Interdisciplinary Information Sciences Vol. 22, No. 1 (2016) 17–29
©Graduate School of Information Sciences, Tohoku University
ISSN 1340-9050 print/1347-6157 online
DOI 10.4036/iis.2016.R.01

Weak Limit Theorem of a Two-phase Quantum Walk with One Defect

Shimpei ENDO[1,*], Takako ENDO[2], Norio KONNO[3], Etsuo SEGAWA[4] and Masato TAKEI[5]

[1] *Laboratoire Kastler Brossel, Ecole Normale Superieure, Paris 75231, France*
[2] *Department of Physics, Ochanomizu University, Tokyo 112-0012, Japan*
[3] *Department of Applied Mathematics, Faculty of Engineering, Yokohama National University, Yokohama 240-8501, Japan*
[4] *Graduate School of Information Sciences, Tohoku University, Sendai 980-8579, Japan*
[5] *Department of Applied Mathematics, Faculty of Engineering, Yokohama National University, Yokohama 240-8501, Japan*

We attempt to analyze a one-dimensional space-inhomogeneous quantum walk (QW) with one defect at the origin, which has two different quantum coins in positive and negative parts. We call the QW "the two-phase QW with one defect", which we treated concerning localization theorems [7]. The two-phase QW with one defect has been expected to be a mathematical model of topological insulator [15] which is an intense issue both theoretically and experimentally [3, 5, 11]. In this paper, we derive the weak limit theorem describing the ballistic spreading, and as a result, we obtain the mathematical expression of the whole picture of the asymptotic behavior. Our approach is based mainly on the generating function of the weight of the passages. We emphasize that the time-averaged limit measure is symmetric for the origin [7], however, the weak limit measure is asymmetric, which implies that the weak limit theorem represents the asymmetry of the probability distribution.

KEYWORDS: quantum walk, weak convergence, generating function, quantum probability, topological insulator

1. Introduction

This is a continuation of the previous work of [7], where we obtained the limit theorems for localization. For their characteristic properties, quantum walks (QWs) have attracted much attention in various fields, such as, quantum search algorithms [2, 23], and topological insulators [15], and so on. For the application of quantum walks, it is of great importance to further develop both analytic and numerical methods. Indeed, during the past decade many researchers have investigated the asymptotic behaviors of QWs from various viewpoints [6, 14, 17, 21, 22, 24]. From a mathematical viewpoint, two types of limit theorems for QWs have been established. The one is localization theorem. Localization is one of the typical properties of discrete-time QWs, which was first studied by Inui *et al.* [13] both mathematically and numerically. The detailed definition of localization is found in [1, 14] for example. The other is the weak limit theorem whose typical expression is described as follows [21]: There exist $C \in [0, 1)$, $a \in (0, 1)$, and a rational polynomial $w(x)$ such that

$$\mu(dx) = C\delta_0(dx) + w(x)f_K(x; a)dx \tag{1.1}$$

where

$$f_K(x; a) = \frac{\sqrt{1-a^2}}{\pi(1-x^2)\sqrt{a^2-x^2}} I_{(-a,a)}(x) \tag{1.2}$$

with

$$I_A(x) = \begin{cases} 1 & (x \in A) \\ 0 & (x \notin A) \end{cases}.$$

Received March 12, 2015; Accepted February 8, 2016; J-STAGE Advance published March 25, 2016
2010 Mathematics Subject Classification: Primary 62F12, Secondary 62F05.
SE acknowledges financial support of Postdoctoral Fellowship for Research Abroad from Japan Society for the Promotion of Science. TE is supported by Toshiko Yuasa Memorial Scholarship Fund. NK is partially supported by the Grant-in-Aid for Scientific Research (C) of Japan Society for the Promotion of Science (Grant No. 21540116). ES acknowledges financial supports of the Grant-in-Aid for Young Scientists (B) of Japan Society for the Promotion of Science (Grant No. 25800088).
*Corresponding author. E-mail: endo.takako@ocha.ac.jp

Here, that the first term, Dirac measure part in Eq. (1.1), $C\delta_0(dx)$, corresponds to localization, and the second term, absolutely continuous part, $w(x)f_K(x;a)dx$, describes the ballistic spreading. We remark that Eq. (1.1) gives

$$1 = C + \int_{-\infty}^{\infty} w(x)f_K(x;a)dx.$$

So far, the weak limit theorem of one-dimensional space-homogeneous QWs, such as Hadamard walk [17], Grover walk [19], have been derived. In 2013, Konno *et al.* [21] have first given the weak limit theorem for the typical inhomogeneous QWs, taking advantage of the generating function of the weights of passages. The method permits the analysis only for the QWs with one defect at the origin, whose quantum coins are the same both in positive and negative parts. Recently, various kinds of methods have been constructed to investigate mathematically the asymptotic behavior of QWs, such as the Fourier analysis [12], the CGMV method [4], the stationary phase method [16], the path counting method [18], and the generating function method [8]. We can expect to analyze various kinds of inhomogeneous QWs by the generating function method, while the Fourier analysis and stationary phase method are useful to study homogeneous QWs. However, the types of QWs that can be analyzed by the generating function method have not been obvious so far. We can also analyze inhomogeneous QWs by the CGMV method, however, the CGMV method allows only for the general discussion of localization for the typical QWs in one dimension. On the other hand, the generating function method offers not only localization theorem, but also the weak limit theorem for QWs.

By using the generating function method, we focus on the ballistic behavior of “the two-phase QW with one defect”. It has been known that the two-phase QW with one defect is deeply related to topological insulator which has attracted much attention of many physicists recently [3, 11, 15] as a key to construct the device of quantum computer. Hence we expect that the two-phase QW with one defect can be utilized to study topological insulator as its ideal mathematical model. By putting a phase in the unitary matrix of the QW in [20], we see that localization happens. Moreover, one-defect QW, whose time-evolution is described by the following two kinds of the unitary matrices, has already been studied in detail [21].

$$U_x = \begin{cases} \begin{bmatrix} a & b \\ c & d \end{bmatrix} & (x \neq 0), \\ \begin{bmatrix} a_0 & b_0 \\ c_0 & d_0 \end{bmatrix} & (x = 0). \end{cases}$$

This is one of the main mathematical motivations why we study the two-phase QW with one defect. Therefore, it would be greatly worth to study the mathematical aspects of the two-phase QW with one defect to exactly grasp the asymptotic behavior. Our main result is the first application of the generating function method to the weak limit theorem of QWs which have two phases with one defect. Combining the time-averaged limit measure [7] with the result in this paper, we obtain the whole mathematical picture of the asymptotic behavior of our two-phase QW.

The rest of this paper is organized as follows. In Section 2, we define the two-phase QW with one defect which is the main target in this paper, and present our main result. In addition, we give a concrete example of our two-phase QW, and show what our analytical result implies. In Section 3, we give the proof of Theorem 2.1.

2. Model and Results

2.1 The two-phase QW with one defect

For the general setting of two-state discrete-time QW in one dimension, the walker has a state at position x in each time t described by a two-dimensional vector as follows:

$$\Psi_t(x) = \begin{bmatrix} \alpha_t(x) \\ \beta_t(x) \end{bmatrix} \quad (x \in \mathbb{Z},\ \alpha_t(x), \beta_t(x) \in \mathbb{C}),$$

where $\mathbb{Z}$ is the set of integers, and $\mathbb{C}$ is the set of complex numbers.

In this paper, we focus on a discrete-time QW with two phases in one dimension whose time-evolution is described by the unitary matrices as follows:

$$U_x = \begin{cases} U_+ = \dfrac{1}{\sqrt{2}}\begin{bmatrix} 1 & e^{i\sigma_+} \\ e^{-i\sigma_+} & -1 \end{bmatrix} & (x \geq 1), \\ U_- = \dfrac{1}{\sqrt{2}}\begin{bmatrix} 1 & e^{i\sigma_-} \\ e^{-i\sigma_-} & -1 \end{bmatrix} & (x \leq -1), \\ U_0 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} & (x = 0), \end{cases} \tag{2.1}$$

where $\sigma_{\pm} \in [0, 2\pi)$.
For the simplicity of analysis, we put the unitary matrix U_0 at $x = 0$ and unified all the determinants to $\det(U_x) = -1$. Here, the time evolution is determined by the recurrence formula

$$\Psi_{t+1}(x) = P_{x+1}\Psi_t(x+1) + Q_{x-1}\Psi_t(x-1) \quad (x \in \mathbb{Z}),$$

where

$$P_x = \begin{cases} \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & e^{i\sigma_+} \\ 0 & 0 \end{bmatrix} & (x \geq 1), \\ \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} & (x = 0), \\ \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & e^{i\sigma_-} \\ 0 & 0 \end{bmatrix} & (x \leq -1), \end{cases} \qquad Q_x = \begin{cases} \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 0 \\ e^{-i\sigma_+} & -1 \end{bmatrix} & (x \geq 1), \\ \begin{bmatrix} 0 & 0 \\ 0 & -1 \end{bmatrix} & (x = 0), \\ \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 0 \\ e^{-i\sigma_-} & -1 \end{bmatrix} & (x \leq -1), \end{cases}$$

with $U_x = P_x + Q_x$. Note that P_x and Q_x correspond to the left and right movements, respectively. The walker steps differently in positive and negative parts each other. In this paper, we call the QW "the two-phase QW with one defect". The model with $\sigma_+ = \sigma_-$ becomes a one-defect QW, which has been analyzed in detail so far [21]. Owing to the defect at the origin, the model has an origin symmetry, and the analysis becomes simple. One of the mathematically interesting future problems is to analyze QW with two phases which does not have defect at the origin, and we will report the analytical results of a two-phase QW without defect at the origin in the upcoming paper. We derived localization theorems [7] for the two-phase QW with one defect, in particular, the time-averaged limit and stationary measures. Hence, by obtaining the weak limit theorem corresponding to the ballistic spreading, we can mathematically express the whole picture of the asymptotic behavior of the two-phase QW with one defect.

