

$$\begin{aligned} \lim_{t \rightarrow \infty} \mathbb{E}(e^{i\xi X_t/t}) &= \langle \Psi_0, \Pi_p(U)\Psi_0 + e^{i\xi \hat{v}_+} \Pi_{ac}(U)\Psi_0 \rangle = \|\Pi_p(U)\Psi_0\|^2 \\ &\quad + \int_{-\infty}^{\infty} e^{i\xi v} d\|E_{\hat{v}_+}(v)\Pi_{ac}(U)\Psi_0\|^2 = \int_{-\infty}^{\infty} e^{i\xi v} d\mu_V(v), \end{aligned}$$

which proves the corollary. □

Example 2.4 Let C_0 be the Hadamard matrix and $C(x)$ satisfy (A.1). As seen in Example 2.3 (iii), (A.2) is satisfied and the spectrum of U_0 is purely absolutely continuous. Let $\Psi_+ \in \mathcal{H}$ satisfy $\Psi_+(0) = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ ($|\alpha|^2 + |\beta|^2 = 1$) and $\Psi_+(x) = 0$ if $x \neq 0$. By Example 2.3,

$$d\|E_{\hat{v}_+}(v)\Pi_{\text{ac}}(U)W_+\Psi_+\|^2 = d\|E_{\hat{v}_0}(v)\Psi_+\|^2 = (1 - c_{\alpha,\beta}v)f_K\left(v; \frac{1}{\sqrt{2}}\right)dv.$$

Let $\Psi_p \in \text{Ran}\Pi_p(U_0)$ be a unit vector and take the initial state Ψ_0 as $\Psi_0 = C_1\Psi_p + C_2W_+\Psi_+$ ($|C_1|^2 + |C_2|^2 = 1$). Suppose that $U = SC$ satisfies (A.3). By Corollary 2.4, X_t/t converges in law to V with a probability distribution μ_V and

$$\mu_V(dv) = |C_1|^2\delta_0(dv) + |C_2|^2(1 - c_{\alpha,\beta}v)f_K\left(v; \frac{1}{\sqrt{2}}\right)dv.$$

3 Wave operator

To prove Theorem 2.1, we use the following general proposition:

Proposition 3.1 *Let U and U_0 be unitary operators on a Hilbert space \mathcal{H} and suppose that $U - U_0 \in \mathcal{T}_1$. The following limit exists:*

$$W_+ = s\text{-}\lim_{t \rightarrow \infty} U^{-t}U_0^t\Pi_{\text{ac}}(U_0)$$

Proof of Theorem 2.1 Since, by Lemma 2.1, $U - U_0 \in \mathcal{T}_1$, the wave operator W_+ exists. If we interchange the roles of U and U_0 , then the proposition says that the limit $s\text{-}\lim_{t \rightarrow \infty} U_0^{-t}U^t\Pi_{\text{ac}}(U)$ also exists, which implies that W_+ is complete. This completes the proof. \square

In the remainder of this section, we suppose that $U - U_0 \in \mathcal{T}_1$ and prove Proposition 3.1. This is done by a discrete analogue of [11, Theorem 6.2]. We use \mathcal{H}_{ac} and \mathcal{H}_p to denote the subspaces of absolute continuity and the direct sum of all eigenspaces of U_0 . Let E_0 be the spectral measure of U_0 with $E_0([0, 2\pi)) = I$. Let

$$\mathcal{H}_{\text{ac},0} = \{\psi \in \mathcal{H}_{\text{ac}} \mid d\|E_0(\lambda)\psi\|^2 = G_\psi(\lambda)^2d\lambda \text{ and } G_\psi \in L^2 \cap L^\infty\},$$

where $L^2 = L^2([0, 2\pi))$ and $L^\infty = L^\infty([0, 2\pi))$. Although the following lemma may be well known, we give proofs for completeness.

Lemma 3.1 $\mathcal{H}_{\text{ac},0}$ is dense in \mathcal{H}_{ac} .

