Quantum Random Walk via Classical Random Walk With Internal States

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Abstract. In recent years quantum random walks have garnered much interest among quantum information researchers. Part of the reason is the prospect that many hard problems can be solved efficiently by employing algorithms based on quantum random walks, in the same way that classical random walks have played a central role in many hugely successful randomized algorithms. In this paper we introduce a new representation for the quantum random walks via the classical random walk with internal states. This new representation allows for a systematic approach to finding closed form expressions for the n-step distributions for a variety of quantum random walk models, and lends itself naturally to large deviation analysis. As an example, we show how to use the new representation to arrive at the same closed form expression for the Hadamard quantum random walk on a line, previously obtained by others. We assert the proposed method works in the most general settings.

1 Introduction

For many hard problems in computer science, the most efficient solution approach known is that of randomized algorithms based on Markov chain or random walk methods [1]. For example, a well-known NP-complete problem is the 3-Satisfiability problem for which the most efficient known algorithm is based on random walk [4]. Randomized algorithms have also been successfully used to estimate the volume of convex bodies [2] and to approximate the permanent [3]. Therefore, it is reasonable to expect that the quantum versions of randomized algorithms which employ appropriate quantum random walk methods, will efficiently solve many hard problems on a quantum computer. In fact, using a quantum random walk method, the black box graph traversal problem can be solved exponentially faster on a quantum computer than on a classical computer [12]. Furthermore, as mentioned in [10], until now many quantum algorithms have been discovered in a rather ad-hoc way. Studying quantum random walks will perhaps provide a systematic way of speeding up a large class of classical randomized algorithms.

To that end, in this paper we study the discrete quantum random walks as defined in Kempe [9] in a new representation. In the classical one dimensional

random walk, the behavior of a (classical) particle moving on a line according to some probabilistic rule is studied. In the simplest model, a particle will move, at every discrete time step, one unit to the left or to the right with probabilities p and $1-p$, respectively, independent of its past positions. Many useful questions can be asked about the dynamics of the particle. One such important question is: how the particle's positions are distributed after t time steps? Similarly, in the quantum random walk model, a (quantum) particle will move *simultaneously*, i.e., *in superposition* both to its left and right with some probabilities. However, this model is not possible as it is easy to show that the sum of probabilities over all its possible positions will not be unitary. Fortunately, it is still possible to construct such a random quantum walk if an extra degree of freedom, e.g., the particle's spin, is incorporated into the model. Mathematically, if the particle's spin is up, then applying an appropriate unitary operator, the particle will move to the right. If the particle's spin is down, then the same operator will move the particle to the left. To achieve the quantum random walk, the particle's spin can be randomized via applying rotation (unitary) operator. We will describe these operators shortly.

In this paper, we will describe a new representation that allows for a systematic approach to finding closed form expressions for the n-step distributions for a variety of quantum random walk models. The new representation is based on the classical random walk with internal states, and for which a rich set of classical analysis tools is readily available. Thus, the new representation also suggests a promising direction for large deviation analysis of quantum random walks. We will show how to use the new representation to arrive at the same closed form expression for the Hadamard quantum random walk on a line, previously obtained by others. We outline how to use it for other quantum random walk models such as two-dimensional random walk and balanced quantum walk.

The rest of our paper is organized as follows. In Section 2, we will provide some related work and a formal model on quantum random on a line, and describe the proposed representation for it in Section 3. Section 4 provides an outline for studying two-dimensional quantum walk and balanced quantum walk based on the new representations, and also carves out a direction for large deviation analysis of the random quantum walks.

2 Preliminary

2.1 Related Work

Quantum random walks have been extensively studied by many researchers. Kempe provided a good introduction to quantum random walk in [9]. The

work of Y. Aharonov et al. [5] provided the first basic model for subsequent various models of quantum random walks. D. Aharonov et al. [6] investigated quantum walks on graphs and their mixing behavior. They showed that, random quantum walks are not stationary processes. Thus, their mixing times are more appropriately measured in terms of how close their $n - step$ distributions are to that of the uniform distribution stemmed from the average of the probability distributions over all time steps. They further showed that the quantum walk on a circle has mixing time $O(n \log n)$. Nayak and Vishwanath [10] also provided a detail analysis of quantum walk on a line via the Fourier analysis on the transformation of the wave equation at each time step. Their results showed that after t time steps, the probability distribution of the particle's position on the line, is almost uniformly over the interval $[-t/2, t/2]$. Romanelli et al. [11] also studied quantum random walk on the line as Markovian processes. They represented the quantum walk by separating the quantum evolution equation into Markovian and interference terms. Based on this, they showed analytically that the quadratic increase in the variance of the quantum walker's position with time is due to the coherence of the quantum evolution.

