

One-dimensional three-state quantum walk

Norio Inui*

Graduate School of Engineering, University of Hyogo, 2167, Shosha, Himeji, Hyogo, 671-2280, Japan

Norio Konno[†] and Etsuo Segawa[‡]

Department of Applied Mathematics, Yokohama National University, 79-5 Tokiwadai, Yokohama, 240-8501, Japan

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We study a generalized Hadamard walk in one dimension with three inner states. The particle governed by the three-state quantum walk moves, in superposition, both to the left and to the right according to the inner state. In addition to these two degrees of freedom, it is allowed to stay at the same position. We calculate rigorously the wave function of the particle starting from the origin for any initial qubit state and show the spatial distribution of probability of finding the particle. In contrast with the Hadamard walk with two inner states on a line, the probability of finding the particle at the origin does not converge to zero even after infinite time steps except special initial states. This implies that the particle is trapped near the origin after a long time with high probability.

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I. INTRODUCTION

Studies of the quantum walks [1–5] are initially motivated by developing techniques for quantum algorithms. For example, the Grover search algorithm [6], which is one of the most famous quantum algorithms, is related to a discrete quantum walk [7,8]. Recently, the quantum walks were connected with a wide variety of field. Knight, Roldán, and Sipe [9] noticed that the coined quantum walk on a line is closely related to an optical interference phenomenon, and an experiment of Bouwmeester *et al.* [10] informed us how to realize the interference features of the quantum walk. Additionally, Kendon and Sanders [11] claimed that the complementarity properties of the quantum walk will be also realized by an extension of the optical quincunx experiment of Bouwmeester *et al.* In condensed-matter physics, Oka *et al.* [12] studied the breakdown of an electric-field-driven system by mapping the Landau-Zener transition dynamics to a quantum walk.

The Hadamard walk plays a key role in studies of the quantum walk, and it has been analyzed in detail. Thus the generalization of the Hadamard walk is one of many fascinating challenges. The simplest classical random walker on a one-dimensional lattice moves to the left *or* to the right with probability 1/2. On the other hand, the quantum walker according to the Hadamard walk on a line moves both to the left and to the right. It is well known that the spatial distribution of the probability of finding a particle governed by the Hadamard walk after a long time is quite different from that of the classical random walk; see [13–16] for examples. However, there are some commonalities. In both walks the probability of finding the probability at a fixed lattice site converges to zero after an infinitely long time.

Let us consider a classical random walker in which it can stay at the same position with nonzero probability in a single time evolution. In the limit of long time, does the probability of finding a walker at a fixed position converge to a positive value? If the probability of staying at the same position in a single step is very close to 1, the walker diffuses very slowly. However, the probability of the existence at a fixed position converges surely to zero if the jumping probability is not zero. The classical random walker which can remain the same position is essentially regarded as the same process as the random walk right or left with probability of 1/2 by scaling the time. Is the same conclusion valid for the quantum walk? The answer is no. We show that the profile of the Hadamard walk changes drastically by appending only one degree of freedom to the inner states.

If the quantum particle in the three-state quantum walk exists at only one site initially, the particle is trapped with high probability near the initial position. Similar localization has been already seen in other quantum walks. The first simulation showing localization was presented by Mackay *et al.* [17] in studying the two-dimensional Grover walk. After that, more refined simulations were performed by Tregenna *et al.* [18] and an exact proof on the localization was given by Inui *et al.* [19]. The second is found in the four-state quantum walk [20,21]. In this walk, a particle moves not only the nearest sites but also the second-nearest sites according to the four inner states. The four-state quantum walk is also a generalized Hadamard walk, and it is similar to the three-state quantum walk. The significant difference between them is that the wave function of the four-state quantum walk does not converge, but that of the three-state quantum walk converges in the limit as time tends to infinity. We focus on the localized stationary distribution of the three-state quantum particle and calculate it rigorously. Moreover, Konno [22] proved that a weak limit distribution of a continuous-time rescaled two-state quantum walk has a similar form to that of the discrete-time one. In fact, both limit density functions for two-state quantum walks have two peaks at the two end points of the supports. As a corollary, it

*Electronic address: inui@eng.u-hyogo.ac.jp

[†]Electronic address: norio@mathlab.sci.ynu.ac.jp

[‡]Electronic address: segawa820@lam.osu.sci.ynu.ac.jp

is easily shown that a weak limit distribution of the corresponding continuous-time three-state quantum walk has the same shape as that of the two-state walk. So localization does not occur in the continuous-time case in contrast with the discrete-time case. In this situation the main aim of this paper is to show that localization occurs for a discrete-time three-state quantum walk rigorously.