Proof For all $\psi \in \mathcal{H}_{\text{ac}}$, there exists a positive function $F \in L^1$ such that $d\|E_0(\lambda)\psi\|^2 = F(\lambda)d\lambda$. Let $B_n = F^{-1}([0, n])$, and let χ_{B_n} be the characteristic function of B_n . We set $G_n = \sqrt{F}\chi_{B_n}$ and $\psi_n = E_0(B_n)\psi$. Then, $G_n \in L^2 \cap L^\infty$ and $\|E_0(B)\psi_n\|^2 = \int_B G_n(\lambda)^2d\lambda$. Hence, $\psi_n \in \mathcal{H}_{\text{ac},0}$ and $\psi = \lim_n \psi_n$. This completes the proof. \square

Lemma 3.2 *Let $\phi \in \mathcal{H}$ and $\psi \in \mathcal{H}_{ac,0}$. Then,*

$$\sum_{t \in \mathbb{Z}} |\langle \phi, U_0^t \psi \rangle|^2 \leq 2\pi \|\phi\|^2 \sup_{\lambda} G_{\psi}(\lambda)^2.$$

Proof Let $\psi \in \mathcal{H}_{ac,0}$ and $\mathcal{L} = L^2([0, 2\pi], G_{\psi}^2(\lambda)d\lambda)$. Let H_0 be the self-adjoint operator defined by $\langle \xi, H_0 \eta \rangle = \int_0^{2\pi} \lambda d\langle \xi, E_0(\lambda)\eta \rangle$ ($\xi, \eta \in \mathcal{H}$). Let $\mathcal{U} : \mathcal{L} \rightarrow \mathcal{H}$ be an injection defined by $\mathcal{U}f = f(H_0)\psi$ ($f \in \mathcal{L}$). Then $\mathcal{U}1 = \psi$ and $\mathcal{U}e^{it\lambda} = U_0^t \psi$ ($t \in \mathbb{N}$). We use Π to denote the orthogonal projection onto $U\mathcal{L}$. Let $\phi \in \mathcal{H}$ and $F = \mathcal{U}^{-1}\Pi\phi \in \mathcal{L}$. Then, we have

$$\langle \phi, U_0^t \psi \rangle = \int_0^{2\pi} e^{it\lambda} \bar{F}(\lambda) G_{\psi}(\lambda)^2 d\lambda = 2\pi \widehat{\bar{F}G_{\psi}^2}(t).$$

Hence, by Parseval’s identity, we obtain

$$\begin{aligned} \sum_{t \in \mathbb{Z}} |\langle \phi, U_0^t \psi \rangle|^2 &= 2\pi \int_0^{2\pi} |\bar{F}(\lambda) G_{\psi}(\lambda)^2|^2 d\lambda \\ &\leq 2\pi \sup_{\lambda} G_{\psi}(\lambda)^2 \int_0^{2\pi} |\bar{F}(\lambda)|^2 G_{\psi}(\lambda)^2 d\lambda \\ &\leq 2\pi \sup_{\lambda} G_{\psi}(\lambda)^2 \|\Pi\phi\|^2. \end{aligned}$$

This completes the proof. □

Let $W_t = U^{-t}U_0^t$.

Lemma 3.3 *Let $t, s \in \mathbb{N}$ ($s \neq t$). Then, $s\text{-}\lim_{r \rightarrow \infty} (W_t - W_s)U_0^r \Pi_{ac}(U_0) = 0$.*

Proof For $t, s \in \mathbb{N}$ ($t > s$), we have $W_t = \sum_{k=s+1}^t (W_k - W_{k-1}) + W_s$ and $W_k - W_{k-1} = U^{-k}(-T)U_0^{k-1}$, where $T = U - U_0 \in \mathcal{T}_1$. Since \mathcal{T}_1 is an ideal, we know that

$$W_t - W_s = \sum_{k=s+1}^t U^{-k}(-T)U_0^{k-1} \in \mathcal{T}_1.$$

In particular, $W_t - W_s$ is compact. Let H_0 be the self-adjoint operator defined in the proof of Lemma 3.2. Since $w\text{-}\lim_{r \rightarrow \infty} e^{irH_0} \Pi_{ac}(H_0) = 0$, we have

$$s\text{-}\lim_{r \rightarrow \infty} (W_t - W_s)U_0^r \Pi_{ac}(U_0) = s\text{-}\lim_{r \rightarrow \infty} (W_t - W_s)e^{irH_0} \Pi_{ac}(H_0) = 0.$$

This completes the proof. □

Proof of Proposition 3.1 By Lemma 3.1, it suffices to prove that, for $\psi \in \mathcal{H}_{ac,0}$,

$$\|(W_t - W_s)\psi\| \rightarrow 0, \quad t, s \rightarrow \infty.$$

Because

$$\|(W_t - W_s)\psi\|^2 = \langle \psi, W_t^*(W_t - W_s)\psi \rangle - \langle \psi, W_s^*(W_t - W_s)\psi \rangle,$$

we need only to prove that

$$\langle \psi, W_t^*(W_t - W_s)\psi \rangle \rightarrow 0, \quad t, s \rightarrow \infty.$$