2.2 Main result: the weak limit theorem

Let $\overline{\mu}_\infty(x)$ be the time-averaged limit measure defined by

$$\overline{\mu}_\infty(x) = \lim_{T\to\infty} \frac{1}{T}\sum_{t=0}^{T-1} P(X_t = x).$$

Then, we introduce C defined by the summation of the time-averaged limit measure $\overline{\mu}_\infty(x)$:

$$C = \sum_{x\in\mathbb{Z}} \overline{\mu}_\infty(x).$$

We see that localization for the QW starting from the origin happens if

$$\overline{\mu}_\infty(0) > 0.$$

Here $\{X_t\}$ is a set for the position of the walker at time t defined by $P(X_t = x) = \|\Psi_t(x)\|^2$, where $P(X_t = x)$ is the probability that the walker exists at position x. Now, we present the weak limit theorem for the missing part $1 - C$ with $0 \leq C < 1$. The proof of Theorem 2.1 is given in Section 3. In general, the weak limit theorem describes the ballistic spreading of the QW [17]. Hereafter, let $\mathbb{R}$ be the set of real numbers.

Theorem 2.1. *Consider the two-phase QW with one defect starting from the origin with the initial coin state* $\varphi_0 = {}^T[\alpha, \beta]$, *where* $\alpha, \beta \in \mathbb{C}$. *Put* $\alpha = ae^{i\phi_1}$, $\beta = be^{i\phi_2}$ *with* $a, b \geq 0$, $a^2 + b^2 = 1$ *and* $\phi_1, \phi_2 \in \mathbb{R}$. *Let* $\sigma = (\sigma_+ - \sigma_-)/2$ *and* $\tilde{\phi}_{12} = \phi_1 - \phi_2$. *For the two-phase QW with one defect,* X_t/t *converges weakly to the random variable* Z *which has the following measure:*

$$\mu(dx) = C\delta_0(dx) + w(x)f_K(x; 1/\sqrt{2})dx,$$

where $f_K(x; 1/\sqrt{2})$ *is defined by Eq. (1.2) and*

$$w(x) = \frac{t_3x^5 + t_2x^4 + t_1x^3 + t_0x^2}{s_2x^4 + s_1x^2 + s_0}, \tag{2.2}$$

with

$$\begin{cases} s_2 = 4\cos^4\sigma, \\ s_1 = 4\cos^2\sigma(1 + 2\sin^2\sigma), \\ s_0 = \cos^2 2\sigma, \end{cases} \qquad \begin{cases} t_3 = 4\cos^2\sigma(b^2 - a^2), \\ t_2 = 4[\cos^2\sigma(1 + \sqrt{2}ab\,\mathrm{sgn}(x)\cos\gamma(x)) + \sqrt{2}ab\,\mathrm{sgn}(x)\sin\gamma(x)\sin 2\sigma], \\ t_1 = 2(b^2 - a^2), \\ t_0 = 2\{1 + \sqrt{2}ab\,\mathrm{sgn}(x)\cos\gamma(x) - \sqrt{2}ab\,\mathrm{sgn}(x)\sin\gamma(x)\sin 2\sigma\}, \end{cases}$$

and

$$\gamma(x) = \begin{cases} \tilde{\phi}_{12} - \sigma_- & (x \geq 0), \\ -\tilde{\phi}_{12} + \sigma_+ & (x < 0). \end{cases}$$

Here we should note that $w(x) f_K(x; 1/\sqrt{2})$ is an absolutely continuous part of the weak limit measure $\mu(dx)$.

If $\sigma_+ = \sigma_-$, then, we see from Eq. (2.2) that the weight function is given by

$$w(x) = \frac{2x^2}{1+2x^2} \begin{cases} 1 + \sqrt{2}\Re(e^{-i\sigma}\alpha\overline{\beta}) + (b^2 - a^2)x & (x \geq 0), \\ 1 - \sqrt{2}\Re(e^{-i\sigma}\alpha\overline{\beta}) + (b^2 - a^2)x & (x < 0), \end{cases} \tag{2.3}$$

which agrees with the result obtained by Theorem 4.1 in [21].

Remark:
Here we should note that the expression of the weight function in Theorem 4.1 in [21] contains a typo, and the correct transcription is

$$w(x) = \frac{|c|^2 x^2}{(|c|^2 - m)^2 + (|c|^2 - m^2)x^2}\left[\gamma(x) - |a_0|^2\left\{(|\alpha|^2 - |\beta|^2) + \frac{2\Re(a_0\alpha\overline{b_0\beta})}{|a_0|^2}\right\}x\right].$$

As we see in Eqs. (2.2) and (2.3), the two different quantum coins give such complexity to the weight function. In our previous paper [7], we reported that the time-averaged distribution of the two-phase QW with one defect is symmetric for the origin, however, we emphasize that the weight function $w(x)$, the main result in this paper, is asymmetric, which suggests that the probability distribution has asymmetry for the origin. One of the interesting future problems is to show the explicit relation between topological insulator and the two-phase QW with one defect, for the two-phase QW with one defect can be considered as an ideal mathematical model of topological insulator which has been considered as a key to construct the device of quantum computer.

2.3 Example

In this subsection, we see a concrete example of our result. We consider the QW defined by the unitary matrices

$$U_x = \begin{cases} U_+ = \dfrac{1}{\sqrt{2}}\begin{bmatrix} 1 & -i \\ i & -1 \end{bmatrix} & (x = 1, 2, \cdots), \\ U_- = \dfrac{1}{\sqrt{2}}\begin{bmatrix} 1 & -1 \\ -1 & -1 \end{bmatrix} & (x = -1, -2, \cdots), \\ U_0 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} & (x = 0). \end{cases}$$

We obtain the QW by putting $\sigma_+ = 3\pi/2$ and $\sigma_- = \pi$ in Eq. (2.1), which we examined its localization effect in Subsection 2.4 in [7]. Hereafter, we will apply our mathematically concrete result, that is, Theorem 2.1, to the QW for the two cases of initial coin state as follows;

(1) Let the initial coin state be $\varphi_0 = {}^T[1, 0]$. According to Theorem 2.1, the weight function of the QW is

$$w(x) = \frac{2(1 - x^3 + x^2 - x)}{x^2 + 4}.$$

Hence, we see

$$\int_{-\frac{1}{\sqrt{2}}}^{\frac{1}{\sqrt{2}}} w(x) f_K(x; 1/\sqrt{2})dx = \frac{3}{5}.$$

In our previous study [7], we obtained the following expression of the time-averaged limit measure $\overline{\mu}_\infty(x)$ (Theorem 2 in [7]):

$$\overline{\mu}_\infty(x) = I_{\{-1/\sqrt{2} \leq \sin\sigma \leq 1\}}(x)\nu^{(+)}(x;\sigma) + I_{\{-1 \leq \sin\sigma \leq 1/\sqrt{2}\}}(x)\nu^{(-)}(x;\sigma),$$

and

$$\nu^{(\pm)}(x;\sigma) = \left(\frac{1 \pm \sqrt{2}\sin\sigma}{3 \pm 2\sqrt{2}\sin\sigma}\right)^2 \{1 \mp 2\Re(ie^{-i\tilde{\sigma}}\alpha\overline{\beta})\}$$
$$\times \left\{\delta_0(x) + (1 - \delta_0(x))(2 \pm \sqrt{2}\sin\sigma)\left(\frac{1}{3 \pm 2\sqrt{2}\sin\sigma}\right)^{|x|}\right\},$$

with $\tilde{\sigma} = (\sigma_+ + \sigma_-)/2$, $\tilde{\phi}_{12} = \phi_1 - \phi_2$. As a result, we derived the coefficient C of the delta function $\delta_0(dx)$ in Eq. (1.1) which expresses localization:

$$C = \sum_x \overline{\mu}_\infty(x) = \frac{4}{25} + 2 \times \frac{12}{25} \sum_{y=1}^{\infty} \left(\frac{1}{5}\right)^y = \frac{2}{5}.$$

