symmetry

Article

A Discontinuity of the Energy of Quantum Walk in Impurities

Kenta Higuchi [1], Takashi Komatsu [2], Norio Konno [3], Hisashi Morioka [4] and Etsuo Segawa [5,*]

[1] Department of Mathematical Sciences, Ritsumeikan University/Noji-Higashi, Kusatsu 525-8577, Japan; ra0039vv@ed.ritsumei.ac.jp
[2] Math. Research Institute Calc for Industry/Minami, Hiroshima 732-0816, Japan; t.komatsu.27@cc.it-hiroshima.ac.jp
[3] Department of Applied Mathematics, Yokohama National University/Hodogaya, Yokohama 240-8501, Japan; konno-norio-bt@ynu.ac.jp
[4] Graduate School of Science and Engineering, Ehime University/Bunkyo-cho 3, Matsuyama, Ehime 790-8577, Japan; morioka@cs.ehime-u.ac.jp
[5] Graduate School of Environment Information Sciences, Yokohama National University/Hodogaya, Yokohama 240-8501, Japan
* Correspondence: segawa-etsuo-tb@ynu.ac.jp

Abstract: We consider the discrete-time quantum walk whose local dynamics is denoted by a common unitary matrix C at the perturbed region $\{0, 1, \ldots, M-1\}$ and free at the other positions. We obtain the stationary state with a bounded initial state. The initial state is set so that the perturbed region receives the inflow ω^n at time n ($|\omega| = 1$). From this expression, we compute the scattering on the surface of -1 and M and also compute the quantity how quantum walker accumulates in the perturbed region; namely, the energy of the quantum walk, in the long time limit. The frequency of the initial state of the influence to the energy is symmetric on the unit circle in the complex plain. We find a discontinuity of the energy with respect to the frequency of the inflow.

Keywords: quantum walk; scattering theory; energy

check for updates

Citation: A Discontinuity of the Energy of Quantum Walk in Impuritie. *Symmetry* **2021**, *13*, 1134. https://doi.org/10.3390/sym13071134

Academic Editor: Motoichi Ohtsu

Received: 29 May 2021
Accepted: 21 June 2021
Published: 24 June 2021

1. Introduction

There is no doubt that a study on scattering theory is one of the most interesting topics of the Schrödinger equation. Recently, it has been revealed that the scatterings of some fundamental stationary Schrödinger equations on the real line with not only delta potentials [1–3] but also continuous potential [4] can be recovered by discrete-time quantum walks. These induced quantum walks are given by the following setting: the non-trivial quantum coins are assigned to some vertices in a finite region on the one-dimensional lattice as the impurities and the free-quantum coins are assigned at the other vertices. The initial state is given so that a quantum walker inflows into the perturbed region at every time step. It is shown that the scattering matrix of the quantum walk on the one-dimensional lattice can be explicitly described by using a path counting in [5] and this path counting method can be described by a discrete analogue of the Feynmann path integral [4]. There are some studies for the scattering theory of quantum walks under slightly general settings and related topics [6–12].

Such a setting is the special setting of [13,14] in that the regions where a quantum walker moves freely coincide with tails in [13,14], and the perturbed region can be regarded as a finite and connected graph in [13,14]. The properties of not only the scattering on the surface of the internal graph but also the stationary state in the internal graph for the Szegedy walk are characterized by [15] with a constant inflow from the tails.

By [14], this quantum walk converges to a stationary state. Therefore, let $\vec{\varphi}(\cdot)$: $\mathbb{Z} \to \mathbb{C}^2$ be the stationary state of the quantum walk on $\mathbb{Z}$. The perturbed region is $\Gamma_M := \{0, 1, \ldots, M-1\}$ and we assign the quantum coin

$$C = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

to each vertex in Γ_M. The inflow into the perturbed region at time n is expressed by ω^n ($|\omega| = 1$). In this paper, we compute (1) the scattering on the surface of the perturbed region Γ_M in the one-dimensional lattice; (2) the energy of the quantum walk. Here, the energy of quantum walk is defined by

$$\mathcal{E}_M(\omega) = \sum_{x=0}^{M-1} ||\vec{\varphi}(x)||^2_{\mathbb{C}^2}.$$

This is the quantity that quantum walkers accumulate to the perturbed region Γ_M in the long time limit. We obtain a necessary and sufficient condition for the perfect transmitting, and also obtain the energy. As a consequence of our result on the energy, we observe a discontinuity of the energy with respect to the frequency of the inflow. Moreover, our result implies that the condition for $\theta(\omega) \in \mathbb{N}$ is equivalent to the condition for the perfect transmitting. Then, we obtain that the situation of the perfect transmitting not only releases quantum walker to the opposite outside but also accumulates quantum walkers in the perturbed region. Note that since this quantum walk can be converted to a quantum walk with absorption walls, the problem is reduced to analysis on a finite matrix E_M, which is obtained by picking up from the total unitary time evolution operator with respect to the perturbed region Γ_M. See [16] for a precise spectral results on E_M.

This paper is organized as follows. In Section 2, we explain the setting of this model and give some related works. In Section 3, an explicit expression for the stationary state is computed using the Chebyshev polynomials. From this expression, we obtain the transmitting and reflecting rates and a necessary and sufficient condition for the perfect transmitting. We also give the energy in the perturbed region. In Section 4, we estimate the asymptotics of the energy to see the discontinuity with respect to the incident inflow.

2. The Setting of our Quantum Walk

The total Hilbert space is denoted by $\mathcal{H} := \ell^2(\mathbb{Z}; \mathbb{C}^2) \cong \ell^2(A)$. Here A is the set of arcs of one-dimensional lattice whose elements are labeled by $\{(x; R), (x; L) \mid x \in \mathbb{Z}\}$, where $(x; R)$ and $(x; L)$ represents the arcs "from $x-1$ to x", and "from $x+1$ to x", respectively. We assign a 2×2 unitary matrix to each $x \in \mathbb{Z}$ so-called local quantum coin

$$C_x = \begin{bmatrix} a_x & b_x \\ c_x & d_x \end{bmatrix}.$$

Putting $|L\rangle := [1, 0]^\top$, $|R\rangle := [0, 1]^\top$ and $\langle L| = [1, 0]$, $\langle R| = [0, 1]$, we define the following matrix valued weights associated with the motion from x to left and right by

$$P_x = |L\rangle\langle L|C_x, \quad Q_x = |R\rangle\langle R|C_x,$$

respectively. Then, the time evolution operator on $\ell^2(\mathbb{Z}; \mathbb{C}^2)$ is described by

$$(U\psi)(x) = P_{x+1}\psi(x+1) + Q_{x-1}\psi(x-1)$$

for any $\psi \in \ell^2(\mathbb{Z}; \mathbb{C}^2)$. Its equivalent expression on $\ell^2(A)$ is described by

$$\begin{aligned} (U'\phi)(x; L) &= a_{x+1}\phi(x+1; L) + b_{x+1}\phi(x+1; R), \\ (U'\phi)(x; R) &= c_{x-1}\phi(x-1; L) + d_{x-1}\phi(x-1; R) \end{aligned} \tag{1}$$

for any $\psi \in \ell^2(A)$. We call a_x and d_x the transmitting amplitudes, and b_x and c_x the reflection amplitudes at x, respectively. If we put $a_x = d_x = 1$ and $b_x = c_x = \sqrt{-1} = i$, then the primitive form of QW in [17] is reproduced. Remark that U and U' are unitarily equivalent such that letting $\eta : \ell^2(\mathbb{Z};\mathbb{C}^2) \to \ell^2(A)$ be

$$(\eta\psi)(x;R) = \langle R|\psi\rangle, \;\; (\eta\psi)(x;L) = \langle L|\psi\rangle$$

then we have $U = \eta^{-1}U'\eta$. The free quantum walk is the quantum walk where all local quantum coins are described by the identity matrix, i.e.,

$$(U_0\psi)(x) = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}\psi(x+1) + \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}\psi(x-1).$$

Then, the walker runs through one-dimensional lattices without any reflections in the free case.

