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Emergence of randomness and arrow of time in quantum walks

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Quantum walks are powerful tools not only for constructing the quantum speedup algorithms but also for describing specific models in physical processes. Furthermore, the discrete time quantum walk has been experimentally realized in various setups. We apply the concept of the quantum walk to the problems in quantum foundations. We show that randomness and the arrow of time in the quantum walk gradually emerge by periodic projective measurements from the mathematically obtained limit distribution under the time-scale transformation.

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I. INTRODUCTION

The discrete time quantum walk (DTQW), which is a quantum analog of the random walk (RW) [1,2], has been expected to be a powerful tool in various fields, especially quantum computation [3–5], physics [6,7], and mathematics [8,9], and has been experimentally realized [10–13]. The important properties are an inverted-bell-shaped limit distribution, which is extremely different from the normal distribution obtained in the RW, and the faster diffusion process than the RW because of a coherent superposition and a quantum interference [14,15]. In this article, we derive the limit distribution of the DTQW with the periodic position measurement (PPM) under the time-scale transformation. We show that randomness and the arrow of time gradually emerge under the time scale transformation from the mathematically obtained limit distribution. The result means that randomness in QWs is quantified and gives us a new insight into the interpretation of the projective measurement.

Our addressed issues on randomness in QWs and the arrow of time have the following background. 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 [1,2], this terminology is abuse of words since the QW is not probabilistic 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 [16], 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 [17–20]. However, the contribution to the quantum walk behavior from environment has not been shown analytically.

Second, we apply the concept of the QW to quantum foundations, especially the problem of quantum measurement.

This problem has been discussed for a long time. Its central question is what is the physical origin of the time asymmetry in quantum measurement [21]. According to the “Copenhagen interpretation,” the projective measurement produces the arrow of time since its description is time asymmetric [22]. Furthermore, it seems to be natural to consider that the description of the quantum dynamics with many projective measurements can be taken as a Markov process since the projective measurement is to forget the measurement outcome [23]. In other words, the arrow of time is uniformly produced by the projective measurements for any time scale. While our proposal is not a complete solution on the arrow of time, this gives us insight from the DTQW. In the article, we discuss the preceding problems with the mathematical model of the DTQW.

The article is organized as follows. In Sec. II, we recapitulate the definition of the DTQW. In Sec. III, we define a specific model of the DTQW with PPM. We show the mathematical result on the limit distribution and give an interpretation of our mathematical result in the randomness and the arrow of time. Section IV is devoted to the summary.

II. DISCRETE TIME QUANTUM WALK

Let us mathematically define the one-dimensional DTQW [24] 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 [1]. 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 article. 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

$$H := a|L\rangle\langle L| + b|L\rangle\langle R| + c|R\rangle\langle L| + d|R\rangle\langle R| \\ = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad (1)$$

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with $|a|^2 + |c|^2 = 1$, $a\bar{b} + c\bar{d} = 0$, $c = -\Delta\bar{b}$, $d = \Delta\bar{a}$, 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:

$$S|x\rangle|L\rangle := |x-1\rangle|L\rangle, \quad (2)$$

$$S|x\rangle|R\rangle := |x+1\rangle|R\rangle. \quad (3)$$

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 step t as

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

where X_t means a random variable at step t since the measurement outcome of the position measurement is probabilistically determined due to the Born rule. Here Tr_c expresses the partial trace for the coin state.

Physically speaking, the DTQW can express the free Dirac equation [25–27] as follows. We assume the specific quantum coin flip,

$$H(\epsilon) = \begin{pmatrix} \cos \epsilon & -i \sin \epsilon \\ -i \sin \epsilon & \cos \epsilon \end{pmatrix}, \quad (5)$$

where the tiny parameter ϵ expresses one lattice size. Let $\Psi_n(x) = [\psi_{n,L}(x), \psi_{n,R}(x)]^T$ be a coin state associated with a position x at step n . More explicitly, the coin state associated with the position x at step n is given by

$$U^t (|0\rangle\langle 0| \otimes \rho_0) U^{t\dagger} = \sum_x [\psi_{n,L}(x) |x, L\rangle\langle x, L| + \psi_{n,R}(x) |x, R\rangle\langle x, R|]. \quad (6)$$

The dynamics of the DTQW is given by

$$\begin{aligned} \Psi_n(x) &= Q(\epsilon)\Psi_{n-1}(x-\epsilon) + P(\epsilon)\Psi_{n-1}(x+\epsilon) \\ &\approx Q(\epsilon) \left(1 - \epsilon \frac{\partial}{\partial x}\right) \Psi_{n-1}(x) \\ &\quad + P(\epsilon) \left(1 + \epsilon \frac{\partial}{\partial x}\right) \Psi_{n-1}(x), \end{aligned} \quad (7)$$

where

$$Q(\epsilon) \approx \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} - i\epsilon \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad (8)$$

$$P(\epsilon) \approx \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} - i\epsilon \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \quad (9)$$