Therefore, we have

$$C + \int_{-\frac{1}{\sqrt{2}}}^{\frac{1}{\sqrt{2}}} w(x) f_K(x; 1/\sqrt{2}) dx = 1.$$

(2) Next, we consider the initial coin state $\varphi_0 = {}^T[i/\sqrt{2}, 1/\sqrt{2}]$. Theorem 2.1 gives the weight function by

$$w(x) = \begin{cases} \dfrac{2(1-\sqrt{2})x^2 + 2 + \sqrt{2}}{x^2+4} & (x \geq 0) \\ \dfrac{(2+\sqrt{2})x^2 + 2 + \sqrt{2}}{x^2+4} & (x < 0) \end{cases}.$$

Hence, we get

$$\int_{-\frac{1}{\sqrt{2}}}^{\frac{1}{\sqrt{2}}} w(x) f_K(x; 1/\sqrt{2}) dx = \frac{1}{5}(3+\sqrt{2}).$$

Here, we derived the time-averaged limit measure $\overline{\mu}_\infty(x)$ by Theorem 2 in [7], and as a result, we obtained the coefficient of the delta function $\delta_0(dx)$ in Eq. (1.1) by

$$C = \sum_x \overline{\mu}_\infty(x) = \frac{4}{25}\left(1 - \frac{1}{\sqrt{2}}\right) + 2 \times \frac{12}{25}\left(1 - \frac{1}{\sqrt{2}}\right) \sum_{y=1}^{\infty} \left(\frac{1}{5}\right)^y = \frac{2}{5}\left(1 - \frac{1}{\sqrt{2}}\right).$$

Thereby, we have

$$C + \int_{-\frac{1}{\sqrt{2}}}^{\frac{1}{\sqrt{2}}} w(x) f_K(x; 1/\sqrt{2}) dx = 1.$$

Here, we show the numerical results of the probability distribution at time $t = 100$, 1000, and 10000 in re-scaled spaces $(x/t, tP_t(x))$ $(t = 100, 1000, 10000)$, where x represents the position of the walker and $P_t(x)$ is the probability that the walker exists on position x at time t. We should note that x/t corresponds to the real axis, and $tP_t(x)$ corresponds to the imaginary axis, respectively. Also, we put the graph of $w(x)f_K(x; 1/\sqrt{2})$, which is related to absolutely continuous part of the weak limit measure $\mu(dx)$, on the picture at each time. We see that the graph of $w(x)f_K(x; 1/\sqrt{2})$ is right on the middle of the probability distribution for each position at each time, which suggests that our result is mathematically proper. We also emphasize that $\overline{\mu}_\infty(x)$ is symmetric for the origin [7], however, $w(x)f_K(x; 1/\sqrt{2})$ does not have an origin symmetry (Figs. 1, 2, 3, 4, 5, 6), which indicates that the weak limit measure represents the asymmetry of the probability distribution (Figs. 1, 2, 3, 4, 5, 6). Furthermore, regardless of the difference of the initial coin state, the distributions become asymmetric.

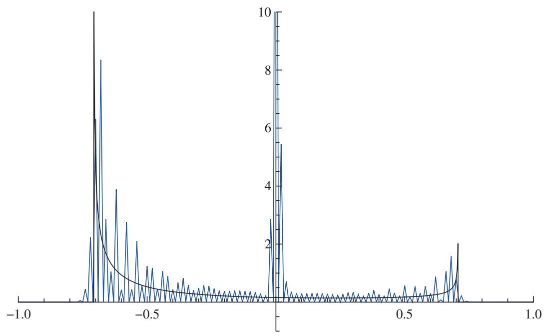

Fig. 1. [$\varphi_0 = {}^T[1, 0]$ case.]
Blue line: Probability distribution in a re-scaled space $(x/100, 100P_{100}(x))$ at time 100, Black curve: $w(x)f_K(x; 1/\sqrt{2})$.

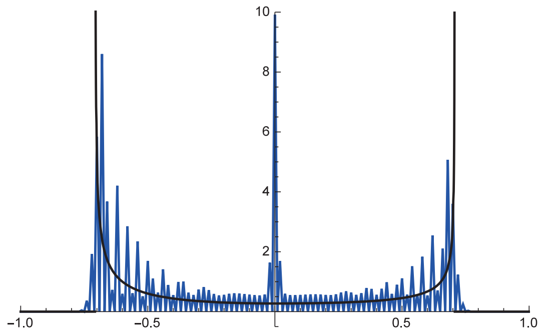

Fig. 2. [$\varphi_0 = {}^T[i/\sqrt{2}, 1/\sqrt{2}]$ case.]
Blue line: Probability distribution in a re-scaled space $(x/100, 100P_{100}(x))$ at time 100, Black curve: $w(x)f_K(x; 1/\sqrt{2})$.

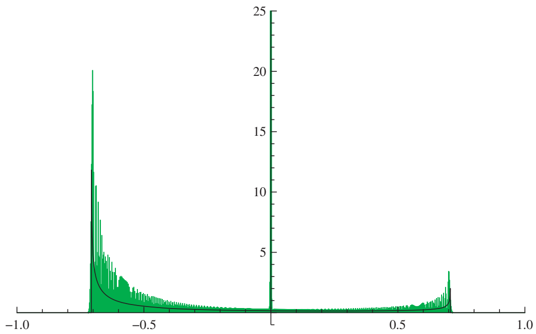

Fig. 3. [$\varphi_0 = {}^T[1, 0]$ case.]
Green line: Probability distribution in a re-scaled space $(x/1000, 1000P_{1000}(x))$ at time 1000, Black curve: $w(x)f_K(x; 1/\sqrt{2})$.

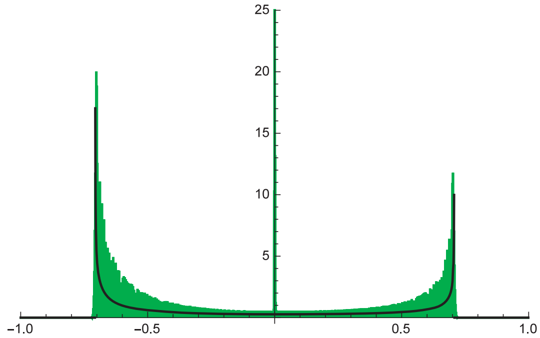

Fig. 4. [$\varphi_0 = {}^T[i/\sqrt{2}, 1/\sqrt{2}]$ case.]
Green line: Probability distribution in a re-scaled space $(x/1000, 1000P_{1000}(x))$ at time 1000, Black curve: $w(x)f_K(x; 1/\sqrt{2})$.

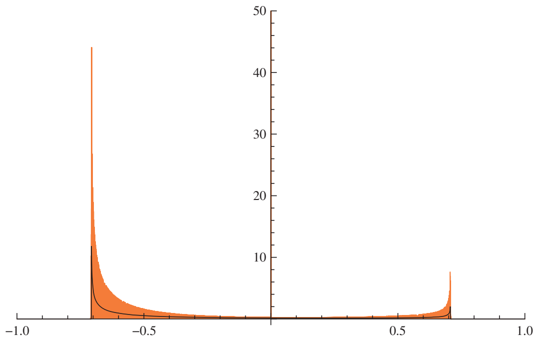

Fig. 5. [$\varphi_0 = {}^T[1, 0]$ case.]
Orange line: Probability distribution in a re-scaled space $(x/10000, 10000P_{10000}(x))$ at time 10000, Black curve: $w(x)f_K(x; 1/\sqrt{2})$.

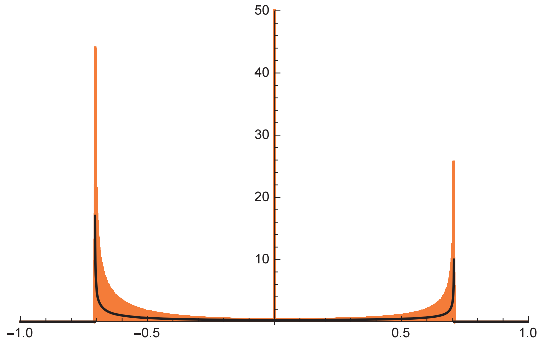

Fig. 6. [$\varphi_0 = {}^T[i/\sqrt{2}, 1/\sqrt{2}]$ case.]
Orange line: Probability distribution in a re-scaled space $(x/10000, 10000P_{10000}(x))$ at time 10000, Black curve: $w(x)f_K(x; 1/\sqrt{2})$.

3. Proof of Theorem 2.1

In this section, we focus on the characteristic function of QW, that is,

$$E\left[e^{i\xi\frac{X_t}{t}}\right] = \int_{x\in\mathbb{Z}} g_{X_t/t}(x)e^{i\xi x}dx, \tag{3.1}$$

where $g_{X_t/t}(x)$ is the density function of random variable X_t/t. In a similar way as Appendix A in [7], we consider how $E[e^{i\xi X_t/t}]$ can be written when $t \to \infty$. Here, we should note that to obtain $g_{X_t/t}(x)$ $(t \to \infty)$ is equivalent to derive $w(x)f_K(x; 1/\sqrt{2})$.