The rest of the paper is organized as follows. After defining the three-state quantum walk, the eigenvalues and eigenvectors of the time evolution operator are calculated and the wave function is shown in Sec. II. A time-averaged probability of finding the particle is introduced in Sec. III, and it is shown that the time-averaged probability of the three-state quantum walk converges to a nonzero value. In Sec. IV, we prove the probability of finding the particle at a fixed itself converges to a nonzero value after infinite long time.

II. DEFINITION OF THE THREE-STATE QUANTUM WALK

The three-state quantum walk (3QW) considered here is a kind of generalized Hadamard walk on a line. The particle ruled by the 3QW is characterized in the Hilbert space which is defined by a direct product of a chirality-state space $|s\rangle \in \{|L\rangle, |0\rangle, |R\rangle\}$ and a position space $|n\rangle \in \{\dots, -2\rangle, -1\rangle, |0\rangle, |1\rangle, |2\rangle, \dots\}$. The chirality states are transformed at each time step by the following unitary transformation:

$$\begin{aligned} |L\rangle &= \frac{1}{3}(-|L\rangle + 2|0\rangle + 2|R\rangle), & |0\rangle &= \frac{1}{3}(2|L\rangle - |0\rangle + 2|R\rangle), \\ |R\rangle &= \frac{1}{3}(2|L\rangle + 2|0\rangle - |R\rangle). \end{aligned}$$

Let $\Psi(n, t) \equiv [\psi_L(n, t), \psi_0(n, t), \psi_R(n, t)]^T$ be the amplitude of the wave function of the particle corresponding to the chiralities L , 0 , and R at the position $n \in \mathbb{Z}$ and the time $t \in \{0, 1, 2, \dots\}$, where T denotes the transpose operator and \mathbb{Z} is the set of integers. We assume that a particle exists initially at the origin. Then the initial quantum states are determined by $[\psi_L(0, 0), \psi_0(0, 0), \psi_R(0, 0)] \equiv [\alpha, \beta, \gamma]$, where $\alpha, \beta, \gamma \in \mathbb{C}$ with $|\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1$. Here \mathbb{C} is the set of complex numbers.

Before we define the time evolution of the wave function, we introduce the following three operators:

$$\begin{aligned} U_L &= \frac{1}{3} \begin{bmatrix} -1 & 2 & 2 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, & U_0 &= \frac{1}{3} \begin{bmatrix} 0 & 0 & 0 \\ 2 & -1 & 2 \\ 0 & 0 & 0 \end{bmatrix}, \\ U_R &= \frac{1}{3} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 2 & 2 & -1 \end{bmatrix}. \end{aligned}$$

If the matrix U_L is applied to the function $\Psi(n, t)$, the only L component is selected after carrying out the superimposition between $\psi_L(n, t)$, $\psi_0(n, t)$, and $\psi_R(n, t)$. Similarly the 0 component and R component are selected in $U_0\Psi(n, t)$ and $U_R\Psi(n, t)$.

We now define the time evolution of the wave function by

$$\Psi(n, t+1) = U_L\Psi(n+1, t) + U_0\Psi(n, t) + U_R\Psi(n-1, t).$$

One finds clearly that the chiralities L and R correspond to the left and right and that the chirality 0 corresponds to the neutral state for the motion.

Using the Fourier analysis, which is often used in the calculations of quantum walks, we obtain the wave function. The spatial Fourier transformation of $\Psi(k, t)$ is defined by

$$\tilde{\Psi}(k, t) = \sum_{n \in \mathbb{Z}} \Psi(n, t) e^{-ikn}.$$

The dynamics of the wave function in the Fourier domain is given by

$$\begin{aligned} \tilde{\Psi}(k, t+1) &= \frac{1}{3} \begin{bmatrix} e^{ik} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-ik} \end{bmatrix} \begin{bmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{bmatrix} \tilde{\Psi}(k, t) \\ &\equiv \tilde{U} \tilde{\Psi}(k, t). \end{aligned} \quad (1)$$