In this paper, we set "impurities" on

$$\Gamma_M := \{0,1,\ldots,M-1\}$$

in the free quantum walk on one-dimensional lattice; that is,

$$C_x = \begin{cases} \begin{bmatrix} a & b \\ c & d \end{bmatrix} & : x \in \Gamma_M, \\ \\ I_2 & : x \notin \Gamma_M. \end{cases} \tag{2}$$

We consider the initial state Ψ_0 as follows.

$$\Psi_0(x) = \begin{cases} e^{i\xi x}|R\rangle & : x \le 0; \\ 0 & : \text{otherwise}, \end{cases}$$

where $\xi \in \mathbb{R}/2\pi\mathbb{Z}$. Note that this initial state belongs to no longer ℓ^2 category. The region Γ_M is obtained a time dependent inflow $e^{-i\xi n}$ from the negative outside. On the other hand, if a quantum walker goes out side of Γ_M, it never come back again to Γ_M. We can regard such a quantum walker as an outflow from Γ_M. Roughly speaking, in the long time limit, the inflow and outflow are balanced and obtain the stationary state with some modification. Indeed, the following statement holds.

Proposition 1 ([14])**.**

1. *This quantum walk converges to a stationary state in the following meaning:*

$$\exists \lim_{n\to\infty} e^{i(n+1)\xi}\Psi_n(x) =: \Phi_\infty(x).$$

2. *This stationary state is a generalized eigenfunction satisfying*

$$U\Phi_\infty = e^{-i\xi}\Phi_\infty.$$

Relation to an absorption problem

Let the reflection amplitude at time n be $\tilde{\gamma}_n(z) := \langle L|\Phi_n(-1)\rangle$ with $z = e^{i\xi}$. We can see that $\tilde{\gamma}_n(z)$ is rewritten by using U' as follows:

$$\begin{aligned} z^{-1}\tilde{\gamma}_{n+1}(z) = {} & \langle \delta_{(-1;L)}, U'\delta_{(0;R)}\rangle + \langle \delta_{(-1;L)}, U'^2\delta_{(0;R)}\rangle z \\ & + \langle \delta_{(-1;L)}, U'^3\delta_{(0;R)}\rangle z^2 + \cdots + \langle \delta_{(-1;L)}, U'^{n+1}\delta_{(0;R)}\rangle z^n \end{aligned}$$

The first term is the amplitude that the inflow at time n cannot penetrate into Γ_M; the m-th term is the amplitude that the inflow at time $n-(m-1)$ penetrates into Γ_M and escapes Γ_M from 0 side at time n. Therefore, each term corresponds to the "absorption" amplitude to -1 with the absorption walls -1 and M with the initial state $\delta_{(0;R)}$. Then

Remark 1. *The reflection amplitude $\langle L|\Phi_\infty(-1)\rangle = \lim_{n\to\infty}\tilde{\gamma}_n(z)$ coincides with the generating function of the absorption amplitude to -1 with respect to time n while the transmitting amplitude $\langle R|\Phi_\infty(M)\rangle = \lim_{n\to\infty}\tilde{\tau}_n(z)$ coincides with the generating function of the absorption amplitude to M with respect to time n.*

Put $\gamma_n := |\langle\delta_{(-1;L)}, U'^n\delta_{(0;R)}\rangle|^2$ and $\tau_n := |\langle\delta_{(M;R)}, U'^n\delta_{(0;R)}\rangle|^2$ which are the absorption/ first hitting probabilities at positions -1 and M, respectively, starting from $(0:R)$. From the above observation, for example, we can express the m-th moments of the absorption/hitting times to -1 and M as follows:

$$\sum_{n\geq 1} n^m\gamma_n = \int_0^{2\pi} \overline{\langle L|\Phi_\infty(-1)\rangle}\left(-i\frac{\partial}{\partial\xi}\right)^m \langle L|\Phi_\infty(-1)\rangle\frac{d\xi}{2\pi}, \tag{3}$$

$$\sum_{n\geq 1} n^m\tau_n = \int_0^{2\pi} \overline{\langle R|\Phi_\infty(M)\rangle}\left(-i\frac{\partial}{\partial\xi}\right)^m \langle R|\Phi_\infty(M)\rangle\frac{d\xi}{2\pi}. \tag{4}$$

Relation to Scattering of quantum walk

The stationary state Φ_∞ is a generalized eigenfunction of U in $\ell^\infty(\mathbb{Z};\mathbb{C}^2)$. The scattering matrix naturally appears in Φ_∞ (see [5]). In the time independent scattering theory, the inflow can be considered as the incident "plane wave", and the impurity causes the scattered wave by transmissions and reflections. Thus, we can see the transmission coefficient and the reflection coefficient in $\Phi_\infty(x)$ for $x\in\mathbb{Z}\setminus\Gamma_M$. For studies of a general theory of scattering, we also mention the recent work by Tiedra de Aldecoa [12].

3. Computation of Stationary State

3.1. Preliminary

Recall that $|L\rangle$ and $|R\rangle$ represent the standard basis of $\mathbb{C}^2$; that is, $|L\rangle = [1,0]^\top$ and $R\rangle = [0,1]^\top$. Let $\chi : \ell^2(\mathbb{Z};\mathbb{C}^2)\to\ell^2(\Gamma_M;\mathbb{C}^2)$ be a boundary operator such that $(\chi\psi)(a) = \psi(a)$ for any $a\in\{(x;R),(x;L)\mid x\in\Gamma_M\}$. Here, the adjoint $\chi^* : \ell^2(\Gamma_M;\mathbb{C}^2)\to\ell^2(\mathbb{Z};\mathbb{C}^2)$ is described by

$$(\chi^*\varphi)(a) = \begin{cases}\varphi(a) & : a\in\{(x;R),(x;L)\mid x\in\Gamma_M\},\\ 0 & : \text{otherwise.}\end{cases}$$