Let $\Xi_t(x)$ be the weight of all the passages of the walker, which moves left l times and moves right m times till time t [21]:

$$\Xi_t(x) = \sum_{l_j, m_j} P_{x_{l_1}}^{l_1} Q_{x_{m_1}}^{m_1} P_{x_{l_2}}^{l_2} Q_{x_{m_2}}^{m_2} \cdots P_{x_{l_t}}^{l_t} Q_{x_{m_t}}^{m_t},$$

where $l + m = t$, $-l + m = x$, $\sum_i l_i = l$, $\sum_j m_j = m$ with $l_i + m_i = 1$, $l_i, m_i \in \{0, 1\}$, and $\sum_{\gamma=l_i,m_j} |x_\gamma| = x$. We give useful concrete expressions of $\tilde{\Xi}_x(z) = \sum_{t\geq 0} \Xi_t(x)z^t$ which play important roles in the proof. Lemma 3.1 is equivalent to Lemma 2 in [7], which we used to derive the time-averaged limit measure for the two-phase QW with one defect. Assume that the quantum walker starts from the origin with the initial coin state $\varphi_0 = {}^T[\alpha, \beta]$ with $\alpha, \beta \in \mathbb{C}$ and $|\alpha|^2 + |\beta|^2 = 1$.

Lemma 3.1. (1) *If* $x = 0$, *we have*

$$\tilde{\Xi}_0(z) = \frac{1}{1 + \tilde{f}_0^{(+)}(z)\tilde{f}_0^{(-)}(z)} \begin{bmatrix} 1 & -\tilde{f}_0^{(+)}(z) \\ \tilde{f}_0^{(-)}(z) & 1 \end{bmatrix}.$$

(2) *If* $|x| \geq 1$, *we have*

$$\tilde{\Xi}_x(z) = \begin{cases} (\tilde{\lambda}^{(+)}(z))^{x-1} \begin{bmatrix} \tilde{\lambda}^{(+)}(z)\tilde{f}_x^{(+)}(z) \\ z \end{bmatrix} [0,-1]\tilde{\Xi}_0(z) & (x \geq 1), \\ (\tilde{\lambda}^{(-)}(z))^{|x|-1} \begin{bmatrix} z \\ \tilde{\lambda}^{(-)}(z)\tilde{f}_x^{(-)}(z) \end{bmatrix} [1,0]\tilde{\Xi}_0(z) & (x \leq -1), \end{cases}$$

where $\tilde{\lambda}^{(+)}(z) = \frac{z}{e^{-i\sigma_+}\tilde{f}_0^{(+)}(z)-\sqrt{2}}$, $\tilde{\lambda}^{(-)}(z) = \frac{z}{\sqrt{2}-e^{i\sigma_-}\tilde{f}_0^{(-)}(z)}$. *Here* $\tilde{f}_x^{(+)}(z)$ *and* $\tilde{f}_x^{(-)}(z)$ *satisfy the following quadratic equations, respectively;*

$$\begin{cases} (\tilde{f}_x^{(+)}(z))^2 - \sqrt{2}e^{i\sigma_+}(1+z^2)\tilde{f}_x^{(+)}(z) + e^{2i\sigma_+}z^2 = 0, \\ (\tilde{f}_x^{(-)}(z))^2 - \sqrt{2}e^{-i\sigma_-}(1+z^2)\tilde{f}_x^{(-)}(z) + e^{-2i\sigma_-}z^2 = 0. \end{cases}$$

Since the coefficients of these quadratic equations are independent of the position x, the solutions $\tilde{f}_x^{(\pm)}(z)$ are also independent of x:

$$\tilde{f}_x^{(\pm)}(z) = \sqrt{2}e^{\pm i\sigma_\pm}z^2\left(1 - \frac{1}{2-\sqrt{2}e^{\mp i\sigma_\pm}\tilde{f}_x^{(\pm)}(z)}\right).$$

Hereafter, we will write $\tilde{f}_x^{(\pm)}(z)$ by $\tilde{f}_0^{(\pm)}(z)$ for simplicity.
Now, from a simple calculation, we obtain $E[e^{i\xi X_t/t}]$ $(t \to \infty)$ written by the square norm of the residue of $\hat{\tilde{\Xi}}_x(z) = \sum_t \tilde{\Xi}_t(x)z^t$ as follows:

Proposition 3.2. *We have*

$$E\left[e^{i\xi\frac{X_t}{t}}\right] \to \int_0^{2\pi} \sum_{\theta \in A} e^{-i\xi\theta'(k)} \|Res(\hat{\tilde{\Xi}}(k:z) : z = e^{i\theta(k)})\|^2 \frac{dk}{2\pi} \quad (t \to \infty), \tag{3.2}$$

where A *is the set of the singular points of* $\hat{\tilde{\Xi}}(k:z) \equiv \sum_{x\in\mathbb{Z}} \tilde{\Xi}_x(z)e^{ikx}$. *Note* $\theta'(k) = \partial\theta(k)/\partial k$.

[Proof of Proposition 3.2]

Hereafter, we will explain how Eq. (3.2) is derived, which is a key of the proof of Theorem 2.1. Put $w_l(k) = Res(\hat{\tilde{\Psi}}(k:z) : z = e^{i\theta^{(l)}(k)})$ with $\Psi_t(x) = \Xi_t(x)\varphi_0$, where $\{e^{i\theta^{(l)}(k)}\}_{l=\pm}$ is the set of the singular points of $\hat{\tilde{\Xi}}(k:z)$. Now we introduce Lemma 3.3, which plays an important role for the proof;

Lemma 3.3. (1) *We have*

$$\left|\frac{\partial\theta^{(+)}(k)}{\partial k} - \frac{\partial\theta^{(-)}(k)}{\partial k}\right| \leq \sqrt{2} \quad (0 < k \leq \pi/2).$$

(2) *There exists* $C^{(0)} \in \mathbb{R}_{>0}$, *such that*

$$\left|\frac{\partial w_\pm(k)}{\partial k}\right| < C^{(0)} \quad (0 < k \leq \pi/2).$$

Noting

$$\left|\frac{\partial\theta^{(+)}(k)}{\partial k} - \frac{\partial\theta^{(-)}(k)}{\partial k}\right| = \frac{2|\cos k|}{\sqrt{1+\cos^2 k}},$$

we obtain (1). Taking into account that the denominator of $\partial w_\pm(k)/\partial k$ can not be 0 and the numerator does not diverge, we get (2), where the expression of $\partial w_\pm(k)/\partial k$ is so complicated and lengthy, and we omit it.
By definition, we have

$$\begin{aligned} E[e^{i\xi X_t/t}] &= \int_0^{2\pi} \langle\hat{\Psi}_t(k), \hat{\Psi}_t(k+\xi/t)\rangle \frac{dk}{2\pi} \\ &= \int_0^{2\pi} \left\langle \sum_l w_l(k)e^{-i(t+1)\theta^{(l)}(k)}, \sum_m w_m(k+\xi/t)e^{-i(t+1)\theta^{(m)}(k+\xi/t)} \right\rangle \frac{dk}{2\pi} \qquad (3.3) \\ &= \int_0^{2\pi} \left\{ \sum_l |w_l(k)|^2 e^{-i\xi(t+1)/t\frac{\partial\theta^{(m)}(k)}{\partial k}} e^{-i(t+1)O(1/t^2)} + O(1/t) \right\} \frac{dk}{2\pi} \\ &\quad + \int_0^{2\pi} \left\{ \sum_l \sum_m \overline{w_l(k)} e^{i(t+1)\theta^{(l)}(k)} w_m(k)e^{-i(t+1)\theta^{(m)}(k)} e^{-i\xi(t+1)/t\frac{\partial\theta^{(m)}(k)}{\partial k}} e^{-i(t+1)O(1/t^2)} + O(1/t) \right\} \frac{dk}{2\pi}. \qquad (3.4) \end{aligned}$$

Here, by using the Fourier analysis, we have

$$\hat{\Psi}_t(k) = \frac{1}{2\pi i}\oint_{|z|=r} \hat{\hat{\Psi}}(k;z)\frac{dz}{z^{t+1}} \quad (0 < r < 1).$$

