Weak limit theorem of a two-phase quantum walk with one defect

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Abstract

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”, which we treated concerning localization theorems [10]. The two-phase QW has been expected to be a mathematical model of the topological insulator [16] 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 [10], however, the weak limit measure is asymmetric, which implies that the weak limit theorem represents the asymmetry of the probability distribution.

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1 Introduction

This paper is a sequential work of [10]. For its characteristic properties, quantum walks (QWs) have attracted much attention of various fields, such as, quantum search algorithms [2, 15], and topological insulators [16]. Owing to such applications of the QWs, it is of great importance to study the QWs both analytically and numerically, and indeed, many researchers have tried to investigate the asymptotic behaviors of QWs from various viewpoints [7, 13, 14, 17, 21, 25] in the past decade. From the mathematical view points, two kinds of limit theorems for QWs have been constructed so far. The one is localization theorem. Localization is one of the typical properties of discrete-time QWs, which was first studied by Inui et al. [12] both mathematically and numerically. The detailed definition of localization is found in [1, 13] for example. The other is the weak limit theorem whose typical expression is described as follows [14]: There exist $C \in [0, 1)$, $a \in (0, 1)$, and a rational polynomial $w(x)$ such that

$$\mu(dx) = C\delta_0(dx) + w(x)f_K(x; a)dx$$

where

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

with

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

We should note that the first term, Dirac measure part in Eq. (1), $C\delta_0(dx)$, corresponds to localization, and the second term, absolutely continuous part, $w(x)f_K(x; a)dx$, corresponds to the ballistic spreading.

We remark that Eq. (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 [6], have been derived. In 2013, Konno et al. [14] 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 [24], the CGMV method [4], the stationary phase method [22], the path counting method [18], and the generating function method [9]. 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, it has not been clear the types of QWs that can be analyzed by the generating function method. We can also analyze inhomogeneous QWs via the CGMV method, still the CGMV method allows only for the general discussion of localization properties for the typical QWs in one dimension. 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”. It has been known that the two-phase QW is deeply related to the topological insulator which has attracted much attention recently of many physicists [3, 11, 16]. Hence we expect that the two-phase QW can be
utilized to study the topological insulator as its mathematical model. Therefore it would be greatly worth to study the mathematical aspects of the two-phase QW to exactly grasp the asymptotic behavior. Our main result is the first application of the generating function method to the weak limit theorem of the two-phase QW. Combining the time-averaged limit measure [10] 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 which is the main target in this paper, and present our main result. In Section 3, we give the proof of Theorem 1.

2 Model and the results

2.1 The two-phase QW

For the general setting of discrete-time QW in one dimension, the walker has a coin 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 $\mathbb{C}$ is the set of complex numbers.

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

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

where $\sigma_\pm \in [0, 2\pi)$. 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

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

with $U_x = P_x + Q_x$. We should note that $P_x$ and $Q_x$ correspond to the left and right movements, respectively. The walker moves differently in positive and negative parts each other. Hereafter, we call the QW “the two-phase QW”. Putting $\sigma_+ = \sigma_-$, the model becomes one-defect QW, which has been analyzed so far in detail [14]. We should note that owing to the defect at the origin, the model has an origin symmetry, and the analysis becomes simple. We will report the analytical results of a QW with two
phases which does not have defect at the origin in the upcoming paper. We derived localization theorems [10] for the two-phase QW, in particular, the time-averaged limit and stationary measures. Therefore, 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 Weak limit theorem

Let $QW$ be the two-phase model starting from the origin with the initial coin state $\varphi_0 = \gamma[\alpha, \beta]$, where $\alpha, \beta \in \mathbb{C}$. Put $\alpha = ae^{\phi_1}$, $\beta = be^{\phi_2}$ with $a, b \geq 0$, $a^2 + b^2 = 1$ and $\phi_1, \phi_2 \in \mathbb{R}$, where $\mathbb{R}$ is the set of real numbers. Let $\sigma = (\sigma_+ - \sigma_-)/2$ and $\hat{\phi}_{12} = \phi_1 - \phi_2$. For the two-phase $QW$, $X_t/t$ 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. (2) and

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

with

$$
s_2 = 4\cos^4 \sigma, \quad s_1 = 4\cos^2 \sigma(1 + 2\sin^2 \sigma), \quad s_0 = \cos^2 2\sigma,
$$

$$
t_3 = 4\cos^2 \sigma(b^2 - a^2), \quad t_2 = 4[\cos^2 \sigma(1 + \sqrt{2}ab \text{sgn}(x) \cos \gamma(x)) + \sqrt{2}ab \text{sgn}(x) \sin \gamma(x) \sin 2\sigma],
$$

$$
t_1 = 2(b^2 - a^2), t_0 = 2\{1 + \sqrt{2}ab \text{sgn}(x) \cos \gamma(x) - \sqrt{2}ab \text{sgn}(x) \sin \gamma(x) \sin 2\sigma\},
$$

and

$$
\gamma(x) = \begin{cases} 
\hat{\phi}_{12} - \sigma_- & (x \geq 0), \\
-\hat{\phi}_{12} + \sigma_+ & (x < 0).
\end{cases} \tag{5}
$$

Here we should note that $w(x)f_K(x; 1/\sqrt{2})$ is an absolutely continuous part.