By direct calculation, we have, for $r > 1$,

$$\begin{aligned} & W_t^*(W_t - W_s) - U_0^{-r} W_t^*(W_t - W_s)U_0^r \\ &= U_0^{-r} W_t^* W_s U_0^r - W_t^* W_s \\ &= \sum_{k=0}^{r-1} \left(U_0^{-k-1} W_t^* W_s U_0^{k+1} - U_0^{-k} W_t^* W_s U_0^k \right). \end{aligned}$$

Since

$$U_0^{-k-1} W_t^* W_s U_0^{k+1} - U_0^{-k} W_t^* W_s U_0^k = U_0^{-k-t-1} (T U^{t-s} - U^{t-s} T) U_0^{s+k},$$

we obtain

$$\begin{aligned} & W_t^*(W_t - W_s) - U_0^{-r} W_t^*(W_t - W_s)U_0^r \\ &= \sum_{k=0}^{r-1} U_0^{-k-t-1} (T U^{t-s} - U^{t-s} T) U_0^{s+k}. \end{aligned}$$

Since, by Lemma 3.3, $s\text{-}\lim_{r \rightarrow \infty} U_0^{-r} W_t^*(W_t - W_s)U_0^r \psi = 0$, we have

$$\begin{aligned} W_t^*(W_t - W_s)\psi &= \sum_{k=0}^{\infty} U_0^{-k-t-1} (T U^{t-s} - U^{t-s} T) U_0^{s+k} \psi \\ &= Z_{t,s}((U_0 T) U^{t-s} - (U_0 U^{t-s}) T) \psi, \end{aligned}$$

where

$$Z_{t,s}(A) = \sum_{k=0}^{\infty} U_0^{-k-t} A U_0^{k+s}.$$

By Lemma 3.4 below, we know that

$$|\langle \psi, W_t^*(W_t - W_s)\psi \rangle| \leq |\langle \psi, Z_{t,s}((U_0T)U^{t-s})\psi \rangle| + |\langle \psi, Z_{t,s}(U_0U^{t-s})T\psi \rangle| \rightarrow 0, \quad t, s \rightarrow \infty.$$

This completes the proof. □

Lemma 3.4 *Let $Y \in \mathcal{T}_1$ and $\{Q(t, s)\}$ be a family of bounded operators with $\sup_{t,s} \|Q(t, s)\| < \infty$. Then, for all $\psi \in \mathcal{H}_{ac,0}$,*

- (1) $\lim_{t,s \rightarrow \infty} \langle \psi, Z_{t,s}(YQ(t, s))\psi \rangle = 0$;
- (2) $\lim_{t,s \rightarrow \infty} \langle \psi, Z_{t,s}(Q(t, s)Y)\psi \rangle = 0$.

Proof Let $Y = \sum_{n=1}^{\infty} \lambda_n |\psi_n\rangle \langle \phi_n|$ be the canonical expansion of the compact operator Y . Since $Y \in \mathcal{T}_1$, $\sum_n \lambda_n < \infty$. Then, by the Cauchy–Schwartz inequality, we have

$$\begin{aligned} |\langle \psi, Z_{t,s}(YQ(t, s))\psi \rangle| &\leq \sum_{n=1}^{\infty} \sum_{k=0}^{\infty} \lambda_n \left| \langle U_0^{k+t}\psi, \psi_n \rangle \langle \phi_n, Q(t, s)U_0^{k+s}\psi \rangle \right| \\ &\leq I_1(t, s)^{1/2} \times I_2(t, s)^{1/2}, \end{aligned}$$

where

$$\begin{aligned} I_1(t) &= \sum_{n=1}^{\infty} \sum_{k=0}^{\infty} \lambda_n \left| \langle \psi_n, U_0^{k+t}\psi \rangle \right|^2, \\ I_2(t, s) &= \sum_{n=1}^{\infty} \sum_{k=0}^{\infty} \lambda_n \left| \langle Q(t, s)^*\phi_n, U_0^{k+s}\psi \rangle \right|^2. \end{aligned}$$