Thus the solution of Eq. (1) is formally given by $\tilde{\Psi}(k, t) = \tilde{U}^t \tilde{\Psi}(k, 0)$. Let $e^{i\theta_j, k}$ and $|\Phi_k^j\rangle$ be the eigenvalues of \tilde{U} and the orthonormal eigenvector corresponding to $e^{i\theta_j, k}$ ($j = 1, 2, 3$). Since the matrix \tilde{U} is a unitary matrix, it is diagonalizable. Therefore the wave function $\tilde{\Psi}(k, t)$ is expressed by

$$\tilde{\Psi}(k, t) = \left(\sum_{j=1}^3 e^{i\theta_j, kt} |\Phi_k^j\rangle \langle \Phi_k^j| \right) \tilde{\Psi}(k, 0),$$

where $\tilde{\Psi}(k, 0) = [\alpha, \beta, \gamma]^T \in \mathbb{C}^3$ with $|\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1$. The eigenvalues are given by

$$\theta_{j,k} = \begin{cases} 0, & j=1, \\ \theta_k, & j=2, \\ -\theta_k, & j=3, \end{cases}$$

$$\cos \theta_k = -\frac{1}{3}(2 + \cos k),$$

$$\sin \theta_k = \frac{1}{3} \sqrt{(5 + \cos k)(1 - \cos k)}, \quad (2)$$

for $k \in [-\pi, \pi)$. The eigenvectors of \tilde{U} , which are orthonormal basis, are obtained after some computation:

$$|\Phi_k^j\rangle = \sqrt{c_k(\theta_{j,k})} \begin{bmatrix} \frac{1}{1 + e^{i(\theta_{j,k}-k)}} \\ \frac{1}{1 + e^{i\theta_{j,k}}} \\ \frac{1}{1 + e^{i(\theta_{j,k}+k)}} \end{bmatrix}, \quad (3)$$

where

$$c_k(\theta) = 2 \left\{ \frac{1}{1 + \cos(\theta - k)} + \frac{1}{1 + \cos \theta} + \frac{1}{1 + \cos(\theta + k)} \right\}^{-1}.$$

In the above calculation, it is most important to emphasize that the eigenvalue 1 is independent of the value k . The eigenvalues of the Hadamard walk are given by $e^{i\theta_k}$ and $e^{i(\pi-\theta_k)}$ with $\sin \theta_k = \sin k/\sqrt{2}$. Therefore the eigenvalues do not take the value 1 except in the special case $k=0$. We have shown that the existence of a strongly degenerated eigenvalue such as 1 in Eq. (2) is a necessary condition for the quantum walk showing the localization [19]. The significant difference between the 3QW and the previous quantum walks showing the

localization such as the Grover walk and the four-state quantum walk is the number of the degenerate eigenvalues of the time evolution matrix. Two degenerate eigenvalues 1 and -1 , which are independent of the value k , exist in both the Grover walk and the four-state quantum walk. In contrast there is only one degenerate eigenvalue in the 3QW, which is independent of the value k . This distinctive property causes the particular time evolution for 3QW.

Let us number each chirality L , 0 , and R using $l=1, 2$, and 3 , respectively. Then the wave function in real space is obtained by the inverse Fourier transform: for $\alpha, \beta, \gamma \in \mathbb{C}$ with $|\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1$,

$$\begin{aligned} \Psi(n, t; \alpha, \beta, \gamma) &= \frac{1}{2\pi} \int_{-\pi}^{\pi} \tilde{\Psi}(k, t) e^{ikn} dk \\ &= \frac{1}{2\pi} \int_{-\pi}^{\pi} \left(\sum_{j=1}^3 e^{i\theta_{j,k}t} |\Phi_k^j\rangle \langle \Phi_k^j| \tilde{\Psi}(k, 0) \right) e^{ikn} dk \\ &= [\Psi(n, t; 1; \alpha, \beta, \gamma), \Psi(n, t; 2; \alpha, \beta, \gamma), \Psi(n, t; 3; \alpha, \beta, \gamma)]^T \\ &= \sum_{j=1}^3 [\Psi_j(n, t; 1; \alpha, \beta, \gamma), \Psi_j(n, t; 2; \alpha, \beta, \gamma), \Psi_j(n, t; 3; \alpha, \beta, \gamma)]^T, \end{aligned} \quad (4)$$

where

$$\Psi_j(n, t; l; \alpha, \beta, \gamma) = \frac{1}{2\pi} \int_{-\pi}^{\pi} c_k(\theta_{j,k}) \varphi_k(\theta_{j,k}, l) e^{i(\theta_{j,k}t + kn)} dk \quad (l=1, 2, 3), \quad (5)$$

with

$$\varphi_k(\theta, l) = \zeta_{l,k}(\theta) [\overline{\alpha \zeta_{1,k}(\theta)} + \overline{\beta \zeta_{2,k}(\theta)} + \overline{\gamma \zeta_{3,k}(\theta)}] \quad (l=1, 2, 3),$$

$$\begin{aligned} \zeta_{1,k}(\theta) &= (1 + e^{i(\theta-k)})^{-1}, & \zeta_{2,k}(\theta) &= (1 + e^{i\theta})^{-1}, \\ \zeta_{3,k}(\theta) &= (1 + e^{i(\theta+k)})^{-1}, \end{aligned} \quad (6)$$

where \bar{z} is conjugate of $z \in \mathbb{C}$. Sometimes we omit the initial qubit state $[\alpha, \beta, \gamma]$ such as $\Psi_j(n, t; l) = \Psi_j(n, t; l; \alpha, \beta, \gamma)$. The probability of finding the particle at position n and time t with the chirality l is given by $P(n, t; l) = |\Psi(n, t; l)|^2$. Thus the probability of finding the particle at position n and time t becomes $P(n, t) = \sum_{l=1}^3 P(n, t; l)$.