We put the principal submatrix of U with respect to the impurities by $E_M := \chi U\chi^*$. The matrix form of E_M with the computational basis $\chi\delta_0|L\rangle, \chi\delta_0|R\rangle, \dots, \chi\delta_{M-1}|L\rangle, \chi\delta_{M-1}|R\rangle$ is expressed by the following $2M\times 2M$ matrix:

$$E_M = \begin{bmatrix} 0 & P & & & \\ Q & 0 & P & & \\ & Q & 0 & \ddots & \\ & & \ddots & \ddots & P \\ & & & Q & 0 \end{bmatrix} \tag{5}$$

We express the $((x;J),(x';J'))$ element of E_M by

$$(E_M)_{(x;J),(x';J')} := \left\langle \chi\delta_x|J\rangle, E_M\chi\delta_{x'}|J'\rangle \right\rangle_{\mathbb{C}^{2M}}.$$

Putting $\psi_n := \chi\Psi_n$, we have

$$\begin{aligned}\psi_{n+1} &= \chi U(\chi^*\chi + (1-\chi^*\chi))\Psi_n \\ &= E_M\psi_n + \chi U(1-\chi^*\chi)\Psi_n \\ &= E_M\psi_n + e^{-i(n+1)\xi}\chi\delta_0|R\rangle.\end{aligned}$$

Then, putting $\phi_n := e^{i(n+1)\xi}\psi_n$, we have

$$e^{-i\xi}\phi_{n+1} = E_M\phi_n + \chi\delta_0|R\rangle. \tag{6}$$

From [14], $\varphi := \exists \lim_{n\to\infty}\phi_n$. Then, the stationary state restricted to Γ_M satisfies

$$(e^{-i\xi} - E_M)\phi_\infty = \chi\delta_0|R\rangle. \tag{7}$$

About the uniqueness of this solution is ensured by the following Lemma since it includes the existence of the inverse of $(e^{-i\xi} - E_M)$.

Lemma 1. *Let E_M be the above with $a \neq 0$.† Then $\sigma(E_M) \subset \{\lambda \in \mathbb{C} \mid |\lambda| < 1\}$.*

Proof. Let $\psi \in \ell^2(\Gamma_M, \mathbb{C}^2)$ be an eigenvector of eigenvalue $\lambda \in \sigma(E_M)$. Then

$$|\lambda|^2||\psi||^2 = ||E_M\psi||^2 = \langle U\chi^*\psi, \chi^*\chi U\chi^*\psi\rangle \leq \langle U\chi^*\psi, U\chi^*\psi\rangle = ||\chi^*\psi||^2 = ||\psi||^2. \tag{8}$$

Here, for the inequality, we used the fact that $\chi^*\chi$ is the projection operator onto

$$\mathrm{span}\{\delta_x|L\rangle, \delta_x|R\rangle \mid x \in \Gamma_M\} \subset \ell^2(\mathbb{Z};\mathbb{C}^2)$$

while for the final equality, we used the fact that $\chi\chi^*$ is the identity operator on $\ell^2(\Gamma_M;\mathbb{C}^2)$. If the equality in (8) holds, then $\chi^*\chi U\chi^*\psi = U\chi^*\psi$ holds. Then, we have the eigenequation $U\chi^*\psi = \lambda\chi^*\psi$ by taking χ^* to both sides of the original eigenequation $\chi U\chi^*\psi = \lambda\psi$. However, there are no eigenvectors having finite supports in a position independent quantum walk on $\mathbb{Z}$ with $a \neq 0$ since its spectrum is described by only a continuous spectrum in general. Thus, $|\lambda|^2 < 1$. □

Now, let us solve this Equation (7). The matrix representation of E_M with the permutation of the labeling such that $(x;R) \leftrightarrow (x;L)$ for any $x \in \Gamma_M$ to (5) is

$$E_M \cong \left[\begin{array}{cc|cc|cc|cc|cc}
0 & 0 & 0 & 0 & & & & & & \\
0 & 0 & b & a & & & & & & \\ \hline
d & c & 0 & 0 & 0 & 0 & & & & \\
0 & 0 & 0 & 0 & b & a & & & & \\ \hline
 & & d & c & \ddots & & \ddots & & & \\
 & & 0 & 0 & & & & & & \\ \hline
 & & & & \ddots & & \ddots & & 0 & 0 \\
 & & & & & & & & b & a \\ \hline
 & & & & & & d & c & 0 & 0 \\
 & & & & & & 0 & 0 & 0 & 0
\end{array}\right].$$

Then, the Equation (7) is expressed by

$$\left[\begin{array}{cc|cc|cc|cc|cc} z & 0 & 0 & 0 & & & & & & \\ \hline 0 & z & -b & -a & & & & & & \\ -d & -c & z & 0 & & & & & & \\ \hline & & 0 & z & -b & -a & & & & \\ & & -d & -c & z & 0 & & & & \\ \hline & & & & \ddots & & \ddots & & & \\ \hline & & & & & & 0 & z & -b & -a \\ & & & & & & -d & -c & z & 0 \\ \hline & & & & & & & & 0 & z \end{array}\right]\left[\begin{array}{c} \varphi(0;R) \\ \varphi(0;L) \\ \hline \varphi(1;R) \\ \varphi(1;L) \\ \hline \vdots \\ \vdots \\ \hline \varphi(M-2;R) \\ \varphi(M-2;L) \\ \hline \varphi(M-1;R) \\ \varphi(M-1;L) \end{array}\right] = \left[\begin{array}{c} 1 \\ 0 \\ \hline 0 \\ 0 \\ \hline \vdots \\ \vdots \\ \hline 0 \\ 0 \\ \hline 0 \\ 0 \end{array}\right].$$

Here, we changed the way of blockwise of E_M and we put $z = e^{-i\xi}$. Putting

$$A_z := \begin{bmatrix} 0 & z \\ -d & -c \end{bmatrix},\ B_z := \begin{bmatrix} -b & -a \\ z & 0 \end{bmatrix},$$

we have

$$\begin{aligned} &\begin{bmatrix} z & 0 \end{bmatrix}\vec{\varphi}(0) = 1,\ \ A_z\vec{\varphi}(0) + B_z\vec{\varphi}(1) = 0,\ \ A_z\vec{\varphi}(1) + B_z\vec{\varphi}(2) = 0, \ldots \\ &\qquad \ldots, A_z\vec{\varphi}(M-2) + B_z\vec{\varphi}(M-1) = 0,\ \ \begin{bmatrix} 0 & z \end{bmatrix}\vec{\varphi}(M-1) = 0, \end{aligned} \tag{9}$$

where $\vec{\varphi}(x) = [\varphi(x;R), \varphi(x;L)]^\top$ for any $x \in \Gamma_M$. The inverse matrix of B_z exists since $z \neq 0$. Then, we have

$$\vec{\varphi}(1) = T\vec{\varphi}(0),\ \vec{\varphi}(2) = T^2\vec{\varphi}(0), \ldots, \vec{\varphi}(M-1) = T^{M-1}\vec{\varphi}(0), \tag{10}$$

where

$$T = -B_z^{-1}A_z = \frac{1}{az}\begin{bmatrix} \Delta|a|^2 & -\Delta a\bar{b} \\ -\Delta\bar{a}b & z^2 + \Delta|b|^2 \end{bmatrix}.$$