If $\sigma_+ = \sigma_-$, then, we see from Eq. (4) that the weight function is given by

$$
w(x) = \frac{2x^2}{1 + 2x^2} \begin{cases} 
1 + \sqrt{2}R(e^{-i\sigma}a\overline{b}) + (b^2 - a^2)x & (x \geq 0), \\
1 - \sqrt{2}R(e^{-i\sigma}a\overline{b}) + (b^2 - a^2)x & (x < 0),
\end{cases} \tag{6}
$$

which agrees with the result obtained by Theorem 4.1 in [14]. Here we should note that the expression of the weight function in Theorem 4.1 in Ref. [14] contains a typo, and the correct transcription is

$$
w(x) = \frac{|c|^2x^2}{(|c|^2 - m)^2 + (|c|^2 - m^2)x^2} \left[\gamma(x) - |a_0|^2 \left\{(|\alpha|^2 - |\beta|^2) + \frac{2R(a_0\overline{a}_0\overline{b})}{|a_0|^2}\right\}x\right].
$$
As we see in Eqs. (4) and (6), the two different quantum coins give such complexity to the weight function. In our previous paper [10], we reported that the time-averaged distribution of the two-phase QW 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 relation in explicit between the topological insulator and the two-phase QW.

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

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

We obtain the QW by putting \( \sigma_+ = 3\pi/2 \) and \( \sigma_- = \pi \) in Eq. (3). Let the initial coin state \( \phi_0 = T[1, 0] \). According to Theorem 1, the weight function of the QW is

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

Hence, we see

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

Here, we should note that we obtained the time-averaged limit measure \( \overline{\nu}_{\infty}(x) \) by Theorem 2 in [10], and as a result, we derived the coefficient of the delta function \( \delta_0(dx) \) in Eq. (1) by

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

where

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

with \( \sigma = (\sigma_+ + \sigma_-)/2 \), \( \tilde{\phi}_{12} = \phi_1 - \phi_2 \), and

\[
\nu^{(\pm)}(x; \sigma) = \left( \frac{1 \pm \sqrt{2}\sin \sigma}{3 \pm 2\sqrt{2}\sin \sigma} \right)^2 \left\{ 1 \pm 2ab \sin(\tilde{\phi}_{12} - \tilde{\sigma}) \right\}
\]

\[
\times \left\{ \delta_0(x) + (1 - \delta_0(x))(2 \pm \sqrt{2}\sin \sigma) \left( \frac{1}{3 \pm 2\sqrt{2}\sin \sigma} \right)^{|x|} \right\}.
\]
Therefore, 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 \( \pi_\infty(x) \) is symmetric for the origin \([10]\), however, \( w(x) f_K(x; 1/\sqrt{2}) \) does not have an origin symmetry \((\text{Figs. 1, 2, 3})\), which indicates that the weak limit measure represents the asymmetry of the probability distribution \((\text{Figs. 1, 2, 3})\).

![Fig. 1](image1.png)  
**Fig. 1.** Blue line: Probability distribution in a re-scaled space \((x/100, 100P_{100}(x))\) at time 100, Black line: \( w(x) f_K(x; 1/\sqrt{2}) \)

![Fig. 2](image2.png)  
**Fig. 2.** Green line: Probability distribution in a re-scaled space \((x/1000, 1000P_{1000}(x))\) at time 1000, Black line: \( w(x) f_K(x; 1/\sqrt{2}) \)

![Fig. 3](image3.png)  
**Fig. 3.** Orange line: Probability distribution in a re-scaled space \((x/10000, 10000P_{10000}(x))\) at time 10000, Black line: \( w(x) f_K(x; 1/\sqrt{2}) \)
3 Proof of Theorem 1

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

\[ E \left[ e^{iξX_t} \right] = \int_{x \in \mathbb{Z}} g_{X_t/t}(x) e^{iξx} dx, \]

where \( g_{X_t/t}(x) \) is the density function of random variable \( X_t/t \). We consider how \( E \left[ e^{iξX_t} \right] \) 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 \( w(x)f_κ(x; 1/\sqrt{2}) \).