By Lemma 3.2, we have

$$I_2(t, s) \leq 2\pi \sup_{\lambda} G_{\psi}(\lambda)^2 \sup_{t,s} \|Q(t, s)\| \sum_n \lambda_n < \infty,$$

where we have used the fact that ϕ_n is a normalized vector. Let $u_k = \sum_{n=1}^{\infty} \lambda_n |\langle \psi_n, U_0^k\psi \rangle|^2$. Then, similar to the above, we observe that $\{u_k\} \in \ell^1(\mathbb{Z})$. Hence, we have

$$\lim_{t \rightarrow \infty} I_1(t) = \lim_{t \rightarrow \infty} \sum_{k=t}^{\infty} u_k = 0.$$

This proves (i). The same proof works for (ii). □

4 Asymptotic velocity

4.1 Proof of Theorem 2.2

Let

$$\mathcal{H}_0 = \bigcup_{m=0}^{\infty} \{ \Psi \in \mathcal{H} \mid \Psi(x) = 0, |x| \geq m \}.$$

We use \mathcal{D} to denote a subspace of vectors $\Psi \in \mathcal{H}$ whose Fourier transform $\hat{\Psi}$ is differentiable in k with

$$\sup_{k \in [0, 2\pi)} \left\| \frac{d}{dk} \hat{\Psi}(k) \right\| < \infty.$$

Note that \mathcal{H}_0 is a core for \hat{x} , and so is \mathcal{D} . Let $D = \mathcal{F} \hat{x} \mathcal{F}^{-1}$. Then, by direct calculation, we know that $(D\hat{\Psi})(k) = i \frac{d}{dk} \hat{\Psi}(k)$ for $\Psi \in \mathcal{D}$. We prove the following theorem:

Theorem 4.1 *Suppose that (A.2) holds. Then,*

$$s\text{-}\lim_{t \rightarrow \infty} \left(\frac{\hat{x}_0(t)}{t} - z \right)^{-1} = (\hat{v}_0 - z)^{-1}, \quad z \in \mathbb{C} \setminus \mathbb{R}. \tag{4.1}$$

Proof For all $\Psi \in \mathcal{H}$ and $\epsilon > 0$, there exists a vector $\Psi_\epsilon \in \mathcal{D}$ such that $\|\Psi - \Psi_\epsilon\| \leq \epsilon$. Because, by the second resolvent identity,

$$\begin{aligned} & \left\| \left(\frac{\hat{x}_0(t)}{t} - z \right)^{-1} \Psi - (\hat{v}_0 - z)^{-1} \Psi \right\| \\ & \leq \frac{2\epsilon}{|\text{Im}z|} + \left\| \left(\frac{\hat{x}_0(t)}{t} - z \right)^{-1} \Psi_\epsilon - (\hat{v}_0 - z)^{-1} \Psi_\epsilon \right\| \\ & \leq \frac{2\epsilon}{|\text{Im}z|} + \frac{1}{|\text{Im}z|} \left\| \left(\hat{v}_0 - \frac{\hat{x}_0(t)}{t} \right) (\hat{v}_0 - z)^{-1} \Psi_\epsilon \right\|, \end{aligned}$$

it suffices to prove that

$$\lim_{t \rightarrow \infty} \left\| \left(\hat{v}_0 - \frac{\hat{x}_0(t)}{t} \right) (\hat{v}_0 - z)^{-1} \Psi \right\| = 0, \quad \Psi \in \mathcal{D}.$$

Note that

$$(\hat{v}_0 - z)^{-1} = \mathcal{F}^{-1} \left(\int_{[0, 2\pi)}^{\oplus} dk \sum_{j=1,2} \left(\frac{i\lambda'_j(k)}{\lambda_j(k)} - z \right)^{-1} |u_j(k)\rangle \langle u_j(k)| \right) \mathcal{F}.$$

Since $\lambda_j(k)$ is analytic and $|\lambda_j(k)| = 1$, we observe from (A.2) that $(\hat{v}_0 - z)^{-1}$ leaves \mathcal{D} invariant. Hence, we only need to prove that

$$\lim_{t \rightarrow \infty} \left\| \left(\hat{v}_0 - \frac{\hat{x}_0(t)}{t} \right) \Psi \right\| = 0, \quad \Psi \in \mathcal{D}.$$

