

THE GENERATOR AND QUANTUM MARKOV SEMIGROUP FOR QUANTUM WALKS

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Abstract

The quantum walks in the lattice spaces are represented as unitary evolutions. We find a generator for the evolution and apply it to further understand the walks. We first extend the discrete time quantum walks to continuous time walks. Then we construct the quantum Markov semigroup for quantum walks and characterize it in an invariant subalgebra. In the meanwhile, we obtain the limit distributions of the quantum walks in one-dimension with a proper scaling, which was obtained by Konno by a different method.

1. Introduction

Quantum walk (QW hereafter) is a quantum analogue of classical random walk. After it was initiated by Meyer [17], it attracted many interests and there are many works developing it in mathematically rigorous way on the one hand and explaining possible practical applications, e.g., in quantum computation (see [2, 7, 9, 11, 12, 14, 17], and references therein for more details).

QW's demonstrate non-intuitive behaviour in several ways comparing to classical random walks. The most outstanding feature is fast diffusing as noted by many authors: the scaling for the central limit theory is n comparing to \sqrt{n} for classical random walks. It is caused from quantum interference. The superposition in QW's is likewise a unique phenomenon that does not exist in classical random walks.

The aim of this paper is to further investigate the QW's by their generators. We find the generator from an evolution map of a QW. As applications we will first extend the discrete time QW's to continuous time walks. We also discuss the quantum Markov semigroup for QW's. The quantum probabilistic aspect of the QW's has been discussed in a separate paper [10]. We remark that there already have been studies of continuous time QW's on the graphs [6, 13, 16, 19,

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21], but we emphasize that the extension here is different from those. It is a natural extension of the discrete time QW on integer lattices in the sense that it agrees with the original discrete time QW for integer times. We note that this concept was already appeared in [8]. Next, not only we construct the quantum Markov semigroup for QW's, we also find an invariant subalgebra on which the dynamics is completely characterized.

Our method is to use Fourier transform, so called a Schrödinger approach, which was introduced by Ambaini et al. [2, 18]. By it we will recover the limit distributions for QW's which was concretely studied by Konno [11, 12] via path integral approach.

This paper is organized as follows. In section 2, we briefly review the QW's and find the unitary evolution map of them. Then, we find a scaled limit distributions of QW's (Theorem 2.1 and Proposition 2.3). In section 3, we observe a superposition phenomena for a typical Hadamard walk. Then we find a continuous time extension. In section 4, we discuss the quantum Markov semigroup for QW's.

2. 1-dimensional quantum walks

In this section we briefly introduce the 1-dimensional QW's. We will see that a QW is a (discrete time) unitary evolution in a suitably chosen Hilbert space.

2.1. 1-dimensional QW's

We first introduce the definition of 1-dimensional quantum walks following [2, 7, 11, 12, 18]. A quantum particle has an intrinsic degree of freedom, called "chirality". This chirality is represented by a 2-dimensional vector: we represent them in \mathbf{C}^2 and call the vectors $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ the left and right chirality, respectively. The spatial movement of the particle is given as follows. At time $n \in \mathbf{N}_0 = \{0, 1, 2, \dots\}$, the probability amplitude of finding the particle at site $x \in \mathbf{Z}$ with chirality state being left or right is given by a two-component vector

$$(2.1) \quad \psi_n(x) = \begin{pmatrix} \psi_n(1; x) \\ \psi_n(2; x) \end{pmatrix} \in \mathbf{C}^2.$$

After one unit of time the chirality is rotated by an a priori given unitary matrix U . According to the final chirality state, if the particle ends up with left chirality, then it moves one step to the left, and if it ends up with right chirality, it moves one step to the right. In order to see this dynamics more precisely let us denote

$$(2.2) \quad U = \begin{pmatrix} l_1 & l_2 \\ r_1 & r_2 \end{pmatrix}$$

and define

$$(2.3) \quad L = \begin{pmatrix} l_1 & l_2 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad R = \begin{pmatrix} 0 & 0 \\ r_1 & r_2 \end{pmatrix}.$$

Then the dynamics for $\psi_n = (\psi_n(x))_{x \in \mathbf{Z}}$ is given by

$$(2.4) \quad \psi_{n+1}(x) = L\psi_n(x+1) + R\psi_n(x-1).$$

This dynamics has been investigated by many authors. There are two main methods to investigate it. One is so called the path integral approach, in which the explicit probability amplitude is computed by using a great deal of combinatorics. This method has been extensively developed by Konno [11, 12]. In particular, Konno obtained the scaled limit distribution of the QW very concretely. The other method is called the Schrödinger approach, which uses Fourier transform taking advantage of space-time homogeneity of QW's. This approach was well-developed in [2, 7, 8, 18]. In this paper we further develop the Schrödinger approach to get a unitary evolution map for the QW in a suitable Hilbert space. Then the generator comes out naturally.

2.2. Evolution of QW's

For each $x \in \mathbf{Z}$, let $\mathcal{H}_x := \mathbf{C}^2$ be a copy of the chirality space. Let

$$(2.5) \quad \mathcal{H} := \bigoplus_{x \in \mathbf{Z}} \mathcal{H}_x$$

be the direct sum Hilbert space, on which the evolution of a QW will be developed. Notice that \mathcal{H} is isomorphic to the Hilbert spaces $l^2(\mathbf{Z}, \mathbf{C}^2)$ and $l^2(\mathbf{Z}) \otimes \mathbf{C}^2$. For each $x \in \mathbf{Z}$, let

$$(2.6) \quad e_x(k) := \frac{1}{\sqrt{2\pi}} e^{ixk}, \quad k \in \mathbf{K} := (-\pi, \pi],$$

\mathbf{K} being understood as a unit circle in \mathbf{R}^2 . The set $\{e_x\}_{x \in \mathbf{Z}}$ defines an orthonormal basis in $L^2(\mathbf{K})$. For each $k \in \mathbf{K}$, let \mathfrak{h}_k be a copy of \mathbf{C}^2 and let

$$(2.7) \quad \hat{\mathcal{H}} := \int_{\mathbf{K}}^{\oplus} \mathfrak{h}_k dk \approx L^2(\mathbf{K}, \mathbf{C}^2) \approx L^2(\mathbf{K}) \otimes \mathbf{C}^2$$

be the direct integral of Hilbert spaces. The Fourier transform between $l^2(\mathbf{Z})$ and $L^2(\mathbf{K})$ naturally extends to a unitary map from \mathcal{H} to $\hat{\mathcal{H}}$ by

$$(2.8) \quad \psi = \left\{ \begin{pmatrix} \psi(1; x) \\ \psi(2; x) \end{pmatrix} \right\}_{x \in \mathbf{Z}} \in \mathcal{H} \mapsto \hat{\psi} = \left\{ \begin{pmatrix} \hat{\psi}(1; k) \\ \hat{\psi}(2; k) \end{pmatrix} \right\}_{k \in \mathbf{K}} \in \hat{\mathcal{H}},$$

where

$$(2.9) \quad \hat{\psi}(i; k) = \sum_{x \in \mathbf{Z}} \psi(i; x) e_x(k), \quad i = 1, 2.$$

Its inverse is given by $\hat{\psi} \mapsto \psi$ with

$$\psi(x) = \int_{-\pi}^{\pi} \frac{1}{\sqrt{2\pi}} e^{-ixk} \hat{\psi}(k) dk \in \mathcal{H}_x.$$

Let us denote by T the left translation in $l^2(\mathbf{Z})$:

$$(2.10) \quad (Ta)(x) = a(x + 1), \quad \text{for } a = (a(x))_{x \in \mathbf{Z}}.$$

T is a unitary map whose adjoint is the right translation:

$$(2.11) \quad (T^*a)(x) = a(x - 1), \quad \text{for } a = (a(x))_{x \in \mathbf{Z}}.$$

The operator T naturally extends to $\mathcal{H} = \bigoplus_{x \in \mathbf{Z}} \mathcal{H}_x$ and for the sake of simplicity we use the same notation T for the extension. Given an operator (2×2 matrix) B on \mathbf{C}^2 , we let

$$(2.12) \quad \tilde{B} := \bigoplus_{x \in \mathbf{Z}} B$$

be the bounded direct sum operator acting on \mathcal{H} .