Let \( Ξ_l(x) \) be the weight of all the passages of the walker, which moves left \( l \) times and moves right \( m \) times till time \( t \) [13]:

\[ Ξ_l(x) = \sum_{l_j, m_j} P_{x_{11}}^{l_1} Q_{x_{12}}^{m_1} P_{x_{12}}^{l_2} Q_{x_{12}}^{m_2} \ldots P_{x_{11}}^{l_l} Q_{x_{12}}^{m_l}, \]

where \( l + m = t \), \(-l + m = x \), \( \sum l_i = l \), \( \sum m_j = m \) with \( l_i + m_i = 1 \), \( l_i, m_i \in \{0, 1\} \), and \( \sum_{x=l_i, m_j} |x_n| = x \). Here, we consider \( z \in \mathbb{C} \) on a unit circle. From a simple calculation, we obtain \( E[e^{iξX_t}] \) \((t \to \infty)\) written by the square norm of the residue of \( ˜Ξ_e(z) = \sum_l Ξ_l(x)z^l \) as follows:

\[ E \left[ e^{iξX_t} \right] = \int_0^{2π} \sum_{θ \in A} e^{-iξ^l(θ)} |\text{Res}( ˜Ξ(k : z) : z = e^{iθ(k)})|^2 \frac{dk}{2π} \quad (t \to \infty), \]

where \( A \) is the set of the singular points of \( ˜Ξ(k : z) \equiv \sum_{z \in \mathbb{Z}} ˜Ξ_e(z)e^{ikz} \). Note \( θ'(k) = \partial θ(k)/\partial k \). We will give a detailed explanation of Eq. (12) in Appendix A. Taking advantage of Eq. (12), we give the proof of Theorem 1.

Now, we give useful concrete expressions of \( ˜Ξ_e(z) \) which play important roles in the proof. Lemma 1 is equivalent to Lemma 2 in [10], which we used to derive the time-averaged limit measure for the two-phase QW. Assume that the quantum walker starts from the origin with the initial coin state \( \varphi_0 = τ[α, β] \) with \( α, β \in \mathbb{C} \) and \( |α|^2 + |β|^2 = 1 \).

Lemma 1 [10] Let \( Δ_x \) be the determinant of \( U_x \). Assume \( a_x, d_x \neq 0 \) for all \( x \in \mathbb{Z} \).

1. If \( x = 0 \), we have

\[ ˜Ξ_0(z) = \frac{1}{1 + ˜ξ_0^{(+)}(z) ˜ξ_0^{(-)}(z)} \begin{bmatrix} 1 & - ˜ξ_0^{(+)}(z) \\ ˜ξ_0^{(-)}(z) & 1 \end{bmatrix}. \]

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

\[ ˜Ξ_x(z) = \begin{cases} \left( ˜ξ^{(+)}(z) \right)^{|x|-1} \begin{bmatrix} 1 & - ˜ξ^{(+)}(z) \\ ˜ξ^{(-)}(z) & 1 \end{bmatrix} [0, -1] ˜Ξ_0(z) \quad (x \geq 1), \\ \left( ˜ξ^{(-)}(z) \right)^{|x|-1} \begin{bmatrix} 1 & - ˜ξ^{(-)}(z) \\ ˜ξ^{(-)}(z) & 1 \end{bmatrix} [1, 0] ˜Ξ_0(z) \quad (x \leq -1), \end{cases} \]

\[ Ξ_0(z) = \begin{bmatrix} 1 & - ˜ξ_0^{(+)}(z) \\ ˜ξ_0^{(-)}(z) & 1 \end{bmatrix}, \]

\[ Ξ_x(z) = \begin{bmatrix} 1 & - ˜ξ^{(+)}(z) \\ ˜ξ^{(-)}(z) & 1 \end{bmatrix} |x| ˜ξ^{(-)}(z) \]

where \( ξ^{(+)}(z) \) and \( ξ^{(-)}(z) \) play important roles in the proof. Lemma 1 is equivalent to Lemma 2 in [10], which we used to derive the time-averaged limit measure for the two-phase QW.
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 \( \tilde{f}_0^+(z) \) and \( \tilde{f}_0^-(z) \) satisfy the following quadratic equations, respectively:

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

Hereafter, we write \( \tilde{f}_x^\pm(z) \) by \( \tilde{f}_0^\pm(z) \), since \( \tilde{f}_x^\pm(z) \) do not depend on the position. Then, we obtain

**Lemma 2** \( \tilde{f}_0^+(z) \) and \( \tilde{f}_0^-(z) \) are expressed in terms of \( \theta \) by

\[
\tilde{f}_0^\pm(e^{i\theta}) = e^{i(\theta - \sigma \pm \phi)} e^{-i\phi(\theta)},
\]

where

\[
\begin{cases}
\sin \phi(\theta) = \text{sgn}(\sin \theta) \sqrt{2 \sin \theta^2 - 1}, \\
\cos \phi(\theta) = \sqrt{2 \cos \theta}.
\end{cases}
\]

From now on, we derive the singular points of \( \hat{\Xi}(k : z) \) and then, compute the residues of \( \hat{\Xi}(k : z) \) at the singular points. Using Lemma 1, we can write down \( \hat{\Xi}(k : z) \) by

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

The first term comes from the positive part of \( \hat{\Xi}_x(z) \), and the second term comes from the negative part of \( \hat{\Xi}_x(z) \), respectively.