III. TIME-AVERAGED PROBABILITY

We focus our attention on the spatial distribution of the probability of finding the particle after a long time. Equation (4) is rather complicated, but the value of $\lim_{t \rightarrow \infty} P(n, t)$ can be exactly calculated in following sections. We start showing a numerical result for the probability of finding the particle at the origin before carrying out the analytical calculation. Fig-

ure 1 shows the time dependence of $P(0, t)$ with initial state $\alpha = i/\sqrt{2}$, $\beta = 0$, and $\gamma = 1/\sqrt{2}$. The probability decreases quickly near $t=0$ and fluctuates near 0.2. The inset in Fig. 1 is plotted as the inversed time, and the amplitude of fluctuation decreases as the time. The horizontal dashed line in Fig. 1 is the value at the origin of the time-averaged probability defined by

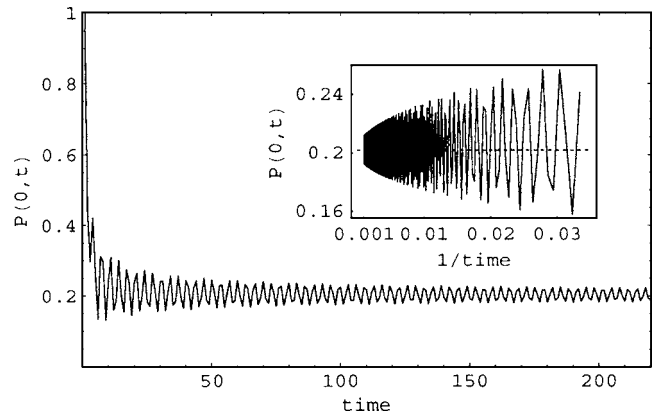


FIG. 1. Time dependence of the probability of finding a particle at the origin starting from an initial state $\alpha = i/\sqrt{2}$, $\beta = 0$, and $\gamma = 1/\sqrt{2}$. The same data are plotted as a function of $1/t$ in the inset. The horizontal dashed line crosses at $(0, 2(5-2\sqrt{6}))$. The amplitude of fluctuation of probability decreases near zero.

$$\bar{P}_\infty(0; \alpha, \beta, \gamma) = \lim_{N \rightarrow \infty} \left(\lim_{T \rightarrow \infty} \frac{1}{T} \sum_{t=0}^{T-1} \sum_{l=1}^3 P_N(0, t; l; \alpha, \beta, \gamma) \right),$$

where $P_N(n, t; l; \alpha, \beta, \gamma)$ is the probability of finding a particle with chirality l at position n and time t on a cyclic lattice containing N sites. The time-averaged probability introduced here has already used to study the quantum walk. In the case of the Hadamard walk on a cycle containing odd sites, the time-averaged probability takes a value $1/N$, which is independent of the initial states [4,23]. Therefore the time-averaged probability converges to zero in the limit $N \rightarrow \infty$. On the other hand, the time-averaged probability of a quantum walk showing localization converges to a nonzero value. For this reason first we calculate the time-averaged probability of the 3QW, and in the next section we will show that the probability $P(n, t)$ itself converges.

From now on we compute the time-averaged probability at the origin in the 3QW on a cycle with N sites. We assume that the number N is odd. The argument of eigenvectors of 3QW with a finite N is $\theta_{j, 2m\pi/N}$ for $m \in [-(N-1)/2, (N-1)/2]$. Since the eigenvalue corresponding to m is the same as the eigenvalue corresponding to $-m$, the wave function is formally expressed by

$$\Psi_N(0, t; l; \alpha, \beta, \gamma) = \sum_{j=1}^3 \sum_{m=0}^{(N-1)/2} c_{j,m,l}(N) e^{i\theta_{N,j,m} t},$$

where $\theta_{N,j,m} = \theta_{j, 2m\pi/N}$. We note here that the coefficient $c_{j,m,l}(N)$ depends on the initial state $[\alpha, \beta, \gamma]$, but we omit it. Then the probability $P_N(0, t; \alpha, \beta, \gamma)$ at the origin is given by

$$P_N(0, t; \alpha, \beta, \gamma) = \sum_{l_1, l_2, j_1, j_2}^3 \sum_{m_1, m_2=0}^{(N-1)/2} \overline{c_{j_1, m_1, l_1}(N)} c_{j_2, m_2, l_2}(N) \times e^{i(\theta_{N, j_2, m_2} - \theta_{N, j_1, m_1}) t}.$$