Our work differs from those in [10] and [11] is that our model assumes little about the physics of the wave packets. Instead, we model the physical process of interest as some appropriate classical random walks with internal states. Thus, we suspect that our model is more general than the ones that are tied to specific wave equations.

2.2 Discrete Quantum Random Walk on a Line

In this section we formally but briefly describe the model for the (discrete) quantum random walk on a line as presented in detail in [9]. Let $\mathcal{H}_P$ be the Hilbert space spanned by the positions of the particle, i.e., $\mathcal{H}_P$ is spanned by the basis states $\{|i>: i \in Z\}$. The position Hilbert space $\mathcal{H}_P$ is further augmented by the coin Hilbert space $\mathcal{H}_C$, to result in the overall particle state in $\mathcal{H}_P \otimes \mathcal{H}_C$. $\mathcal{H}_C = \{|\downarrow>, |\uparrow>\}$ represents the outcome of a "coin toss" and corresponds directly to the particle's spin: "up" or "down". This augmentation is necessary to provide an extra degree of freedom to make the quantum random walk physically possible. Specifically, just like a coin-flip in the classical random walk, the first step of the quantum random walk is a rotation in the coin-space for the purpose of randomizing the particle's spin. In the second step, a translation operator is applied to the particle's quantum state, which will move the particle according to its current spin values.

Depending on the desired quantum walk model, an appropriate rotation operator can be used. We consider a frequently used operator, also called the

Hadamard coin H:

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

Next, the translation of the particle can be described using the following unitary operator:

$$S = |\uparrow><\uparrow| \otimes \sum_s |s+1><s| + |\downarrow><\downarrow| \otimes \sum_s |s-1><s|$$

Overall, each step of the walk is accomplished by the unitary operator:

$$U = S(H \otimes I),$$

which implements a coin toss followed by a move.

Given that the initial particle's position and spin are in the pure states, e.g., $|0>$ and $|\uparrow>$, H will ensure that after the first coin-flip followed by a translation, the particle will have an equal chance of being on the left or right if measured properly. Mathematically,

$$|\uparrow> \otimes |0> \xrightarrow{H} \frac{1}{\sqrt{2}}(|0> + |1>) \otimes |0> \tag{1}$$

$$\xrightarrow{S} \frac{1}{\sqrt{2}}(|\uparrow> \otimes |1> + |\downarrow> \otimes |-1>) \tag{2}$$

Now measuring the coin state in the standard basis at this point, we will have the probabilities $P(|\uparrow> \otimes |1>) = P(|\downarrow> \otimes |-1>) = \frac{1}{2}$.

3 Representation of Quantum Random Walks with Classical Random Walk with Internal States

The classical random walks with internal states are fully described in Hughes [7]. In a walk with M internal states at each site, at any step the walker may move to a new site, with or without an accompanying change of state, or he may pause at his present site, with or without a change of state. An advantage of using random walk with internal states to model a problem, is that many analytic tools have been developed for these models. In what follows, we show how to model the Hadamard quantum walk with this model.

In the case of the Hadamard quantum walk, our first observation is that each time we apply $U = S(H \otimes I)$, a pure state splits into two according to the following rules:

$$U(\pm|\uparrow> \otimes |s>) = \frac{1}{\sqrt{2}}(\pm|\uparrow> \otimes |s+1>) + \frac{1}{\sqrt{2}}(\pm|\downarrow> \otimes |s-1>)$$

$$U(\pm|\downarrow> \otimes |s>) = \frac{1}{\sqrt{2}}(\pm|\uparrow> \otimes |s+1>) + \frac{1}{\sqrt{2}}(\mp|\downarrow> \otimes |s-1>)$$