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

\[
\begin{cases}
\tilde{\lambda}^\pm(e^{i\theta}) = \mp \{ \text{sgn}(\sin \theta) \sqrt{2 \cos^2 \theta - 1} + i \sqrt{2} \sin \theta \}, \\
\tilde{f}_0^\pm(e^{i\theta}) = - \text{sgn}(\cos \theta) e^{i(\theta \pm \phi)} \{ \sqrt{2} \cos \theta - \sqrt{2 \cos^2 \theta - 1} \}.
\end{cases}
\]

We should also note that the singular points derived from \( \tilde{\Xi}_0(z) \) correspond to localization. On the other hand, the principal singular points in this paper come from

\[
1 - e^{ik} \tilde{\lambda}^+(z) = 0,
\]

and

\[
1 - e^{-ik} \tilde{\lambda}^-(z) = 0.
\]

The solutions of Eqs. \((17)\) and \((18)\) satisfy the next conditions. For Eq. \((17)\), we see

\[
cos k = \text{sgn}(\cos \theta^+(k)) \sqrt{2 \cos^2 \theta^+(k) - 1},
\]
\[
\sin k = \sqrt{2} \sin \theta^+(k), \quad (20)
\]
and for Eq. (13), we have
\[
\cos k = - \sgn(\cos \theta^-(k)(k)) \sqrt{2 \cos^2 \theta^-(k) - 1}, \quad (21)
\]
\[
\sin k = \sqrt{2} \sin \theta^-(k). \quad (22)
\]

To compute the RHS of Eq. (12) and derive \( g_{X,t}(x) \) \((t \to \infty)\) comparing Eq. (12) with Eq. (11), we put \(-\partial \theta^\pm(k)/\partial k = x_\pm\). Then, we derivate Eqs. (19) and (21) with respect to \(k\), and we obtain \(\sin k, \cos k, \sin \theta^\pm(k),\) and \(\cos \theta^\pm(k)\) as follows. From Eqs. (19) and (20), we have

\[
\begin{align*}
\cos k &= - \sgn(\cos k) \frac{x_+}{\sqrt{1 - x_+^2}}, \quad \cos \theta^+(k) = - \sgn(\cos k) \frac{1}{\sqrt{2(1 - x_+^2)}}, \\
\sin k &= \sgn(\sin k) \frac{1 - 2x_+^2}{1 - x_+^2}, \quad \sin \theta^+(k) = \sgn(\sin k) \frac{1 - 2x_+^2}{2(1 - x_+^2)}. 
\end{align*}
\]

From Eqs. (21) and (22), we see

\[
\begin{align*}
\cos k &= \sgn(\cos k) \frac{x_-}{\sqrt{1 - x_-^2}}, \quad \cos \theta^-(k) = \sgn(\cos k) \frac{1}{\sqrt{2(1 - x_-^2)}}, \\
\sin k &= \sgn(\sin k) \frac{1 - 2x_-^2}{1 - x_-^2}, \quad \sin \theta^-(k) = \sgn(\sin k) \frac{1 - 2x_-^2}{2(1 - x_-^2)}. 
\end{align*}
\]

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

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

where

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

and

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

In the next stage, we derive the residue of \(\hat{\Xi}(k ; z)\) at \(e^{i \theta^\pm(k)}\). At first, substituting the singular points to \(\tilde{f}_0^\pm(z)\), we obtain

1. \(\tilde{f}_0^+(e^{i \theta^+(k)}) = - \sgn(\cos k) e^{i \theta^+(k) + \sigma_+} \frac{\sqrt{1 - x_+^2}}{1 + |x|}, \quad \tilde{f}_0^-(e^{i \theta^+(k)}) = - \sgn(\cos k) e^{i \theta^+(k) - \sigma_-} \frac{\sqrt{1 - x_-^2}}{1 + |x|}.\)
2. \( \tilde{f}_0^+(e^{i\theta^-(k)}) = \text{sgn}(\cos k) e^{i((\theta^-(k) + \sigma_+)/2)} \frac{\sqrt{1 - x^2}}{1 + |x|} \), \( \tilde{f}_0^-(e^{i\theta^-(k)}) = \text{sgn}(\cos k) e^{i((\theta^-(k) - \sigma_-)/2)} \frac{\sqrt{1 - x^2}}{1 + |x|} \).