The coefficient $c_{j,m,l}(N)$ can be derived from the product of eigenvectors. Although lengthy calculations are required to express the coefficient $c_{j,m,l}(N)$ explicitly, it is shown below that the coefficient $c_{j,m,l}(N)$ except $j=1$ does not contribute $P_N(t)$. Noting that the equation

$$\lim_{T \rightarrow \infty} \frac{1}{T} \sum_{t=0}^{T-1} e^{i\theta t} = \begin{cases} 1, & \theta = 0, \\ 0, & \theta \neq 0, \end{cases}$$

we have

$$\begin{aligned} \bar{P}_N(0; \alpha, \beta, \gamma) &= \sum_{l=1}^3 \left(\left| \sum_{m=0}^{(N-1)/2} c_{1,m,l}(N) \right|^2 + \left| \sum_{j=2}^3 c_{j,0,l}(N) \right|^2 \right. \\ &\quad \left. + \sum_{j=2}^3 \sum_{m=1}^{(N-1)/2} |c_{j,m,l}(N)|^2 \right). \end{aligned} \quad (7)$$

The difference between the first term and the other terms is caused by the difference of the degree of degenerate eigenvalues.

Let $\phi_k^j(N)$ be the eigenvector corresponding to the eigenvalue $e^{i\theta_{j,k} t}$ of the time-evolution matrix of the 3QW with a matrix size $3N \times 3N$. The eigenvectors are easily obtained by

$$|\phi_m^j(N)\rangle = \frac{1}{\sqrt{3N}} [|\Phi_m^j\rangle, \omega |\Phi_m^j\rangle, \omega^2 |\Phi_m^j\rangle, \dots, \omega^{N-1} |\Phi_m^j\rangle],$$

where $\omega = e^{2\pi i/N}$. Since the coefficient $c_{j,m,l}(N)$ is proportional to the product of eigenvectors, the orders with respect to N of the first term and the second term in Eq. (7) are $O(1)$ and $O(N^{-1})$, respectively. Thus we can neglect the second term in the limit of $N \rightarrow \infty$. Using the eigenvectors in Eq. (3), we have

$$\bar{P}_\infty(0; \alpha, \beta, \gamma) = (5 - 2\sqrt{6})(1 + |\alpha + \beta|^2 + |\beta + \gamma|^2 - 2|\beta|^2).$$

The time-averaged probability takes the maximum value $2(5 - 2\sqrt{6})$ at $\beta=0$, which is indicated by the horizontal dashed line in Fig. 1. The components of $\bar{P}_\infty(0; \alpha, \beta, \gamma)$ corresponding to $l=1, 2, 3$ are, respectively, given by

$$\bar{P}_\infty(0; 1; \alpha, \beta, \gamma) = \frac{|\sqrt{6}\alpha - 2(\sqrt{6}-3)\beta + (12-5\sqrt{6})\gamma|^2}{36},$$

$$\bar{P}_\infty(0; 2; \alpha, \beta, \gamma) = \frac{(\sqrt{6}-3)^2 |\alpha + \beta + \gamma|^2}{9},$$

$$\bar{P}_\infty(0; 3; \alpha, \beta, \gamma) = \frac{|\sqrt{6}\gamma - 2(\sqrt{6}-3)\beta + (12-5\sqrt{6})\alpha|^2}{36}. \quad (8)$$

We stress here that the time-averaged probability is not always positive. If $\alpha = 1/\sqrt{6}$, $\beta = -2/\sqrt{6}$, and $\gamma = 1/\sqrt{6}$, then the time-averaged probability becomes zero—that is, $\bar{P}_\infty(0; 1/\sqrt{6}, -2/\sqrt{6}, 1/\sqrt{6}) = 0$.

IV. STATIONARY DISTRIBUTION OF THE PARTICLE

We showed that the time-averaged probability of the 3QW converges to a nonzero value except in special initial states. This result, however, does not mean that a particle is observed with almost the same probability at the origin after a long-time evolution. Indeed the probabilities of finding a particle in the Grover walk and the four-state quantum walk, whose time-averaged probabilities converge to nonzero values, do not converge, because the time-averaged probabilities in both cases depend on the parity of the time. Figure 1 suggests that the probability $P(n, t) = P(n, t; \alpha, \beta, \gamma)$ itself converges in a limit of $t \rightarrow \infty$. In this section we calculate the limit $P_*(n) \equiv \lim_{t \rightarrow \infty} P(n, t)$ rigorously and consider the dependence of $P_*(n)$ on the position n .