Thus we can embed the Hadamard walk into a random walk with internal states (see B. D. Hughes et al [8]) by letting the states

$$(s, \uparrow, +1), \quad (s, \uparrow, -1), \quad (s, \downarrow, +1), \quad (s, \downarrow, -1) \quad \text{for } s \in \mathbb{Z}$$

represent respectively the pure states

$$(|\uparrow> \otimes |s>), \quad -(|\uparrow> \otimes |s>), \quad (|\downarrow> \otimes |s>) \quad \text{and} \quad -(|\downarrow> \otimes |s>)$$

of the Hadamard random walk. Here $s \in \mathbb{Z}$ are sites, and "1" $= (\uparrow, +1)$, "2" $= (\uparrow, -1)$, "3" $= (\downarrow, +1)$ and "4" $= (\downarrow, -1)$ are the four internal states. The splitting of the pure states in the quantum walk corresponds to the following transition probabilities of a random walk with internal states.

$$P[(s+1,\uparrow,+1) \mid (s,\uparrow,+1)] = P[(s-1,\downarrow,+1) \mid (s,\uparrow,+1)] = \frac{1}{2}$$

$$P[(s+1,\uparrow,-1) \mid (s,\uparrow,-1)] = P[(s-1,\downarrow,-1) \mid (s,\uparrow,-1)] = \frac{1}{2}$$

$$P[(s+1,\uparrow,+1) \mid (s,\downarrow,+1)] = P[(s-1,\downarrow,-1) \mid (s,\downarrow,+1)] = \frac{1}{2}$$

$$P[(s+1,\uparrow,-1) \mid (s,\downarrow,-1)] = P[(s-1,\downarrow,+1) \mid (s,\downarrow,-1)] = \frac{1}{2}$$

Notice that the above transition probabilities are translation invariant in $s \in \mathbb{Z}$. As in Kempe [9], let the walk begin at $|\downarrow> \otimes |0> = (0,\downarrow,+1) = (0,3)$ Following the notations in Hughes, let us define the two matrices

$$p(1) = P[(s+1,m) \mid (s,m')]_{(m,m')} = \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \end{pmatrix}$$

and

$$p(-1) = P[(s-1,m) \mid (s,m')]_{(m,m')} = \begin{pmatrix} 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 \end{pmatrix}$$

where m and m' go over all internal states. The initial conditions are encoded in the column vector $V = (0,0,1,0)^T$, and the n step probabilities are represented by the column vector $P_n(s) = (P_n(s,1), P_n(s,2), P_n(s,3), P_n(s,4))^T$ with $P_0(s) = \delta_0(s)V$.

Now, the quantum walk is assumed to begin at a pure state, and the density matrix expands covering more and more quantum states, each element of it splitting into two at each iteration. We allow the quantum walk to proceed without cancellations as the cancellations can be done at any moment. In order to find the distribution after n time steps, we count in all the cancellations and renormalize to get

$$\mu_n(s) = 2^n (P_n(s,1) - P_n(s,2))^2 + 2^n (P_n(s,3) - P_n(s,4))^2$$

for all $s \in \mathbb{Z}$. The generating function of $P_n(s)$ is a vector defined as

$$P(s;\xi) = \sum_{n=0}^{\infty} P_n(s) \xi^n$$

and therefore

$$P(s;\xi) = \delta_0(s)V + \xi p(1) P(s-1;\xi) + \xi p(-1) P(s+1;\xi)$$

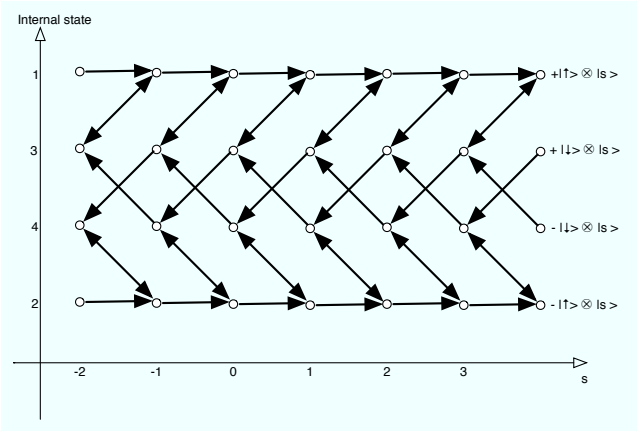


Fig. 1. *The random walk over $\mathbb{Z}$ with four internal states that embeds the Hadamard quantum walk.*