Noting Lemma 11, we see

\[
\frac{e^{ik}}{1 - e^{ik}\lambda^+(z)} \left[ \tilde{f}_0^+(z)\tilde{\lambda}^+(z) \right] [0, -1] \tilde{\Xi}_0(z) = \frac{1}{\Lambda_0(z)} e^{ik} \left[ \tilde{f}_0^+(z)\tilde{\lambda}^+(z) \right] - z \left( f_0^-(z) + \beta \right),
\]

and the square norm of residue of the first term of Eq. (15) is written as

\[
\left| \text{Res} \left( \frac{e^{ik}}{1 - e^{ik}\lambda^+(z)} \right) \left[ \tilde{f}_0^+(z)\tilde{\lambda}^+(z) \right] [0, -1] \tilde{\Xi}_0(z) : z = e^{i\theta^+(k)} \right|^2
\]

\[
= \left| \text{Res} \left( \frac{1}{1 - e^{ik}\lambda^+(z)} : z = e^{i\theta^+(k)} \right) \right|^2 \frac{1}{|\Lambda_0(e^{i\theta^+(k)})|^2} \left[ \tilde{f}_0^+(e^{i\theta^+(k)})\tilde{\lambda}^+(e^{i\theta^+(k)}) \right] - e^{i\theta^+(k)} \left( f_0^-(e^{i\theta^+(k)}) + \beta \right) \]

\[
\times |\lambda - \beta f_0^-(e^{i\theta^-(k)})|^2.
\]

In a similar way, we can write down the second term of Eq. (15) by

\[
\left| \text{Res} \left( \frac{e^{ik}}{1 - e^{ik}\lambda^-(z)} \right) \left[ f_0^-(z)\tilde{\lambda}^-(z) \right] [1, 0] \tilde{\Xi}_0(z) : z = e^{i\theta^-(k)} \right|^2
\]

\[
= \left| \text{Res} \left( \frac{1}{1 - e^{ik}\lambda^-(z)} : z = e^{i\theta^-(k)} \right) \right|^2 \frac{1}{|\Lambda_0(e^{i\theta^-(k)})|^2} \left[ \tilde{f}_0^-(e^{i\theta^-(k)})\tilde{\lambda}^-(e^{i\theta^-(k)}) \right] + e^{i\theta^-(k)} \left( \tilde{f}_0^-(e^{i\theta^-(k)}) + \beta \right) \]

\[
\times |\alpha - \beta f_0^+(e^{i\theta^-(k)})|^2.
\]

Hence, we obtain

\[
\| \text{Res}(\tilde{\Xi}(k) : z = e^{i\theta^+(k)}) \|^2 = \left| \text{Res} \left( \frac{1}{1 - e^{ik}\lambda^+(z)} : z = e^{i\theta^+(k)} \right) \right|^2 \frac{1}{|\Lambda_0(e^{i\theta^+(k)})|^2} \times \left[ \tilde{f}_0^+(e^{i\theta^+(k)})\tilde{\lambda}^+(e^{i\theta^+(k)}) \right]^2 |\alpha f_0^-(e^{i\theta^+(k)}) + \beta|^2
\]

\[
+ \left| \text{Res} \left( \frac{1}{1 - e^{ik}\lambda^-(z)} : z = e^{i\theta^-(k)} \right) \right|^2 \frac{1}{|\Lambda_0(e^{i\theta^-(k)})|^2} \times \left[ \tilde{f}_0^-(e^{i\theta^-(k)})\tilde{\lambda}^-(e^{i\theta^-(k)}) \right]^2 |\alpha - \beta f_0^+(e^{i\theta^-(k)})|^2.
\]

Henceforth, we will express the items below in terms of \( x_+ \) or \( x_- \), and then substitute the items in Eq. (15).

1. \( \left| \text{Res} \left( \frac{1}{1 - e^{ik}\lambda^+(z)} : z = e^{i\theta^+(k)} \right) \right|^2 \) and \( \left| \text{Res} \left( \frac{1}{1 - e^{ik}\lambda^-(z)} : z = e^{i\theta^-(k)} \right) \right|^2 \),
2. \[ \frac{1}{|\tilde{\Lambda}_0(e^{i\theta})|^2} \]

3. \[ |\alpha f_0^+(e^{i\theta}) + \beta|^2 \] and \[ |\alpha - \beta f_0^-(e^{i\theta})|^2 \]

4. \[ \left\| \tilde{\chi}^+(e^{i\theta}) f_0^+(e^{i\theta}) \right\|^2 \] and \[ \left\| \tilde{\chi}^-(e^{i\theta}) f_0^-(e^{i\theta}) \right\|^2 \]

