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On the Quantum Walk [1]

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Abstract

Quantum walks are powerful tools not only to construct the quantum speedup algorithms but also to describe specific models in physical processes. Furthermore, the discrete time quantum walk has been experimentally realized in various setups. We show the limit distribution of the discrete time quantum walk with the periodic position measurement under the time scale transformation.

1 Introduction

A quantum walk (QW) [1–3], the quantum mechanical analogue of the classical random walk (RW), is a useful tool to promote various fields. For instance, the QW is an important primitive in universal quantum computation [4, 5] and efficient quantum algorithms [6–10]. The realization of topological phases [11] and quantum phase transitions [12] in optical lattice systems by the QW have been discussed. The relation between the Landau-Zener transition and the QW was found in Ref. [13]. The QW provides a new clue to more fundamental problems such as the photosynthesis and efficient energy transfer in biomolecules [14,15]. There are several important properties of the QW: (i) the inverted-bell like limit distribution, (ii) the quadratic speed-up of the variance to the classical RW, and (iii) the localization due to the quantum coherence and interference. The physical, mathematical, and computational properties of the QW are summarized in Refs. [16–19].

There remains the following open problems on the discrete time quantum walks (DTQWs). First, it is well known that randomness results from environment in the RW. Although some researchers often call the QW a quantum "random" walk due to its original definition [2][3], this terminology is abuse of words since the QW is not probabilis-

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[3]While we introduce the QW as the quantization of the RW, the QW was independently defined from different motivations; to construct the stochastic process in quantum probability theory [1], the quantization of the RW based on the time symmetric property [2], and the quantization of the cellular automaton in the context of the quantum lattice gases [3]. More precisely, these definitions [1–3] are not equivalent. Thereafter, Ambainis *et al.* mathematically define the DTQW to combine the above notations [30], which is used throughout this paper. Note that, this definition is consistent with the Gudder definition [1]. Furthermore, the continuous time QW [45] is different from the DTQW and corresponds to the hopping dynamics in the Hubbard model. The difference of both QWs still remains the open problems in mathematics and physics.

tic but deterministic due to the time evolution for the closed quantum system. As far as we know, no one has yet analyzed a quantification of randomness in QWs. Environment, of which the description corresponds to that of quantum measurement in quantum mechanics [22], seems intuitively to be the origin of randomness. In such studies, the description of the periodic quantum measurement is used and the quantum-classical transition, which means an immediate change from the QW to the RW due to the decoherence effect, is shown [23–26]. However, the contribution to the quantum walk behavior from environment has not been shown analytically. In this paper, we focus on this issue. , a nontrivial *stochastic* process which gives the distributions of DTQWs did not be found. Using the probabilisitic perspects of the weak value [27], it might be possible to find this relationship [28,29].

2 Discrete Time Quantum Walk

Let us mathematically define the one-dimensional DTQW [30] as follows. First, we prepare the position and the coin states denoted as $|x\rangle\langle x|$ and ρ_0, respectively, corresponding to the quantization of the RW [2]. Here, we assume that the position is the one-dimensional discretized lattice denoted as $\mathbb{Z}$ and the coin state is a qubit with the orthonormal basis, $|L\rangle = (1,0)^T$ and $|R\rangle = (0,1)^T$, where T is transposition. To simplify the discussion, we assume that the initial state is localized at the origin ($x = 0$) with the mixed state $\rho_0 = (|L\rangle\langle L| + |R\rangle\langle R|)/2$ as the coin state throughout this paper. Second, the time evolution of the QW is described by a unitary operator U. A quantum coin flip corresponding to the coin flip in the RW is described by a unitary operator $H \in U(2)$ acting on the coin state given by

$$H := a|L\rangle\langle L| + b|L\rangle\langle R| + c|R\rangle\langle L| + d|R\rangle\langle R|, \tag{1}$$