Therefore, we obtain the dynamics of the DTQW from the beginning,

$$\Psi_\tau(x) \approx e^{-i(\sigma_x + \sigma_z \frac{\partial}{\partial x})t} \Psi_0(x), \quad (10)$$

where σ_x and σ_z are the Pauli x and z matrices and $t = \epsilon\tau$. This equation corresponds to the Dirac equation by taking the coin state as the spinor. 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 [10], the Cs atoms trapped in the

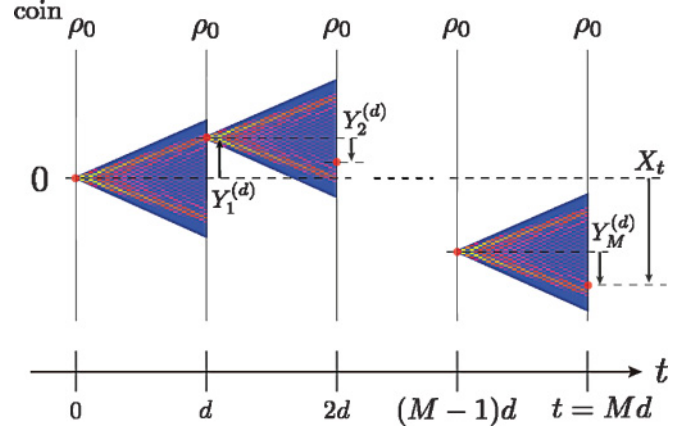


FIG. 1. (Color online) Quantum walk with the periodic position measurement. The schematic figure of the DTQW with PPMs is explained in the text.

optical lattice [11], the photons by employing the fiber network loop [12], and the $^{40}\text{Ca}^+$ atoms in the ion trap [13].

III. DISCRETE TIME QUANTUM WALK WITH PERIODIC POSITION MEASUREMENT

In this section, we show the relationship between the DTQW and decoherence and give the interpretation to quantum foundations. From here on, we define a simple model of the QW with environment as illustrated in Fig. 1. After step d 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 reprepare 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 [28]. We denote the sequence of the random variables on the DTQW between measurements by step d 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 distributed (i.i.d.) sequence. The random variable for the QW with the PPM is denoted as $X_t = Y_1^{(d)} + Y_2^{(d)} + \dots + Y_M^{(d)}$. When the measurement step d is independent of the final time t , the sequence of the blocks of the DTQW by step d can be taken as a 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 $\beta = 0.5$, $t = \text{step } 100$, and $d = t^\beta$, we take the position measurement 10 times by 10 steps and then obtain the probability distribution shown in Fig. 2. 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. 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

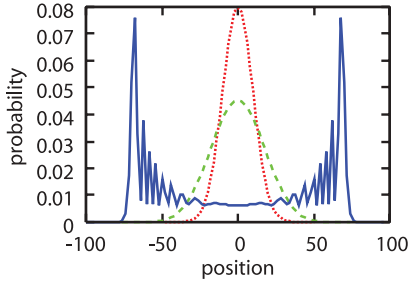


FIG. 2. (Color online) Example of the probability distributions at the 100th step. The case of $\beta = 0$ corresponds to the RW (dotted line), $\beta = 1$ corresponds to the DTQW (solid line), and $\beta = 0.5$ corresponds to the quantum-classical crossover (dashed line). The coin parameters are $a = b = c = -d = 1/\sqrt{2}$, which is called the Hadamard (quantum) walk. In the case of $\beta = 0.5$, the distribution is Gaussian but the variance is larger than that of the RW, $\beta = 0$.

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 step d between measurements and the number of the measurements M with the final time $t = dM$. If $d \sim t^\beta$, then, as $t \rightarrow \infty$, we have the limit distribution as follows:

$$\frac{X_t^{(\beta)}}{t^{(1+\beta)/2}} \Rightarrow \begin{cases} N(0,1) & \text{for } \beta = 0, \\ N(0, 1 - \sqrt{1 - |a|^2}) & \text{for } 0 < \beta < 1, \\ K(|a|) & \text{for } \beta = 1, \end{cases} \quad (11)$$

where “ \Rightarrow ” means the convergence in distribution and $N(m, \sigma^2)$ expresses 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 $r \in (0, 1)$,

$$f(x; r) = \frac{\sqrt{1 - r^2}}{\pi(1 - x^2)\sqrt{r^2 - x^2}} I_{(-r, r)}(x), \quad (12)$$

where $I_{(-r, r)}(x)$ is the indicator function, that is, $I_A(x) = 1$ ($x \in A$), $= 0$ ($x \notin A$). The proof is seen in the Appendix. This theorem is our main result and is illustrated in Fig. 3. The theorem tells us that the QW with the position measurement always has the normal limit distribution. It should be noted that