1. Computation of \[ \left| Res \left( \frac{1}{1 - e^{ik\chi}(z)} : z = e^{i\theta(z)} \right) \right|^2 \]
   and \[ \left| Res \left( \frac{1}{1 - e^{-ik\chi}(z)} : z = e^{i\theta(z)} \right) \right|^2 \]
   Let \[ g^\pm(z) = 1 - e^{\pm ik\chi}(z) \]. Expanding \[ g^\pm(z) \] around \[ z = e^{i\theta(z)} \], we have

\[ Res \left( \frac{1}{1 - e^{\pm ik\chi}(z)} : z = e^{i\theta(z)} \right) = \frac{1}{\partial g^\pm(z)} \]

From Eqs. [16], we see

\[ \left. \frac{\partial g^\pm(z)}{\partial z} \right|_{z = e^{i\theta(z)}} = \pm \frac{\text{sgn}(\cos k)}{\sqrt{1 - x^2}} e^{-i(\theta(z) \mp k)} \left\{ \text{sgn}(\cos k \sin k) \right\} \]

which imply

\[ \left| Res \left( \frac{1}{1 - e^{ik\chi}(z)} : z = e^{i\theta(z)} \right) \right|^2 = x_+^2 \]

\[ \left| Res \left( \frac{1}{1 - e^{-ik\chi}(z)} : z = e^{i\theta(z)} \right) \right|^2 = x_-^2 \]

2. Computation of \[ \frac{1}{|\tilde{\Lambda}_0(e^{i\theta})|^2} \]

Noting Lemma [1], we have for any \( \theta \in \mathbb{R} \),

\[ |\tilde{\Lambda}_0(e^{i\theta})|^2 = 1 + 2Re \left\{ \tilde{\chi}^+(e^{i\theta}) \tilde{\chi}^-(e^{i\theta}) \right\} + |f_0^+(e^{i\theta})|^2 |f_0^-(e^{i\theta})|^2 \]

where \( \mathbb{R} \) is the set of the real numbers. Hence, substituting the singular points into Eq. [24], we obtain

\[ \left\{ \left| \frac{1}{\tilde{\Lambda}_0(e^{i\theta}(k))} \right|^2 = \frac{(1 + x_+)^2}{2(1 + x_+^2) (1 + \cos 2\sigma) + \text{sgn}(\sin k \cos k) \sqrt{1 - 2x_+^2} \sin 2\sigma} \right\} \]

\[ \left\{ \left| \frac{1}{\tilde{\Lambda}_0(e^{i\theta}(k))} \right|^2 = \frac{(1 - x_-)^2}{2(1 + x_-^2) (1 + \cos 2\sigma) - \text{sgn}(\sin k \cos k) \sqrt{1 - 2x_-^2} \sin 2\sigma} \right\} \]

3. Computation of \[ |\alpha f_0^-(e^{i\theta}(k)) + \beta|^2 \] and \[ |\alpha - \beta f_0^+(e^{i\theta}(k))|^2 \].
Let the initial coin state $\varphi_0 = T[\alpha, \beta]$, where $\alpha = a e^{i\phi_1}$, $\beta = b e^{i\phi_2}$ with $a, b \geq 0$ and $a^2 + b^2 = 1$. Noting

$$|\alpha f_0^-(e^{i\theta^+(k)})\rangle + |\beta\rangle|^2 = |\alpha|^2 |f_0^-(e^{i\theta^+(k)})\rangle|^2 + |\beta|^2 + 2\Re\{\alpha \overline{\beta} f_0^-(e^{i\theta^+(k)})\},$$

and

$$|\alpha - \beta f_0^+(e^{i\theta^-(k)})\rangle|^2 = |\alpha|^2 - 2\Re\{\alpha \overline{\beta} f_0^-(e^{i\theta^+(k)})\} + |\beta|^2 |f_0^+(e^{i\theta^-(k)})\rangle|^2,$$

we obtain

$$\begin{cases}
|\alpha f_0^-(e^{i\theta^+(k)})\rangle + |\beta\rangle|^2 = a^2\left(1 - \frac{x_+}{1 + x_+}\right) + b^2 + \frac{\sqrt{2ab}}{1 - x_+} \{\cos \gamma_+ + \text{sgn}(\sin k \cos k)\sqrt{1 - 2x_+^2} \sin \gamma_+\}, \\
|\alpha - \beta f_0^+(e^{i\theta^-(k)})\rangle|^2 = a^2 - \frac{\sqrt{2ab}}{1 - x_-} \{\cos \gamma_- - \text{sgn}(\sin k \cos k)\sqrt{1 - 2x_-^2} \sin \gamma_-\} + b^2 \frac{1 + x_-}{1 - x_-},
\end{cases} \tag{28}$$

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

4. Computation of $\begin{bmatrix} \tilde{\lambda}^+(e^{i\theta^+(k)}) f_0^+(e^{i\theta^+(k)}) \\ - e^{i\theta^+(k)} \end{bmatrix}$ and $\begin{bmatrix} \tilde{\lambda}^-(e^{i\theta^-(k)}) f_0^-(e^{i\theta^-(k)}) \\ e^{i\theta^-(k)} \end{bmatrix}$.