where $|a|^2 + |c|^2 = 1$, $a\bar{b} + c\bar{d} = 0$, $c = -\Delta\bar{b}$, $d = \Delta\bar{a}$, and $|\Delta| := |\det U| = 1$, noting that $abcd \neq 0$ except for the trivial case. Thereafter, the position shift S is described as the move due to the coin state;

$$S|x\rangle|L\rangle := |x-1\rangle|L\rangle \tag{2}$$

$$S|x\rangle|R\rangle := |x+1\rangle|R\rangle. \tag{3}$$

Therefore, the unitary operator describing the one-step time evolution for the QW is defined as $U = S(I \otimes H)$. We repeat this procedure keeping the quantum coherence between the position and coin states. Finally, we obtain the probability distribution on the position x at t step as

$$\Pr(X_t = x) = \mathrm{Tr}\left[\left(\mathrm{Tr}_c\, U^t \left(|0\rangle\langle 0| \otimes \rho_0\right) U^{t\dagger}\right) |x\rangle\langle x|\right], \tag{4}$$

where X_t means a random variable at t step since the measurement outcome of the position measurement is probabilistically determined due to the Born rule.

Physically speaking, the DTQW can be described by the free Dirac equation [31–33]. In fact, this was discussed by Schrödinger under the *Zitterbewegung* of the relativistic electron [34] and was also implied by the introduction of the path integral [35]. In other words, the DTQW helps us analyze the trembling motion of the relative electron, photon, neutrino, and so on. Also, by developing quantum technologies to build up the precise measurement techniques and highly control the quantum system, it is possible to experimentally realize the DTQWs such as the *trans*-crotonic acid using the nuclear magnetic resonance [21], the Cs atoms trapped in the optical lattice [36], the photons by employing the fiber network loop [37], and the $^{40}Ca^{+}$ atoms in the ion trap [38].

3 Limit Distributions for DTQW with Periodic Position Measurement

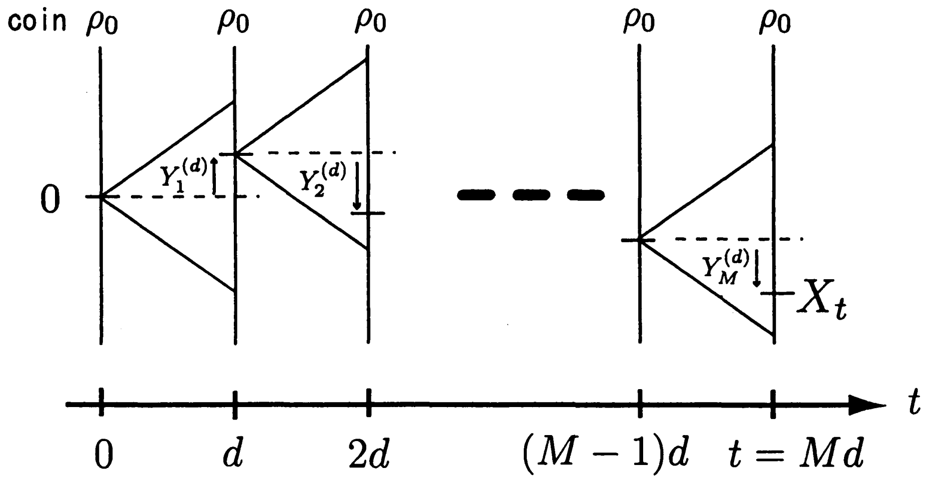

Figure 1: **Quantum walk with the periodic position measurement.** After d step of the DTQW, we only measure the position of the particle, that is, we take the projective measurement on the position state after taking the partial trace on the coin state. For simplicity, after the position measurement, we re-prepare the initial coin state ρ_0. We repeat this procedure M times.