Here $\Delta = \det(P+Q) = \det\begin{bmatrix} a & b \\ c & d \end{bmatrix}$. For the boundaries, there exists κ such that

$$\vec{\varphi}(0) = \begin{bmatrix} z^{-1} & \kappa \end{bmatrix},\ \begin{bmatrix} 0 & z \end{bmatrix}\vec{\varphi}(M-1) = 0. \tag{11}$$

By (10) and (11), κ satisfies

$$\left\langle \begin{bmatrix} 0 \\ 1 \end{bmatrix}, T^{M-1}\begin{bmatrix} z^{-1} \\ \kappa \end{bmatrix} \right\rangle = 0 \tag{12}$$

which is equivalent to

$$\kappa = -\frac{z^{-1}(T^{M-1})_{2,1}}{(T^{M-1})_{2,2}}.$$

Now, the problem is reduced to considering the n-th power of T because the eigenvector is expressed by $\vec{\varphi}(n) = T^n\vec{\varphi}(0)$. Since T is a just 2×2 matrix, we can prepare the following lemma.

Lemma 2. *Let A be a 2-dimensional matrix denoted by*

$$A = \begin{bmatrix} \alpha & \beta \\ \gamma & \delta \end{bmatrix}.$$

1. $(\alpha-\delta)^2+4\beta\gamma=0$ *and* $A\neq\epsilon I$ *for some* ϵ *case. Let* $\lambda=(\alpha+\delta)/2$*. Then*

$$A^n=\begin{bmatrix}\lambda^n+\frac{\alpha-\delta}{2}n\lambda^{n-1} & \beta n\lambda^{n-1}\\ \gamma n\lambda^{n-1} & \lambda^n-\frac{\alpha-\delta}{2}n\lambda^{n-1}\end{bmatrix}$$

2. *Otherwise. Let* $\zeta_n:=(\det(A)^{1/2})^{n-1}U_{n-1}(\frac{\mathrm{tr}(A)}{2\det(A)^{1/2}})$ *for* $n\geq 1$*. Then*

$$A^n=\begin{bmatrix}\zeta_{n+1}-\delta\zeta_n & \beta\zeta_n\\ \gamma\zeta_n & \zeta_{n+1}-\alpha\zeta_n\end{bmatrix},$$

where $U_n(\cdot)$ *is the n-th Chebyshev polynomial of the second kind.*

Remark 2. *The condition "*$(\alpha-\delta)^2+4\beta\gamma=0$ *and* $A\neq\epsilon I$*" is equivalent to the non-diagonalizability of A.*

Remark 3. *For* $A=T$ *case, the condition of 1. is reduced to*

$$\omega:=\Delta^{-1/2}z\in\{\epsilon_1|a|+\epsilon_2 i|b|\mid\epsilon_1,\epsilon_2\in\{\pm1\}\}=:\partial B.$$

Remark 4. *For* $A=T$ *case, the variable of the Chebyshev polynomial in 2. is reduced to*

$$\mathrm{tr}(T)/(2\det(T)^{1/2})=(\omega+\omega^{-1})/(2|a|).$$

Moreover, if $\omega=e^{ik}$*, the Chebyshev polynomial is described by* $U_{-1}(\cdot)=0$*,*

$$U_n(\cos k/|a|)=\frac{\lambda_+^{n+1}-\lambda_-^{n+1}}{\lambda_+-\lambda_-}\quad(n\geq 0).$$

Here, $\lambda_\pm$ *in RHS are the roots of the quadratic equation*

$$\lambda^2-\frac{2\cos k}{|a|}\lambda+1=0$$

with $|\lambda_-|\leq|\lambda_+|$*.*

3.2. Transmitting and Reflecting Rates

Let us divide the unit circle in the complex plain as follows:

$$B_{in}=\{e^{ik}\mid|\cos k|<|a|\},\ \partial B=\{e^{ik}\mid|\cos k|=|a|\},\ B_{out}=\{e^{ik}\mid|\cos k|>|a|\}. \quad (13)$$

By the unitarity of $\begin{bmatrix}a & b\\ c & d\end{bmatrix}$ and using the Chebyshev recursion; $U_{n+1}(x)=2xU_n(x)-U_{n-1}(x)$, we insert (1) and (2) in Lemma 2 into (10), and we have an explicit expression for the stationary state as follows.

Theorem 1. *Let the stationary state restricted to* $\Gamma_M=\{0,1,\ldots,M-1\}$ *be* ϕ_∞ *and* $\vec{\varphi}(n):=[\phi_\infty(n;R)\ \phi_\infty(n;L)]^\top$*. Then we have*

$$\vec{\varphi}(n)=\begin{cases}\frac{z^{-1}(\alpha\Delta^{-1/2})^{-n}}{\omega\zeta'_M-|a|\zeta'_{M-1}}\begin{bmatrix}\omega\zeta'_{M-n}-|a|\zeta'_{M-n-1}\\ \alpha b\zeta'_{M-n-1}\end{bmatrix} & :\omega\notin\partial B\\[2em] \frac{\Delta^{-1/2}\lambda^n}{\epsilon_R|a|+i\epsilon_I M|b|}\begin{bmatrix}\epsilon_R\alpha(\epsilon_R|a|+i\epsilon_I|b|(M-n))\\ b(M-n-1)\end{bmatrix} & :\omega\in\partial B\end{cases} \quad (14)$$

for $n = 0, 1, \ldots, M-1$, *where* $\alpha = a/|a|$ *and* $\zeta'_m = U_{m-1}(\frac{\omega+\omega^{-1}}{2|a|})$ $(m \geq 0)$, $\lambda = \mathrm{sgn}(\epsilon_R)\alpha^{-1}$ $\Delta^{1/2}$. *Here* $\epsilon_R = \mathrm{sgn}(Re(\omega))$ *and* $\epsilon_I = \mathrm{sgn}(Im(\omega))$

Since the transmitting and reflecting rates are computed by

$$T(\omega) = \left| \left\langle \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \vec{\varphi}(M-1) \right\rangle \times d \right|^2,$$
$$R(\omega) = \left| \left\langle \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \vec{\varphi}(0) \right\rangle \times a + \left\langle \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \vec{\varphi}(0) \right\rangle \times b \right|^2,$$

we obtain explicit expressions for them as follows.

Corollary 1. *Assume* $abcd \neq 0$. *For any* $\omega \in \mathbb{R}/(2\pi\mathbb{Z})$, *we have*

$$T(\omega) = \frac{|a|^2}{|a|^2 + |b|^2 \zeta'^2_M} \tag{15}$$
$$R(\omega) = \frac{|b|^2 \zeta'^2_M}{|a|^2 + |b|^2 \zeta'^2_M} \tag{16}$$

Note that the unitarity of the time evolution can be confirmed by $T + R = 1$. By Corollary 1, we can find a necessary and sufficient conditions for the perfect transmitting; that is , $T = 1$.