The wave function given by Eq. (4) is an infinite superposition of the wave function $e^{i(\theta_{j,k} t + kn)}$. If the argument $\theta_{j,k}$ given in Eq. (2) for $j=2, 3$ is not absolute zero, then $e^{i\theta_{j,k} t}$ oscillates with high frequency in k space for large t . On the other hand, $c_k(\theta_{j,k}) \varphi_k(\theta_{j,k}, l)$ in Eq. (5) changes smoothly with respect to k . Therefore we expect that the integration for $j=2, 3$ in Eq. (5) becomes small as the time increases due to cancellation and converges to zero in the limit of $t \rightarrow \infty$ —that is,

$$\lim_{t \rightarrow \infty} \sum_{j=2}^3 \Psi_j(n, t; l; \alpha, \beta, \gamma) = 0, \quad (9)$$

for $l=1, 2, 3$ and $\alpha, \beta, \gamma \in \mathbb{C}$ with $|\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1$. This conjecture can be rigorously proved using the Riemann-Lebesgue lemma (see the Appendix). Consequently, the probability $P_*(n) = P_*(n; \alpha, \beta, \gamma)$ is determined by the eigenvector corresponding to the eigenvalue 1—that is, $\theta_{1,k} = 0$ [see Eq. (2)]—and l th component of $P_*(n; l) = P_*(n; l; \alpha, \beta, \gamma)$ is given by

$$P_*(n; l; \alpha, \beta, \gamma) = |\Psi_1(n, t; l; \alpha, \beta, \gamma)|^2. \quad (10)$$

Note that $\Psi_1(n, t; l; \alpha, \beta, \gamma)$ does not depend on time t , since $\theta_{1,k} = 0$. By transforming integration in the left-hand side in Eq. (10) into a complex integral, we have

$$P_*(n; 1; \alpha, \beta, \gamma) = |2\alpha I(n) + \beta J_+(n) + 2\gamma K_+(n)|^2,$$

$$P_*(n; 2; \alpha, \beta, \gamma) = \left| \alpha J_-(n) + \frac{\beta}{2} L(n) + \gamma J_+(n) \right|^2,$$

$$P_*(n; 3; \alpha, \beta, \gamma) = |2\alpha K_-(n) + \beta J_-(n) + 2\gamma I(n)|^2, \quad (11)$$

where $c = -5 + 2\sqrt{6} \in (-1, 0]$ and

$$I(n) = \frac{2c^{|n|+1}}{c^2 - 1}, \quad L(n) = I(n-1) + 2I(n) + I(n+1),$$

$$J_+(n) = I(n) + I(n+1), \quad J_-(n) = I(n-1) + I(n),$$

$$K_+(n) = I(n+1), \quad K_-(n) = I(n-1), \quad (12)$$

for any $n \in \mathbb{Z}$. We should remark that it is confirmed that $\bar{P}_\infty(0; l; \alpha, \beta, \gamma) = P_*(0; l; \alpha, \beta, \gamma)$ for $l=1, 2, 3$ by using Eqs. (8), (11), and (12).

Here we give an example. From Eqs. (11) and (12), we obtain

$$P_*(0; i/\sqrt{2}, 0, 1/\sqrt{2}) = \frac{4c^2(5c^2 + 2c + 5)}{(1 - c^2)^2} = 2(5 - 2\sqrt{6}) = 0.202 \dots, \quad (13)$$

$$P_*(n; i/\sqrt{2}, 0, 1/\sqrt{2}) = \frac{2(5c^4 + 2c^3 + 10c^2 + 2c + 5)}{(1 - c^2)^2} c^{2|n|}, \quad (14)$$

for any $|n| \geq 1$. Furthermore,

$$0 < \sum_{n \in \mathbb{Z}} P_*(n; i/\sqrt{2}, 0, 1/\sqrt{2}) = 1/\sqrt{6} = 0.408 \dots < 1. \quad (15)$$

That is, $P_*(n; i/\sqrt{2}, 0, 1/\sqrt{2})$ is not a probability measure. The above value depends on the initial qubit state—for example,

$$\sum_{n \in \mathbb{Z}} P_*(n; 1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3}) = 3 - \sqrt{6} = 0.550 \dots,$$