By a simple calculation, we have

$$\begin{bmatrix} \tilde{\lambda}^+(e^{i\theta^+(k)}) f_0^+(e^{i\theta^+(k)}) \\ - e^{i\theta^+(k)} \end{bmatrix}^2 = |\tilde{\lambda}^+(e^{i\theta^+(k)})|^2 |f_0^+(e^{i\theta^+(k)})|^2 + 1 = \frac{2}{1 + x_+} \quad (x_+ > 0),$$

$$\begin{bmatrix} \tilde{\lambda}^-(e^{i\theta^-(k)}) f_0^-(e^{i\theta^-(k)}) \\ e^{i\theta^-(k)} \end{bmatrix}^2 = 1 + |\tilde{\lambda}^-(e^{i\theta^-(k)})|^2 |f_0^-(e^{i\theta^-(k)})|^2 = \frac{2}{1 - x_-} \quad (x_- < 0). \tag{29}$$

Here, we should remark

$$- \frac{\partial \theta^\pm(k)}{\partial k} = x_\pm \tag{30}.$$ 

Eq. (30) implies

$$x_+ = \frac{|\cos k|}{\sqrt{1 + \cos^2 k}} \quad x_- = - \frac{|\cos k|}{\sqrt{1 + \cos^2 k}}. \tag{31}$$

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

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

Combining Eqs. (23) and (24) with Eq. (31), and noting Eq. (30), we get

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

and therefore, we obtain

$$\frac{dk}{dx} = \begin{cases} \text{sgn}(\sin k \cos k) f_K(x; 1/\sqrt{2})\pi dx & (x > 0), \\
 - \text{sgn}(\sin k \cos k) f_K(x; 1/\sqrt{2})\pi dx & (x < 0). \tag{32} \end{cases}$$
Substituting the items given in 1. to 4. into Eq. (25) and combining with Eq. (12), we arrive at Theorem 1.

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Appendix A

In Appendix A, we explain how Eq. (12), which is a key relation of the proof of Theorem 1, is derived. Put $w_l(k) = \text{Res}(\tilde{\Psi}_t(k : z = e^{i\theta_l(k)})$ with $\Psi_t(x) = \Xi_t(x)\varphi_0$. By definition, we have

$$E\left[e^{i\xi\tilde{\lambda}}\right] = \sum_j P(X_t = j)e^{i\xi\tilde{\lambda}}$$

$$= \sum_j \|\Xi_t(j)\varphi_0\|^2 e^{i\xi\tilde{\lambda}}$$

$$= \sum_{x,y} \phi_0^*\Xi_t(y)\Xi_t(x)\varphi_0 e^{i\xi\tilde{\lambda}}$$

$$= \sum_{x,y} \langle\Psi_t(y),\Psi_t(x)\rangle e^{i\xi\tilde{\lambda}} \int_0^{2\pi} e^{i(x-y)\xi t} \frac{dk}{2\pi}$$

$$= \int_0^{2\pi} \left\langle\tilde{\Psi}_t(k),\tilde{\Psi}_t(k + \frac{\xi}{t})\right\rangle \frac{dk}{2\pi}$$

$$= \int_0^{2\pi} \left\{ \sum_l w_l(k)e^{-i(t+1)\theta_l(k)}\sum_m w_m(k + \frac{\xi}{t})e^{-i(t+1)\theta_m(k + \frac{\xi}{t})} \right\} \frac{dk}{2\pi}$$

$$= \int_0^{2\pi} \left\{ \sum_l |w_l(k)|^2 e^{-i\frac{\xi}{t}l\theta_l(k)} e^{-i(t+1)O(\frac{1}{t^2})} + O\left(\frac{1}{t}\right) \right\} \frac{dk}{2\pi}$$

$$+ \int_0^{2\pi} \left\{ \sum_l \sum_m w_l(k)e^{-i(t+1)\theta_l(k)} w_m(k)e^{-i(t+1)\theta_m(k)} e^{-i\frac{\xi}{t}l\theta_l(k)} e^{-i(t+1)O(\frac{1}{t^2})} + O\left(\frac{1}{t}\right) \right\} \frac{dk}{2\pi}. \tag{A.3}$$

Here we should note that we use the residue theorem when we calculate Eq. (A.1) to Eq. (A.2), and Maclaurin's expansion for $w_m(k + \frac{\xi}{t})$ when we calculate Eq. (A.2) to Eq. (A.3). By the Riemann-Lebesgue Theorem, the second term of Eq. (A.3) vanishes when $t \to \infty$, and we get the desired equation.