Corollary 2. *Assume* $abcd \neq 0$. *Let* $\omega = e^{ik}$ *with some real value k. Then the perfect transmitting happens if and only if*

$$\arccos\left(\frac{\cos k}{|a|}\right) \in \left\{ \frac{\ell}{M}\pi \mid \ell \in \{0, \pm 1, \ldots, \pm(M-1)\} \right\}.$$

On the other hand, the perfect reflection never occurs.

Remark that if $\omega \notin B_{in}$, then the perfect transmitting never happens.

3.3. Energy in the Perturbed Region

Taking the square modulus to $\vec{\varphi}(n)$ in Theorem 1, the relative probability at position $n \in \Gamma_M = \{0, \ldots, M-1\}$ can be computed as follows.

Proposition 2. *Assume* $abcd \neq 0$. *Then, the relative probability is described by*

$$||\vec{\varphi}(n)||^2 = \begin{cases} \frac{1}{|a|^2+|b|^2\zeta'^2_M}\left(|a|^2 + |b|^2\zeta'^2_{M-n-1} + |b|^2\zeta'^2_{M-n}\right) & : \omega \notin \partial B \\ \\ \frac{1}{|a|^2+M^2|b|^2}\left\{|a|^2 + |b|^2(M-n)^2 + |b|^2(M-n-1)^2\right\} & : \omega \in \partial B \end{cases} \tag{17}$$

Proof. Let us consider the case for $\omega \notin \partial B$. Using the property of the Chebyshev polynomial, we have $\zeta'_{m+1}\zeta'_{m-1} = \zeta'^2_m - 1$ and $(\omega + \omega^{-1})/|a| \cdot \zeta'_m = \zeta'_{m+1} + \zeta'_{m-1}$. It holds that

$$\begin{aligned}(\omega + \omega^{-1})\zeta'_m\zeta'_{m-1} &= |a|(\zeta'_{m+1} + \zeta'_{m-1})\zeta'_{m-1} \\ &= |a|(\zeta'^2_m + \zeta'^2_{m-1} - 1).\end{aligned}$$

Since $\zeta'_m \in \mathbb{R}$, we have

$$\begin{aligned} q(m) := |\omega\zeta'_m - |a|\zeta'_{m-1}|^2 &= {\zeta'}^2_m + |a|^2{\zeta'}^2_{m-1} - |a|^2(\omega+\omega^{-1})\zeta'_m\zeta'_{m-1} \\ &= |b|^2{\zeta'}^2_m + |a|^2, \end{aligned}$$

Then, we have

$$\begin{aligned} ||\vec{\varphi}(n)||^2 &= \frac{1}{q(M)}(q(M-n) + |b|^2{\zeta'}^2_{M-n-1}) \\ &= \frac{|b|^2{\zeta'}^2_{M-n} + |a|^2 + |b|^2{\zeta'}^2_{M-n-1}}{|b|^2{\zeta'}^2_M + |a|^2}. \end{aligned}$$

□

Then, we can see how much quantum walkers accumulate in the perturbed region $\Gamma_M = \{0, \ldots, M-1\}$ by

$$\mathcal{E}_M(\omega) =: \sum_{n=0}^{M-1} ||\vec{\varphi}(n)||^2.$$

We call it the energy of quantum walk. The dependency of the energy on ω is symmetric on the unit circle in the complex plain.

Corollary 3. *Let $\mathcal{E}_M(\omega)$ be the above and assume $abcd \neq 0$. Then we have*

$$\mathcal{E}_M(\omega) = \frac{1}{|a|^2 + |b|^2{\zeta'}^2_M}\left\{M|a|^2 + \frac{|b|^2}{(\lambda_+ - \lambda_-)^2}\left({\zeta'}^2_{M+1} - {\zeta'}^2_{M-1} - 4M\right)\right\} \tag{18}$$

In particular, $\mathcal{E}_M(\cdot)$ is continuous at every $\omega_* \in \partial B$ and

$$\mathcal{E}_M(\omega_*) = \frac{1}{3}\,\frac{M}{|a|^2 + |b|^2M^2}\left(3|a|^2 + |b|^2 + 2|b|^2M^2\right).$$

Proof. Using the properties of the Chebyshev polynomial for example, $U_n^2 - U_{n+1}U_{n-1} = 1$, $T_n = (U_n - U_{n-2})/2$, we have

$$(\lambda_+^{m-1} + \lambda_-^{m-1})\zeta'_M = 2T_{m-1}U_{m-1} = {\zeta'}^2_m - {\zeta'}^2_{m-1} + 1.$$

Then, we have

$$\begin{aligned} \sum_{n=0}^{m-1} {\zeta'_n}^2 &= \sum_{n=0}^{m-1}\left(\frac{\lambda_+^m - \lambda_-^m}{\lambda_+ - \lambda_-}\right)^2 \\ &= \frac{1}{(\lambda_+ - \lambda_-)^2}\left\{(\lambda_+^{m-1} + \lambda_-^{m-1})\zeta'_m - 2m\right\} \\ &= \frac{1}{(\lambda_+ - \lambda -)^2}({\zeta'}^2_m - {\zeta'}^2_{m-1} - 2m + 1) \end{aligned} \tag{19}$$

Then, we have

$$\begin{aligned} \sum_{n=0}^{M-1} ||\vec{\varphi}(n)||^2 &= \frac{1}{|a|^2 + |b|^2{\zeta'}^2_M}\left(M|a|^2 + |b|^2\sum_{n=0}^{M-1}{\zeta'}^2_{M-n-1} + {\zeta'}^2_{M-n}\right) \\ &= \frac{1}{|a|^2 + |b|^2{\zeta'}^2_M}\left\{M|a|^2 + \frac{|b|^2}{(\lambda_+ - \lambda_-)^2}\left({\zeta'}^2_{M+1} - {\zeta'}^2_{M-1} - 4M\right)\right\} \end{aligned}$$

Here, we used (19) in the last equality.

If $\omega \in \partial B$, then by directly computation taking summation of (17) over $n \in \Gamma_M = \{0, 1, \ldots, M-1\}$, we obtain the conclusion. Let us see $\mathcal{E}_M(\cdot)$ is continuous at ∂B. We put $x := (1/|a|)\cos k$ and $\zeta'_m(x) := \zeta'_m$. Remark that $\omega \to \omega_*$ implies $|x| \to 1$. In the following, we consider $x \to 1$ case. The Taylor expansion of $\zeta'_m(x)$ around $x = 1$ is

$$\zeta'_m(1-\epsilon) = m - \frac{m}{3}(m^2-1)\epsilon + O(\epsilon^2).$$

The reason for obtaining the expansion until ϵ^1 order is

$$\zeta'^2_{M+1} - \zeta'^2_{M-1} - 4M = O(\epsilon^2).$$

around $x = 1$. Note that $(\lambda_+ - \lambda_-)^2 = 4(x^2-1)$. Then

$$(\lambda_+ - \lambda_-)^2 = -8\epsilon + O(\epsilon)$$

around $x = 1$. Then inserting all of them into (18), we obtain

$$\lim_{\omega \to \omega_*} \mathcal{E}_M(\omega) = \frac{M}{|a|^2 + |b|^2 M^2}\left(|a|^2 + \frac{|b|^2}{3} + \frac{2|b|^2}{3}M^2\right).$$