From now on, we define a simple model of the QW with environment as illustrated in Fig. 1. After d step of the DTQW, we only measure the position of the particle, that is, we take the projective measurement on the position state after taking the partial trace on the coin state. For simplicity, after the position measurement, we re-prepare the initial coin state ρ_0. We repeat this procedure M times. The probability distribution at the final time $t = dM$ is concerned in the following. This model is called the DTQW with the PPM[4]. We denote the sequence of the random variables on the DTQW between measurements by d step as $\{Y_i^{(d)}\}$. The position measurement corresponds to the collision with another particle, that is, environment, as in the classical sense. Furthermore, since the initial coin states are the same for each block of the DTQW, $\{Y_i^{(d)}\}$ is an independent identically

[4]Our model is different from the "decoherence QW" analyzed by Zhang [26]. In the decoherence QW, one often take the joint measurement of the position and the coin. The limit distribution of the case of $\beta = 0$, that is, the measurement period is independent of the final time, is the normal distribution with the convergence time order 1/2. There remains the open problem to similarly analyze the extended Zhang model.

distributed (i.i.d.) sequence. The random variable for the QW with the PPM is denoted as $X_t = Y_1^{(d)} + Y_2^{(d)} + \cdots + Y_M^{(d)}$. When the measurement step d is independent of the final time t, the sequence of the blocks of the DTQW by d step can be taken as the Markov process since $\{Y_i^{(d)}\}$ is an i.i.d. sequence. This case can correspond to the RW. To extract more detailed information, we assume that the measurement step d depends on the final time t as $d \sim t^{\beta}$ with $\beta \in [0,1]$, which is called a time scale transformation. Because of $M \sim t^{1-\beta}$, this means that the number of the position measurements is changed by the final time t. For example, in the case of $\beta = 0.5$, $t = 100$ step, and $d = t^{\beta}$, we take the position measurement 10 times in 10 steps. In the following, we denote the random variable X_t as $X_t^{(\beta)}$. Then, we present the following theorem on the limit distribution for any $\beta \in [0,1]$.

Theorem 1 (Shikano, Chisaki, Segawa, and Konno [39]). *Let $\{Y_i^{(d)}\}$ be an i.i.d. sequence of the DTQW on $\mathbb{Z}$ with the initial localized position $x = 0$, the initial coin qubit $\rho_0 = (|L\rangle\langle L| + |R\rangle\langle R|)/2$, and the quantum coin flip $H = a|L\rangle\langle L| + b|L\rangle\langle R| + c|R\rangle\langle L| + d|R\rangle\langle R| \in U(2)$ noting that $abcd \neq 0$. Let $X_t = \sum_{i=1}^{M} Y_i^{(d)}$ be a random variable on a position with d step between measurements and the number of the measurements M with the final time $t = dM$. If $d \sim t^{\beta}$, then, as $t \to \infty$, we have the limit distribution as follows:*

$$\frac{X_t^{(\beta)}}{t^{(1+\beta)/2}} \Rightarrow \begin{cases} N(0,1) & \text{for } \beta = 0 \\ N(0, 1-\sqrt{1-|a|^2}) & \text{for } 0 < \beta < 1 \\ K(|a|) & \text{for } \beta = 1, \end{cases} \tag{5}$$

where "$\Rightarrow$" means the convergence in distribution and $N(m,\sigma^2)$ is the normal distribution with the mean m, the variance σ^2. Note that, the random variable $K(r)$ has the probability density function $f(x;r)$ with a parameter $r \in (0,1)$:

$$f(x;r) = \frac{\sqrt{1-r^2}}{\pi(1-x^2)\sqrt{r^2-x^2}} I_{(-r,r)}(x). \tag{6}$$

Here, $I_{(-r,r)}(x)$ is the indicator function, that is, $I_A(x) = 1$ $(x \in A), = 0$ $(x \notin A)$.

Proof. Since the case of $\beta = 0$ is corresponded to the random walk, we obtain the Gaussian distribution as the limit distribution from the well-known central limit theorem. Furthermore, since the case of $\beta = 1$ is corresponded to the simple quantum walk, its limit distribution has already shown by Konno [40, 41]. In the follows, we only consider the limit distribution in the case of $0 < \beta < 1$.