With these preparations we can rewrite the dynamics of a QW as an evolution map in the Hilbert space \mathcal{H} . Notice that the equation (2.4) is the same as

$$(2.13) \quad \psi_{n+1}(x) = L(T\psi_n)(x) + R(T^*\psi_n)(x), \quad x \in \mathbf{Z},$$

which we can write in a single equation:

$$(2.14) \quad \psi_{n+1} = (\tilde{L}T + \tilde{R}T^*)\psi_n.$$

It is not hard to see that the operator $\tilde{L}T + \tilde{R}T^*$ is a unitary operator on \mathcal{H} . Thus the solution to (2.14) is easily seen to be

$$(2.15) \quad \psi_n = (\tilde{L}T + \tilde{R}T^*)^n \psi_0.$$

This is the time evolution of the QW that we are looking for. One may write the unitary $\tilde{L}T + \tilde{R}T^*$ as $T\tilde{L} + T^*\tilde{R}$ by noticing $\tilde{L}T = T\tilde{L}$ and $\tilde{R}T^* = T^*\tilde{R}$, if one stresses the order that the movement (space translation) follows the action of chirality rotation.

Now we find the evolution of the QW in a Fourier transform space. Notice that the translation operator T is represented as a multiplication operator by e^{-ik} in the Fourier transform space. Thus, the evolution in (2.15) has the representation in Fourier transform space as follows:

$$(2.16) \quad \begin{aligned} \hat{\psi}_n(k) &= (e^{-ik}L + e^{ik}R)^n \hat{\psi}_0(k) \\ &= \begin{pmatrix} e^{-ik}l_1 & e^{-ik}l_2 \\ e^{ik}r_1 & e^{ik}r_2 \end{pmatrix}^n \hat{\psi}_0(k). \end{aligned}$$

This representation has been already obtained in [2, 7, 8, 18]. Notice that for each $k \in \mathbf{K}$ the matrix

$$(2.17) \quad U(k) := \begin{pmatrix} e^{-ik}l_1 & e^{-ik}l_2 \\ e^{ik}r_1 & e^{ik}r_2 \end{pmatrix}$$

is a unitary matrix in \mathbf{C}^2 , and hence the evolution in (2.16) is again unitary in $\hat{\mathcal{H}}$, as it should be.

The probability density to find out the particle at a site $x \in \mathbf{Z}$ at time n is simply

$$(2.18) \quad \|\psi_n(x)\|^2 = |\psi_n(1;x)|^2 + |\psi_n(2;x)|^2,$$

or it can also be given by

$$(2.19) \quad \left\| \int_{-\pi}^{\pi} \frac{1}{\sqrt{2\pi}} e^{-ixk} \hat{\psi}_n(k) dk \right\|^2 = \frac{1}{2\pi} \left\{ \left| \int_{-\pi}^{\pi} e^{-ixk} \hat{\psi}_n(1;k) dk \right|^2 + \left| \int_{-\pi}^{\pi} e^{-ixk} \hat{\psi}_n(2;k) dk \right|^2 \right\}.$$

Konno has obtained the explicit form of the density (2.18) by using previously mentioned path integral approach. It uses a good deal amount of combinatorics and the resulting formula looks rather complicated [11, 12]. Nevertheless, by using his formula, Konno has successfully obtained the asymptotic distributions of the scaled QW's. On the other hand, by using the formula in (2.19), Ambainis et al. also explained many properties of QW's [2, 18]. In particular, when one is interested in the asymptotic behavior of QW's it turns out that the formula in (2.19) is extremely convenient because we have a nice tool so called the method of stationary phase [3, 4]. The asymptotic behavior of the probability amplitudes by this method was investigated by Ambainis et al. [2, 18]. In the next subsection we will find the limit distribution of the scaled QW by computing the limit of characteristic functions. We notice that Grimmett et al. obtained also the weak limit of the scaled QW's by using the method of moments in the Schrödinger approach [7]. In [8], Katori et al. further developed this method and they re-established the limit distribution. The moment problem is closely related to the interacting Fock spaces via quantum probability theory, which we have discussed in other paper [10].

2.3. Limit distributions

In this subsection we study the limit distribution of the scaled QW. Let $\{X_n^{(U;\psi_0)}\}_{n \geq 0}$ be the random variables distributed on the integer space \mathbf{Z} according to the QW whose evolution is given by (2.15). That is,

$$(2.20) \quad \mathbf{P}(X_n^{(U;\psi_0)} = x) = \|\psi_n(x)\|^2.$$

Before we state the result we notice that a multiplication by a phase factor to U does not affect the distribution of $\{X_n^{(U;\psi_0)}\}$. Thus, for a technical reason in the

proof, we will assume that

$$(2.21) \quad \det U = 1.$$

Thereby we caution the reader that if the matrix U in a given model does not satisfy (2.21), we will first adjust it by multiplying some phase factor so that (2.21) is satisfied.

THEOREM 2.1. *There is a random variable $Z^{(U;\psi_0)}$ on the real line such that in distribution*

$$(2.22) \quad \lim_{n \rightarrow \infty} \frac{X_n^{(U;\psi_0)}}{n} = Z^{(U;\psi_0)}.$$

If $l_1 l_2 r_1 r_2 \neq 0$, the distribution $\mu^{(U;\psi_0)}$ of $Z^{(U;\psi_0)}$ has a density function: it is supported on $(-|l_1|, |l_1|)$ and has the form:

$$(2.23) \quad \rho^{(U;\psi_0)}(y) = \frac{\sqrt{1 - |l_1|^2}}{\pi(1 - y^2)\sqrt{|l_1|^2 - y^2}} g^{(U;\psi_0)}(y)$$

with $g^{(U;\psi_0)}(y)$ being a dependent part to the initial condition. On the other hand, if one of l_1 or l_2 is zero, then the distribution $\mu^{(U;\psi_0)}$ is a point mass: for

$$\psi_0 = \left\{ \begin{pmatrix} \psi_0(1; x) \\ \psi_0(2; x) \end{pmatrix} \right\}_{x \in \mathbf{Z}},$$

$$(2.24) \quad \mu^{(U;\psi_0)} = \begin{cases} (\sum_{x \in \mathbf{Z}} |\psi_0(1; x)|^2) \delta_{-1} + (\sum_{x \in \mathbf{Z}} |\psi_0(2; x)|^2) \delta_1, & \text{if } l_2 = 0 \\ \delta_0, & \text{if } l_1 = 0 \end{cases}$$

Remark 2.2. (a) The function $g^{(U;\psi_0)}(y)$ depends heavily on the initial state ψ_0 . In Proposition 2.3 below we will see a concrete form of $g^{(U;\psi_0)}(y)$ for QW's that are initially localized at the origin. The above formula was first shown by Konno [11, 12]. Grimmett et al. also obtained the formula for the (biased) Hadamard QW's [7]. Katori et al. recovered it from the method of moments [8]. Recently Ahlbrecht et al. discussed the asymptotic behaviour of QW's by using a perturbative method [1].

(b) In relevance with the limit theory, we would like to mention some recent results. Sunada and Tate investigated the limit theory of the quantum walk (starting at one point, say the origin) much more closely dividing the region into three areas: allowed region (inside the interval $(-|l_1|, |l_1|)$), around the wall ($|x| \sim \pm |l_1|$), and hidden region ($|l_1| < |x| < 1$). In particular, for the hidden region, they obtained the large deviation principle, i.e., the probability in the hidden region decreases exponentially with a concrete rate function. See [22] for the details. In [15], Machida investigated that by allowing various initial conditions, in the limit we can recover some of the well known distributions such as semicircular law, arcsine law, Gaussian, and uniform distributions.

The proof of Theorem 2.1 will be given in the Appendix. Although it was shown already, our Shrödinger approach should be a good contrast to the path integral approach. As mentioned, the method of stationary phase plays the key role for asymptotics of the integral of rapidly varying functions.

Next we consider the situation that the particle is initially located at the origin. We will get more concrete form of the limit density function.