□

4. Asymptotics of Energy

If $\omega \in \partial B$, then by Corollary 3, it is immediately obtained that

$$\lim_{M \to \infty} \frac{\mathcal{E}_M(\omega)}{M} = \frac{2}{3}. \tag{20}$$

Let us consider the case of $\omega \in B_{in} \cup B_{out}$ as follows. Note that

$$\lambda_\pm = \begin{cases} \mathrm{sgn}(\cos k)e^{\pm\theta} & : \omega \in B_{out}, \\ e^{\pm i\theta} & : \omega \in B_{in}, \end{cases}$$

where $(1/|a|)\cos k = \cosh\theta$ ($\omega \in B_{out}$), while $(1/|a|)\cos k = \cos\theta$ ($\omega \in B_{in}$) such that $\sin\theta > 0$ and $\sinh\theta > 0$. To observe the asymptotics of $\mathcal{E}_M(\omega)$ for $\omega \notin \partial B$, we rewrite $\mathcal{E}_M(\omega)$ as follows:

$$\mathcal{E}_M(\omega) = \begin{cases} \frac{1}{|a|^2\sinh^2\theta + |b|^2\sinh^2 M\theta}\left\{(-|b|^2 + |a|^2\sinh^2\theta)M + \frac{|b|^2}{4}\frac{\sinh 2M\theta \sinh 2\theta}{\sinh^2\theta}\right\} & : \omega \in B_{out} \\ \frac{1}{|a|^2\sin^2\theta + |b|^2\sin^2 M\theta}\left\{(|b|^2 + |a|^2\sin^2\theta)M - \frac{|b|^2}{4}\frac{\sin 2M\theta \sin 2\theta}{\sin^2\theta}\right\} & : \omega \in B_{in} \end{cases} \tag{21}$$

From now on, let us consider the asymptotics of $\mathcal{E}_M(\omega)$ for large M. We summarize our results on the asymptotics of $\mathcal{E}_M(\omega)$ in Table 1. In the following, we regard $\mathcal{E}_M(\omega)$ as a function of θ, M; that is $\mathcal{E}(M, \theta)$ because θ can be expressed by ω and consider the asymptotics for large M.

4.1. $\omega \in B_{out}$

Let us see that

$$\lim_{M \to \infty} \mathcal{E}_M(\omega) = \frac{\cosh\theta}{\sinh\theta} = \frac{\left|\frac{\cos k}{a}\right|}{\sqrt{\left|\frac{\cos k}{a}\right|^2 - 1}}. \tag{22}$$

Note that $\sinh M\theta \sim e^{M\theta}/2 \gg M$. Then by (21), we have

$$\mathcal{E}_M(\omega) \sim \frac{1}{|b|^2 e^{2M\theta}} \times \frac{|b|^2}{4} \frac{e^{2M\theta} \sinh 2\theta}{\sinh^2\theta} = \frac{\cosh\theta}{\sinh\theta}.$$

By (22), if $\omega \to \omega_* \in \partial B$, then $\mathcal{E}_M(\omega) \sim 1/\theta \to \infty$. To connect it to the limit for the case of $\omega_* \in \partial B$ described by (20) continuously, we consider $M \to \infty$ and $\theta \to 0$ simultaneously, so that $M\theta \sim \theta_* \in (0, \infty)$. Let us see that

$$\mathcal{E}_M(\omega) \sim \frac{1}{\sinh^2\theta_*}\left(-1 + \frac{\sinh 2\theta_*}{2\theta_*}\right)M \tag{23}$$

Noting that $\sinh m\theta = \sinh m\theta_* \neq 0$, for $m = 1, 2$ and $\sinh\theta \sim \theta_*/M$, we have

$$\begin{aligned}\mathcal{E}_M(\omega) &\sim \frac{1}{|b^2|\sinh^2\theta_*}\left\{-|b|^2 M + \frac{|b|^2}{4}\frac{\sinh 2\theta_* \times (2\theta_*/M)}{(\theta_*/M)^2}\right\} \\ &= \frac{1}{\sinh^2\theta_*}\left(-1 + \frac{\sinh 2\theta_*}{2\theta_*}\right)M\end{aligned}$$

Therefore, if we design the parameter θ_* so that

$$\frac{2}{3} = \frac{1}{\sinh^2\theta_*}\left(-1 + \frac{\sinh 2\theta_*}{2\theta_*}\right), \tag{24}$$

then the energy of B_{out} continuously closes to that of ∂B in the sufficient large system size M.

4.2. $\omega \in B_{in}$

In this paper, since we determine θ satisfying $\sin\theta > 0$, we set $\theta \in (0, \pi)$. Remark that $\mathcal{E}_M(\omega^{-1}) = \mathcal{E}_M(\omega)$ for any $\omega \in B_{in}$ because $e^{i\theta}$ is invariant under this deformation.

By (21), if $\sin\theta \asymp \sin M\theta \asymp 1$, we have

$$\mathcal{E}_M(\omega) \sim \left(\frac{|a|^2\sin^2\theta + |b|^2}{|a|^2\sin^2\theta + |b^2|\sin^2 M\theta}\right)M, \tag{25}$$

for sufficiently large M, which implies that

$$M \lesssim \mathcal{E}_M(\omega) \lesssim \left(1 + \frac{|b|^2}{|a|^2\sin^2\theta}\right)M \tag{26}$$

if $\theta \notin \{0, \pi\}$ is fixed. Then, we conclude that $\mathcal{E}_M(\omega) = O(M)$ if $\theta \notin \mathbb{Z}\pi$ is fixed for $\omega \in B_{in}$. On the other hand, if we design θ so that the condition of the perfect transmitting is satisfied; $\theta = \pi\ell/M$, $|\ell| \in \{1, \ldots, M-1\}$ (see Corollary 1) and choose ℓ which is very close to 0 or M, then $|\sin\theta| \ll 1$. Note that if $|\sin\theta| \to 0$, which means $\omega \to \omega_* \in \partial B$, then the coefficient of the upper bound in (26) diverges.

Then, from now on, let us consider the following three cases having a magnitude relation between θ and M;

$$\text{(i) } 1 \ll M \ll 1/\sin\theta;\quad \text{(ii) } M \asymp 1/\sin\theta;\quad \text{(iii) } 1/\sin\theta \ll M.$$

1. Case (i): $1 \ll M \ll 1/\sin\theta$
   Let us start to evaluate RHS of (21). Since

$$\frac{\sin 2M\theta\sin 2\theta}{4\sin^2\theta} \sim M\left\{1 - \frac{1}{3}(1 + 2M^2)\theta\right\},$$

the "{ }" part in RHS of (21) can be evaluated by $2|b|^2M^3\theta^2/3$. The denominator of (21) is evaluated by $1/(|b|^2M^2\theta^2)$. Combining them, we have

$$\mathcal{E}_M(\omega) \sim \frac{2M}{3} \tag{27}$$

This is consistent with (20).