By the definition of the spatial Fourier transformation of $Y_1^{(d)}$, $E(e^{i\xi Y_1^{(d)}})$ can be denoted as

$$E(e^{i\xi Y_1^{(d)}}) = \int_0^{2\pi} \frac{1}{2} \mathrm{Tr}[\widehat{H}^d(k+\xi) \cdot \widehat{H}^{-d}(k)] \frac{dk}{2\pi} \tag{7}$$

with $\widehat{H}(k) = (e^{ik}|R\rangle\langle R| + e^{-ik}|L\rangle\langle L|)H$. Since $(Y^{(d)})_j$ is i.i.d sequence, we can describe the characteristic function $E(e^{i\xi X_t})$ as following lemma.

Lemma 1 (Segawa and Konno [42]).

$$E(e^{i\xi X_t}) = \left\{ \int_0^{2\pi} \frac{1}{2} \mathrm{Tr}[\widehat{H}^d(k+\xi) \cdot \widehat{H}^{-d}(k)] \frac{dk}{2\pi} \right\}^M . \tag{8}$$

Let eigenvalues and corresponding eigenvectors of $\widehat{H}(k)$ be $e^{i\varphi_l(k)}$ and $|v_l(k)\rangle$, respectively ($l \in \{\pm\}$). By using Lemma 1, we evaluate $E(e^{i\xi X_t^{(\beta)}/t^\theta})$ with respect to time step t as follows.

$$\frac{1}{2}\mathrm{Tr}[\widehat{H}^{t^\beta}(k+\xi/t^\theta)\cdot \widehat{H}^{-t^\beta}(k)] = \frac{1}{2}\sum_{l,m\in\{\pm\}} e^{it^\beta\{\varphi_l(k+\xi/t^\theta)-\varphi_m(k)\}}V_{lm}(k,\xi/t^\theta), \tag{9}$$

where $V_{lm}(k,\xi) = \langle v_m(k)|\left(|v_l(k+\xi)\rangle\langle v_l(k+\xi)|\right)|v_m(k)\rangle$. We can express $e^{it^\beta\{\varphi_l(k+\xi/t^\theta)-\varphi_m(k)\}}$ and $V_{lm}(k,\xi/t^\theta)$ under an assumption $\theta > \beta$:

$$e^{it^\beta\{\varphi_l(k+\xi/t^\theta)-\varphi_m(k)\}} = e^{it^\beta(\varphi_l(k)-\varphi_m(k))} \times e^{i\xi t^{\beta-\theta}\varphi_l'(k)+O(t^{\beta-2\theta})}, \tag{10}$$

where $\varphi_l'(k) = d\varphi_l(k)/dk$, and

$$\begin{aligned} V_{lm}(k,\xi/t^\theta) &= \langle v_m(k)|\left(|v_l(k)\rangle\langle v_l(k)| + \frac{\xi}{t^\theta}\left(|v_l(k)\rangle\langle v_l(k)|\right)' + O(t^{-2\theta})\right)|v_m(k)\rangle \\ &= \delta_{lm} + \frac{\xi}{t^\theta}\langle v_m(k)|\left(|v_l'(k)\rangle\langle v_l(k)| + |v_l(k)\rangle\langle v_l'(k)|\right)|v_m(k)\rangle + O(t^{-2\theta}) \\ &= \delta_{lm}\left(1+\frac{\xi}{t^\theta}(\langle v_l'(k)|v_l(k)\rangle + \langle v_l(k)|v_l'(k)\rangle)\right) + O(t^{-2\theta}) \\ &= \delta_{lm}\left(1+\frac{\xi}{t^\theta}(\langle v_l(k)|v_l(k)\rangle)'\right) + O(t^{-2\theta}) = \delta_{lm} + O(t^{-2\theta}). \end{aligned} \tag{11}$$