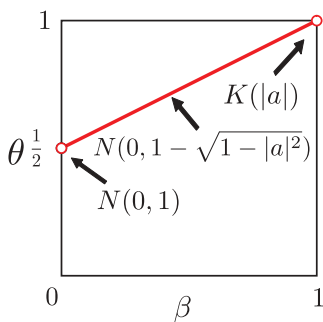


FIG. 3. (Color online) Limit distributions of the quantum walk with the PPM under the time-scale transformation. The relationship between the order of the convergence time θ and the measurement time period β in Eq. (11) is illustrated. Here, this relationship is given by $\theta = (1 + \beta)/2$.

the case of $\beta = 1$ is the DTQW without position measurement. 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 $1 \text{ step} \ll 10^{-21} \text{ s}$ in the case of the relativistic electron [25]. 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 [10–13].

Also, the theorem tells us that the projective measurement does not always lead quantum systems to be classical. According to the Copenhagen doctrine, the properties of the projective measurement are to forget a measurement outcome and cause the quantum-classical transition, which is often called the “state reduction.” Therefore, the description about the quantum dynamics with many projective measurements seems to be always taken as a Markov process [23]. However, from the difference of the time-scale order, the limit distribution does not correspond to that of a Markov process like the Brownian motion with the time-scale transformation, although we undertake the projective measurements in the case of $0 < \beta < 1$. From the preceding fact, we give an insight to the arrow of time. Except for $\beta = 1$, we undertake the position measurement for the DTQW infinite times. In other words, our obtained entropy by position measurement is always infinity as $t \rightarrow \infty$ but its increasing rate depends on the time-scale parameter β . Therefore, our result (11) shows that the projective measurement does not uniformly produce the arrow of time for any time scale. Note that this always leads to the arrow of time according to the Copenhagen doctrine [22].

IV. CONCLUSION

We have analytically obtained the limit distribution of the DTQW on \mathbb{Z} with PPMs (11). 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 have applied the concept of the QW to the problem of quantum measurement and shown that the quantum dynamics with the projective measurements cannot be taken as a Markov process under some specified time scales; that is, this is not time-scale invariant. Our results show that randomness and the arrow of time in QWs gradually emerge. Furthermore, we prove the limit distribution in the cases of the general coin state and the continuous-time QW [29].

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APPENDIX: PROOF OF THEOREM 1

In this appendix, we give the proof of the theorem basically using the spatial Fourier transform [30,31] and the Taylor expansions.

Proof. Since the case of $\beta = 0$ can be taken as the RW, we obtain the normal distribution as the limit distribution from the well-known central limit theorem. Furthermore, since the case of $\beta = 1$ corresponds to the DTQW, its limit distribution has already shown in Refs. [14,15]. In the following, we only consider the limit distribution in the case of $0 < \beta < 1$.

Since $\{Y_i^{(d)}\}$ is the i.i.d. sequence and $X_t = \sum_{i=1}^M Y_i^{(d)}$, we can describe $E(e^{i\xi X_t}) = \{E(e^{i\xi Y_1^{(d)}})\}^M$, where $E(Z)$ is the expectation value of the random variable Z and $E(e^{i\xi Z})$ is called the characteristic function of Z , as

$$E(e^{i\xi X_t}) = \left\{ \int_0^{2\pi} \frac{1}{2} \text{Tr}[\hat{H}^d(k + \xi) \hat{H}^{-d}(k)] \frac{dk}{2\pi} \right\}^M, \quad (\text{A1})$$

where $\hat{H}(k) = (e^{ik}|R\rangle\langle R| + e^{-ik}|L\rangle\langle L|)H$, which is the spatial Fourier transform. Note that the details of this method are seen in Ref. [30] used in a different context. Let the eigenvalue of $\hat{H}(k)$ be $e^{i\varphi_l(k)}$ ($l \in \{\pm\}$). Then we can rewrite the integrand of Eq. (A1) for replacing ξ with ξ/t^θ and d with t^β in the following: When $\theta > \beta$, we have

$$\begin{aligned} & \frac{1}{2} \text{Tr}[\hat{H}^{t^\beta}(k + \xi/t^\theta) \hat{H}^{-t^\beta}(k)] \\ & \approx \frac{1}{2} \sum_{l,m \in \{\pm\}} e^{it^\beta[\varphi_l(k+\xi/t^\theta) - \varphi_m(k)]} \delta_{l,m} \\ & \approx \frac{1}{2} \sum_{l,m \in \{\pm\}} e^{it^\beta[\varphi_l(k) - \varphi_m(k)]} e^{i\xi t^{\beta-\theta} \frac{d\varphi_l(k)}{dk}} \delta_{l,m} \\ & = \frac{1}{2} [e^{i\xi t^{\beta-\theta} h(k)} + e^{-i\xi t^{\beta-\theta} h(k)}] \\ & \approx 1 - \frac{\xi^2}{2t^{2(\theta-\beta)}} [h(k)]^2, \end{aligned} \quad (\text{A2})$$