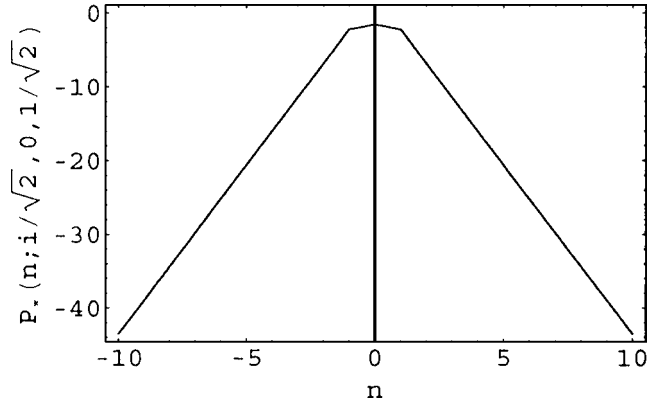


FIG. 2. Distribution of probability of finding a particle $P_*(n)$ at the position n in the 3QW with the initial state $\alpha = i/\sqrt{2}$, $\beta = 0$, and $\gamma = 1/\sqrt{2}$ on a semilogarithmic scale. The probability decreases exponentially for large $|n|$.

$$\sum_{n \in \mathbb{Z}} P_*(n; 1/\sqrt{3}, -1/\sqrt{3}, 1/\sqrt{3}) = (3 - \sqrt{6})/9 = 0.061 \dots$$

Note that in the case of the classical symmetric random walk starting from the origin, it is known that $P_*(n) = 0$ for any $n \in \mathbb{Z}$; therefore, we have $\sum_{n \in \mathbb{Z}} P_*(n) = 0$. The same conclusion can be obtained for the discrete-time and continuous-time two-state quantum walks [13,14,22].

Figure 2 shows the probability $P_*(n; i/\sqrt{2}, 0, 1/\sqrt{2})$ in logarithmic scale. The probability decreases exponentially for large $|n|$, and its asymptotic behavior is expressed by $P_*(n; i/\sqrt{2}, 0, 1/\sqrt{2}) \propto c^{2|n|}$ in the limit of $n \rightarrow \pm\infty$ as Eq. (14) indicates.

We here mention the time dependence of $P(n, t)$. The particle is observed near the origin with high probability. However, this does not imply that the particle cannot escape from the region near the origin. Figure 3 shows the change of $P(n, t)$ in a space-time. The particle is observed at the dark region with high probability. One clearly finds three dark

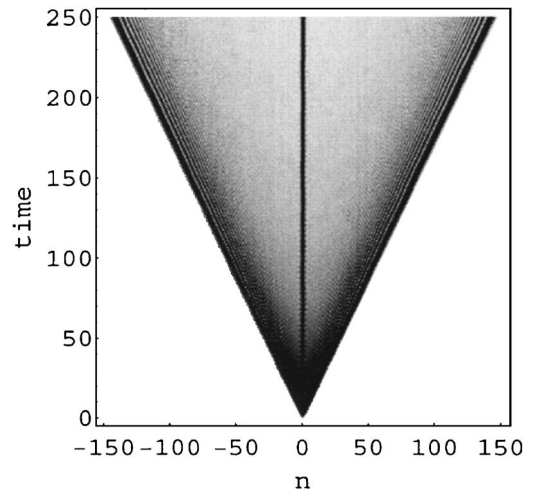


FIG. 3. Density plot of probability of finding a particle $P(n, t)$ in the space-time. The initial state is $\alpha = i/\sqrt{2}$, $\beta = 0$, and $\gamma = 1/\sqrt{2}$. The particle is observed on darker regions with high probability.

regions. The first is a region near a center line connecting to the origin, and we can confirm the localization near the origin. The second and third regions are boundaries of the triangle. These regions show trajectories of two peaks moving outside in the space-time, which are also seen in the Hadamard walk. As a result, we conclude that the particle in the 3QW splits the region into three parts in superposition.

V. CONCLUSIONS AND DISCUSSION

The unique properties which are not observed in other quantum walks can be found in the 3QW. The particle starting from the origin splits the space-time region into three pieces in superposition. Two of three leave for infinite points and the remainder stays at the origin. In contrast with the ordinary Hadamard walk, the probability of finding the particle at the origin does not vanish for large time and converges to $2(5-2\sqrt{6})=0.202\dots$, which is the maximum among possible combinations of α , β , and γ

A simple reason why the 3QW is different from other quantum walks is the difference in the degree of degenerate eigenvalues. The necessary condition of localization is the existence of degenerate eigenvalues. Furthermore, each degree of degeneration must be proportional to the dimension of the Hilbert space. In addition, if the degenerate eigenvalue is 1 only, then the probability of finding the particle can converge in the limit of $t \rightarrow \infty$. The Grover walk and the four-state quantum walk exhibit localization, but the probability of finding the particle oscillates, because of the existence of degenerate eigenvalues 1 and -1 . On the other hand, the degenerate eigenvalue in the 3QW unrelated to the wave number is only 1; therefore, the probability converges.