Appendix B

In Appendix B, 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. According to [10], we have
\[
\begin{align*}
\hat{\lambda}^{(\pm)}(w) &= \pm \frac{i}{\sqrt{2}} \{(w + w^{-1}) - \sqrt{(w + w^{-1})^2 - 2}\}, \\
\tilde{f}_0^{(\pm)}(w) &= -\frac{\sqrt{\sigma^2}}{\sqrt{2}} \{(w - w^{-1}) + \sqrt{(w - w^{-1})^2 + 2}\}.
\end{align*}
\]
Putting \( w = i(1 - \epsilon)e^{i\theta} \) \((\epsilon \in \mathbb{R}, \ |\epsilon| \ll 1)\), we consider how \( \lim_{\epsilon \to 0} \sqrt{(w + w^{-1})^2 - 2} \) can be specified in terms of \( \theta \) according to the range of \( \cos \theta \) or \( \sin \theta \). Noting \( |\epsilon| \ll 1 \), we can approximates \( \hat{\lambda}^{(\pm)}(w) \) as [10]
\[
\tilde{\lambda}^{(+)}(w) = \frac{i}{\sqrt{2}} \left\{ (1 - \epsilon)ie^{i\theta} - (1 - \epsilon)^{-1}ie^{-i\theta} - \sqrt{(1 - \epsilon)ie^{i\theta} - (1 - \epsilon)^{-1}ie^{-i\theta})^2 - 2} \right\} \\
\sim -\frac{i}{\sqrt{2}} \left\{ 2\sin \theta + 2\epsilon \cos \theta + \delta \sqrt{4\sin^2 \theta - 2} \right\},
\] (B.1)
where we put \( \delta \in \mathbb{R} \) and \( \delta^2 = 1 \). Noting \( |\tilde{\lambda}^{(+)}(w)| < 1 \), Eq. (B.1) suggests that we need to take into consideration the next two cases [10].

1. \( |\sin \theta| \geq 1/\sqrt{2} \) case.
   Eq. (B.1) implies
   \[
   \frac{1}{2} \left\{ 2\sin \theta + 2\delta \sqrt{\sin^2 \theta - 1/2} \right\}^2 < 1.
   \]
   Thus, we have
   \[
   2\sin^2 \theta + 2\sin \theta \delta \sqrt{\sin^2 \theta - 1/2} < 1.
   \]
   Consequently, we obtain \( \delta = -\text{sgn}(\sin \theta) \).

2. \( |\sin \theta| < 1/\sqrt{2} \) case.
   Eq. (B.1) also implies
   \[
   \frac{1}{2} \left\{ 2\sin \theta + 2\delta \sqrt{\sin^2 \theta - 1/2} \right\}^2 + 4\epsilon^2 \cos^2 \theta < 1.
   \]
   Thus, we see
   \[
   4\epsilon^2 \cos^2 \theta + 8\epsilon \cos \theta \delta \sqrt{1/2 - \sin^2 \theta} < 0.
   \]
   Consequently, we obtain \( \delta = -\text{sgn}(\cos \theta) \).

As a result, the square root is expressed as
\[
\lim_{\epsilon \to 0} \sqrt{(w + w^{-1})^2 - 2} = \begin{cases}
-2 \text{sgn}(\sin \theta) \sqrt{\sin^2 \theta - \frac{1}{2}} \quad (|\sin \theta| \geq 1/\sqrt{2}) , \\
-2i \text{sgn}(\cos \theta) \sqrt{\frac{1}{2} - \sin^2 \theta} \quad (|\sin \theta| \leq 1/\sqrt{2}).
\end{cases}
\] (B.2)
Next, we determine in detail \( \tilde{\lambda}^{(\pm)}(z) \) and \( \tilde{f}_0^{(\pm)}(z) \). When we focus on the weak limit theorem for our two-phase QW, we 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, \( |\tilde{f}_0^{(\pm)}(z)| \neq 1 \). Hence Eq. (B.2) gives
\[
\begin{align*}
\tilde{\lambda}^{(\pm)}(z) &= \mp \{ \text{sgn}(\cos \theta) \sqrt{2} \cos \theta - 1 + i\sqrt{2} \sin \theta \}, \quad (|\sin \theta| \leq 1/\sqrt{2}) \\
\tilde{f}_0^{(\pm)}(z) &= \text{sgn}(\cos \theta) e^{i(\theta \pm \sigma z)} \{ \sqrt{2} \cos \theta - \sqrt{2} \cos^2 \theta - 1 \},
\end{align*}
\]
where \( z = e^{i\theta} \).