2. Case (ii): $M \asymp 1/|\sin\theta|$
Under this condition, the parameter θ lives around 0 or π if M is large. Since we consider $\theta \in (0, \pi)$, we can evaluate $\sin\theta$ by $\sin\theta \sim \theta$, or $\sin\theta \sim (\pi - \theta)$ for large M. We define $\theta' = \theta$ if $0 < \theta < \pi/2$ and $\theta' = \pi - \theta$ if $\pi/2 \le \theta < \pi$. Because $M\sin\theta \asymp 1$ by the assumption, we have $M\theta' \asymp 1$. Therefore, we put $M\theta' = \theta_* + \epsilon$ with $\theta_* \asymp 1$ and $|\epsilon| \ll 1$. Then up to the value θ_*, let us see

$$\mathcal{E}_M(\omega) \sim \begin{cases} \frac{1}{\sin^2\theta_*}\left(1 - \frac{\sin 2\theta_*}{2\theta_*}\right)M & : \theta_* \notin \mathbb{Z}\pi, \\ \frac{|b|^2}{|a|^2\theta_*^2}M^3 & : \theta_* \in \mathbb{Z}\pi \text{ and } \epsilon M \ll 1 \\ \frac{M}{\epsilon^2} & : \theta_* \in \mathbb{Z}\pi \text{ and } \epsilon M \gg 1 \end{cases} \tag{28}$$

Note that if $\theta_* \notin \mathbb{Z}\pi$, then $\sin\theta = \sin\theta' \sim \theta_*/M$ and $\sin^2 M\theta = \sin^2 M\theta' \sim \sin^2\theta_* \neq 0$, $\sin 2M\theta = \sin 2M\theta' \sim \sin 2\theta_*$ and so on. Inserting them into (21), we have

$$\begin{aligned}\mathcal{E}_M(\omega) &\sim \frac{1}{|a|^2\theta_*^2/M^2 + |b|^2\sin^2\theta_*}\left\{(|a|^2\theta_*^2/M^2 + |b|^2)M - \frac{|b|^2}{4}\frac{\sin 2\theta_* \cdot 2\theta_*/M}{\theta_*^2/M^2}\right\} \\ &\sim \frac{1}{\sin^2\theta_*}\left(1 - \frac{\sin 2\theta_*}{2\theta_*}\right)M\end{aligned}$$

On the other hand, if $\theta_* \in \mathbb{Z}\pi$, since $\sin\theta \sim \theta_*/M$ and $\sin M\theta_* \sim \epsilon$, by (21), we have

$$\begin{aligned}\mathcal{E}_M(\omega) &\sim \frac{1}{|a|^2\theta^2 + |b|^2\epsilon^2}\left\{|b|^2M - \frac{|b|^2}{4}\frac{2\epsilon \cdot 2\theta_*/M}{(\theta_*/M)^2}\right\} \\ &\sim \frac{|b|^2M}{|a|^2\theta'^2 + |b|^2\epsilon^2} \\ &\sim \begin{cases} \frac{|b|^2}{|a|^2\theta_*^2}M^3 & : \epsilon \ll \theta_*/M \\ M/\epsilon^2 & : \epsilon \gg \theta_*/M \end{cases}\end{aligned}$$

3. Case (iii): $1/|\sin\theta| \ll M$
The "{ }" part in (21) is estimated by $(|b|^2 + |a|^2\sin^2\theta)M$ because $M\theta \gg 1$. Then, we have

$$\mathcal{E}_M(\omega) \sim \left(\frac{|a|^2\sin^2\theta + |b|^2}{|a|^2\sin^2\theta + |b^2|\sin^2 M\theta}\right)M, \tag{29}$$

for sufficiently large M which is the same as (25). Let us consider the following case study:

$$\text{(a)}\ \max\{|\sin\theta|, |\sin M\theta|\} \asymp 1;\quad \text{(b)}\ |\sin\theta|, |\sin M\theta| \ll 1.$$

(a) Let us see $\mathcal{E}_M(\omega) = O(M)$ in this case. If $\sin\theta \asymp \sin\theta M \asymp 1$, then the coefficient of M in (29) is a finite value, then we have (26). On the other hand, if each of $\sin\theta$ or $\sin M\theta \ll 1$, then (29) implies

$$\mathcal{E}_M(\omega) \sim \begin{cases} \frac{1}{\sin^2 M\theta}M & : \sin\theta \ll \sin M\theta \asymp 1 \\ (1 + \frac{|b|^2}{|a|^2\sin^2\theta})M & : \sin M\theta \ll \sin\theta \asymp 1 \end{cases} \tag{30}$$

(b) Since $|\sin M\theta| \ll 1$, we evaluate $|\sin M\theta|$ by

$$|\sin M\theta| \sim \min\{|M\theta|,\ |\pi - M\theta|, \dots, |M\pi - M\theta|\} =: \delta.$$

Then, there exists a natural number m such that $|\theta - m\pi/M| = \delta/M$. Note that $|\sin\theta|$ is also sufficiently small. Then, the natural number m must be $m/M \ll 1$ if $0 < \theta < \pi/2$ and $(M-m)/M \ll 1$ if $\pi/2 \le \theta < \pi$. Putting $m' := \min\{m, M-m\}$, we have

$$|\sin\theta| \sim |\frac{m'}{M}\pi \pm \frac{\delta}{M}| \sim \frac{\delta}{M}.$$

Therefore, $|\sin\theta| \ll |\sin M\theta| \ll 1$ holds. Then, (29) implies

$$\mathcal{E}_M(\omega) \sim \frac{M}{\delta^2}.$$

We summarize the above statements in the following theorem by setting $\theta = O(1/M)$, $\epsilon = 1/M^\alpha$ as a special but natural design of the parameters.

Theorem 2. *Let us set $\omega \in B_{in}$ so that*

$$\theta = \theta(M) = \left(x\pi + \frac{1}{M^\alpha}\right)\frac{1}{M}$$

with the parameters $x \in (0, M) \subset \mathbb{R}$ and $\alpha \ge 0$. If $x \to 0$ or $x \to M$ with fixed M, then $\mathcal{E}_M(\omega) = O(M)$. On the other hand, if we take $M \to \infty$ and fix $x' = \min\{x, M-x\} \asymp 1$, then we have

$$\mathcal{E}_M(\omega) = \begin{cases} O(M^3) & : x' \text{ is natural number and } \alpha \ge 1, \\ O(M^{1+2\alpha}) & : x' \text{ is natural number and } 0 \le \alpha < 1, \\ O(M) & : \text{otherwise.} \end{cases}$$

Table 1. Asymptotics of the energy of $\mathcal{E}_M(\omega)$: $\cos\theta = (\omega + \omega^{-1})/(2|a|)$, $M\theta = \theta_* + \epsilon$.