By direct calculation, we have

$$\begin{aligned} & \left\| \left(\hat{v}_0 - \frac{\hat{x}_0(t)}{t} \right) \Psi \right\|^2 \\ &= \int_0^{2\pi} dk \left\| \sum_{j=1,2} \left(\frac{i\lambda'_j(k)}{\lambda_j(k)} \right) \langle u_j(k), \hat{\Psi}(k) \rangle u_j(k) - \hat{U}(k)^{-t} \frac{D}{t} \hat{U}(k)^t \hat{\Psi}(k) \right\|^2 \\ &= \int_0^{2\pi} \frac{dk}{t^2} \left\| \sum_{j=1,2} \lambda_j(k)^t \hat{U}(k)^{-t} \left(i \frac{d}{dk} \langle u_j(k), \hat{\Psi}(k) \rangle u_j(k) \right) \right\|^2. \end{aligned}$$

By the definition of \mathcal{D} and (A.2), we know that

$$\sup_{k \in [0, 2\pi)} \left\| \left(i \frac{d}{dk} \langle u_j(k), \hat{\Psi}(k) \rangle u_j(k) \right) \right\| < \infty.$$

Hence, we have

$$\left\| \left(\hat{v}_0 - \frac{\hat{x}_0(t)}{t} \right) \Psi \right\| = O(t^{-1}),$$

which completes the proof. □

4.2 Proof of Theorem 2.3

The proof falls naturally into two parts:

Theorem 4.2 *Let U be a unitary operator on \mathcal{H} . $\hat{x}(t) = U^{-t} \hat{x} U^t$ satisfies*

$$s\text{-}\lim_{t \rightarrow \infty} \exp \left(i \xi \frac{\hat{x}(t)}{t} \right) \Pi_p(U) = \Pi_p(U), \quad \xi \in \mathbb{R}.$$

Theorem 4.3 *Let $U = SC$ and $U_0 = SC_0$ satisfy (A.1) and (A.2). Then,*

$$s\text{-}\lim_{t \rightarrow \infty} \exp \left(i \xi \frac{\hat{x}(t)}{t} \right) \Pi_{ac}(U) = \exp(i \xi \hat{v}_+) \Pi_{ac}(U), \quad \xi \in \mathbb{R}.$$

Proof of Theorem 2.3 By (A.3), we have

$$\begin{aligned} \text{s-} \lim_{t \rightarrow \infty} \exp\left(i\xi \frac{\hat{x}(t)}{t}\right) &= \text{s-} \lim_{t \rightarrow \infty} \exp\left(i\xi \frac{\hat{x}(t)}{t}\right) (\Pi_p(U) + \Pi_p(U)) \\ &= \Pi_p(U) + \exp(i\xi \hat{v}_+) \Pi_{ac}(U). \end{aligned}$$

This prove the theorem. \square

It remains to prove Theorems 4.2 and 4.3.

Proof of Theorem 4.2 Let $\mathcal{H}_p(U)$ be the direct sum of all eigenspaces of U . It suffices to prove that, for $\Psi \in \mathcal{H}_p(U)$,

$$\text{s-} \lim_{t \rightarrow \infty} \exp\left(i\xi \frac{\hat{x}(t)}{t}\right) \Psi = \Psi.$$

Let λ_n be the eigenvalues of U and take an ONB $\{\eta_n\}_{n=1}^\infty$ of \mathcal{H}_p such that $U\eta_n = \lambda_n\eta_n$. We have $\Pi_p(U) = \sum_n |\eta_n\rangle\langle\eta_n|$. Let $\epsilon > 0$. For sufficiently large N , $\Psi_N = \sum_{n=1}^N \langle\eta_n, \Psi\rangle\eta_n$ satisfies $\|\Psi - \Psi_N\| \leq \epsilon$. Then,

$$\left\| \exp\left(i\xi \frac{\hat{x}(t)}{t}\right) \Psi - \Psi \right\| \leq 2\epsilon + \left\| \exp\left(i\xi \frac{\hat{x}(t)}{t}\right) \Psi_N - \Psi_N \right\|.$$

By direct calculation, we have

$$\begin{aligned} \left\| \exp\left(i\xi \frac{\hat{x}(t)}{t}\right) \Psi_N - \Psi_N \right\| &= \left\| \left(\exp\left(i\xi \frac{\hat{x}}{t}\right) - 1 \right) U^t \Psi_N \right\| \\ &= \left\| \sum_{n=1}^N \lambda_n^t \langle\eta_n, \Psi\rangle \left(\exp\left(i\xi \frac{\hat{x}}{t}\right) - 1 \right) \eta_n \right\| \\ &\leq \sum_{n=1}^N |\langle\eta_n, \Psi\rangle| \left\| \left(\exp\left(i\xi \frac{\hat{x}}{t}\right) - 1 \right) \eta_n \right\|. \quad (4.2) \end{aligned}$$