Now, we have the following expression by using the residue theorem;

$$\hat{\Psi}_t(k) = -\sum_{l=\pm} Res(\hat{\hat{\Psi}}(k:z) : z = e^{i\theta^{(l)}(k)})(e^{i\theta^{(l)}(k)})^{-t-1} + \frac{1}{2\pi i}\oint_{|z|=R} \hat{\hat{\Psi}}(k;z)\frac{dz}{z^{t+1}} \tag{3.5}$$

with $R > 1$. Due to Lemma 3.1, we see

$$\begin{aligned}\hat{\hat{\Psi}}(k:z) = &\frac{e^{ik}}{(1-e^{ik}\tilde{\lambda}^{(+)}(z))(1+\tilde{f}_0^{(+)}(z)\tilde{f}_0^{(-)}(z))}\begin{bmatrix} -\tilde{\lambda}^{(+)}(z)\tilde{f}_0^{(+)}(z)(\tilde{f}_0^{(-)}(z)\alpha+\beta) \\ -z(\tilde{f}_0^{(-)}(z)\alpha+\beta)\end{bmatrix} \\ &+ \frac{e^{-ik}}{(1-e^{-ik}\tilde{\lambda}^{(-)}(z))(1+\tilde{f}_0^{(+)}(z)\tilde{f}_0^{(-)}(z))}\begin{bmatrix} z(\alpha-\tilde{f}_0^{(+)}(z)\beta) \\ \tilde{\lambda}^{(-)}(z)\tilde{f}_0^{(-)}(z)(\alpha-\tilde{f}_0^{(+)}(z)\beta)\end{bmatrix} \\ &+ \frac{1}{1+\tilde{f}_0^{(+)}(z)\tilde{f}_0^{(-)}(z)}\begin{bmatrix}\alpha-\tilde{f}_0^{(+)}(z)\beta \\ \tilde{f}_0^{(-)}(z)\alpha+\beta\end{bmatrix}.\end{aligned}$$

According to [21], we obtain

$$\tilde{f}^{(\pm)}(w) = -\frac{we^{\pm i\sigma_\pm}}{\sqrt{2}}\left\{(w-w^{-1})+\sqrt{(w-w^{-1})^2+2}\right\},$$

and

$$\tilde{\lambda}^{(\pm)}(w) = \pm\frac{i}{\sqrt{2}}\left\{(w+w^{-1})-\sqrt{(w+w^{-1})^2-2}\right\}.$$

By putting $w = Re^{i\theta}$ ($R \in \mathbb{R}_{\geq 0}$), we see that there exist $C^{(1)}, C^{(2)} \in \mathbb{R}_{>0}$ such that

$$|\tilde{f}^{(\pm)}(w)| \sim C^{(1)}R^2$$

and

$$|\tilde{\lambda}^{(\pm)}(Re^{i\theta})| \sim C^{(2)}.$$

Thereby, we have

$$|\hat{\hat{\Psi}}(k:Re^{i\theta})| \sim \left|\begin{bmatrix}1\\ \frac{1}{R}\end{bmatrix}+\begin{bmatrix}\frac{1}{R}\\ 1\end{bmatrix}+\frac{1}{R^2}\begin{bmatrix}1\\1\end{bmatrix}\right| = \left|\left(1+\frac{1}{R}+\frac{1}{R^2}\right)\begin{bmatrix}1\\1\end{bmatrix}\right|,$$

which leads to

$$\frac{1}{2\pi i}\int_0^{2\pi} |\hat{\hat{\Psi}}(k:Re^{i\theta})|\frac{Rd\theta}{|Re^{i\theta}|^{t+1}} \leq C^{(3)}\int_0^{2\pi}\frac{d\theta}{R^t} \quad (C^{(3)} \in \mathbb{R}_{>0}).$$

Accordingly, we get

$$\lim_{R\to\infty}\frac{1}{2\pi i}\int_0^{2\pi} |\hat{\hat{\Psi}}(k:Re^{i\theta})|\frac{Rd\theta}{|Re^{i\theta}|^{t+1}} = 0.$$

Therefore, we obtain by Eq. (3.5)

$$\hat{\Psi}_t(k) = -\sum_{l=\pm} Res(\hat{\hat{\Psi}}(k:z) : z = e^{i\theta^{(l)}(k)})(e^{i\theta^{(l)}(k)})^{-t-1} \quad (R\to\infty),$$

which also can be obtained by [10] (pp. 264–265).
Using Maclaurin's expansion for $w_m(k+\xi/t)e^{-i(t+1)\theta^{(m)}(k+\xi/t)}$, that is,

$$w_m(k+\xi/t)e^{-i(t+1)\theta^{(m)}(k+\xi/t)} = \left(w_m(k)+\frac{\xi}{t}\frac{\partial w_m(k)}{\partial k}+\frac{\xi^2}{2t^2}\frac{\partial^2 w_m(k)}{\partial k^2}+\cdots\right)e^{-i(t+1)\left\{\theta^{(m)}(k)+\frac{\xi}{t}\frac{\partial\theta^{(m)}(k)}{k}+\frac{\xi^2}{2t^2}\frac{\partial^2\theta^{(m)}(k)}{\partial k^2}+\cdots\right\}},$$

and noting Lemma 3.3, we obtain Eq. (3.4). By the Riemann-Lebesgue Theorem, the second term of Eq. (3.4) vanishes when $t\to\infty$, and we get the desired equation. □

Taking advantage of Eq. (3.2), we give the proof of Theorem 2.1. From now on, we derive the singular points of $\hat{\hat{\Xi}}(k:z)$ and then, compute the residues of $\hat{\hat{\Xi}}(k:z)$ at the singular points. Using Lemma 3.1, we obtain the expression of $\hat{\hat{\Xi}}(k:z)$ as follows:

$$\hat{\tilde{\Xi}}(k:z) = \left\{ \frac{e^{ik}}{1 - e^{ik}\tilde{\lambda}^{(+)}(z)} \begin{bmatrix} \tilde{\lambda}^{(+)}(z)\tilde{f}_0^{(+)}(z) \\ z \end{bmatrix} [0,-1] + \frac{e^{-ik}}{1 - e^{-ik}\tilde{\lambda}^{(-)}(z)} \begin{bmatrix} z \\ \tilde{\lambda}^{(-)}(z)\tilde{f}_0^{(-)}(z) \end{bmatrix} [1,0] + I \right\} \tilde{\Xi}_0(z). \tag{3.6}$$

The first term comes from the positive part of $\tilde{\Xi}_x(z)$, and the second term comes from the negative part of $\tilde{\Xi}_x(z)$, respectively. In addition, the third term describes localization.

Here, we should remark that if $|z| < 1$, then $|\tilde{\lambda}^{(\pm)}(z)| < 1$. Thus, the infinite series $\sum_x (\tilde{\lambda}^{(+)}(z))^{|x|-1} e^{ikx}$ and $\sum_x (\tilde{\lambda}^{(-)}(z))^{|x|-1} e^{-ikx}$ converge. Now, as we see in Appendix A, we have

$$\tilde{\lambda}^{(\pm)}(e^{i\theta}) = \mp\{\mathrm{sgn}(\cos\theta)\sqrt{2\cos^2\theta - 1} + i\sqrt{2}\sin\theta\}, \tag{3.7}$$

$$\tilde{f}_0^{(\pm)}(e^{i\theta}) = \mathrm{sgn}(\cos\theta) e^{i(\theta \pm \sigma_\pm)}\{\sqrt{2}|\cos\theta| - \sqrt{2\cos^2\theta - 1}\}. \tag{3.8}$$

Expressions (3.7) and (3.8) can also be obtained by the statements just after Eq. (24) in [21]. The principal singular points in this paper come from

$$1 - e^{ik}\tilde{\lambda}^{(+)}(z) = 0, \tag{3.9}$$

and

$$1 - e^{-ik}\tilde{\lambda}^{(-)}(z) = 0. \tag{3.10}$$

The solutions of Eqs. (3.9) and (3.10) satisfy the next conditions. By Eq. (3.9), we have

$$\cos k = -\mathrm{sgn}(\cos\theta^{(+)}(k))\sqrt{2\cos^2\theta^{(+)}(k) - 1}, \tag{3.11}$$

$$\sin k = \sqrt{2}\sin\theta^{(+)}(k), \tag{3.12}$$

and Eq. (3.10) suggests

$$\cos k = \mathrm{sgn}(\cos\theta^{(-)}(k))\sqrt{2\cos^2\theta^{(-)}(k) - 1}, \tag{3.13}$$

$$\sin k = \sqrt{2}\sin\theta^{(-)}(k). \tag{3.14}$$

By comparing Eq. (3.2) with Eq. (3.1), we put $-\partial\theta^{(\pm)}(k)/\partial k = x_\pm$ to compute the RHS of Eq. (3.2) and derive $g_{X_t/t}(x)$ ($t \to \infty$). Then, we derivate Eqs. (3.11) and (3.13) with respect to k, and $\sin k$, $\cos k$, $\sin\theta^{(\pm)}(k)$, and $\cos\theta^{(\pm)}(k)$ are described as follows:

From Eqs. (3.11) and (3.12), we have

$$\begin{cases} \cos k = \mathrm{sgn}(\cos k)\dfrac{x_+}{\sqrt{1 - x_+^2}}, \ \cos\theta^{(+)}(k) = -\mathrm{sgn}(\cos k)\dfrac{1}{\sqrt{2(1 - x_+^2)}}, \\ \sin k = \mathrm{sgn}(\sin k)\sqrt{\dfrac{1 - 2x_+^2}{1 - x_+^2}}, \ \sin\theta^{(+)}(k) = \mathrm{sgn}(\sin k)\sqrt{\dfrac{1 - 2x_+^2}{2(1 - x_+^2)}}. \end{cases} \tag{3.15}$$