Taking the Fourier transform of $P(s;\xi)$ and $p(l)$, get $\widehat{P}(k;\xi) = \sum_s e^{isk} P(s;\xi)$ and

$$L(k) = \sum_l e^{ilk} p(l) = \frac{1}{2} \begin{pmatrix} e^{ik} & 0 & e^{-ik} & 0 \\ 0 & e^{ik} & 0 & e^{-ik} \\ e^{ik} & 0 & 0 & e^{-ik} \\ 0 & e^{ik} & e^{-ik} & 0 \end{pmatrix}$$

Hence, obtaining as in Hughes, $\widehat{P}(k;\xi) = V + \xi L(k)\widehat{P}(k;\xi)$ and

$$\widehat{P}(k;\xi) = (I - \xi L(k))^{-1} V,$$

where I is the identity matrix. We invert the discrete Fourier transform, obtaining

$$P(s;\xi) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-isk} (I - \xi L(k))^{-1} V dk$$

Expanding $(I - \xi L(k))^{-1}$ in powers of ξ, find

$$P_n(s) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-isk} L(k)^n V dk$$

Thus we have proved the following theorem.

Theorem 1 *The distribution of the Hadamard quantum walk is*

$$\mu_n(s) = \frac{1}{2^n} \left[\frac{1}{2\pi} (1,-1,0,0) \left(\int_{-\pi}^{\pi} e^{-isk} (2L(k))^n dk \right) V \right]^2$$

$$+ \frac{1}{2^n} \left[\frac{1}{2\pi} (0,0,1,-1) \left(\int_{-\pi}^{\pi} e^{-isk} (2L(k))^n dk \right) V \right]^2$$

In the above theorem, the eigenvalues of

$$2L(k) = \begin{pmatrix} e^{ik} & 0 & e^{-ik} & 0 \\ 0 & e^{ik} & 0 & e^{-ik} \\ e^{ik} & 0 & 0 & e^{-ik} \\ 0 & e^{ik} & e^{-ik} & 0 \end{pmatrix}$$

are

$$\lambda_1 = 0, \quad \lambda_2 = 2\cos(k) \quad \text{and} \quad \lambda_{3,4} = \pm\sqrt{1+\cos^2(k)} + i\sin(k)$$

and the corresponding matrix of right eigenvectors

$$R(k) = \begin{pmatrix} -e^{-2ik} & 1 & -\sqrt{1+\cos^2(k)} - \cos(k) & \sqrt{1+\cos^2(k)} - \cos(k) \\ -e^{-2ik} & 1 & \sqrt{1+\cos^2(k)} + \cos(k) & -\sqrt{1+\cos^2(k)} + \cos(k) \\ 1 & 1 & -e^{ik} & -e^{ik} \\ 1 & 1 & e^{ik} & e^{ik} \end{pmatrix}$$

giving us the closed form for the diagonalized $(2L(k))^n = R(k)\Lambda(k)^n R(k)^{-1}$. Inverting $R(k)$ obtain

$$R^{-1}(k) = \begin{pmatrix} \frac{-e^{ik}}{4\cos(k)} & \frac{-e^{ik}}{4\cos(k)} & \frac{e^{ik}}{4\cos(k)} & \frac{e^{ik}}{4\cos(k)} \\ \frac{e^{ik}}{4\cos(k)} & \frac{e^{ik}}{4\cos(k)} & \frac{e^{-ik}}{4\cos(k)} & \frac{e^{-ik}}{4\cos(k)} \\ -\frac{1}{4\sqrt{1+\cos^2(k)}} & \frac{1}{4\sqrt{1+\cos^2(k)}} & \frac{\cos(k)-\sqrt{1+\cos^2(k)}}{4\sqrt{1+\cos^2(k)}}e^{-ik} & -\frac{\cos(k)-\sqrt{1+\cos^2(k)}}{4\sqrt{1+\cos^2(k)}}e^{-ik} \\ \frac{1}{4\sqrt{1+\cos^2(k)}} & -\frac{1}{4\sqrt{1+\cos^2(k)}} & -\frac{\cos(k)+\sqrt{1+\cos^2(k)}}{4\sqrt{1+\cos^2(k)}}e^{-ik} & \frac{\cos(k)+\sqrt{1+\cos^2(k)}}{4\sqrt{1+\cos^2(k)}}e^{-ik} \end{pmatrix}$$