PROPOSITION 2.3. *Suppose that the initial condition is a qubit state $\begin{pmatrix} a \\ b \end{pmatrix}$, $a, b \in \mathbf{C}$, $|a|^2 + |b|^2 = 1$, located at the origin. Then the density of the limit distribution in Theorem 2.1 in the case $l_1 l_2 r_1 r_2 \neq 0$ is given by the following formula.*

$$\rho^{(U; \psi_0)}(y) = \frac{\sqrt{1 - |l_1|^2}}{\pi(1 - y^2)\sqrt{|l_1|^2 - y^2}} (1 - \beta^{(U; \psi_0)}(y)) 1_{(-|l_1|, |l_1|)}(y)$$

with

$$\beta^{(U; \psi_0)} = |a|^2 - |b|^2 + \frac{\bar{l}_1 l_2 \bar{a} b + l_1 \bar{l}_2 a \bar{b}}{|l_1|^2}.$$

Remark 2.4. The formula in Proposition 2.3 is exactly what Konno obtained by the path integral approach [11, 12].

The proof of Proposition 2.3 will also be given in the Appendix.

3. Continuous time QW's

In this section we extend the discrete time QW's to continuous time QW's. It is done from our development in Section 2 and we remark that it is a different kind of version for continuous time QW's from those appearing in the literature [13, 16, 19]. As we have seen in the last section, the distribution of QW's depends heavily on the initial condition. In particular, the QW's reveal the superposition of states. In the next subsection we will see the superposition phenomena in the simplest case of Hadamard walk.

3.1. Superposition of QW's

Let us consider the Hadamard QW with the unitary matrix for the rotation of chirality given by

$$(3.1) \quad U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}.$$

We notice here that we have changed the rows of the matrix from the usual Hadamard matrix. It is just to make $\det U = 1$ and it only makes the exchange of left and right movements of the quantum walker. We will consider for the initial conditions not only the case that the walker starts at the origin but also the case that it is spatially distributed.

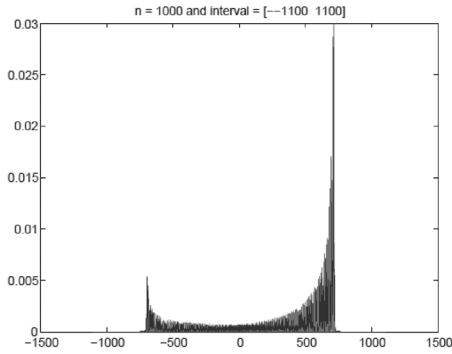


FIGURE 3.1

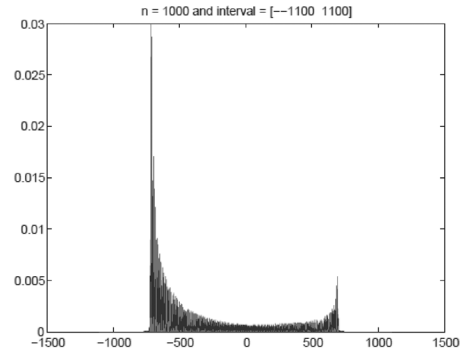


FIGURE 3.2

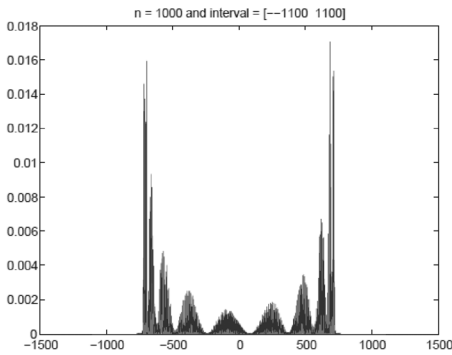


FIGURE 3.3

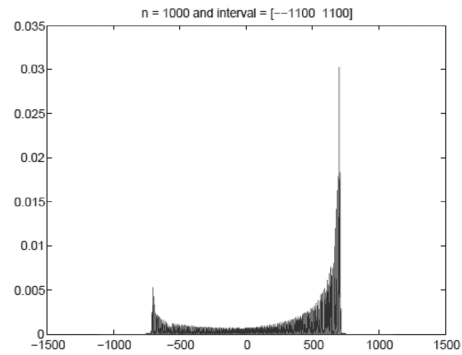


FIGURE 3.4

Figure 3.1 shows the spatial distribution of the QW at time $n = 1000$ starting at the point $x = 10$ with initial qubit state $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$, i.e., $\psi_0 = \left\{ \begin{pmatrix} 0 \\ 1 \end{pmatrix} \delta_{10}(x) \right\}_{x \in \mathbf{Z}}$, or $\hat{\psi}_0(k) = \frac{1}{\sqrt{2\pi}} \begin{pmatrix} 0 \\ e^{10ik} \end{pmatrix}$. Similarly Figure 3.2 shows the distribution at $n = 1000$ with $\psi_0 = \left\{ \begin{pmatrix} 1 \\ 0 \end{pmatrix} \delta_{-10}(x) \right\}_{x \in \mathbf{Z}}$. Figure 3.3 shows the distribution at $n = 1000$ with $\psi_0 = \left\{ \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} \delta_{10}(x) + \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} \delta_{-10}(x) \right\}_{x \in \mathbf{Z}}$, the mixture of the previous two examples. It shows the superposition of the QW. Finally Figure 3.4 shows the distribution at $n = 1000$ for $\psi_0 = \left\{ \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} \delta_0(x) + \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} \delta_0(x) \right\}_{x \in \mathbf{Z}}$. We see

that if it were the classical random walk, then the distribution for the initial condition in Figure 3.3 would be the mean of the distributions of the Figure 3.1 and 3.2. But the distribution for the QW is totally different from this behavior and the result in Figure 3.3 shows that in QW's the walks have interference to each other, like in a two slit experiment in quantum mechanics. Figure 3.4 shows that it is still different from the behavior of the QW who starts at the origin with mixed qubit state of the two walkers of Figure 3.3. Notice that the two walkers positioned at $x = 10$ and $x = -10$ might be viewed as positioned "almost" at the origin if one looks at them from a "long" distance of size 1000. But the results of Figure 3.3 and 3.4 show that it is different from the intuition.

3.2. Continuous time QW's

We recall the evolution of QW in (2.16):

$$\hat{\psi}_n(k) = U(k)^n \hat{\psi}_0(k),$$

where

$$(3.2) \quad U(k) = \begin{pmatrix} e^{-ik}l_1 & e^{-ik}l_2 \\ e^{ik}r_1 & e^{ik}r_2 \end{pmatrix}.$$

By (A.7) the unitary matrix $U(k)$ is diagonalized as

$$U(k) = S(k - \theta_1) \begin{pmatrix} e^{i\gamma(k-\theta_1)} & 0 \\ 0 & e^{-i\gamma(k-\theta_1)} \end{pmatrix} S(k - \theta_1)^{-1}.$$

Thus we can rewrite it as

$$(3.3) \quad U(k) = e^{iH(k)},$$

where $H(k)$ is a self-adjoint operator defined by

$$(3.4) \quad H(k) = S(k - \theta_1) \begin{pmatrix} \gamma(k - \theta_1) & 0 \\ 0 & -\gamma(k - \theta_1) \end{pmatrix} S(k - \theta_1)^{-1}.$$

The evolution of QW can now be denoted by

$$(3.5) \quad \hat{\psi}_n(k) = e^{inH(k)} \hat{\psi}_0(k).$$

Now it is strightforward to extend the QW to a continuous time QW:

DEFINITION 3.1. Let U be a 2×2 unitary matrix. The continuous time QW on \mathbf{Z} is defined by the unitary evolution (in Fourier space) defined by

$$(3.6) \quad \hat{\psi}_t(k) = e^{itH(k)} \hat{\psi}_0(k),$$

where $H(k)$ is the self-adjoint operator given in (3.4).

Remark 3.2. (a) As mentioned before, this continuous extension of QW is different from the usual ones on the graphs, where the generator comes from the

discrete Laplacian. Moreover, the intrinsic chiral state is not concerned in those models, but here the continuous time QW has still the chiral states.