From Eqs. (3.13) and (3.14), we see

$$\begin{cases} \cos k = \mathrm{sgn}(\cos k)\dfrac{x_-}{\sqrt{1 - x_-^2}}, \ \cos\theta^{(-)}(k) = \mathrm{sgn}(\cos k)\dfrac{1}{\sqrt{2(1 - x_-^2)}}, \\ \sin k = \mathrm{sgn}(\sin k)\sqrt{\dfrac{1 - 2x_-^2}{1 - x_-^2}}, \ \sin\theta^{(-)}(k) = \mathrm{sgn}(\sin k)\sqrt{\dfrac{1 - 2x_-^2}{2(1 - x_-^2)}}. \end{cases} \tag{3.16}$$

Therefore, we obtain the set of the singular points of $\hat{\tilde{\Xi}}(k:z)$ as follows:

$$A = \{e^{i\theta^{(+)}(k)}, e^{i\theta^{(-)}(k)}\},$$

with

$$e^{i\theta^{(+)}(k)} = -\frac{\mathrm{sgn}(\cos k)}{\sqrt{2(1 - x_+^2)}} + i\,\mathrm{sgn}(\sin k)\sqrt{\frac{1 - 2x_+^2}{2(1 - x_+^2)}},$$

and

$$e^{i\theta^{(-)}(k)} = \frac{\mathrm{sgn}(\cos k)}{\sqrt{2(1 - x_-^2)}} + i\,\mathrm{sgn}(\sin k)\sqrt{\frac{1 - 2x_-^2}{2(1 - x_-^2)}}.$$

In the next stage, we derive the residue of $\hat{\tilde{\Xi}}(k;z)$ at the singular points. At first, substituting the singular points to Eq. (3.8), we have

(1) $\tilde{f}_0^{(+)}(e^{i\theta^{(+)}(k)}) = -\mathrm{sgn}(\cos k)e^{i(\theta^+(k)+\sigma_+)}\dfrac{\sqrt{1-x_+^2}}{1+|x_+|}$, $\tilde{f}_0^{(-)}(e^{i\theta^{(+)}(k)}) = -\mathrm{sgn}(\cos k)e^{i(\theta^{(+)}(k)-\sigma_-)}\dfrac{\sqrt{1-x_+^2}}{1+|x_+|}$,

(2) $\tilde{f}_0^{(+)}(e^{i\theta^{(-)}(k)}) = \mathrm{sgn}(\cos k)e^{i(\theta^{(-)}(k)+\sigma_+)}\dfrac{\sqrt{1-x_-^2}}{1+|x_-|}$, $\tilde{f}_0^{(-)}(e^{i\theta^{(-)}(k)}) = \mathrm{sgn}(\cos k)e^{i(\theta^{(-)}(k)-\sigma_-)}\dfrac{\sqrt{1-x_-^2}}{1+|x_-|}$.

Noting Lemma 3.1, we see

$$\frac{e^{ik}}{1-e^{ik}\tilde{\lambda}^{(+)}(z)}\begin{bmatrix}\tilde{f}_0^{(+)}(z)\tilde{\lambda}^{(+)}(z)\\ z\end{bmatrix}[0,-1]\tilde{\Xi}_0(z) = -\frac{1}{\tilde{\Lambda}_0(z)}\frac{e^{ik}}{1-e^{ik}\tilde{\lambda}^{(+)}(z)}\begin{bmatrix}\tilde{f}_0^{(+)}(z)\tilde{\lambda}^{(+)}(z)\\ z\end{bmatrix}(\alpha\tilde{f}_0^{(-)}(z)+\beta),$$

and the square norm of residue of the first term of Eq. (3.6) is written as

$$\begin{aligned}&\left|Res\left(\frac{e^{ik}}{1-e^{ik}\tilde{\lambda}^{(+)}(z)}\begin{bmatrix}\tilde{f}_0^{(+)}(z)\tilde{\lambda}^{(+)}(z)\\ z\end{bmatrix}[0,-1]\tilde{\Xi}_0(z) : z=e^{i\theta^{(+)}(k)}\right)\right|^2\\ &\quad=\left|Res\left(\frac{1}{1-e^{ik}\tilde{\lambda}^{(+)}(z)} : z=e^{i\theta^{(+)}(k)}\right)\right|^2\frac{1}{|\tilde{\Lambda}_0(e^{i\theta^{(+)}(k)})|^2}\left\|\begin{bmatrix}\tilde{f}_0^{(+)}(e^{i\theta^{(+)}(k)})\tilde{\lambda}^{(+)}(e^{i\theta^{(+)}(k)})\\ e^{i\theta^{(+)}(k)}\end{bmatrix}\right\|^2|\alpha\tilde{f}_0^{(-)}(e^{i\theta^{(+)}(k)})+\beta|^2.\end{aligned}$$

In a similar fashion, we can write down the second term of Eq. (3.6) by

$$\begin{aligned}&\left|Res\left(\frac{e^{-ik}}{1-e^{-ik}\tilde{\lambda}^{(-)}(z)}\begin{bmatrix}z\\ \tilde{f}_0^{(-)}(z)\tilde{\lambda}^{(-)}(z)\end{bmatrix}[1,0]\tilde{\Xi}_0(z) : z=e^{i\theta^{(-)}(k)}\right)\right|^2\\ &\quad=\left|Res\left(\frac{1}{1-e^{-ik}\tilde{\lambda}^{(-)}(z)} : z=e^{i\theta^{(-)}(k)}\right)\right|^2\frac{1}{|\tilde{\Lambda}_0(e^{i\theta^{(-)}(k)})|^2}\left\|\begin{bmatrix}e^{i\theta^{(-)}(k)}\\ \tilde{f}_0^{(-)}(e^{i\theta^{(-)}(k)})\tilde{\lambda}^{(-)}(e^{i\theta^{(-)}(k)})\end{bmatrix}\right\|^2\\ &\quad\times|\alpha-\beta\tilde{f}_0^{(+)}(e^{i\theta^{(-)}(k)})|^2.\end{aligned}$$

Thereby, we obtain

$$\begin{aligned}\|Res(\hat{\tilde{\Xi}}(k:z) : z=e^{i\theta^{(\pm)}(k)})\|^2 &= \left|Res\left(\frac{1}{1-e^{ik}\tilde{\lambda}^{(+)}(z)} : z=e^{i\theta^{(+)}(k)}\right)\right|^2\frac{1}{|\tilde{\Lambda}_0(e^{i\theta^{(+)}(k)})|^2}\\ &\times\left\|\begin{bmatrix}\tilde{f}_0^{(+)}(e^{i\theta^{(+)}(k)})\tilde{\lambda}^{(+)}(e^{i\theta^{(+)}(k)})\\ e^{i\theta^{(+)}(k)}\end{bmatrix}\right\|^2|\alpha\tilde{f}_0^{(-)}(e^{i\theta^{(+)}(k)})+\beta|^2\\ &+\left|Res\left(\frac{1}{1-e^{-ik}\tilde{\lambda}^{(-)}(z)} : z=e^{i\theta^{(-)}(k)}\right)\right|^2\frac{1}{|\tilde{\Lambda}_0(e^{i\theta^{(-)}(k)})|^2}\\ &\times\left\|\begin{bmatrix}e^{(i\theta^{(\pm)}(k))}\\ \tilde{f}_0^{(-)}(e^{i\theta^{(-)}(k)})\tilde{\lambda}^{(-)}(e^{i\theta^{(-)}(k)})\end{bmatrix}\right\|^2|\alpha-\beta\tilde{f}_0^{(+)}(e^{i\theta^{(-)}(k)})|^2.\end{aligned}\tag{3.17}$$

Henceforth, we will express the items below with respect to x_+ or x_-, and then substitute the items in Eq. (3.17).

- $\left|Res\left(\dfrac{1}{1-e^{ik}\tilde{\lambda}^{(+)}(z)} : z=e^{i\theta^{(+)}(k)}\right)\right|^2$ and $\left|Res\left(\dfrac{1}{1-e^{-ik}\tilde{\lambda}^{(-)}(z)} : z=e^{i\theta^{(-)}(k)}\right)\right|^2$,
- $\dfrac{1}{|\tilde{\Lambda}_0(e^{i\theta^{(\pm)}(k)})|^2}$,
- $|\alpha\tilde{f}_0^{(-)}(e^{i\theta^{(+)}(k)})+\beta|^2$ and $|\alpha-\beta\tilde{f}_0^{(+)}(e^{i\theta^{(-)}(k)})|^2$,
- $\left\|\begin{bmatrix}\tilde{\lambda}^{(+)}(e^{i\theta^{(+)}(k)})\tilde{f}_0^{(+)}(e^{i\theta^{(+)}(k)})\\ e^{i\theta^{(+)}(k)}\end{bmatrix}\right\|^2$ and $\left\|\begin{bmatrix}e^{i\theta^{(-)}(k)}\\ \tilde{\lambda}^{(-)}(e^{i\theta^{(-)}(k)})\tilde{f}_0^{(-)}(e^{i\theta^{(-)}(k)})\end{bmatrix}\right\|^2$.