Finally we discuss a relation between the limit distribution for the original 3QW, X_t , as time $t \rightarrow \infty$ and that of the rescaled X_t/t in the same limit. When we consider the 3QW starting from a mixture of three pure states $[1, 0, 0]^T$, $[0, 1, 0]^T$, and $[0, 0, 1]^T$ with probability $1/3$, respectively, we can obtain a weak limit probability distribution $f(x)$ for the rescaled 3QW X_t/t as $t \rightarrow \infty$ in the following:

$$f(x) = \frac{1}{3} \delta_0(x) + \frac{\sqrt{8} I_{(-1/\sqrt{3}, 1/\sqrt{3})}(x)}{3\pi(1-x^2)\sqrt{1-3x^2}}, \quad (16)$$

for $x \in [-1, 1]$, where $\delta_0(x)$ denotes the point mass at the origin and $I_{(a,b)}(x) = 1$, if $x \in (a, b)$, $=0$, otherwise. The above derivation is due to the method by Grimmett *et al.* [15]. We should note that the first term on the right-hand side of Eq. (16) corresponds to localization of the original 3QW. In fact, from Eq. (11), we have

$$\frac{1}{3} \sum_{n \in \mathbb{Z}} [P_*(n; 1, 0, 0) + P_*(n; 0, 1, 0) + P_*(n; 0, 0, 1)] = \frac{1}{3}.$$

The last value $1/3$ is nothing but the coefficient $1/3$ of $\delta_0(x)$. Moreover, the second term on the right-hand side of Eq. (16)

has a similar form to a weak limit density function for the same rescaled Hadamard walk with two inner states starting from a uniform random mixture of two pure states $[1, 0]^T$ and $[0, 1]^T$:

$$f_H(x) = \frac{I_{(-1/\sqrt{2}, 1/\sqrt{2})}(x)}{\pi(1-x^2)\sqrt{1-2x^2}},$$

for $x \in [-1, 1]$; see [13–15]. This case does not have a δ measure term corresponding to a localization. A more detailed study of this line of thought will appear in our forthcoming paper.

APPENDIX: PROOF OF Eq. (9)

Here we give an outline of the proof of Eq. (9). A direct computation gives

$$\sum_{j=2}^3 \begin{bmatrix} \Psi_j(n, t; 1; \alpha, \beta, \gamma) \\ \Psi_j(n, t; 2; \alpha, \beta, \gamma) \\ \Psi_j(n, t; 3; \alpha, \beta, \gamma) \end{bmatrix} = M \begin{bmatrix} \alpha \\ \beta \\ \gamma \end{bmatrix},$$

where $M = (m_{ij})_{1 \leq i, j \leq 3}$ with

$$m_{11} = 3J_{n,t} + \frac{1}{2} \{J_{n-1,t} + J_{n+1,t} + (K_{n-1,t} - K_{n+1,t})\},$$

$$m_{33} = 3J_{n,t} + \frac{1}{2} \{J_{n-1,t} + J_{n+1,t} - (K_{n-1,t} - K_{n+1,t})\},$$

$$m_{12} = -\{J_{n,t} + J_{n+1,t} + (K_{n,t} - K_{n+1,t})\},$$

$$m_{32} = -\{J_{n,t} + J_{n-1,t} + (K_{n,t} - K_{n+1,t})\},$$

$$m_{13} = -2J_{n+1,t}, \quad m_{31} = -2J_{n-1,t},$$

$$m_{21} = -\{J_{n,t} + J_{n-1,t} + (K_{n-1,t} - K_{n,t})\},$$

$$m_{23} = -\{J_{n,t} + J_{n+1,t} + (K_{n+1,t} - K_{n,t})\},$$

$$m_{22} = 4J_{n,t}$$

and

$$J_{n,t} = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{\cos(kn)}{5 + \cos k} \cos(\theta_k t) dk,$$

$$K_{n,t} = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{\cos(kn)}{\sqrt{(5 + \cos k)(1 - \cos k)}} \sin(\theta_k t) dk.$$

From the Riemann-Lebesgue lemma, we can show that

$$\lim_{t \rightarrow \infty} J_{n,t} = 0, \quad \lim_{t \rightarrow \infty} (K_{n,t} - K_{n+1,t}) = 0,$$

for any $n \in \mathbb{Z}$. Therefore we have the desired conclusion.

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