(b) From (3.6), one notices that the quantum walk unitary evolution satisfies the Schrödinger equation (in the Fourier transform space $\hat{\mathcal{H}} = L^2(\mathbf{K}, \mathbf{C}^2)$):

$$(3.7) \quad \frac{\partial \hat{\psi}_t}{\partial t} = iH\hat{\psi}_t, \quad \hat{\psi}_t \in \hat{\mathcal{H}},$$

where the Hamiltonian operator H is given by

$$(3.8) \quad H = \int_{\mathbf{K}}^{\oplus} H(k) dk.$$

If we pull back the equation in the real Hilbert space $\mathcal{H} = l^2(\mathbf{Z}, \mathbf{C}^2)$, then it is written as

$$(3.9) \quad \frac{\partial \psi_t}{\partial t} = iK\psi_t, \quad \psi_t \in \mathcal{H},$$

where the Hamiltonian operator K works as

$$(K\psi)(x) = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} e^{-ixk} H(k) \hat{\psi}(k) dk, \quad \psi \in \mathcal{H},$$

where $\hat{\psi}$ is the Fourier transform of ψ .

Example 3.3. We consider again the Hardamard walk of the previous subsection but in the continuous time. We take the initial condition of Figure

$$3.3, \text{ i.e., } \psi_0 = \left\{ \left(\begin{array}{c} 0 \\ \frac{1}{\sqrt{2}} \end{array} \right) \delta_{10}(x) + \left(\begin{array}{c} \frac{1}{\sqrt{2}} \\ 0 \end{array} \right) \delta_{-10}(x) \right\}_{x \in \mathbf{Z}}, \text{ or } \hat{\psi}_0(k) = \frac{1}{2\sqrt{\pi}} \begin{pmatrix} e^{-10ik} \\ e^{10ik} \end{pmatrix}.$$

Figure 3.5 shows a series of snapshots of the distribution of $X_t^{(U; \psi_0)}$ at times $t = 99.25, 99.5, 99.75$, and 100.

4. Quantum Markov semigroup for QW's

In this section we study the quantum Markov semigroup [20] associated to the continuous time QW's. The notion of a quantum Markov semigroup arose to describe the irreversible evolution of an open quantum system. A quantum Markov semigroup is a semigroup of completely positive, identity preserving, normal linear maps on the algebra of all bounded linear operators on a Hilbert space. Here we restrict ourselves to the evolution of observables in a closed quantum system. For the details, we refer to [5] and references therein.

It turns out to be convenient to work on the Fourier transform Hilbert space $\hat{\mathcal{H}} = \int_{\mathbf{K}}^{\oplus} h_k dk$, where h_k is a copy of \mathbf{C}^2 for each $k \in \mathbf{K} = (-1, 1]$, considered as a unit circle in \mathbf{R}^2 . Let $\mathcal{M} \subset \mathcal{B}(\hat{\mathcal{H}})$ be a Banach subalgebra consisting of the

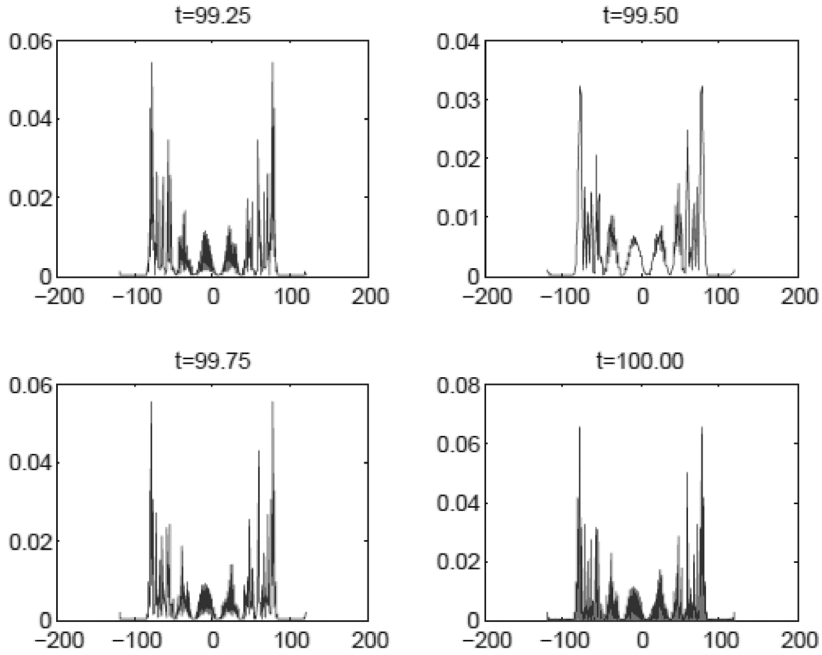


FIGURE 3.5

operators

$$(4.1) \quad A := \int_{\mathbf{K}}^{\oplus} A(k) dk \in \mathcal{M},$$

where $A(k)$ is a 2×2 matrix for each $k \in \mathbf{K}$ and they satisfy

$$\sup_k \|A(k)\| < \infty.$$

Given a unitary matrix $U = \begin{pmatrix} l_1 & l_2 \\ r_1 & r_2 \end{pmatrix}$, recall the unitary matrix $U(k)$ in (3.2).

Notice that it defines a unitary operator on $\hat{\mathcal{H}}$, belonging to \mathcal{M} , via the form $\int_{\mathbf{K}}^{\oplus} U(k) dk$ in the representation of (4.1). Recall the operator $H(k)$ in (3.4). By taking normalized eigenvectors of $U(k)$ we can take $S(k)$ in (3.4) as a unitary operator (see (A.6)):

$$(4.2) \quad S(k) = \begin{pmatrix} \frac{1}{\sqrt{1 + |\alpha_+(k)|^2}} & \frac{1}{\sqrt{1 + |\alpha_-(k)|^2}} \\ \frac{\alpha_+(k)}{\sqrt{1 + |\alpha_+(k)|^2}} & \frac{\alpha_-(k)}{\sqrt{1 + |\alpha_-(k)|^2}} \end{pmatrix},$$

where

$$(4.3) \quad \alpha_{\pm}(k) = ie^{i(k+\theta_1-\theta_2)}(|l_1|/|l_2| \sin k \pm \sqrt{1 + (|l_1|/|l_2| \sin k)^2}).$$

In the above $\theta_2 \in \mathbf{K}$ is such that $l_2 = |l_2|e^{i\theta_2}$ and we have used the relation $\cos \gamma(k) = |l_1| \cos k$. Then $H(k)$ is given by

$$(4.4) \quad H(k) = S(k - \theta_1) \begin{pmatrix} \gamma(k - \theta_1) & 0 \\ 0 & -\gamma(k - \theta_1) \end{pmatrix} S(k - \theta_1)^*.$$

Because $\cos^{-1}|l_1| \leq \gamma(k) \leq \pi - \cos^{-1}|l_1|$ uniformly for $k \in \mathbf{K}$, the operator norm $\|H(k)\|$ (as an operator on \mathbf{C}^2) is bounded by $\pi - \cos^{-1}|l_1|$ uniformly for $k \in \mathbf{K}$. Thus the self-adjoint operator $H := \int_{\mathbf{K}}^{\oplus} H(k) dk$ is a bounded operator on $\hat{\mathcal{H}}$ and belongs to \mathcal{M} . We define a semigroup V_t on $\mathcal{B}(\hat{\mathcal{H}})$ by

$$(4.5) \quad V_t(A) := e^{iHt} A e^{-iHt}, \quad A \in \mathcal{B}(\hat{\mathcal{H}}).$$