1. Computation of $\left|Res\left(\dfrac{1}{1-e^{ik}\tilde{\lambda}^{(+)}(z)} : z=e^{i\theta^{(+)}(k)}\right)\right|^2$ and $\left|Res\left(\dfrac{1}{1-e^{-ik}\tilde{\lambda}^{(-)}(z)} : z=e^{i\theta^{(-)}(k)}\right)\right|^2$:

Let $g^{(\pm)}(z) = 1-e^{\pm ik}\tilde{\lambda}^{(\pm)}(z)$. Expanding $g^{(\pm)}(z)$ around $z=e^{i\theta^{(\pm)}(k)}$, we have

$$Res\left(\frac{1}{1-e^{\pm ik}\tilde{\lambda}^{(\pm)}(z)} : z=e^{i\theta^{(\pm)}(k)}\right) = \left.\frac{1}{\dfrac{\partial g^{(\pm)}(z)}{\partial z}}\right|_{z=e^{i\theta^{(\pm)}(k)}}.$$

From Eq. (3.7), we see

$$\left.\frac{\partial g^{(\pm)}(z)}{\partial z}\right|_{z=e^{i\theta^{(\pm)}(k)}} = \pm\frac{\mathrm{sgn}(\cos k)}{\sqrt{1-x_{\pm}^2}}\, e^{-i(\theta^{(\pm)}(k)\mp k)}\left\{\mathrm{sgn}(\cos k\sin k)\frac{\sqrt{1-2x_{\pm}^2}}{x_{\pm}}+i\right\},$$

which imply

$$\begin{cases} \left|Res\left(\dfrac{1}{1-e^{ik}\tilde{\lambda}^{(+)}(z)} : z=e^{i\theta^{(+)}(k)}\right)\right|^2 = x_+^2, \\ \left|Res\left(\dfrac{1}{1-e^{-ik}\tilde{\lambda}^{(-)}(z)} : z=e^{i\theta^{(-)}(k)}\right)\right|^2 = x_-^2. \end{cases}$$

2. Computation of $\dfrac{1}{|\tilde{\Lambda}_0(e^{i\theta^{(\pm)}(k)})|^2}$: Noting Lemma 3.1, we have for any $\theta\in\mathbb{R}$,

$$|\tilde{\Lambda}_0(e^{i\theta})|^2 = 1+2\Re\{\tilde{f}_0^{(+)}(e^{i\theta})\tilde{f}_0^{(-)}(e^{i\theta})\}+|\tilde{f}_0^{(+)}(e^{i\theta})|^2|\tilde{f}_0^{(-)}(e^{i\theta})|^2, \tag{3.18}$$

where $\mathbb{R}$ is the set of real numbers. Hence, substituting the singular points into Eq. (3.18), we obtain

$$\begin{cases} \dfrac{1}{|\tilde{\Lambda}_0(e^{i\theta^{(+)}(k)})|^2} = \dfrac{(1+x_+)^2}{2\{1+x_+^2(1+\cos 2\sigma)+\mathrm{sgn}(\sin k\cos k)\sqrt{1-2x_+^2}\sin 2\sigma\}}, \\ \dfrac{1}{|\tilde{\Lambda}_0(e^{i\theta^{(-)}(k)})|^2} = \dfrac{(1-x_-)^2}{2\{1+x_-^2(1+\cos 2\sigma)-\mathrm{sgn}(\sin k\cos k)\sqrt{1-2x_-^2}\sin 2\sigma\}}. \end{cases}$$

3. Computation of $|\alpha\tilde{f}_0^{(-)}(e^{i\theta^{(+)}(k)})+\beta|^2$ and $|\alpha-\beta\tilde{f}_0^{(+)}(e^{i\theta^{(-)}(k)})|^2$.
Let the initial coin state $\varphi_0={}^T[\alpha,\beta]$, where $\alpha=ae^{i\phi_1}$, $\beta=be^{i\phi_2}$ with $a,b\geq 0$ and $a^2+b^2=1$. Taking account of

$$|\alpha\tilde{f}_0^{(-)}(e^{i\theta^{(+)}(k)})+\beta|^2 = |\alpha|^2|\tilde{f}_0^{(-)}(e^{i\theta^{(+)}(k)})|^2+|\beta|^2+2\Re\{\alpha\overline{\beta}\tilde{f}_0^{(-)}(e^{i\theta^{(+)}(k)})\},$$

and

$$|\alpha-\beta\tilde{f}_0^{(+)}(e^{i\theta^{(-)}(k)})|^2 = |\alpha|^2-2\Re\{\overline{\alpha}\beta\tilde{f}_0^{(+)}(e^{i\theta^{(-)}(k)})\}+|\beta|^2|\tilde{f}_0^{(+)}(e^{i\theta^{(-)}(k)})|^2,$$

we obtain

$$\begin{cases} |\alpha\tilde{f}_0^{(-)}(e^{i\theta^{(+)}(k)})+\beta|^2 = a^2\dfrac{1-x_+}{1+x_+}+b^2+\dfrac{\sqrt{2}ab}{1+x_+}\left\{\cos\gamma_+ +\mathrm{sgn}(\sin k\cos k)\sqrt{1-2x_+^2}\sin\gamma_+\right\}, \\ |\alpha-\beta\tilde{f}_0^{(+)}(e^{i\theta^{(-)}(k)})|^2 = b^2\dfrac{1+x_-}{1-x_-}+a^2-\dfrac{\sqrt{2}ab}{1-x_-}\left\{\cos\gamma_- -\mathrm{sgn}(\sin k\cos k)\sqrt{1-2x_-^2}\sin\gamma_-\right\}, \end{cases}$$

where $\gamma_+=\tilde{\phi}_{12}-\sigma_-$ and $\gamma_-=\tilde{\phi}_{21}+\sigma_+$ with $\tilde{\phi}_{12}=\phi_1-\phi_2$.

4. Computation of $\left\|\begin{bmatrix}\tilde{\lambda}^{(+)}(e^{i\theta^{(+)}(k)})\tilde{f}_0^{(+)}(e^{i\theta^{(+)}(k)}) \\ e^{i\theta^{(+)}(k)}\end{bmatrix}\right\|^2$ and $\left\|\begin{bmatrix}e^{i\theta^{(-)}(k)} \\ \tilde{\lambda}^{(-)}(e^{i\theta^{(-)}(k)})\tilde{f}_0^{(-)}(e^{i\theta^{(-)}(k)})\end{bmatrix}\right\|^2$.

By a simple calculation, we have

$$\begin{cases} \left\|\begin{bmatrix}\tilde{\lambda}^{(+)}(e^{i\theta^{(+)}(k)})\tilde{f}_0^{(+)}(e^{i\theta^{(+)}(k)}) \\ e^{i\theta^{(+)}(k)}\end{bmatrix}\right\|^2 = |\tilde{\lambda}^{(+)}(e^{i\theta^{(+)}(k)})|^2|\tilde{f}_0^{(+)}(e^{i\theta^{(+)}(k)})|^2+1 = \dfrac{2}{1+x_+} \quad (x_+>0), \\ \left\|\begin{bmatrix}e^{i\theta^{(-)}(k)} \\ \tilde{\lambda}^{(-)}(e^{i\theta^{(-)}(k)})\tilde{f}_0^{(-)}(e^{i\theta^{(-)}(k)})\end{bmatrix}\right\|^2 = 1+|\tilde{\lambda}^{(-)}(e^{i\theta^{(-)}(k)})|^2|\tilde{f}_0^{(-)}(e^{i\theta^{(-)}(k)})|^2 = \dfrac{2}{1-x_-} \quad (x_-<0). \end{cases}$$

Here, we remark

$$-\frac{\partial\theta^{(\pm)}(k)}{\partial k} = x_{\pm}, \tag{3.19}$$

which imply

$$x_+ = \frac{|\cos k|}{\sqrt{1+\cos^2 k}}, \quad x_- = -\frac{|\cos k|}{\sqrt{1+\cos^2 k}}. \tag{3.20}$$

Hence, we can regard x_+ and x_- as a variable x:

$$x = \begin{cases} x_+ & (x>0), \\ x_- & (x<0). \end{cases}$$

Combining Eqs. (3.15) and (3.16) with Eq. (3.20), and noting Eq. (3.19), we get

$$\frac{dx}{dk} = \mp \operatorname{sgn}(x)\operatorname{sgn}(\sin k\cos k)(1-x^2)\sqrt{1-2x^2},$$

and therefore, we obtain

$$dk = \begin{cases} -\operatorname{sgn}(\sin k\cos k) f_K(x;1/\sqrt{2})\pi dx & (x>0), \\ \operatorname{sgn}(\sin k\cos k) f_K(x;1/\sqrt{2})\pi dx & (x<0). \end{cases}$$

Substituting the items given in 1. to 4. into Eq. (3.17) and combining with Eq. (3.2), we arrive at Theorem 2.1.