	$\mathbf{1 \ll M \ll 1/\theta}$	$\mathbf{1 \ll M \asymp 1/\theta}$	$\mathbf{1/\theta \ll M}$
$\omega \in \partial B$	-	-	$O(M)$
$\omega \in B_{out}$	$O(M)$		$\begin{cases} O(\theta^{-1}) & : 1/\theta \gg 1 \\ O(1) & : 1/\theta \asymp 1 \end{cases}$
$\omega \in B_{in}$	$O(M)$	$\begin{cases} O(M^3/{\theta_*}^2) & : \theta_* \in \mathbb{Z}\pi, \epsilon M \ll 1 \\ O(M\epsilon^{-2}) & : \theta_* \in \mathbb{Z}\pi, \epsilon M \gg 1 \\ O(M) & : \theta_* \notin \mathbb{Z}\pi \end{cases}$	

5. Conclusions

We considered the quantum walk on the line with the perturbed region $\{0, 1, \dots, M\}$; that is, an non-trivial quantum coin is assigned at the perturbed region and the free quantum coin is assigned at the other region. We set an ℓ^∞ initial state so that free quantum walkers are inputted at each time step to the perturbed region. A closed form of the stationary state of this dynamical system was obtained and we computed the energy of the quantum walk in the perturbed region. This energy represents how quantum walker feels "comfortable" in the perturbed region. We showed that the "feeling" of quantum walk depends on the frequency of the initial state. We can divide the region of the frequency into three parts to classify the asymptotics of the energy for large M; B_{in}, B_{out}, δB. The region B_{in} coincides with the continuous spectrum of the quantum walk with $M \to \infty$ [5]. We showed that quantum walkers prefer to the initial state whose frequency corresponds to the continuous spectrum in the infinite system. More precisely, the energy of the quantum walk in the perturbed region is estimated by $O(1)$ if $\theta \in B_{out}$, while one is estimated by $O(M)$ if

$\theta \in \delta B$ and *almost all* pseudo momentum θ gives $O(M)$-energy, but some momentum gives $O(M^3)$ if $\theta \in B_{in}$ (Theorem 2). Such an initial state exactly exists but it is quite rare from the view point of the Lebesgue measure. The most comfortable initial state for quantum walkers has the frequency whose pseudo momentum θ lives in some neighborhood of the boundary ∂B and accomplishes the perfect transmitting. If the momentum of the initial state exceeds the boundary ∂B from the internal region B_{in}, then the energy is immediately reduced to $O(1)$. It suggests that the control of the frequency of the initial state to give the maximal energy in the perturbed region is quite sensitive from the view point of an implementation.

The spectrum of the boundary ∂B for $M \to \infty$ produces the two singular points of the density function of the Konno limit distribution and is characterized by the Airy functions. In [16], details of the spectrum behavior around ∂B is discussed. Indeed, a kind of "speciality" also appears as the non-diagonalizability of T when $\theta \in \partial B$ in our work (Lemma 2). Note that the infinite system does not have any *edges*, which means every node is "impurity", while our quantum walker feels the *edges* of the impurities; nodes 0 and M. Therefore, to see the effect of such a finiteness on the behavior of the quantum walker comparing with the infinite system, computing how a quantum walker is distributed in the perturbed region is interesting which may be possible from the explicit expression of the stationary state in Theorem 1. Moreover, to consider the escaping time from the perturbed region seems to be useful to estimate the finesse as the interferometer motivated by quantum walk and it would be possible to extract some information from (3) and (4). This remains one of the interesting problems for the future.

Author Contributions: Conceptualization, E.S.; Formal analysis, E.S., H.M., T.K., K.H. and N.K. All authors have read and agreed to the published version of the manuscript.

Funding: HM was supported by the grant-in-aid for young scientists No. 16K17630, JSPS. ES acknowledges financial supports from the Grant-in-Aid of Scientific Research (C) No. JP19K03616, Japan Society for the Promotion of Science and Research Origin for Dressed Photon.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Higuchi, Y.; Konno, N.; Sato, I.; Segawa, E. Quantum graph walk I: mapping to quantum walks. *Yokohama Math. J.* **2013**, *59*, 33–53.
2. Matsue, K.; Matsuoka, L.; Ogurisu, O.; Segawa, E. Resonant-tunneling in discrete-time quantum walk. *Quantum Stud. Math. Found.* **2018**, *6*, 35–44. [CrossRef]
3. Tanner, G. From quantum graphs to quantum random walks, Non-Linear Dynamics and Fundamental Interactions, NATO Science Series II: Mathematics. *Phys. Chem.* **2006**, *213*, 69–87.
4. Higuchi, K. Feynman-type representation of the scattering matrix on the line via a discrete-time quantum walk. *J. Phys. A-Math. Theor.* **2021**, *33*, 23.
5. Konno, N.; Komatsu, T.; Morioka, H.; Segawa, E. Generalized eigenfunctions for quantum walks via path counting approach. *Rev. Math. Phys.* **2021**, *33*, 2150019.
6. Konno, N.; Komatsu, T.; Morioka, H.; Segawa, E. Asymptotic properties of generalized eigenfunctions for multi-dimensional quantum walks. *arXiv*, **2021**, arXiv.2104.00836.
7. Morioka, H. Generalized eigenfunctions and scattering matrices for position-dependent quantum walks. *Rev. Math. Phys.* **2019**, *31*, 1950019. [CrossRef]
8. Morioka, H.; Segawa, E. Detection of edge defects by embedded eigenvalues of quantum walks. *Quantum Inf. Process*. **2019**, *18*, 283. [CrossRef]
9. Richard, S.; Suzuki, A.; de Aldecoa, R.T. Quantum walks with an anisotropic coin I: spectral theory. *Lett. Math. Phys.* **2018**, *108*, 331–357. [CrossRef]
10. Richard, S.; Suzuki, A.; de Aldecoa, R.T. Quantum walks with an anisotropic coin II: scattering theory. *Lett. Math. Phys. First Online* **2018**. [CrossRef]
11. Suzuki, A. Asymptotic velocity of a position-dependent quantum walk. *Quantum Inf. Process* **2016**, *15*, 103–119. [CrossRef]
12. de Aldecoa, R.T. Stationary scattering theory for unitary operators with an application to quantum walks. *J. Funct. Anal.* **2020**, *279*, 108704. [CrossRef]

13. Feldman, E.; Hillery, M. Quantum walks on graphs and quantum scattering theory, Coding Theory and Quantum Computing, edited by D. Evans, J. Holt, C. Jones, K. Klintworth, B. Parshall, O. Pfister, and H. Ward. *Contemp. Math.* **2005**, *381*, 71–96.
14. Higuchi, Y.; Segawa, E. Dynamical system induced by quantum walks. *J. Physiscs A Math. Theor.* **2009**, *52*, 395202. [CrossRef]
15. Mohamed, S.; Higuchi, Y.; Segawa, E. Electric circuit induced by quantum walks. *J. Stat. Phys.* **2020**, *181*, 603–617.
16. Kuklinski, P. Conditional probability distributions of finite absorbing quantum walks. *Phys. Rev. A* **2020**, *101*, 032309. [CrossRef]
17. Feynman, R.P.; Hibbs, A.R. *Quantum Mechanics and Path Integrals*; emended edition; Dover Publications, Inc.: Mineola, NY, USA, 2010.