Since $\lim_{t \rightarrow \infty} |1 - e^{i\xi x/t}| = 0$, $|1 - e^{i\xi x/t}| \leq 2$ and $\sum_x \|\eta_n(x)\|_{\mathbb{C}^2}^2 = \|\eta_n\|^2 < \infty$, we have

$$\lim_{t \rightarrow \infty} \left\| \left(\exp\left(i\xi \frac{\hat{x}}{t}\right) - 1 \right) \eta_n \right\|^2 = \lim_{t \rightarrow \infty} \sum_{x \in \mathbb{Z}} |e^{i\xi x/t} - 1|^2 \|\eta_n(x)\|_{\mathbb{C}^2}^2 = 0,$$

which, combined with (4.2), completes the proof. \square

Lemma 4.1 $[U_0, \exp(i\xi \hat{v}_0)] = 0$.

Proof By direct calculation, we have

$$\begin{aligned}
 [U_0, \exp(i\xi \hat{v}_0)] &= s\text{-}\lim_{t \rightarrow \infty} \left[U_0, \exp\left(i\xi \frac{\hat{x}_0(t)}{t}\right) \right] \\
 &= s\text{-}\lim_{t \rightarrow \infty} U_0 \left\{ \exp\left(i\xi \frac{\hat{x}_0(t)}{t}\right) - \exp\left(i\xi \frac{\hat{x}_0(t+1)}{t}\right) \right\} = 0.
 \end{aligned}$$

Proof of Theorem 4.3 By (A.1) and (A.2), Theorems 2.1 and 2.2 hold. Then, W_+ is a unitary operator from $\mathcal{H}_{ac}(U_0)$ to $\mathcal{H}_{ac}(U)$. Hence, we have

$$\exp(i\xi \hat{v}_+) \Pi_{ac}(U) = W_+ \exp(i\xi \hat{v}_0) W_+^* \Pi_{ac}(U).$$

By direct calculation, we observe that

$$\begin{aligned}
 I(t) &:= \exp\left(i\xi \frac{\hat{x}(t)}{t}\right) \Pi_{ac}(U) - \exp(i\xi \hat{v}_+) \Pi_{ac}(U) \\
 &= W_t \exp\left(i\xi \frac{\hat{x}_0(t)}{t}\right) W_t^* \Pi_{ac}(U) - W_+ \exp(i\xi \hat{v}_0) W_+^* \Pi_{ac}(U) \\
 &=: \sum_{j=1}^3 I_j(t),
 \end{aligned}$$

where

$$\begin{aligned}
 I_1(t) &= W_t \exp\left(i\xi \frac{\hat{x}_0(t)}{t}\right) (W_t^* - W_+^*) \Pi_{ac}(U), \\
 I_2(t) &= W_t \left(\exp\left(i\xi \frac{\hat{x}_0(t)}{t}\right) - \exp(i\xi \hat{v}_0) \right) W_+^* \Pi_{ac}(U), \\
 I_3(t) &= (W_t - W_+) \exp(i\xi \hat{v}_0) W_+^* \Pi_{ac}(U).
 \end{aligned}$$

Because W_t and $\exp(i\xi \hat{x}_0(t)/t)$ are uniformly bounded, we know from Theorems 2.1 and 2.2 that $s\text{-}\lim_{t \rightarrow \infty} I_1(t) = s\text{-}\lim_{t \rightarrow \infty} I_2(t) = 0$. Hence, we have

$$\begin{aligned}
 I(t) &= (W_t - W_+) \exp(i\xi \hat{v}_0) W_+^* \Pi_{ac}(U) + o(1) \\
 &= (W_t - W_+) \Pi_{ac}(U_0) \exp(i\xi \hat{v}_0) W_+^* \Pi_{ac}(U) \\
 &\quad + (W_t - W_+) [\exp(i\xi \hat{v}_0), \Pi_{ac}(U_0)] W_+^* \Pi_{ac}(U) + o(1),
 \end{aligned}$$

where we have used the fact that $\text{Ran} W_+^* = \mathcal{H}_{ac}(U_0)$. Since, by Lemma 4.1, $[\exp(i\xi \hat{v}_0), \Pi_{ac}(U_0)] = 0$, we obtain from Theorem 2.1, that $s\text{-}\lim_{t \rightarrow \infty} I(t) = 0$. This completes the proof. □

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