Notice that V_t has the representation

$$(4.6) \quad V_t(A) = e^{t\mathcal{L}}(A),$$

where the generator $\mathcal{L} \in \mathcal{B}(\hat{\mathcal{H}})$ is defined by

$$(4.7) \quad \mathcal{L}(A) := i[H, A].$$

By the way that the operator H is defined, it is clear that V_t leaves the subalgebra \mathcal{M} invariant. Moreover, if $A \in \mathcal{M}$ is represented by $A = \int_{\mathbf{K}}^{\oplus} A(k) dk$, then

$$(4.8) \quad V_t(A) = \int_{\mathbf{K}}^{\oplus} V_{k,t}(A(k)) dk,$$

where

$$(4.9) \quad V_{k,t}(A(k)) = e^{itH(k)} A(k) e^{-itH(k)} = e^{t\mathcal{L}_k}(A(k)),$$

with the local generator \mathcal{L}_k defined by

$$(4.10) \quad \mathcal{L}_k(A(k)) = i[H(k), A(k)].$$

The semigroup $\{V_t\}_{t \geq 0}$ is a quantum Markov semigroup on $\mathcal{B}(\hat{\mathcal{H}})$ [20]. In particular it preserves the identity and positivity. Our main purpose in this section is to characterize the action of the semigroup $\{V_t\}_{t \geq 0}$ on the invariant subalgebra. For it let us recall the Pauli matrices:

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

THEOREM 4.1. *For each $k \in \mathbf{K}$, there is a 3×3 unitary matrix $W(k)$ such that by defining $C(k) := W(k) \begin{pmatrix} 0 & 0 & 0 \\ 0 & 2\gamma(k) & 0 \\ 0 & 0 & -2\gamma(k) \end{pmatrix} W(k)^*$, we have*

$$V_{k,t}(\sigma_0) = \sigma_0, \quad \text{and} \quad \begin{pmatrix} V_{k,t}(\sigma_1) \\ V_{k,t}(\sigma_2) \\ V_{k,t}(\sigma_3) \end{pmatrix} = e^{iC(k-\theta_1)t} \begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \end{pmatrix}.$$

Therefore, for each $A \in \mathcal{M}$ of the form in (4.1) we have

$$V_t(A) = \int_{\mathbf{K}}^{\oplus} \sum_{l=0}^3 a_l(k) V_{k,t}(\sigma_l) dk,$$

where the coefficients are such that $A(k) = \sum_{l=0}^3 a_l(k) \sigma_l$ for each $k \in \mathbf{K}$.

Proof. By direct computation, we can rewrite $H(k)$ as

$$(4.11) \quad \begin{aligned} H(k) &= \gamma(k - \theta_1) S(k - \theta_1) \sigma_3 S(k - \theta_1)^* \\ &= \gamma(k - \theta_1) \sum_{l=1}^3 h_l(k - \theta_1) \sigma_l, \end{aligned}$$

with

$$(4.12) \quad \begin{aligned} h_1(k) &= \frac{1}{\sqrt{1 + (|l_1|/|l_2| \sin k)^2}} (-\sin(k + \theta_1 - \theta_2)), \\ h_2(k) &= \frac{1}{\sqrt{1 + (|l_1|/|l_2| \cos k)^2}} (\cos(k + \theta_1 - \theta_2)), \\ h_3(k) &= \frac{1}{\sqrt{1 + (|l_1|/|l_2| \sin k)^2}} (-|l_1|/|l_2| \sin k). \end{aligned}$$

Notice that

$$\frac{d}{dt} V_{k,t}(B) = V_{k,t}(\mathcal{L}_k(B)) = iV_{k,t}([H(k), B])$$

for all 2×2 matrix B . From this and (4.11), and by using the commutation relations of Pauli matrices, we have

$$(4.13) \quad \begin{aligned} \frac{d}{dt} V_{k,t}(\sigma_0) &= 0, \\ \frac{d}{dt} \begin{pmatrix} V_{k,t}(\sigma_1) \\ V_{k,t}(\sigma_2) \\ V_{k,t}(\sigma_3) \end{pmatrix} &= 2 \begin{pmatrix} h_1(k - \theta_1) \\ h_2(k - \theta_2) \\ h_3(k - \theta_1) \end{pmatrix} \times \begin{pmatrix} V_{k,t}(\sigma_1) \\ V_{k,t}(\sigma_2) \\ V_{k,t}(\sigma_3) \end{pmatrix}, \end{aligned}$$

where the product in the second line means the vector product of three dimensional vectors. It is easy to solve the linear equation (4.13):

$$(4.14) \quad V_{k,t}(\sigma_0) = \sigma_0$$

$$\begin{pmatrix} V_{k,t}(\sigma_1) \\ V_{k,t}(\sigma_2) \\ V_{k,t}(\sigma_3) \end{pmatrix} = W(k - \theta_1) \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{2\gamma(k-\theta_1)it} & 0 \\ 0 & 0 & e^{-2\gamma(k-\theta_1)it} \end{pmatrix} W(k - \theta_1)^* \begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \end{pmatrix},$$

where $W(k)$ is a 3×3 matrix whose columns are the normalized eigenvectors of the matrix

$$\begin{pmatrix} 0 & -2h_3(k) & 2h_2(k) \\ 2h_3(k) & 0 & -2h_1(k) \\ -2h_2(k) & 2h_1(k) & 0 \end{pmatrix},$$

whose eigenvalues are $0, \pm 2\gamma(k)i$. Now let $A = \int_{\mathbf{K}}^{\oplus} A(k) dk \in \mathcal{M}$. Since the Pauli matrices together with the identity form a basis of the algebra of 2×2 matrices there are constants $a_l(k), l = 0, 1, 2, 3$, such that $A(k) = \sum_{l=0}^3 a_l(k)\sigma_l$ for each $k \in \mathbf{K}$. Thus the evolution of A under V_t is given by

$$(4.15) \quad V_t(A) = \int_{\mathbf{K}}^{\oplus} V_{k,t}(A(k)) dk$$

$$= \int_{\mathbf{K}}^{\oplus} \sum_{l=0}^3 a_l(k) V_{k,t}(\sigma_l) dk,$$

with $V_{k,t}(\sigma_l), l = 0, 1, 2, 3$, being given in (4.14). It completely characterizes the action of the quantum Markov semigroup on \mathcal{M} . \square

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A. Appendix: Limit distributions

In this appendix, we will prove Theorem 2.1 and Proposition 2.3 for the limit distributions of 1-dimensional QW's. We start with the case $l_1 l_2 r_1 r_2 \neq 0$. The key idea is to diagonalize the matrix $U(k)$ defined in (2.17). Recall the unitary matrix $U = \begin{pmatrix} l_1 & l_2 \\ r_1 & r_2 \end{pmatrix}$. By (2.21), we have the relations:

$$(A.1) \quad |l_1|^2 + |r_1|^2 = |l_2|^2 + |r_2|^2 = |l_1|^2 + |l_2|^2 = |r_1|^2 + |r_2|^2 = 1;$$

$$r_1 = -\bar{l}_2, \quad r_2 = \bar{l}_1.$$

Let $\theta_1 \in \mathbf{K}$ be the unique number satisfying

$$(A.2) \quad l_1 = |l_1|e^{i\theta_1}.$$

Then the characteristic equation for $U(k)$ reads:

$$(A.3) \quad \lambda^2 - 2|l_1| \cos(k - \theta_1)\lambda + 1 = 0.$$

Let $\gamma(k)$ be the nonnegative symmetric function defined on $\mathbf{K} = (-\pi, \pi]$ such that

$$(A.4) \quad \cos \gamma(k) = |l_1| \cos k, \quad k \in \mathbf{K}.$$

In the sequel $\gamma(k)$ is also naturally understood as a periodic function of period 2π defined on \mathbf{R} . Then the solutions to (A.3), i.e., the eigenvalues of $U(k)$ are

$$(A.5) \quad \lambda_+(k) := e^{i\gamma(k-\theta_1)} \quad \text{and} \quad \lambda_-(k) := e^{-i\gamma(k-\theta_1)}.$$

The corresponding (unnormalized) eigenvectors are:

$$(A.6) \quad e_+(k - \theta_1) \equiv \begin{pmatrix} u_+(k - \theta_1) \\ v_+(k - \theta_1) \end{pmatrix} := \begin{pmatrix} e^{-i(k-\theta_1)} \\ -\frac{e^{i\theta_1}}{l_2} (|l_1|e^{-i(k-\theta_1)} - e^{i\gamma(k-\theta_1)}) \end{pmatrix},$$

$$e_-(k - \theta_1) \equiv \begin{pmatrix} u_-(k - \theta_1) \\ v_-(k - \theta_1) \end{pmatrix} := \begin{pmatrix} e^{-i(k-\theta_1)} \\ -\frac{e^{i\theta_1}}{l_2} (|l_1|e^{-i(k-\theta_1)} - e^{-i\gamma(k-\theta_1)}) \end{pmatrix}.$$