For $s \in \mathbb{Z}$ and $n \geq 0$, let us define $D_{\uparrow,n}(s) = \frac{1}{2\pi}(1,-1,0,0)\left(\int_{-\pi}^{\pi} e^{-isk}(2L(k))^n dk\right)V$ and $D_{\downarrow,n}(s) = \frac{1}{2\pi}(0,0,1,-1)\left(\int_{-\pi}^{\pi} e^{-isk}(2L(k))^n dk\right)V$ as the functions in Theorem 1. Then for the initial internal state $V = (0,0,1,0)^T$ as in [9] (i.e. the initial pure state $|\downarrow> \otimes |0>$ being equivalent to $\delta_0(s)V$ in the random walk model), we have the following closed form solution.

Corollary 1 *The distribution of the Hadamard quantum walk is expressed in the closed form as*

$$\mu_n(s) = \frac{D_{\uparrow,n}^2(s) + D_{\downarrow,n}^2(s)}{2^n},$$

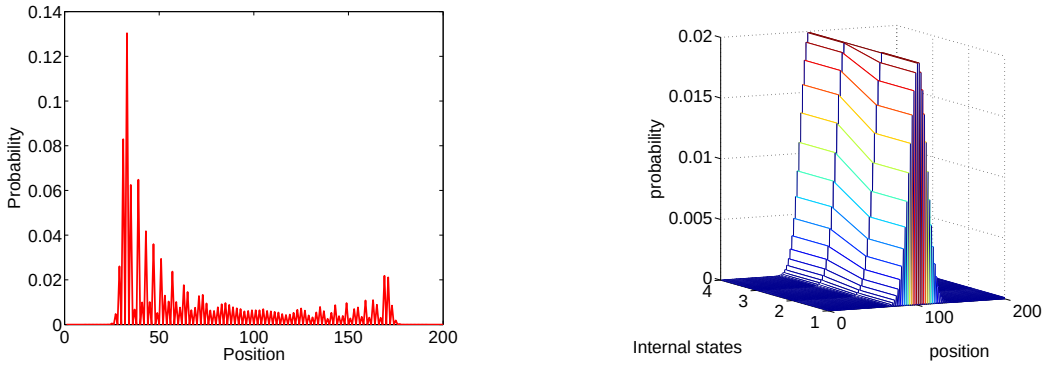
where

$$D_{\uparrow,n}(s) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{e^{-i(s+1)k}}{2\sqrt{1+\cos^2(k)}}\left[\lambda_3^n - \lambda_4^n\right]dk$$

and

$$D_{\downarrow,n}(s) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{e^{-isk}\left[(\lambda_4^n - \lambda_3^n)\cos(k) + (\lambda_3^n + \lambda_4^n)\sqrt{1+\cos^2(k)}\right]}{2\sqrt{1+\cos^2(k)}}dk$$

The above closed form solution was initially derived in [10] in 2000. Generated by our representation, Figs. 3(a) and 3(b) show the overall distribution of the particle positions and the joint distribution of internal states and positions after 100 time steps, starting at $s = 100$. The fact that the joint distribution of internal state and positions approaching Gaussian will be key to large deviation analysis. We will briefly discuss this later.



(a) (b)

Fig. 2. *(a) Probability distribution of the particle's position after 100 time steps, starting at* $s = 100$*; (b) Joint distribution of internal states and positions.*

4 Other Applications

In this section, we suggest the generalities of the proposed representation by outlining how it can be applied to the balanced quantum walk and two-dimensional quantum walk, and the large deviation analysis.