Since $\varphi'(k) \equiv \varphi_+'(k) = -\varphi_-'(k)$, we obtain by combining Eq. (9) with Eqs. (10) and (11),

$$\begin{aligned} &\frac{1}{2}\mathrm{Tr}[\widehat{H}^{t^\beta}(k+\xi/t^\theta)\cdot\widehat{H}^{-t^\beta}(k)] \\ &= \frac{1}{2}\sum_{l,m\in\{\pm\}} e^{it^\beta(\varphi_l(k)-\varphi_m(k))} \times e^{i\xi t^{\beta-\theta}\varphi_l'(k)+O(t^{\beta-2\theta})}(\delta_{lm}+O(t^{-2\theta})) \\ &= \frac{1}{2}\sum_{l\in\{\pm\}} e^{i\xi t^{\beta-\theta}\varphi_l'(k)+O(\beta-2\theta)} + O(t^{-2\theta}) \\ &= \frac{1}{2}\left(e^{i\xi t^{\beta-\theta}\varphi'(k)+O(t^{\beta-2\theta})} + e^{-i\xi t^{\beta-\theta}\varphi'(k)+O(t^{\beta-2\theta})} + O(t^{-2\theta})\right) \\ &= \frac{1}{2}\{1 + i\xi t^{\beta-\theta}\varphi'(k) - \frac{(\xi\varphi'(k))^2}{2t^{2(\theta-\beta)}} \\ &\qquad + 1 - i\xi t^{\beta-\theta}\varphi'(k) - \frac{(\xi\varphi'(k))^2}{2t^{2(\theta-\beta)}} + o(t^{-2(\theta-\beta)})\} \\ &= 1 - \frac{\xi^2}{2t^{2(\theta-\beta)}}(\varphi'(k))^2 + o(t^{-2(\theta-\beta)}). \end{aligned} \tag{12}$$

By Lemma 1 and Eq. (12), if $2(\theta-\beta) = 1-\beta$, we obtain

$$\begin{aligned} E(e^{i\xi X_t^{(\beta)}/t^\theta}) &= \left(\int_0^{2\pi} 1 - \frac{\xi^2}{2t^{2(\theta-\beta)}}(\varphi'(k))^2 + o(t^{-2(\theta-\beta)})\frac{dk}{2\pi}\right)^{t^{1-\beta}} \\ &= \left(1 - \frac{\xi^2}{2t^{2(\theta-\beta)}}\sigma^2 + o(t^{-2(\theta-\beta)})\right)^{t^{1-\beta}} \\ &\to e^{-\xi^2\sigma^2(a)/2} \text{ as } t \to \infty, \end{aligned} \tag{13}$$

where

$$\sigma^2(a) = \int_0^{2\pi} (\varphi'(k))^2 \frac{dk}{2\pi} = 1 - \sqrt{1 - |a|^2}. \tag{14}$$

This is the required result. The proof of $\sigma^2(a) = 1 - \sqrt{1 - |a|^2}$ is shown in the appendix. □

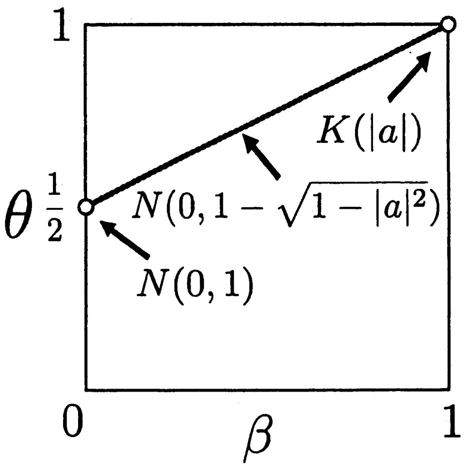

Figure 2: **Limit distributions of the quantum walk with the periodic position measurement under the time scale transformation.** Relationship between the convergence time order θ and the measurement time period β in equation (5).