Then $U(k)$ is diagonalized as

$$(A.7) \quad U(k) = S(k - \theta_1) \begin{pmatrix} e^{i\gamma(k-\theta_1)} & 0 \\ 0 & e^{-i\gamma(k-\theta_1)} \end{pmatrix} S(k - \theta_1)^{-1},$$

where $S(k - \theta_1)$ is the matrix whose columns are $e_+(k - \theta_1)$ and $e_-(k - \theta_1)$. The solution $\hat{\psi}_n(k)$ in (2.16) then becomes

$$(A.8) \quad \hat{\psi}_n(k) = S(k - \theta_1) \begin{pmatrix} e^{in\gamma(k-\theta_1)} & 0 \\ 0 & e^{-in\gamma(k-\theta_1)} \end{pmatrix} S(k - \theta_1)^{-1} \hat{\psi}_0(k).$$

In order to get the asymptotic limit (2.22), we use the method of stationary phase, which we state as a lemma (see [3, 4] for more details.).

LEMMA A.1 ([4, p. 220]). *Suppose that $f \in C[a, b]$ and $\alpha \in C^2[a, b]$ with α real. Consider the integral of the form:*

$$(A.9) \quad I(n) := \int_a^b \exp\{in\alpha(t)\} f(t) dt.$$

Suppose further that $\alpha'(c) = 0$ in a unique point $c \in [a, b]$ and $\alpha''(c) \neq 0$. Then as $n \rightarrow \infty$, we have the asymptotic behavior of $I(n)$:

$$(A.10) \quad I(n) = \exp\{in\alpha(c)\} f(c) \sqrt{\frac{2}{n|\alpha''(c)|}} \exp\left\{\frac{i\pi\mu}{4}\right\} + o(n^{-1/2}),$$

where $\mu = \text{sign } \alpha''(c)$.

Proof of Theorem 2.1. The case $l_1 l_2 r_1 r_2 \neq 0$. We compute the characteristic function of $X_n^{(U; \psi_0)}/n$:

$$(A.11) \quad \varphi_n^{(U; \psi_0)}(\zeta) := \mathbf{E}[e^{i\zeta X_n^{(U; \psi_0)}/n}].$$

By using (2.19), (A.6), (A.8), and by a translation by θ_1 in the integral, we get

$$(A.12) \quad \varphi_n^{(U; \psi_0)}(\zeta) = \sum_{x \in \mathbf{Z}} e^{i\zeta x/n} \left\{ \left| \int_{-\pi}^{\pi} \frac{1}{\sqrt{2\pi}} e^{-ixk} (l_+(k)e^{in\gamma(k)} + l_-(k)e^{-in\gamma(k)}) dk \right|^2 + \left| \int_{-\pi}^{\pi} \frac{1}{\sqrt{2\pi}} e^{-ixk} (m_+(k)e^{in\gamma(k)} + m_-(k)e^{-in\gamma(k)}) dk \right|^2 \right\},$$

where

$$(A.13) \quad \begin{aligned} l_+(k) &= u_+(k) \left\langle \begin{pmatrix} 1 \\ 0 \end{pmatrix}, S(k)^{-1} \hat{\psi}_0(k + \theta_1) \right\rangle, \\ l_-(k) &= u_-(k) \left\langle \begin{pmatrix} 0 \\ 1 \end{pmatrix}, S(k)^{-1} \hat{\psi}_0(k + \theta_1) \right\rangle, \end{aligned}$$

and

$$(A.14) \quad \begin{aligned} m_+(k) &= v_+(k) \left\langle \begin{pmatrix} 1 \\ 0 \end{pmatrix}, S(k)^{-1} \hat{\psi}_0(k + \theta_1) \right\rangle, \\ m_-(k) &= v_-(k) \left\langle \begin{pmatrix} 0 \\ 1 \end{pmatrix}, S(k)^{-1} \hat{\psi}_0(k + \theta_1) \right\rangle. \end{aligned}$$

We estimate the asymptotic integrals separately. For that, define

$$(A.15) \quad \begin{aligned} I_{\pm}(n) &:= \int_{-\pi}^{\pi} \frac{1}{\sqrt{2\pi}} e^{-ixk} (l_{\pm}(k)e^{\pm in\gamma(k)}) dk \\ J_{\pm}(n) &:= \int_{-\pi}^{\pi} \frac{1}{\sqrt{2\pi}} e^{-ixk} (m_{\pm}(k)e^{\pm in\gamma(k)}) dk. \end{aligned}$$

In the sum over $x \in \mathbf{Z}$ in (A.12), we find the contribution that gives

$$(A.16) \quad \frac{x}{n} = y$$

for a constant $y \geq 0$. The case $y < 0$ is similar. Then the integral $I_+(n)$ is rewritten as

$$(A.17) \quad I_+(n) = \int_{-\pi}^{\pi} e^{in(\gamma(k)-yk)} \frac{1}{\sqrt{2\pi}} l_+(k) dk.$$

In order to use Lemma A.1 we let

$$(A.18) \quad \alpha(k) := \gamma(k) - yk.$$

Then by definition of $\gamma(k)$ in (A.4) we see that at two points $c_1(y)$ and $c_2(y)$, $c_2(y) = \pi - c_1(y)$ with $0 \leq c_1(y) < \pi/2$, we have

$$\alpha'(c_1(y)) = 0 = \alpha'(c_2(y)).$$

Also we easily compute

$$\alpha''(c_i(y)) = (1 - |l_1|^2) \frac{\cos \gamma(c_i(y))}{(\sin \gamma(c_i(y)))^3}, \quad i = 1, 2.$$

Thus, asymptotically,

$$I_+(n) \sim I_+^{(1)}(n)e^{(\pi/4)i} + I_+^{(2)}(n)e^{-(\pi/4)i}$$

with

$$I_+^{(j)}(n) = \frac{1}{\sqrt{n\pi}} \frac{1}{\sqrt{1 - |l_1|^2}} |\sin \gamma(c_1(y))| |\tan \gamma(c_1(y))|^{1/2} \\ \times e^{in(\gamma(c_j(y)) - c_j(y)y)} I_+(c_j(y)), \quad j = 1, 2.$$

Also for those x and n satisfying (A.16)

$$I_-(n) \sim I_-^{(1)}(n)e^{-(\pi/4)i} + I_-^{(2)}(n)e^{+(\pi/4)i}$$

with (we use symmetry of γ)

$$I_-^{(j)}(n) = \frac{1}{\sqrt{n\pi}} \frac{1}{\sqrt{1 - |l_1|^2}} |\sin \gamma(c_1(y))| |\tan \gamma(c_1(y))|^{1/2} \\ \times e^{-in(\gamma(c_j(y)) - c_j(y)y)} I_-(-c_j(y)), \quad j = 1, 2.$$

Similarly we can compute the asymptotics of $J_{\pm}(n)$. Under the condition (A.16) we have

$$J_+(n) \sim J_+^{(1)}(n)e^{(\pi/4)i} + J_+^{(2)}(n)e^{-(\pi/4)i}$$

with

$$J_+^{(j)}(n) = \frac{1}{\sqrt{n\pi}} \frac{1}{\sqrt{1 - |l_1|^2}} |\sin \gamma(c_1(y))| |\tan \gamma(c_1(y))|^{1/2} \\ \times e^{in(\gamma(c_j(y)) - c_j(y)y)} m_+(c_j(y)), \quad j = 1, 2.$$

And

$$J_-(n) \sim J_-^{(1)}(n)e^{-(\pi/4)i} + J_-^{(2)}(n)e^{+(\pi/4)i}$$

with

$$J_-^{(j)}(n) = \frac{1}{\sqrt{n\pi}} \frac{1}{\sqrt{1 - |l_1|^2}} |\sin \gamma(c_1(y))| |\tan \gamma(c_1(y))|^{1/2} \\ \times e^{-in(\gamma(c_j(y)) - c_j(y)y)} m_-(-c_j(y)), \quad j = 1, 2.$$