using the Taylor expansion for sufficiently large t . Here, $\delta_{l,m}$ is the Kronecker δ and $h(k) \equiv \frac{d\varphi_+(k)}{dk} = -\frac{d\varphi_-(k)}{dk}$. By Eqs. (A1)

and (A2), only if $2(\theta - \beta) = 1 - \beta$, then there exists the limit distribution as follows:

$$\begin{aligned} E[e^{i\xi X_t^{(\beta)}/t^\theta}] & \approx \left\{ \int_0^{2\pi} \left(1 - \frac{\xi^2}{2t^{2(\theta-\beta)}} [h(k)]^2 \right) \frac{dk}{2\pi} \right\}^{t^{1-\beta}} \\ & = \left[1 - \frac{\xi^2}{2t^{2(\theta-\beta)}} \sigma(a)^2 \right]^{t^{1-\beta}} \\ & \rightarrow e^{-\xi^2 \sigma(a)^2/2} \text{ as } t \rightarrow \infty, \end{aligned} \quad (\text{A3})$$

where

$$\sigma(a)^2 \equiv \int_0^{2\pi} [h(k)]^2 \frac{dk}{2\pi}. \quad (\text{A4})$$

In the following, we derive $\sigma(a)^2$. Generally, a quantum coin flip $H \in \text{U}(2)$ is expressed by four parameters r, ϕ, ψ, δ with $r \in (0, 1)$, $\phi, \psi, \delta \in \mathbb{R}$ such that

$$H(r, \phi, \psi, \delta) = \begin{pmatrix} r e^{i\phi} & \sqrt{1-r^2} e^{i\psi} \\ -\sqrt{1-r^2} e^{-i(\psi-\delta)} & r e^{-i(\phi-\delta)} \end{pmatrix}. \quad (\text{A5})$$

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

$$\det[H(r, \phi + k, \psi + k, \delta) - zI] = 0. \quad (\text{A6})$$

So we have

$$\begin{aligned} & \det[H(r, \phi + k, \psi + k, \delta) - zI] \\ & = [r e^{i(\phi+k)} - z][r e^{-i(\phi+k-\delta)} - z] + (1-r^2) e^{i\delta} \\ & = z^2 - 2r e^{i\delta/2} \cos(\delta' + k) z + e^{i\delta} = 0, \end{aligned} \quad (\text{A7})$$

where $\delta' \equiv \phi - \delta/2$. Putting the solutions $e^{i\varphi_+(k)}$ and $e^{i\varphi_-(k)}$ into Eq. (A7), we obtain

$$e^{i\varphi_+(k)} + e^{i\varphi_-(k)} = 2r e^{i\delta/2} \cos(\delta' + k), \quad (\text{A8})$$

$$\varphi_+(k) + \varphi_-(k) = \delta + 2m\pi, \quad (\text{A9})$$

where $m \in \mathbb{Z}$. By Eqs. (A8) and (A9), we have

$$\cos[\varphi_+(k) - \delta/2] = r \cos(\delta' + k). \quad (\text{A10})$$

By differentiating both sides of Eq. (A10) with respect to k ,

$$\left[\frac{d\varphi_+(k)}{dk} \right]^2 = [h(k)]^2 = \frac{r^2 \sin^2(\delta' + k)}{1 - r^2 \cos^2(\delta' + k)}. \quad (\text{A11})$$

Therefore, we derive Eq. (A4) as

$$\begin{aligned} \sigma(a)^2 & = \int_0^{2\pi} [h(k)]^2 \frac{dk}{2\pi} = \int_0^{2\pi} \frac{|a|^2 \sin^2 k}{1 - |a|^2 \cos^2 k} \frac{dk}{2\pi} \\ & = 1 - \sqrt{1 - |a|^2}. \end{aligned} \quad (\text{A12})$$

This shows that $\sigma(a)^2$ only depends on the parameter a of the quantum coin flip. Therefore, the proof is completed. ■

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the quantum lattice gases [33]. Thereafter, Ambainis *et al.* mathematically define the DTQW to combine the preceding notations [24] and this definition is used throughout this article. Furthermore, the continuous-time QW [34] is different from the DTQW and corresponds to the hopping dynamics in the Hubbard model. The differences of both QWs still remain open problems in mathematics and physics.

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