This theorem is our main result and is illustrated in Fig. 2. The theorem tells us that the QW with the position measurement always has the normal limit distribution. The position measurement produces randomness in the QW such as the Brownian motion. Therefore, we always obtain that the limit distribution is the normal distribution since we always face the decoherence effect due to environment in the realistic experimental setup. It is extremely difficult to experimentally show the properties of the QW as some physical process since we only obtain the distribution after many steps due to 1 step $\ll 10^{-21}$ sec in the case of the relative electron [31]. However, the projective measurement does not uniformly produce randomness from the case of $0 < \beta < 1$. In other words, the parameter β may be an indicator of decoherence in QWs. It is possible to evaluate the degree of decoherence from the behavior of the variance in the experimentally realized QW [21,36–38].

4 Summary

We have analytically obtained the limit distribution of the DTQW on $\mathbb{Z}$ with PPMs (5). From this mathematical result, we have shown that the origin of randomness is the position measurement like the Brownian motion but there does not always exist the quantum-classical transition in the DTQW by the position measurement since the degree of randomness is not time scale invariant. Also, we have constructed the quantification of the DTQW with PPMs. Furthermore, we will prove the limit distribution in the extended cases of the general coin state and the continuous time QW [44].

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A Proof of Eq. (14)

Quantum coin $H \in U(2)$ is expressed by four parameters r, ϕ, ψ, δ with $r \in [0,1]$, ϕ, ψ, $\delta \in \mathbb{R}$ such that

$$H \equiv H(r,\phi,\psi,\delta) = \begin{bmatrix} re^{i\phi} & \sqrt{1-r^2}e^{i\psi} \\ -\sqrt{1-r^2}e^{-i(\psi-\delta)} & re^{-i(\phi-\delta)} \end{bmatrix}$$

The eigenvalues of $\widehat{H}(k)$ is given by the solution for

$$\det[H(r,\phi+k,\psi+k,\delta)-tI]=0. \tag{15}$$

So, we have

$$\begin{aligned} &\det[H(r,\phi+k,\psi+k,\delta)-tI] \\ &= (re^{i(\phi+k)}-t)(re^{-i(\phi+k-\delta)}-t)+(1-r^2)e^{i\delta} \\ &= t^2 - r(e^{i(\phi+k)}+e^{-i(\phi+k-\delta)})t + e^{i\delta} \\ &= t^2 - re^{i\delta/2}(e^{i(\phi+k-\delta/2)}+e^{-i(\phi+k-\delta/2)})t + e^{i\delta} \\ &= t^2 - 2re^{i\delta/2}\cos(\delta'+k)+e^{i\delta}=0, \end{aligned} \tag{16}$$

where $\delta' = \phi - \delta/2$. Putting the solutions, $e^{i\alpha(k)}$ and $e^{i\beta(k)}$, for Eq. (16), we obtain

$$e^{i\alpha(k)} + e^{i\beta(k)} = 2re^{i\delta/2}\cos(\delta'+k) \tag{17}$$

$$\alpha(k)+\beta(k) = \delta + 2m\pi, \tag{18}$$

where $m \in \mathbb{Z}$. By the above equations Eqs. (17) and (18), we have

$$\cos(\alpha(k)-\delta/2) = r\cos(\delta'+k). \tag{19}$$

By differentiating both sides of Eq. (19) with respect to k,

$$\left(\frac{d\alpha}{dk}\right)^2 = \frac{r^2\sin^2(\delta'+k)}{1-r^2\cos^2(\delta'+k)}. \tag{20}$$

Therefore, we derive Eq. (14) as

$$\begin{aligned} \sigma^2 &= \int_0^{2\pi}\left(\frac{d\alpha}{dk}\right)^2\frac{dk}{2\pi} = \int_0^{2\pi}\frac{|a|^2\sin^2 k}{1-|a|^2\cos^2 k}\frac{dk}{2\pi} \\ &= 1-\sqrt{1-|a|^2}. \end{aligned} \tag{21}$$

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