We now apply these asymptotic estimates to (A.12). Then as a Riemann integral, the sum over $x \in \mathbf{Z}$ becomes an integral over y . Moreover, by Lemma A.1, since the leading term appears at the points that satisfy $\alpha' = 0$, we see from (A.18) that the integral over y is supported on the range of α' , which is $[-|l_1|, |l_1|]$. Finally, by using Riemann-Lebesgue lemma, we see that the characteristic function has the limit:

$$(A.19) \quad \lim_{n \rightarrow \infty} \phi_n^{(U; \psi_0)}(\xi) = \int e^{i\xi y} \rho^{(U; \psi_0)}(y) dy,$$

where the density function $\rho^{(U; \psi_0)}(y)$ is supported in $[-|l_1|, |l_1|]$ and is represented by

$$(A.20) \quad \rho^{(U; \psi_0)}(y) = \frac{1}{\pi(1 - |l_1|^2)} \sin^2 \gamma(c_1(y)) |\tan \gamma(c_1(y))| g^{(U; \psi_0)}(y),$$

with

$$(A.21) \quad g^{(U; \psi_0)}(y) = \{|l_+(c_1(y))|^2 + |l_+(c_2(y))|^2 + |l_-(-c_1(y))|^2 \\ + |l_-(-c_2(y))|^2 + |m_+(c_1(y))|^2 + |m_+(c_2(y))|^2 \\ + |m_-(-c_1(y))|^2 + |m_-(-c_2(y))|^2\}.$$

Let us now compute the factor in the density that does not depend on the initial condition. By differentiating (A.4) and from the definition of $c_1(y)$ we have

$$(A.22) \quad |l_1| \sin c_1(y) = y \sin \gamma(c_1(y)).$$

By (A.4) and (A.22) we get

$$(A.23) \quad \sin^2 \gamma(c_1(y)) = \frac{1 - |l_1|^2}{1 - y^2} \quad \text{and} \quad \cos^2 \gamma(c_1(y)) = \frac{|l_1|^2 - y^2}{1 - y^2}.$$

Inserting these into (A.20) we get the first half part in the density (2.23). The remaining part that depends on the initial condition is obtained by direct computation. We have represented the values of $l_{\pm}(\pm c_j(y))$ and $m_{\pm}(\pm c_j(y))$ for $j = 1, 2$ in Lemma A.3 below. By this we get the remaining part $g^{(U; \psi_0)}(y)$ in (A.21) and the proof for the case $l_1 l_2 r_1 r_2 \neq 0$ is completed.

The case that $l_1 = 0$ or $l_2 = 0$. In this case the behaviour of QW is very simple. We can directly compute the distribution of $X_n^{(U; \psi_0)}$ from the defining relation (2.4). Let $\psi_0 = \left\{ \begin{pmatrix} \psi_0(1; x) \\ \psi_0(2; x) \end{pmatrix} \right\}_{x \in \mathbf{Z}}$ be the initial condition. We first

consider the case $l_2 = 0$. Then, at time n , we have

$$\begin{pmatrix} \psi_n(1; x) \\ \psi_n(2; x) \end{pmatrix} = \begin{pmatrix} l_1^n \psi_0(1; x+n) \\ r_2^n \psi_0(2; x-n) \end{pmatrix}.$$

Therefore

$$\mathbf{P}(X_n^{(U; \psi_0)} = x) = |\psi_0(1; x+n)|^2 + |\psi_0(2; x-n)|^2,$$

and hence

$$\begin{aligned} \mathbf{E}(e^{i\xi X_n^{(U; \psi_0)}}) &= \sum_{x \in \mathbf{Z}} e^{i\xi x} (|\psi_0(1; x+n)|^2 + |\psi_0(2; x-n)|^2) \\ &= e^{-i\xi n} \sum_{x \in \mathbf{Z}} e^{i\xi x} |\psi_0(1; x)|^2 + e^{i\xi n} \sum_{x \in \mathbf{Z}} e^{i\xi x} |\psi_0(2; x)|^2. \end{aligned}$$

Thus, by dominated convergence theorem, we have

$$\lim_{n \rightarrow \infty} \mathbf{E}(e^{i\xi X_n^{(U; \psi_0)}/n}) = e^{-i\xi} \sum_{x \in \mathbf{Z}} |\psi_0(1; x)|^2 + e^{i\xi} \sum_{x \in \mathbf{Z}} |\psi_0(2; x)|^2.$$

We conclude that for $l_2 = 0$ the limit distribution is

$$\mu^{(U; \psi_0)} = \left(\sum_{x \in \mathbf{Z}} |\psi_0(1; x)|^2 \right) \delta_{-1} + \left(\sum_{x \in \mathbf{Z}} |\psi_0(2; x)|^2 \right) \delta_1.$$

Next we consider the case $l_1 = 0$. Then, at time n , we have

$$\begin{pmatrix} \psi_n(1; x) \\ \psi_n(2; x) \end{pmatrix} = \begin{cases} (l_2 r_1)^{m-1} \begin{pmatrix} l_2 \psi_0(2; x+1) \\ r_1 \psi_0(1; x-1) \end{pmatrix}, & \text{if } n = 2m-1 \\ (l_2 r_1)^m \begin{pmatrix} \psi_0(1; x) \\ \psi_0(2; x) \end{pmatrix}, & \text{if } n = 2m. \end{cases}$$

Therefore

$$\mathbf{P}(X_n^{(U; \psi_0)} = x) = \begin{cases} |\psi_0(1; x-1)|^2 + |\psi_0(2; x+1)|^2 & \text{if } n \text{ is odd} \\ |\psi_0(1; x)|^2 + |\psi_0(2; x)|^2 & \text{if } n \text{ is even} \end{cases}$$

and hence

$$\begin{aligned} \mathbf{E}(e^{i\xi X_n^{(U; \psi_0)}}) &= \begin{cases} \sum_{x \in \mathbf{Z}} e^{i\xi x} (|\psi_0(1; x-1)|^2 + |\psi_0(2; x+1)|^2) & \text{if } n \text{ is odd} \\ \sum_{x \in \mathbf{Z}} e^{i\xi x} (|\psi_0(1; x)|^2 + |\psi_0(2; x)|^2) & \text{if } n \text{ is even} \end{cases} \\ &= \begin{cases} e^{i\xi} \sum_{x \in \mathbf{Z}} e^{i\xi x} |\psi_0(1; x)|^2 + e^{-i\xi} \sum_{x \in \mathbf{Z}} e^{i\xi x} |\psi_0(2; x)|^2 & \text{if } n \text{ is odd} \\ \sum_{x \in \mathbf{Z}} e^{i\xi x} (|\psi_0(1; x)|^2 + |\psi_0(2; x)|^2) & \text{if } n \text{ is even.} \end{cases} \end{aligned}$$

By dominated convergence theorem again, we have

$$\lim_{n \rightarrow \infty} \mathbf{E}(e^{i\xi X_n^{(U; \psi_0)}/n}) = \sum_{x \in \mathbf{Z}} (|\psi_0(1; x)|^2 + |\psi_0(2; x)|^2) = 1.$$

We conclude that for $l_1 = 0$ the limit distribution is

$$\mu^{(U; \psi_0)} = \delta_0.$$

The proof is completed. \square

Proof of Proposition 2.3. If the particle is located at the origin with a chiral state $\begin{pmatrix} a \\ b \end{pmatrix}$, then the Fourier transform of it is just a constant:

$$(A.24) \quad \hat{\psi}_0(k) \equiv \begin{pmatrix} \hat{\psi}_0(1; k) \\ \hat{\psi}_0(2; k) \end{pmatrix} = \frac{1}{\sqrt{2\pi}} \begin{pmatrix} a \\ b \end{pmatrix}.$$

By using this and Lemma A.3 we can directly compute the function $g^{(U; \psi_0)}(y)$ in (A.21), which gives exactly the factor $(1 - \beta^{(U; \psi_0)}y)$ in the statement of the proposition. By Theorem 2.1 the proof is completed. \square

Now we present the values of functions that are used to get $g^{(U; \psi_0)}(y)$ in Theorem 2.1, i.e., the part of limit density function that depends on the initial conditions. It is obtained by directly computing $l_{\pm}(\pm c_j(y))$ and $m_{\pm}(\pm c_j(y))$ for $j = 1, 2$. For this we first need to compute $S(k)^{-1}$ at $k = \pm c_j(y)$, $j = 1, 2$.