Balanced Quantum Walk.
As seen in Fig. 3(a), the n-step distribution is asymmetric. This is due to the asymmetry of H. For the balance walk, Kemp [9] suggested to use the following rotation operator (coin):

$$Y = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}$$

Using the same approach, expand the result of an iteration, at every step there will be eight terms. Thus, we can represent eight internal states:

$$\pm(|\uparrow> \otimes |s>), \quad \pm i(|\uparrow> \otimes |s>), \quad \pm(|\downarrow> \otimes |s>) \quad \text{and} \quad \pm i(|\downarrow> \otimes |s>)$$

for a given location $s \in \mathbb{Z}$. Here each internal state is determined by the spin, the plus or minus in front, and the multiplication by i. The corresponding walk with internal states is reducible with the states associated with $\pm(|\uparrow> \otimes |s>)$ and $\pm i(|\downarrow> \otimes |s>)$ being disconnected from the states associated with $\pm i(|\uparrow> \otimes |s>)$ and $\pm(|\downarrow> \otimes |s>)$. In other words, the four internal states

$$\text{“1”} = (\uparrow, +1), \quad \text{“2”} = (\downarrow, +i), \quad \text{“3”} = (\uparrow, -1), \quad \text{and} \quad \text{“4”} = (\downarrow, -i)$$

are disconnected from

$$\text{“5”} = (\uparrow, +i), \quad \text{“6”} = (\downarrow, -1), \quad \text{“7”} = (\uparrow, -i), \quad \text{and} \quad \text{“8”} = (\downarrow, +1)$$

Once again, following the notation in Hughes [7], we define the following matrices

$$p(1) = P[(s+1,m) \mid (s,m')]_{(m,m')} = \frac{1}{2}\left(\begin{array}{cccc|cccc} 1&0&0&0&0&0&0&0\\ 0&0&1&0&0&0&0&0\\ 0&0&1&0&0&0&0&0\\ 1&0&0&0&0&0&0&0\\ \hline 0&0&0&0&1&0&0&0\\ 0&0&0&0&0&0&1&0\\ 0&0&0&0&0&0&1&0\\ 0&0&0&0&1&0&0&0 \end{array}\right)$$

and

$$p(-1) = P[(s-1,m) \mid (s,m')]_{(m,m')} = \frac{1}{2}\left(\begin{array}{cccc|cccc} 0&1&0&0&0&0&0&0\\ 0&1&0&0&0&0&0&0\\ 0&0&0&1&0&0&0&0\\ 0&0&0&1&0&0&0&0\\ \hline 0&0&0&0&0&1&0&0\\ 0&0&0&0&0&1&0&0\\ 0&0&0&0&0&0&0&1\\ 0&0&0&0&0&0&0&1 \end{array}\right)$$

We can write the Fourier transform of $p(l)$ as

$$L(k) = \sum_l e^{ilk} p(l) = \frac{1}{2}\left(\begin{array}{c|c} \ell(k) & 0\\ \hline 0 & \ell(k) \end{array}\right), \text{ where } \ell(k) = \begin{pmatrix} e^{ik} & e^{-ik} & 0 & 0\\ 0 & e^{-ik} & e^{ik} & 0\\ 0 & 0 & e^{ik} & e^{-ik}\\ e^{ik} & 0 & 0 & e^{-ik} \end{pmatrix}$$

Given the representation above, the closed form expression for the balanced quantum walk can be obtained in exactly the same way as that of the presented Hadamard walk.

Two-Dimensional Quantum Walk.
For a two-dimensional quantum walk, one potentially use two coins, and the outcome of a new coin toss is in $\mathcal{H}_C \otimes \mathcal{H}_C$, i.e., we use the rotation transformation $H \otimes H$. It is straightforward to verify that, using the same approach, there will be eight internal states, with four states with be disconnected from the other four just like the balanced walk. Furthermore, the forward and backward probability matrices, and the closed form solutions can be easily obtained using the same approach as before.

Large Deviation Analysis.
In the Markov chain we use to represent the quantum walk with, for every internal state j, the distribution $P_n(s,j)$ over all $s \in \mathbb{Z}$ as shown in Fig. 3(b), converges to that of a scaled Gaussian, i.e. one quarter of a normal density. In order to represent the quantum walks we consider the cancellations between pairs of internal states, the asymptotic expression for the quantum walk can

therefore be represented via the large deviation functions $I_j(n)$ for the tail probabilities $\sum_{s \geq an} P_n(s,j) \sim e^{-I_j(a)n}$.

5 Conclusions

We introduced a new representation for the quantum random walks via the classical random walk with internal states. This new representation allowed for a systematic approach to finding closed form expressions for the n-step distributions for a variety of quantum random walk models, and naturally lend itself to large deviation analysis.

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