REFERENCES

[1] A. Ahlbrecht, V. B. Scholz, and A. H. Werner, "Disordered quantum walks in one lattice dimension," *Journal of Mathematical Physics*, **52**: 102201 (2011).

[2] A. Ambainis, A. Backurs, N. Nahimovs, R. Ozols, and A. Rivosh, "Search by quantum walks on two-dimensional grid without amplitude amplification," *Springer, Lecture Notes in Computer Science*, **7582**: 87–97 (2013).

[3] A. A. Burkov and L. Balents, "Weyl semimetal in a topological insulator multilayer," *Physical Review Letters*, **107**: 127205 (2011).

[4] M. J. Cantero, F. A. Grunbaum, L. Moral, and L. Velazquez, "One-dimensional quantum walks with one defect," *Reviews in Mathematical Physics*, **24**: 1250002 (2012).

[5] Y. L. Chen, J. G. Analytis, J.-H. Chu, Z. K. Liu, S.-K. Mo, X. L. Qi, H. J. Zhang, D. H. Lu, X. Dai, Z. Fang, S. C. Zhang, I. R. Fisher, Z. Hussain, and Z.-X. Shen, "Experimental realization of a three-dimensional topological insulator, Bi 2Te3" *Science*, **325**: 178–181 (2009).

[6] C.-I. Chou and C.-L. Ho, "Localization and recurrence of quantum walk in periodic potential on a line," *Chinese Physics B*, **23**: 110302 (2013).

[7] S. Endo, T. Endo, N. Konno, E. Segawa, and M. Takei, "Limit theorems of a two-phase quantum walk with one defect," *Quantum Information and Computation*, **15**: 1373–1396 (2015).

[8] T. Endo and N. Konno, "The time-averaged limit measure of the Wojcik model," *Quantum Information and Computation*, **15**: 0105–0133 (2015).

[9] T. Endo and N. Konno, "Weak Convergence of the Wojcik model," *Yokohama Mathematical Journal*, **61**: 87–111 (2015).

[10] P. Flajolet and R. Sedgewick, Analytic combinatorics, Cambridge University Press (2009).

[11] L. Fu and C. L. Kane, "Superconducting Proximity Effect and Majorana fermions at the surface of a topological insulator," *Physical Review Letters*, **100**: 096407 (2008).

[12] G. Grimmett, S. Janson, and P. F. Scudo, "Weak limits for quantum random walks," *Physical Review E*, **69**: 026119 (2004).

[13] N. Inui, Y. Konishi, and N. Konno, "Localization of two-dimensional quantum walks," *Physical Review A*, **69**: 052323 (2003).

[14] A. Joye and M. Merkli, "Dynamical localization of quantum walks in random environments," *Journal of Statistical Physics*, **140**: 1025–1053 (2010).

[15] T. Kitagawa, M. S. Rudner, E. Berg, and E. Demler, "Exploring topological phases with quantum walks," *Physical Review A*, **82**: 033429 (2010).

[16] C. K. Ko and H. J. Yoo, "The generator and quantum Markov semigroup for quantum walks," *Kodai Mathematical Journal*, **36**: 363–385 (2013).

[17] N. Konno, "A new type of limit theorems for the one-dimensional quantum random walk," *Journal of the Mathematical Society of Japan*, **57**: 1179–1195 (2005).

[18] N. Konno, "A path integral approach for disordered quantum walks in one dimension," *Fluctuation and Noise Letters*, **5**: 529–537 (2005).

[19] N. Konno, "Quantum walks," *Quantum Potential Theory, Lecture Notes in Mathematics*, **1954**: 309–452 (2008).

[20] N. Konno, "Localization of an inhomogeneous discrete-time quantum walk on the line," *Quantum Information Processing*, **9**: 405–418 (2010).

[21] N. Konno, T. Luczak, and E. Segawa, "Limit measures of inhomogeneous discrete-time quantum walks in one dimension," *Quantum Information Processing*, **12**: 33–53 (2013).

[22] N. Konno and H. J. Yoo, "Limit theorems for open quantum random walks," *Journal of Statistical Physics*, **150**: 299–319 (2013).

[23] N. Shenvi, J. Kempe, and K. B. Whaley, "A quantum random walk search algorithm," *Physical Review A*, **67**: 052307 (2003).

[24] A. Wojcik, T. Luczak, P. Kurzynski, A. Grudka, T. Gdala, and M. Bednarska-Bzdega, "Trapping a particle of a quantum walk on the line," *Physical Review A*, **85**: 012329 (2012).

Appendix A

In Appendix A, we consider how $\tilde{f}_x^{(\pm)}(z)$ and $\tilde{\lambda}^{(\pm)}$ are fixed when we focus on the ballistic behavior of the two-phase QW with one defect. The protocol is similar to that of Appendix C in [9]. According to [7], we have

$$\tilde{\lambda}^{(\pm)}(w) = \pm\frac{i}{\sqrt{2}}\{(w+w^{-1}) - \sqrt{(w+w^{-1})^2-2}\}, \quad \tilde{f}_0^{(\pm)}(w) = -\frac{we^{\pm i\sigma_\pm}}{\sqrt{2}}\{(w-w^{-1}) + \sqrt{(w-w^{-1})^2+2}\}.$$

By putting $w = i(1-\varepsilon)e^{i\theta}$ ($\varepsilon \in \mathbb{R}$, $|\varepsilon| \ll 1$), we consider how $\lim_{\varepsilon\to 0}\sqrt{(w+w^{-1})^2-2}$ can be specified with respect to θ depending on the range of $\cos\theta$ or $\sin\theta$. Taking account of $|\varepsilon| \ll 1$, we have

$$\tilde{\lambda}^{(\pm)}(w) \sim \mp \frac{i}{\sqrt{2}} \{2\sin\theta + 2i\varepsilon\cos\theta + \delta\sqrt{4\sin^2\theta - 2}\}, \tag{3.21}$$

where we put $\delta \in \mathbb{R}$ with $\delta^2 = 1$ [7]. For $|\tilde{\lambda}^{(\pm)}(w)| < 1$, Eq. (3.21) suggests that we need to take into consideration the two cases as follows [7]:

(1) Case of $|\sin\theta| \geq 1/\sqrt{2}$.
Eq. (3.21) implies

$$\frac{1}{2}\left\{2\sin\theta + 2\delta\sqrt{\sin^2\theta - 1/2}\right\}^2 < 1,$$

which leads to

$$2\sin^2\theta + 2\sin\theta\delta\sqrt{\sin^2\theta - 1/2} < 1.$$

Thereby, we obtain $\delta = -\mathrm{sgn}(\sin\theta)$.

(2) Case of $|\sin\theta| < 1/\sqrt{2}$.
Eq. (3.21) suggests

$$\frac{1}{2}\left[\left\{2\varepsilon\cos\theta + 2\delta\sqrt{1/2 - \sin^2\theta}\right\}^2 + 4\sin^2\theta\right] < 1,$$

and we see

$$4\varepsilon^2\cos^2\theta + 8\varepsilon\cos\theta\delta\sqrt{1/2 - \sin^2\theta} < 0.$$

Hence, we obtain $\delta = -\mathrm{sgn}(\cos\theta)$.

From the above discussion, we have the square root by [7]

$$\lim_{\varepsilon\to 0}\sqrt{(w + w^{-1})^2 - 2} = \begin{cases} -2\,\mathrm{sgn}(\sin\theta)\sqrt{\sin^2\theta - \dfrac{1}{2}} & (|\sin\theta| \geq 1/\sqrt{2}), \\ -2i\,\mathrm{sgn}(\cos\theta)\sqrt{\dfrac{1}{2} - \sin^2\theta} & (|\sin\theta| \leq 1/\sqrt{2}). \end{cases} \tag{3.22}$$

In the next stage, we determine concrete expressions of $\tilde{\lambda}^{(\pm)}(z)$ and $\tilde{f}_0^{(\pm)}(z)$. If we focus on the weak limit theorem for our two-phase QW, we need to choose the square root so that $1/(1 - e^{ik}\tilde{\lambda}^{(+)}(z))$ and $1/(1 - e^{-ik}\tilde{\lambda}^{(-)}(z))$ have the singular points, that is, $|\tilde{f}_0^{(\pm)}(z)| \neq 1$. Therefore, we see by Eq. (3.22)

$$\begin{cases} \tilde{\lambda}^{(\pm)}(z) = \mp\{\mathrm{sgn}(\cos\theta)\sqrt{2\cos^2\theta - 1} + i\sqrt{2}\sin\theta\}, \\ \tilde{f}_0^{(\pm)}(z) = \mathrm{sgn}(\cos\theta)e^{i(\theta\pm\sigma_\pm)}\{\sqrt{2}|\cos\theta| - \sqrt{2\cos^2\theta - 1}\}, \end{cases} \quad (|\sin\theta| \leq 1/\sqrt{2})$$

with $z = e^{i\theta}$, which are the desired transcriptions.