LEMMA A.2. *Suppose that $l_1 l_2 r_1 r_2 \neq 0$. The values $S(k)^{-1}$ at $k = \pm c_j(y)$, $j = 1, 2$, are as follows:*

$$S(c_1(y))^{-1} = \frac{l_2 e^{i(c_1(y) - \theta_1)}}{2} \begin{pmatrix} \frac{1-y}{l_2 e^{-i\theta_1}} & \frac{-1}{|l_1|} \left(y + i \frac{\sqrt{|l_1|^2 - y^2}}{\sqrt{1 - |l_1|^2}} \right) \\ \frac{1+y}{l_2 e^{-i\theta_1}} & \frac{1}{|l_1|} \left(y + i \frac{\sqrt{|l_1|^2 - y^2}}{\sqrt{1 - |l_1|^2}} \right) \end{pmatrix}$$

$$S(c_2(y))^{-1} = \frac{l_2 e^{i(c_2(y) - \theta_1)}}{2} \begin{pmatrix} \frac{1-y}{l_2 e^{-i\theta_1}} & \frac{-1}{|l_1|} \left(y - i \frac{\sqrt{|l_1|^2 - y^2}}{\sqrt{1 - |l_1|^2}} \right) \\ \frac{1+y}{l_2 e^{-i\theta_1}} & \frac{1}{|l_1|} \left(y - i \frac{\sqrt{|l_1|^2 - y^2}}{\sqrt{1 - |l_1|^2}} \right) \end{pmatrix}$$

$$S(-c_1(y))^{-1} = \frac{l_2 e^{-i(c_1(y) + \theta_1)}}{2} \begin{pmatrix} \frac{1+y}{l_2 e^{-i\theta_1}} & \frac{1}{|l_1|} \left(y + i \frac{\sqrt{|l_1|^2 - y^2}}{\sqrt{1 - |l_1|^2}} \right) \\ \frac{1-y}{l_2 e^{-i\theta_1}} & \frac{-1}{|l_1|} \left(y + i \frac{\sqrt{|l_1|^2 - y^2}}{\sqrt{1 - |l_1|^2}} \right) \end{pmatrix}$$

$$S(-c_2(y))^{-1} = \frac{l_2 e^{-i(c_2(y) + \theta_1)}}{2} \begin{pmatrix} \frac{1+y}{l_2 e^{-i\theta_1}} & \frac{1}{|l_1|} \left(y - i \frac{\sqrt{|l_1|^2 - y^2}}{\sqrt{1 - |l_1|^2}} \right) \\ \frac{1-y}{l_2 e^{-i\theta_1}} & \frac{-1}{|l_1|} \left(y - i \frac{\sqrt{|l_1|^2 - y^2}}{\sqrt{1 - |l_1|^2}} \right) \end{pmatrix}$$

Proof. We use the definition of $S(k)$ by using the eigenvectors of $U(k)$ in (A.6) and compute the values at $\pm c_j(y)$, $j = 1, 2$, as it was done in (A.23). □

It is then straightforward to compute $l_{\pm}(\pm c_j(y))$ and $m_{\pm}(\pm c_j(y))$. Notice that the Fourier transform of the initial vector is denoted by $\hat{\psi}_0 = \left\{ \begin{pmatrix} \hat{\psi}_0(1; k) \\ \hat{\psi}_0(2; k) \end{pmatrix} \right\}_{k \in \mathbf{K}}$.

LEMMA A.3. *Suppose that $l_1 l_2 r_1 r_2 \neq 0$. The values of $l_{\pm}(\pm c_j(y))$ and $m_{\pm}(\pm c_j(y))$, $j = 1, 2$, are as follows.*

$$\begin{aligned} l_+(c_1(y)) &= \frac{l_2 e^{-i\theta_1}}{2} \left(\frac{1-y}{l_2 e^{-i\theta_1}} \hat{\psi}_0(1; c_1(y) + \theta_1) \right. \\ &\quad \left. - \frac{1}{|l_1|} \left(y + i \frac{\sqrt{|l_1|^2 - y^2}}{1 - |l_1|^2} \right) \hat{\psi}_0(2; c_1(y) + \theta_1) \right) \\ l_+(c_2(y)) &= \frac{l_2 e^{-i\theta_1}}{2} \left(\frac{1-y}{l_2 e^{-i\theta_1}} \hat{\psi}_0(1; c_2(y) + \theta_1) \right. \\ &\quad \left. - \frac{1}{|l_1|} \left(y - i \frac{\sqrt{|l_1|^2 - y^2}}{1 - |l_1|^2} \right) \hat{\psi}_0(2; c_2(y) + \theta_1) \right) \\ l_-(-c_1(y)) &= \frac{l_2 e^{-i\theta_1}}{2} \left(\frac{1-y}{l_2 e^{-i\theta_1}} \hat{\psi}_0(1; -c_1(y) + \theta_1) \right. \\ &\quad \left. - \frac{1}{|l_1|} \left(y + i \frac{\sqrt{|l_1|^2 - y^2}}{1 - |l_1|^2} \right) \hat{\psi}_0(2; -c_1(y) + \theta_1) \right) \\ l_-(-c_2(y)) &= \frac{l_2 e^{-i\theta_1}}{2} \left(\frac{1-y}{l_2 e^{-i\theta_1}} \hat{\psi}_0(1; -c_2(y) + \theta_1) \right. \\ &\quad \left. - \frac{1}{|l_1|} \left(y - i \frac{\sqrt{|l_1|^2 - y^2}}{1 - |l_1|^2} \right) \hat{\psi}_0(2; -c_2(y) + \theta_1) \right) \end{aligned}$$

$$\begin{aligned}
m_+(c_1(y)) &= \frac{1 - |l_1|^2}{2|l_1|} \left(\frac{-1}{l_2 e^{-i\theta_1}} \left(y - i\sqrt{\frac{|l_1|^2 - y^2}{1 - |l_1|^2}} \right) \hat{\psi}_0(1; c_1(y) + \theta_1) \right. \\
&\quad \left. + \frac{|l_1|}{1 - |l_1|^2} (1 + y) \hat{\psi}_0(2; c_1(y) + \theta_1) \right) \\
m_+(c_2(y)) &= \frac{1 - |l_1|^2}{2|l_1|} \left(\frac{-1}{l_2 e^{-i\theta_1}} \left(y + i\sqrt{\frac{|l_1|^2 - y^2}{1 - |l_1|^2}} \right) \hat{\psi}_0(1; c_2(y) + \theta_1) \right. \\
&\quad \left. + \frac{|l_1|}{1 - |l_1|^2} (1 + y) \hat{\psi}_0(2; c_2(y) + \theta_1) \right) \\
m_-(-c_1(y)) &= \frac{1 - |l_1|^2}{2|l_1|} \left(\frac{-1}{l_2 e^{-i\theta_1}} \left(y - i\sqrt{\frac{|l_1|^2 - y^2}{1 - |l_1|^2}} \right) \hat{\psi}_0(1; -c_1(y) + \theta_1) \right. \\
&\quad \left. + \frac{|l_1|}{1 - |l_1|^2} (1 + y) \hat{\psi}_0(2; -c_1(y) + \theta_1) \right) \\
m_-(-c_2(y)) &= \frac{1 - |l_1|^2}{2|l_1|} \left(\frac{-1}{l_2 e^{-i\theta_1}} \left(y + i\sqrt{\frac{|l_1|^2 - y^2}{1 - |l_1|^2}} \right) \hat{\psi}_0(1; -c_2(y) + \theta_1) \right. \\
&\quad \left. + \frac{|l_1|}{1 - |l_1|^2} (1 + y) \hat{\psi}_0(2; -c_2(y) + \theta_1) \right).
\end{aligned}$$

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